Dynamical Systems Methods Applied to the Michaelis-Menten and Lindemann Mechanisms

by

Matthew Stephen Calder

A thesis
presented to the University of Waterloo
in fulfilment of the
thesis requirement for the degree of
Doctor of Philosophy
in
Applied Mathematics

Waterloo, Ontario, Canada, 2009

Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners. I understand that my thesis may be made electronically available to the public.

Matthew Stephen Calder

Abstract

In the first part of this thesis, we will explore an iterative procedure to determine the detailed asymptotic behaviour of solutions of a certain class of nonlinear vector differential equations which approach a nonlinear sink as time tends to infinity. This procedure is indifferent to resonance in the eigenvalues. Some attention will be given to finding approximations to solutions which are themselves flows. Moreover, we will address the writing of one component in terms of another in the case of a planar system.

In the second part of this thesis, we will explore the Michaelis-Menten mechanism of a single enzyme-substrate reaction. The focus is an analysis of the planar reduction in phase space or, equivalently, solutions of the scalar reduction. In particular, we will prove the existence and uniqueness of a slow manifold between the horizontal and vertical isoclines. Also, we will determine the concavity of all solutions in the first quadrant. Moreover, we will establish the asymptotic behaviour of all solutions near the origin, which generally is not given by a Taylor series. Finally, we will determine the asymptotic behaviour of the slow manifold at infinity. Additionally, we will study the planar reduction. In particular, we will find non-trivial bounds on the length of the pre-steady-state period, determine the asymptotic behaviour of solutions as time tends to infinity, and determine bounds on the solutions valid for all time.

In the third part of this thesis, we explore the (nonlinear) Lindemann mechanism of unimolecular decay. The analysis will be similar to that for the Michaelis-Menten mechanism with an emphasis on the differences. In the fourth and final part of this thesis, we will present some open problems.

Acknowledgements

There are many people who have guided me over the years to where I am now. From high school, the three most influential teachers I would like to thank (in alphabetical order) are Mark Bramham, Vincent Gedge, and Stan Kolesnik. From university, the three most influential professors I would like to thank (in alphabetical order) are Achim Kempf, David Siegel (my always patient and helpful supervisor), and John Wainwright.

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Chapter 1

Introduction to the Thesis

Consider the vector ordinary differential equation

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \tag{1.1}$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state vector, t is time, $\dot{} = \frac{d}{dt}$, the matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is Hurwitz[1], and the nonlinear vector field $\mathbf{b} \in C^2(\mathbb{R}^n, \mathbb{R}^n)$ satisfies $\mathbf{b}(\mathbf{0}) = \mathbf{0}$ and $\mathbf{D}\mathbf{b}(\mathbf{0}) = \mathbf{0}$. All solutions with initial condition $\mathbf{x}_0$ sufficiently close to the origin will approach the origin asymptotically as $t \to \infty$. It is very desirable to obtain the asymptotic behaviour of the solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$ as $t \to \infty$ with sufficient detail when $\|\mathbf{x}_0\|$ is sufficiently small. In Part I of this thesis, we will explore an iterative procedure, which is indifferent to resonance in the eigenvalues, to construct asymptotic expansions of $\boldsymbol{\phi}_t(\mathbf{x}_0)$ as $t \to \infty$ with any desired accuracy. This detailed asymptotic behaviour, for example, will enable us to construct phase portraits with more detail than the linearization. Moreover, the detailed behaviour will have implications for concavity results, parameter estimation and reduction methods in chemical kinetics, and it will show the limitations of using traditional power series.

The famous Michaelis-Menten mechanism for an enzyme reaction is given symbolically by

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E,$$

where S is the substrate, E is the enzyme, C is the complex, P is the product, and k_{-1}, k_1, and k_2 are the reaction-rate constants. This leads to the planar system of dimensionless ordinary differential equations

$$\dot{x} = -x + (1 - \eta + x)\, y, \quad \varepsilon\dot{y} = x - (1 + x)\, y, \tag{1.2}$$

[1]That is, all the eigenvalues have real parts that are strictly negative.

where x is a scaled substrate concentration, y is a scaled complex concentration, $\dot{} = \frac{d}{dt}$, $\varepsilon > 0$ is a parameter (generally assumed to be small but in this thesis it can be of any size), and $\eta \in (0, 1)$ is another parameter. In Part II of this thesis, we will derive many new and interesting properties of the planar system. Observe that the planar system (1.2) is indeed in the form of (1.1).

The (nonlinear) Lindemann mechanism for unimolecular decay is given symbolically by

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \overset{k_2}{\to} P,$$

where A is the molecule that decays, B is the activated complex, and P is the product of the decay. This mechanism yields the dimensionless planar system

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = x^2 - y - \varepsilon xy, \tag{1.3}$$

where x is a scaled concentration of A, y is a scaled concentration of B, $\varepsilon > 0$ is a parameter (which can be of any size), and $\dot{} = \frac{d}{dt}$. In Part III of this thesis, we will derive many properties of this planar system. Note that this system is not in the form of (1.1) since the matrix for the linear part is not Hurwitz.

In this introductory chapter, we will explore a few "toy problems." These problems will be similar in spirit to some of the problems we will encounter in this thesis and thus will serve to give the reader a taste of things to come. However, the simplicity of these problems enables us to approach them in a manner that may be different than the approach we would take in a more complicated example.

1.1 Toy Problem 1

Consider the initial value problem

$$\dot{x} = -x - x^2, \quad x(0) = 1, \tag{1.4}$$

where $\dot{} = \frac{d}{dt}$. We will pretend that we cannot solve the initial value problem exactly. Our goal is to obtain non-trivial bounds on the solution $x(t)$ and to establish the (non-trivial) leading-order behaviour.

1.1.1 Bounds on $x(t)$

Observe that $x = 0$ is a solution of the differential equation and $\dot{x} < 0$ when $x = 1$. It follows that $x(t)$ satisfies

$$0 \leq x(t) \leq 1 \quad \text{for all} \quad t \geq 0. \tag{1.5}$$

We can use these simple bounds in conjunction with the differential equation to obtain better bounds. Combining (1.4) and (1.5), we see that

$$-2x(t) \leq \dot{x}(t) \leq -x(t) \quad \text{for all} \quad t \geq 0.$$

That is,

$$\dot{x}(t) + 2x(t) \geq 0 \quad \text{and} \quad \dot{x}(t) + x(t) \leq 0 \quad \text{for all} \quad t \geq 0.$$

If we multiply each inequality by an appropriate exponential integrating factor, replace t by s, and re-arrange, we get

$$\frac{d}{ds}\left(\mathsf{e}^{2s}x(s)\right) \geq 0 \quad \text{and} \quad \frac{d}{ds}\left(\mathsf{e}^{s}x(s)\right) \leq 0 \quad \text{for all} \quad s \geq 0.$$

Now, integrate with respect to s from 0 to t, use the initial condition $x(0) = 1$, and re-arrange the result. This yields

$$\mathsf{e}^{-2t} \leq x(t) \leq \mathsf{e}^{-t} \quad \text{for all} \quad t \geq 0. \tag{1.6}$$

This process can be repeated to obtain even better bounds.

1.1.2 Leading-Order Behaviour of $x(t)$

The initial value problem (1.4) can be written as the integral equation

$$x(t) = \mathsf{e}^{-t} - \mathsf{e}^{-t}\int_0^t \mathsf{e}^{s}x(s)^2\,ds.$$

Importantly, we can re-write this as

$$x(t) = c\,\mathsf{e}^{-t} + \mathsf{e}^{-t}\int_t^\infty \mathsf{e}^{s}x(s)^2\,ds,$$

where

$$c := 1 - \int_0^\infty \mathsf{e}^{s}x(s)^2\,ds.$$

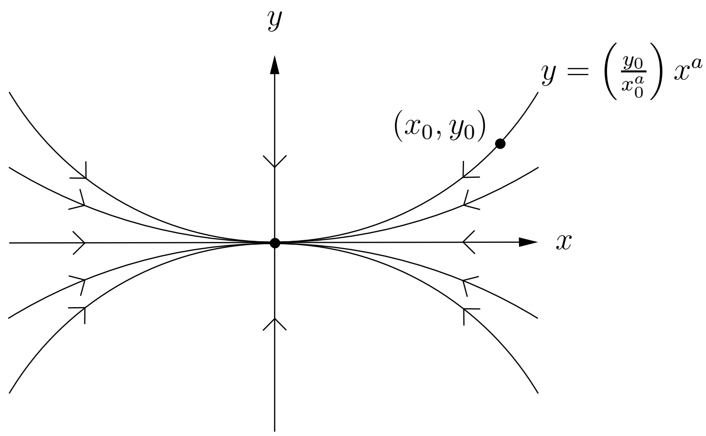

Figure 1.1: A phase portrait for the planar system (1.7).

Note that, by virtue of (1.6),

$$\tfrac{1}{3}\,\mathsf{e}^{-3t} \le \int_t^\infty \mathsf{e}^s x(s)^2\,ds \le \mathsf{e}^{-t} \quad \text{for all} \quad t \ge 0.$$

It follows that we can write

$$c\,\mathsf{e}^{-t} \le x(t) \le \mathsf{e}^{-t} \quad \text{for all} \quad t \ge 0 \quad \text{and} \quad x(t) = c\,\mathsf{e}^{-t} + \mathcal{O}\big(\mathsf{e}^{-2t}\big) \quad \text{as} \quad t \to \infty$$

for some $c \in \big(0, \frac{2}{3}\big)$. (Appealing to the bounds (1.6) and the fact that $x(t) \not\equiv \mathsf{e}^{-2t}$ and $x(t) \not\equiv \mathsf{e}^{-t}$, we cannot have $c = 0$ or $c = \frac{2}{3}$.) The techniques we will develop in Chapter 3 can be used to show that $c = \frac{1}{2}$.

1.2 Toy Problem 2

Consider the linear system

$$\dot{x} = -x, \quad \dot{y} = -ay, \tag{1.7}$$

where $a > 1$ is a constant and $\dot{} = \frac{d}{dt}$. The corresponding scalar differential equation is

$$y' = \frac{ay}{x}, \tag{1.8}$$

where $' = \frac{d}{dx}$. See Figure 1.1, which gives the phase portrait. We will restrict attention to $x > 0$.

1.2.1 Antifunnel

The solution $y = 0$ to the scalar differential equation (1.8) is an exceptional solution which appears to attract all other scalar solutions. Define the region

$$\Gamma_b := \left\{ \ (x, y) \ : \ x > 0, \ \ -x\,\mathrm{e}^{-bx} \le y \le x\,\mathrm{e}^{-bx} \ \right\} \quad (b > 0)\,, \tag{1.9}$$

which is an example of an antifunnel. (See §A.3 for a discussion on antifunnels.) It can be shown using the Antifunnel Theorem (see Theorem A.4) and other techniques that any solution to (1.7) with $x(0) > 0$ will eventually enter and remain inside the so-called trapping region Γ_b. Moreover, the solution $y = 0$ is the only solution to (1.8) contained entirely in Γ_b. In Parts II and III of this thesis, we will deal with planar systems, namely (1.2) and (1.3), having trapping regions which contain a unique attracting solution (called a slow manifold).

1.2.2 Fraser Iterative Scheme

Consider the scalar differential equation (1.8). If we choose an initial function $y_0(x)$, we can define an iterative scheme

$$y_{n+1}(x) := \frac{x y_n'(x)}{a} \quad (n \in \mathbb{N}_0)\,,$$

where $\mathbb{N}_0 := \{0, 1, 2, \ldots\}$. This can be referred to as the Fraser iterative scheme, after Simon Fraser who used the scheme to approximate the slow manifold for both the Michaelis-Menten mechanism and the Lindemann mechanism. See, for example, [43].

Finding the Iterates using a Generating Function

Define the exponential generating function

$$w(x, \tau) := \sum_{n=0}^{\infty} \frac{y_n(x)}{n!}\,\tau^n,$$

where $\{y_n(x)\}_{n=0}^{\infty}$ are the Fraser iterates. Note that

$$y_n(x) = \frac{\partial^n w}{\partial \tau^n}(x, 0) \quad \text{for all} \quad n \in \mathbb{N}_0.$$

See, for example, pages 60–61 of [77] and [128] for a discussion on generating functions.

Observe that

$$\frac{\partial w}{\partial x}(x, \tau) = \sum_{n=0}^{\infty} \frac{y_n'(x)}{n!}\,\tau^n \quad \text{and} \quad \frac{\partial w}{\partial \tau}(x, \tau) = \sum_{n=0}^{\infty} \frac{y_{n+1}(x)}{n!}\,\tau^n.$$

Since $ay_{n+1}(x) = xy_n'(x)$, we see that $w(x,\tau)$ satisfies the partial differential equation and initial condition

$$x\,\frac{\partial w}{\partial x} - a\,\frac{\partial w}{\partial \tau} = 0, \quad w(x,0) = y_0(x).$$

We will use the method of characteristics (see §A.12 of Appendix A) to solve this. Consider the initial value problem

$$\left(\frac{dx}{dr}, \frac{d\tau}{dr}, \frac{dw}{dr}\right) = (x, -a, 0)\,, \quad (x(0), \tau(0), w(0)) = (s, 0, y_0(s))\,,$$

which describes a curve parameterized by r in the solution surface $w(x,\tau)$. Solving gives

$$x = s\,\mathsf{e}^{r}, \quad \tau = -ar, \quad w = y_0(s).$$

Solving the first two equations for s in terms of x and τ gives $s = x\,\mathsf{exp}\left(\frac{\tau}{a}\right)$. Thus, the generating function is given by

$$w(x,\tau) = y_0\left(x\,\mathsf{exp}\left(\frac{\tau}{a}\right)\right).$$

Initial Iterate $y_0(x) = x^c$

Suppose that we choose $y_0(x) := x^c$, where $c > 0$. Then, the generating function is given by

$$w(x,\tau) = x^c\,\mathsf{exp}\left(\frac{c\tau}{a}\right).$$

Thus, the Fraser iterates are given by

$$y_n(x) = \left(\frac{c}{a}\right)^n x^c \quad (n \in \mathbb{N}_0)\,.$$

Clearly, if $c < a$ then the Fraser iterates converge pointwise to the solution $y = 0$ and if $c > a$ then the iterates diverge.

Initial Iterate $y_0(x) = \mathsf{e}^x$

Suppose now that $y_0(x) := \mathsf{e}^x$. Then, the generating function is given by

$$w(x,\tau) = \mathsf{exp}\left(x\,\mathsf{exp}\left(\frac{\tau}{a}\right)\right).$$

Interestingly, we can write this as

$$w(x,\tau) = \mathsf{e}^x\left[\sum_{n=0}^{\infty} \frac{\phi_n(x)}{a^n n!}\,\tau^n\right],$$

where $\{\phi_n(x)\}_{n=0}^{\infty}$ are the exponential polynomials (which are also called the Touchard polynomials). See, for example, [7] or pages 63–67 of [103]. Consequently, the Fraser iterates are

$$y_n(x) = \frac{\mathsf{e}^x \phi_n(x)}{a^n} \quad (n \in \mathbb{N}_0).$$

Observe that

$$y_n(1) = \frac{\mathsf{e} B_n}{a^n} \quad \text{and} \quad \frac{y_{n+1}(1)}{y_n(1)} = \left(\frac{1}{a}\right)\left(\frac{B_{n+1}}{B_n}\right) \quad (n \in \mathbb{N}_0),$$

where $\{B_n\}_{n=0}^{\infty}$ are the Bell numbers. Since $\lim\limits_{n\to\infty} \dfrac{B_{n+1}}{B_n} = \infty$, it follows that $\lim\limits_{n\to\infty} y_n(1) = \infty$.

1.3 Toy Problem 3

Consider now the nonlinear planar system

$$\dot{x} = -x + xy, \quad \dot{y} = -ay - xy, \tag{1.10}$$

where $a > 1$ is a constant and $\dot{} = \frac{d}{dt}$. This system could arise, for example, from applying the Law of Mass Action (see §A.1 of Appendix A) to the chemical mechanism

$$X + Y \xrightarrow{1} 2X, \quad X \xrightarrow{1} P_1, \quad Y \xrightarrow{a} P_2,$$

where P_1 and P_2 are arbitrary products. The corresponding scalar differential equation is

$$y' = \frac{(a+x)\,y}{x\,(1-y)}, \tag{1.11}$$

where $' = \frac{d}{dx}$. We will consider only $x > 0$. See Figure 1.2.

1.3.1 Antifunnel

The solution $y = 0$, as with the linearized system, is an exceptional solution which attracts all other solutions. In fact, the region Γ_b, which was defined in (1.9), is a trapping region for the nonlinear system just like it is for the linear system. Again, the solution $y = 0$ (the slow manifold) is the only scalar solution which is contained entirely inside Γ_b.

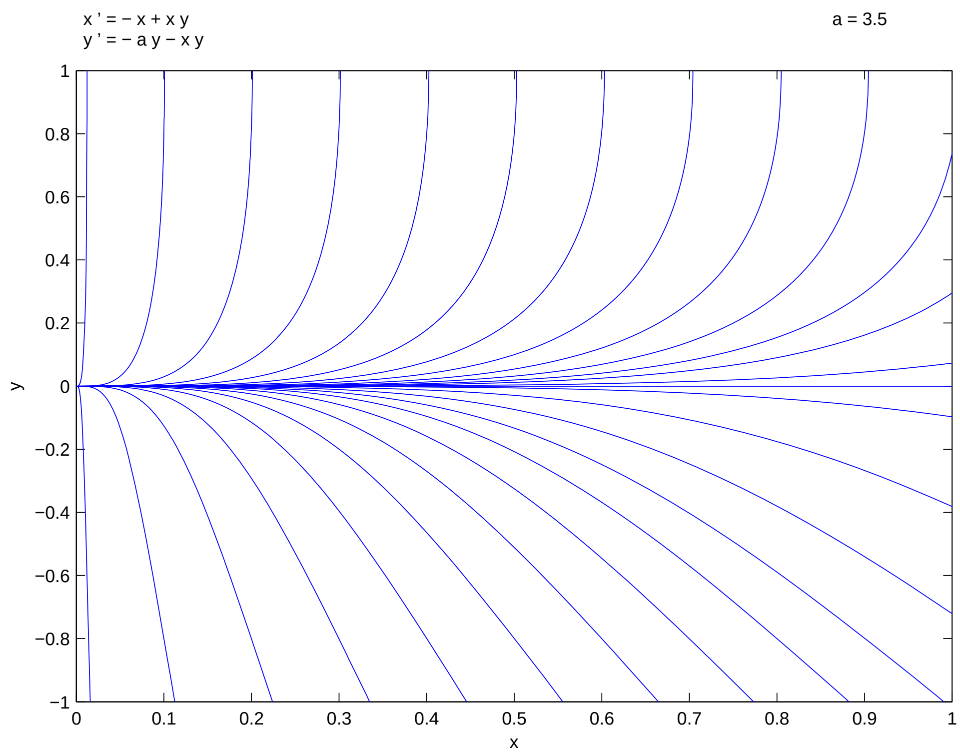

Figure 1.2: A phase portrait for the nonlinear planar system (1.10) for $a = 3.5$.

1.3.2 Exact solution of the scalar differential equation

The scalar differential equation (1.11) can be solved exactly in terms of the Lambert W function (see §A.16 of Appendix A). Write the differential equation as

$$\left[\frac{1}{y(s)} - 1\right] y'(s) = \frac{a}{s} + 1 \quad \text{for} \quad s > 0.$$

If we integrate with respect to s from x_0 to x and apply the initial condition $y(x_0) = y_0$, where $x_0, y_0 > 0$ for simplicity, we get

$$\ln\left(\frac{y(x)}{y_0}\right) - y(x) + y_0 = a \ln\left(\frac{x}{x_0}\right) + x - x_0.$$

Taking the exponential of both sides and re-arranging,

$$-y(x)\,\mathrm{e}^{-y(x)} = -\left(\frac{y_0}{x_0^a\,\mathrm{e}^{x_0+y_0}}\right) x^a\,\mathrm{e}^x.$$

By definition of the Lambert W function, we obtain the explicit solution

$$y(x) = -W\left(-\left[\frac{y_0}{x_0^a \, \mathsf{e}^{x_0+y_0}}\right] x^a \, \mathsf{e}^x\right).$$

Since $W(x) = x + \mathsf{o}(x)$ as $x \to 0$, we can say

$$y(x) = \left[\frac{y_0}{x_0^a \, \mathsf{e}^{x_0+y_0}}\right] x^a + \mathsf{o}(x^a) \quad \text{as} \quad x \to 0^+.$$

Observe that if $a \notin \{2, 3, \ldots\}$ then $y(x)$ is not representable as a Taylor series at $x = 0$. However, applying the power series method to the scalar differential equation (1.11) yields the zero series.

1.4 Comments on this Thesis

1.4.1 Structure

This thesis is divided into four parts. Part I deals with iterative schemes which determine the asymptotic behaviour of solutions of a certain class of nonlinear vector differential equations as they approach a sink. Part II deals with properties of the Michaelis-Menten mechanism of a single enzyme-substrate reaction. Part III deals with the Lindemann mechanism of unimolecular decay. Part IV consists of a chapter on open problems as well as the appendix. Each part (except Part IV) has an introductory chapter (where the problem and literature are introduced), a main chapter (where the fundamental results are established), and additional specialized chapters.

This thesis is intended to be reader-friendly and leisurely yet rigorous. Simple examples are included frequently where appropriate. Most chapters conclude with a brief summary of essential material in the chapter. Moreover, Appendix A includes a review of some results and concepts which are used in the thesis. Finally, Appendix B includes some interesting results or approaches which have not been fully explored, have led to issues which have not been overcome, or otherwise do not fit in anywhere else.

1.4.2 Goals and Themes

There are many goals and themes that are common in this thesis.

- Obtaining (non-trivial) leading-order behaviour as $t \to \infty$ for solutions $\mathbf{x}(t)$ of certain nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$.

- Obtaining simple bounds on solutions $\mathbf{x}(t)$ of certain nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$ valid for all $t \geq 0$. Differential inequalities are a common tool used for this purpose.

- Obtaining asymptotic expansions for x_2 in terms of x_1 as $x_1 \to 0$ for solutions $\mathbf{x}(t)$ of certain planar nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$.

- Handling resonance in the eigenvalues for certain nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$.

- Finding approximations to solutions of certain nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$ which are also flows.

- Establishing concavity for solutions of certain scalar nonlinear differential equations $y' = f(x, y)$.

- Utilizing isoclines (other than the horizontal and vertical) to analyze certain scalar nonlinear differential equations $y' = f(x, y)$.

- Proving the existence and uniqueness of a solution in a trapping region for certain scalar nonlinear differential equations $y' = f(x, y)$. To achieve these results, we use antifunnels.

- Estimating the time for solutions $\mathbf{x}(t)$ to enter a trapping region for certain nonlinear differential equations $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$.

- The Lambert W function makes many fundamental appearances.

Part I

Asymptotics Near a Nonlinear Sink

Chapter 2

Introduction

Part I of this thesis is concerned with the determination of asymptotic behaviour of solutions of systems of ordinary differential equations as they approach a nonlinear sink.[1] Many known applicable results may quickly come to mind, such as the Hartman-Grobman Theorem, Poincaré's Theorem, and normal form theory. However, a certain limitation of the Hartman-Grobman Theorem, Poincaré's Theorem, and normal form theory also quickly comes to mind, namely resonance. The techniques of this part of the thesis, fortunately, are not hindered by resonance.

Remark 2.1: Part III of this thesis deals with a system that has a non-hyperbolic equilibrium. In particular, this equilibrium point is a saddle node. Some attention is given to determining the asymptotic behaviour of solutions as they approach this equilibrium. See §A.8 of Appendix A which gives a brief overview of the classification of equilibrium points.

2.1 The Problem

Let $n \in \mathbb{N}$ and consider the constant matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ and vector field $\mathbf{b} : \mathbb{R}^n \to \mathbb{R}^n$. The system of ordinary differential equations under consideration is

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n, \quad \dot{} = \frac{d}{dt},$$

where $\mathbf{A}$ and $\mathbf{b}$ have certain properties which we will outline below.

[1] An equilibrium point is a sink if the linearization matrix at this point only has eigenvalues with strictly negative real parts. Consequently, all nearby solutions approach the equilibrium point asymptotically. The "nonlinear" of "nonlinear sink" merely emphasizes the fact that it results from a nonlinear differential equation.

2.1.1 The Matrix A

The matrix $\mathbf{A}$ is assumed to be Hurwitz with eigenvalues $\{\lambda_i\}_{i=1}^n$ which have respective negative real parts $\{\mu_i\}_{i=1}^n$. Moreover, we will assume a specific ordering of the eigenvalues.

Assumption 2.2: The real parts of the eigenvalues of the matrix $\mathbf{A}$ satisfy

$$\mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1 < 0. \tag{2.1}$$

A very crucial ratio is given by

$$\kappa := \frac{\mu_n}{\mu_1}, \tag{2.2}$$

which quantifies the spacing of the eigenvalues. Observe that $\kappa \geq 1$. The significance of the ratio between eigenvalues has been noted before. See, for example, $II.3 of [16].

Remark 2.3: In this chapter, as well as other chapters in this part of the thesis, the constants $\{\mu_i\}_{i=1}^n$ are understood to be the real parts of the eigenvalues of $\mathbf{A}$ and satisfy (2.1). Furthermore, the constant κ is understood to be the ratio in (2.2).

2.1.2 The Vector Field b

The $\mathbf{b}(\mathbf{x})$ term in the differential equation encapsulates the nonlinear part. We will need to make an assumption on the minimum amount of smoothness possessed by $\mathbf{b}(\mathbf{x})$. Moreover, we need to specify the basic decay rate of $\mathbf{b}(\mathbf{x})$ and $\mathbf{Db}(\mathbf{x})$, where the notation $\mathbf{D} := \frac{\partial}{\partial \mathbf{x}}$ denotes the derivative operator. In particular, the Jacobian of $\mathbf{b}$ is given by

$$\mathbf{Db} = \left\{ \frac{\partial b_i}{\partial x_j} \right\}_{i,j=1}^n = \begin{pmatrix} \frac{\partial b_1}{\partial x_1} & \cdots & \frac{\partial b_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial b_n}{\partial x_1} & \cdots & \frac{\partial b_n}{\partial x_n} \end{pmatrix}.$$

Note that we will be using the notation $B_r(\mathbf{p})$ and B_r to denote, respectively, the open balls in $\mathbb{R}^n$ of radius r centred at $\mathbf{p}$ and $\mathbf{0}$.

Assumption 2.4: Consider the vector field $\mathbf{b}$.

(a) There is some neighbourhood $\mathcal{N} \subset \mathbb{R}^n$ with $\mathbf{0} \in \mathcal{N}$ and $\mathbf{b} \in C^1(\mathcal{N}, \mathbb{R}^n)$.

(b) There are $\delta, k > 0$ such that $B_\delta \subset \mathcal{N}$ and

$$\|\mathbf{b}(\mathbf{x})\| \leq k \|\mathbf{x}\|^\alpha \quad \text{for all} \quad \mathbf{x} \in B_\delta, \tag{2.3}$$

where $\alpha > 1$ is a fixed parameter.

(c) There are $\delta, k > 0$ such that $B_\delta \subset \mathcal{N}$ and

$$\|\mathbf{Db}(\mathbf{x})\| \leq k \|\mathbf{x}\|^\beta \quad \text{for all} \quad \mathbf{x} \in B_\delta, \tag{2.4}$$

where $\beta > 0$ is a fixed parameter.

Observe that these assumptions imply

$$\mathbf{b}(\mathbf{0}) = \mathbf{0} \quad \text{and} \quad \mathbf{Db}(\mathbf{0}) = \mathbf{0}$$

which, among other things, means that the origin is an equilibrium point of the given system. Since $\mathbf{A}$ is Hurwitz, we can conclude that the origin is asymptotically stable.

Definition 2.5: Consider the matrix $\mathbf{A}$ and vector field $\mathbf{b}$. If $1 \leq \kappa < \alpha$, we will say that the eigenvalues of $\mathbf{A}$ are *closely-spaced* relative to the vector field $\mathbf{b}$. If $\kappa \geq \alpha$, we will say that the eigenvalues of $\mathbf{A}$ are *widely-spaced* relative to the vector field $\mathbf{b}$.

The distinction of closely-spaced and widely-spaced eigenvalues turns out to be of fundamental importance. Moreover, note that this distinction does not make reference to resonance in the eigenvalues.

Remarks 2.6:

(i) In this chapter, as well as other chapters in this part of the thesis, the constants α and β are understood to be as in (2.3) and (2.4).

(ii) The constants δ, k in (2.3) are only used to establish a decay rate. We will be dealing with many precise estimates (and combinations of estimates) which are introduced by saying something like "there are constants $\delta, k > 0$ such that..." The scope of where these constants retain their meaning is usually clear from the context. The important point is that there are some constants such that a given inequality is true.

(iii) Sometimes an optimal[2] choice for α and β is clear, for example $b(x) = x^2$, and sometimes an optimal choice is not clear, for example $b(x) = x^2 \ln(x)$ with $b(0) = 0$. In the former example,

[2] As we will see, higher values of α and β yield better approximations to the solution. Moreover, our choice of α might be the difference of the eigenvalues being closely-spaced (the "easy" case) or widely-spaced (the "hard" case).

we can take $\alpha = 2$ and $\beta = 1$. In the latter example, however, any $\alpha \in (1, 2)$ will satisfy (2.3) and any $\beta \in (0, 1)$ will satisfy (2.4) with no optimal choices for the decay rates.

(iv) Suppose that $\mathbf{b} \in C^r(\mathcal{N}, \mathbb{R}^n)$, where $r \in \{2, 3, \ldots\}$, with[3] $D^\xi b_i(\mathbf{0}) = 0$ for all $i \in \{1, 2, \ldots, n\}$ and $|\xi| \le r - 1$. Then, if we wish, we can take $\alpha = r$ and $\beta = r - 1$. This follows from Taylor's Theorem. In the scalar case, $n = 1$, for each $m \in \{0, \ldots, r-1\}$ we have

$$b^{(m)}(x) = \sum_{i=0}^{r-m-1} \frac{b^{(m+i)}(0)}{i!}\, x^i + \mathcal{O}\big(x^{r-m}\big) = \mathcal{O}\big(x^{r-m}\big) \quad \text{as} \quad x \to 0.$$

In particular, setting $m = 0$ and $m = 1$ gives $b(x) = \mathcal{O}(x^r)$ and $b'(x) = \mathcal{O}\big(x^{r-1}\big)$ as $x \to 0$.

(v) For a given α, it need not be the case that $\beta = \alpha - 1$. After all, one cannot differentiate asymptotic expressions in general. Consider $b(x) := x^4 \sin\big(\frac{1}{x}\big)$ with it understood that $b(0) = 0$. Now, for $x \neq 0$ we have

$$b'(x) = 4\,x^3 \sin\big(\tfrac{1}{x}\big) - x^2 \cos\big(\tfrac{1}{x}\big) \quad \text{and} \quad b''(x) = 12\,x^2 \sin\big(\tfrac{1}{x}\big) - 6\,x \cos\big(\tfrac{1}{x}\big) - \sin\big(\tfrac{1}{x}\big)\,.$$

Observe that $b \in C^1$ but $b \notin C^2$. Moreover, $|b(x)| \le |x|^4$ for all x. However, $\left|\frac{b'(x)}{x^3}\right|$ is unbounded in any neighbourhood of the origin. Hence we can take $\alpha = 4$ (which is the natural choice for α) but we cannot take $\beta = 3$. The optimal choices are $\alpha = 4$ and $\beta = 2$.

2.1.3 The System $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$

Consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{2.5}$$

where $\mathbf{x} \in \mathbb{R}^n$ and $\dot{} = \frac{d}{dt}$. The system has the origin as an equilibrium point. As is customary, we will denote by $\boldsymbol{\phi}_t(\mathbf{x}_0)$ the flow of (2.5). That is, $\boldsymbol{\phi}_t(\mathbf{x}_0)$ is the solution of the initial value problem as a function of the initial condition $\mathbf{x}_0$. The goal of this part of the thesis is to determine the detailed behaviour of solutions to (2.5) near the origin. That is, we want to find asymptotic expansions of $\boldsymbol{\phi}_t(\mathbf{x}_0)$ as $t \to \infty$ when $\|\mathbf{x}_0\|$ is sufficiently small.

[3] We are using multi-index notation to indicate all the possible derivatives of order at most $r - 1$.

2.1.4 Integral Equation

Equivalently, the initial value problem (2.5) can be re-written as an integral equation. Multiply the differential equation by the integrating factor $\mathsf{e}^{-t\mathbf{A}}$ and then replace t by s, giving

$$\mathsf{e}^{-s\mathbf{A}}\left[\dot{\mathbf{x}}(s) - \mathbf{A}\mathbf{x}(s)\right] = \mathsf{e}^{-s\mathbf{A}}\mathbf{b}(\mathbf{x}(s)).$$

Simplifying the left-hand side,

$$\frac{d}{ds}\left(\mathsf{e}^{-s\mathbf{A}}\mathbf{x}(s)\right) = \mathsf{e}^{-s\mathbf{A}}\mathbf{b}(\mathbf{x}(s)).$$

If we integrate with respect to s from 0 to t, we get

$$\mathsf{e}^{-t\mathbf{A}}\mathbf{x}(t) - \mathbf{x}_0 = \int_0^t \mathsf{e}^{-s\mathbf{A}}\mathbf{b}(\mathbf{x}(s))\,ds.$$

Solving for $\mathbf{x}(t)$, we are left with the integral equation

$$\mathbf{x}(t) = \mathsf{e}^{t\mathbf{A}}\mathbf{x}_0 + \int_0^t \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{b}(\mathbf{x}(s))\,ds. \tag{2.6}$$

2.1.5 Resonance

The techniques developed in this part of the thesis will work regardless of resonance, but we still need to be mindful of when resonance might occur. The reader may wish to consult §A.9 of Appendix A which reviews resonance.

Proposition 2.7: *Resonance in the eigenvalues of $\boldsymbol{A}$ can only occur if $\kappa \geq 2$.*

Proof: Suppose that there is resonance. By definition of resonance, there is an index $j \in \{1, \dots, n\}$ and set of coefficients $\{m_i\}_{i=1}^n \subset \mathbb{N}_0$ such that

$$\lambda_j = \sum_{i=1}^n m_i\lambda_i \quad \text{and} \quad \sum_{i=1}^n m_i \geq 2.$$

Taking the real part of the first equation and re-writing (2.1), we have

$$\mu_j = \sum_{i=1}^n m_i\mu_i \quad \text{and} \quad 0 < -\mu_1 \leq \cdots \leq -\mu_n.$$

It follows that

$$-\mu_n \geq -\mu_j = \sum_{i=1}^n m_i(-\mu_i) \geq \left(\sum_{i=1}^n m_i\right)(-\mu_1) \geq 2(-\mu_1).$$

That is, $\mu_n \leq 2\mu_1$ which is equivalent to $\kappa \geq 2$. □

2.2 Functions Defined By Integrals

In this part of the thesis, we will be dealing heavily with exponential estimates and improper integrals. Most importantly, we will be constructing approximations to solutions of (2.5) whose definitions involve improper integrals. Two good references for this material are §14.4-14.9 of [3] and §6.5 of [81].

We will be dealing with a certain class of functions defined by improper integrals. Let $\delta > 0$ be a constant and define the set

$$\Omega_\delta := \{ \ (t, \mathbf{x}) \ \ : \ t \geq 0, \ \mathbf{x} \in \mathbb{R}^n, \ \ \|\mathbf{x}\| < \delta \ \} .$$

Suppose that for the function $\mathbf{F} \in C^1(\Omega_\delta, \mathbb{R}^n)$, there are $k, \rho > 0$ such that

$$\|\mathbf{F}(t, \mathbf{x})\| \leq k \,\mathsf{e}^{-\rho t} \quad \text{for all} \quad (t, \mathbf{x}) \in \Omega_\delta.$$

Hence, we consider the function

$$\mathbf{f}(t, \mathbf{x}) := \int_t^\infty \mathbf{F}(s, \mathbf{x}) \, ds, \quad (t, \mathbf{x}) \in \Omega_\delta.$$

Observe that, for all $(t, \mathbf{x}) \in \Omega_\delta$,

$$\left\| \int_t^\infty \mathbf{F}(s, \mathbf{x}) \, ds \right\| \leq \int_t^\infty \|\mathbf{F}(s, \mathbf{x})\| \ ds \leq \int_t^\infty \left(k \,\mathsf{e}^{-\rho s} \right) \ ds = \left(\frac{k}{\rho} \right) \mathsf{e}^{-\rho t} \leq \frac{k}{\rho}.$$

It follows from the Weierstrass M-Test that the integral converges uniformly on Ω_δ and $\mathbf{f}$ is continuous on Ω_δ. Furthermore, if there are $\ell, \eta > 0$ such that

$$\left\| \frac{\partial \mathbf{F}}{\partial \mathbf{x}}(t, \mathbf{x}) \right\| \leq \ell \,\mathsf{e}^{-\eta t} \quad \text{for all} \quad (t, \mathbf{x}) \in \Omega_\delta,$$

then we can differentiate $\mathbf{f}(t, \mathbf{x})$ under the integral sign, giving

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}}(t, \mathbf{x}) = \int_t^\infty \frac{\partial \mathbf{F}}{\partial \mathbf{x}}(s, \mathbf{x}) \, ds, \quad (t, \mathbf{x}) \in \Omega_\delta,$$

where the integral converges uniformly in Ω_δ. See, for example, Theorems 14-19, 14-22, and 14-24 of [3].

There is one other possibility we should mention. Suppose that for the function $\mathbf{F}$ above, we have instead $\mathbf{x} \in \mathbb{C}^n$ and $\mathbf{F}(t, \mathbf{x}) \in \mathbb{C}^n$ with $\mathbf{F}$ complex analytic at $\mathbf{0}$. Then, $\mathbf{f}$ is complex analytic at $\mathbf{0}$ and derivatives of $\mathbf{f}$ of any order can found by differentiating under the integral sign. It follows from this that $\mathbf{f}$ is real analytic in $\mathbf{x}$ at $\mathbf{0}$. See, for example, §6.5 of [81].

2.3 Important Exponential Estimates

2.3.1 The Need for σ

Many of the results that follow in this part of the thesis are established by considering exponential estimates of functions of time. In particular, these estimates are of the form

$$|u(t)| \leq k\,\mathsf{e}^{(a+\sigma)t} \quad \text{for} \quad t \geq 0,$$

where a is some constant inherent to the problem at hand and $\sigma > 0$ is some constant included to accommodate the possible effects of repeated eigenvalues and resonance. Typically, σ is taken to be as small as one desires. In the above example, if $a < 0$ we would assume that $\sigma < -a$ so as to preserve the decaying property of the exponential. However, any positive value of σ would not change the truth of the statement.

Why exactly is the σ necessary? When there is resonance or there are repeated eigenvalues, solutions of ordinary differential equations may have terms of the form $t^m\mathsf{e}^{at}$. We will look at the necessity of σ more closely.

Let $u(t) := t^m\mathsf{e}^{at}$, where $m \in \mathbb{N}$ and $a < 0$ are constants. We will make a few observations about the decay rate of $u(t)$.

- There does not exist a constant $k > 0$ such that $|u(t)| \leq k\,\mathsf{e}^{at}$ for all $t \geq 0$. This is because $\left|u(t)\,\mathsf{e}^{-at}\right| = t^m$ is unbounded as $t \to \infty$.

- For any $\sigma > 0$, there exists a constant $k > 0$ such that $|u(t)| \leq k\,\mathsf{e}^{(a+\sigma)t}$ for all $t \geq 0$. This is because $\left|u(t)\,\mathsf{e}^{-(a+\sigma)t}\right| = t^m\mathsf{e}^{-\sigma t}$ is bounded for all $t \geq 0$.

- There does not exist a $k > 0$ such that $|u(t)| \leq k\,\mathsf{e}^{(a+\sigma)t}$ for all $t \geq 0$ and for all $\sigma > 0$. This is because $\left|u(t)\,\mathsf{e}^{-(a+\sigma)t}\right| = t^m\mathsf{e}^{-\sigma t}$ achieves the maximum value $\left(\frac{m}{\sigma\mathsf{e}}\right)^m$ for a given $\sigma > 0$ and this maximum value is unbounded as $\sigma \to 0^+$.

Remarks 2.8:

(i) Note the position of the $\sigma > 0$ in the second and third observations above. In this thesis, the (arbitrary) choice of $\sigma > 0$ is made at the beginning of the calculation of exponential estimates.

(ii) Let $u(t)$ be an arbitrary function. Suppose that for any $\sigma > 0$ there is a $k > 0$ (which depends on σ) such that

$$|u(t)| \leq k\,\mathsf{e}^{(a+\sigma)t} \quad \text{for all} \quad t \geq 0.$$

Then,

$$\frac{\ln|u(t)|}{t} \leq a + \sigma + \frac{\ln k}{t}.$$

Since $\sigma > 0$ is arbitrary and k is a constant (with respect to t), it follows that

$$\limsup_{t\to\infty} \frac{\ln|u(t)|}{t} \leq a.$$

This is an equivalent way of indicating the exponential decay rate of $u(t)$. It is the prevalent way in, for example, Chapter 13 of [28]. In this thesis, however, the exponential way is of practical benefit. Note that if $u(t) = 0$ for some $t \geq 0$ we take $\ln|u(t)| = -\infty$ by extending the logarithmic function.

2.3.2 Decay Rate of the Matrix Exponential

For obvious reasons, the decay rate of the matrix exponential $\mathsf{e}^{t\mathbf{A}}$ will be of fundamental importance to us. Intuitively, we would expect that, for large time, the size of the matrix exponential $\mathsf{e}^{t\mathbf{A}}$ decays at a rate determined by the slowest eigenvalue in real part. In turn, the decay rate of $\boldsymbol{\phi}_t(\mathbf{x}_0)$ should have this same decay rate. This is indeed the case.

Claim 2.9: *Let* $\mathbf{\Lambda} := \mathit{diag}(\mu_1, \ldots, \mu_n)$*. Then,*

$$\mathsf{e}^{\mu_n t} \leq \left\|\mathsf{e}^{t\mathbf{\Lambda}}\right\| \leq \mathsf{e}^{\mu_1 t} \quad \textit{and} \quad \mathsf{e}^{-\mu_1 t} \leq \left\|\mathsf{e}^{-t\mathbf{\Lambda}}\right\| \leq \mathsf{e}^{-\mu_n t} \quad \textit{for all} \quad t \geq 0.$$

Proof: We will only prove the bounds on $\left\|\mathsf{e}^{t\mathbf{\Lambda}}\right\|$ for $t \geq 0$ since the bounds for $\left\|\mathsf{e}^{-t\mathbf{\Lambda}}\right\|$ are similarly proven. Now, we know

$$\mathsf{e}^{t\mathbf{\Lambda}} = \mathsf{diag}\left(\mathsf{e}^{\mu_1 t}, \ldots, \mathsf{e}^{\mu_2 t}\right) \quad \text{and} \quad \mathsf{e}^{t\mathbf{\Lambda}}\mathbf{x} = \left(\mathsf{e}^{\mu_1 t}x_1, \ldots, \mathsf{e}^{\mu_n t}x_n\right)^T.$$

It follows that, for $t \geq 0$,

$$\left\|\mathsf{e}^{t\mathbf{\Lambda}}\right\| = \max_{\|\mathbf{x}\|=1}\left\{\left\|\mathsf{e}^{t\mathbf{\Lambda}}\mathbf{x}\right\|\right\} = \max_{\|\mathbf{x}\|=1}\left\{\sqrt{\sum_{i=1}^{n}\mathsf{e}^{2\mu_i t}x_i^2}\right\} \leq \max_{\|\mathbf{x}\|=1}\left\{\mathsf{e}^{\mu_1 t}\sqrt{\sum_{i=1}^{n}x_i^2}\right\} = \mathsf{e}^{\mu_1 t}.$$

Furthermore, if we choose $\mathbf{x} = (0, \ldots, 0, 1)^T$ we see that

$$\left\| \mathsf{e}^{t\boldsymbol{\Lambda}} \right\| = \max_{\|\mathbf{x}\|=1} \left\{ \sqrt{\sum_{i=1}^{n} \mathsf{e}^{2\mu_i t} x_i^2} \right\} \geq \mathsf{e}^{\mu_n t}.$$

□

If $\mathbf{A}$ is not diagonal, there may be terms like $t^i \mathsf{e}^{\lambda_j t}$ in the matrix exponential and so we need to introduce σ in the basic decay rate of $\mathsf{e}^{t\mathbf{A}}$. What follows is a standard result for the decay rate of $\mathsf{e}^{t\mathbf{A}}$. However, we append a condition which tells us when we can ignore the σ. As we shall see, the presence (or absence) of σ in the decay rate of $\mathsf{e}^{t\mathbf{A}}$ has a ripple effect on many calculations which appear in the following chapters.

Lemma 2.10: *Consider the matrix $\boldsymbol{A}$ and let $\sigma > 0$.*

(a) There is a $k > 0$ such that

$$\left\| \mathsf{e}^{t\boldsymbol{A}} \right\| \leq k\, \mathsf{e}^{(\mu_1 + \sigma)t} \quad \textit{for all} \quad t \geq 0. \tag{2.7}$$

(b) There is a $k > 0$ such that

$$\left\| \mathsf{e}^{-t\boldsymbol{A}} \right\| \leq k\, \mathsf{e}^{(-\mu_n + \sigma)t} \quad \textit{for all} \quad t \geq 0. \tag{2.8}$$

(c) If $\boldsymbol{A}$ is diagonalizable, then we may take $\sigma = 0$ in (2.7) *and* (2.8).

Proof:

(a) It follows from the fact that the elements of $\mathsf{e}^{t\mathbf{A}}$ are linear combinations of terms of the form $t^i \mathsf{e}^{\lambda_j t}$, where $i \in \{0, \ldots, n-1\}$ and $j \in \{1, \ldots, n\}$.

(b) Similar to the previous part.

(c) If $\mathbf{A}$ is diagonalizable, there exists an invertible matrix $\mathbf{P}$ such that $\mathbf{A} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{-1}$, where $\boldsymbol{\Lambda} := \mathsf{diag}\,(\lambda_1, \ldots, \lambda_n)$. A standard result tells us that $\mathsf{e}^{t\mathbf{A}} = \mathbf{P}\mathsf{e}^{t\boldsymbol{\Lambda}}\mathbf{P}^{-1}$. By Claim 2.9,

$$\left\| \mathsf{e}^{t\mathbf{A}} \right\| \leq \|\mathbf{P}\| \left\| \mathbf{P}^{-1} \right\| \mathsf{e}^{\mu_1 t} \quad \text{and} \quad \left\| \mathsf{e}^{-t\mathbf{A}} \right\| \leq \|\mathbf{P}\| \left\| \mathbf{P}^{-1} \right\| \mathsf{e}^{-\mu_n t} \quad \text{for all} \quad t \geq 0.$$

□

Remark 2.11: Suppose that $\mathbf{A}$ is not diagonalizable. Let $\mathbf{J}$ be the Jordan canonical form. (Jordan forms are mentioned in §A.15 of Appendix A.) Then, there exists an invertible matrix $\mathbf{P}$ such that $\mathbf{A} = \mathbf{PJP}^{-1}$. Consequently, $\mathrm{e}^{t\mathbf{A}} = \mathbf{P}\mathrm{e}^{t\mathbf{J}}\mathbf{P}^{-1}$. Since $\mathbf{A}$ is not diagonalizable, $\mathbf{J}$ has a Jordan block which is not a diagonal matrix. Hence, there will be at least one term of the form $t^i\mathrm{e}^{\lambda_j t}$ for $i \in \{1, \ldots, n-1\}$ and $j \in \{1, \ldots, n\}$. See, for example, Chapter 3 of [28] and Chapter 1 of [100].

2.3.3 Decay Rate of the Flow

The matrix $\mathbf{A}$ is Hurwitz and hence all solutions of the linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$ approach the origin asymptotically. In particular, for any $\sigma \in (0, -\mu_1)$ there is a constant $k > 0$ such that

$$\left\|\mathrm{e}^{t\mathbf{A}}\mathbf{x}_0\right\| \leq k\,\mathrm{e}^{(\mu_1+\sigma)t}\,\|\mathbf{x}_0\| \quad \text{for all} \quad t \geq 0.$$

This carries over to solutions of the nonlinear system, although we cannot conclude global asymptotic stability.

Theorem 2.12: *Consider the system* (2.5) *with flow* $\boldsymbol{\phi}_t(\boldsymbol{x}_0)$. *For any* $\sigma \in (0, -\mu_1)$, *there are constants*[4] $\delta, k > 0$ *such that*

$$\|\boldsymbol{\phi}_t(\boldsymbol{x}_0)\| \leq k\,\mathrm{e}^{(\mu_1+\sigma)t}\,\|\boldsymbol{x}_0\| \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta. \tag{2.9}$$

Proof: We will assume that $\|\mathbf{x}_0\| > 0$ for if this were not the case the result would be trivial. This proof is more or less standard but we are careful to include the initial condition in the estimate which is not standard. See, for example, pages 314 and 315 of [28]. In [28], they used Gronwall's Inequality at a key step (they had a slight difference in assumptions) but we will instead use a modification.[5]

From the integral equation (2.6),

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq \left\|\mathrm{e}^{t\mathbf{A}}\right\|\|\mathbf{x}_0\| + \int_0^t \left\|\mathrm{e}^{(t-s)\mathbf{A}}\right\|\|\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0))\|\,ds. \tag{2.10}$$

Applying the estimates (2.3) and (2.7) to the inequality (2.10), there are constants $\delta_1, k_1, k_2 > 0$ such that

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq k_1\mathrm{e}^{(\mu_1+\sigma)t}\,\|\mathbf{x}_0\| + k_2\int_0^t \mathrm{e}^{(\mu_1+\sigma)(t-s)}\,\|\boldsymbol{\phi}_s(\mathbf{x}_0)\|^\alpha\,ds, \tag{2.11}$$

[4] The constant k is understood to be independent of $\mathbf{x}_0$.

[5] Such modifications are examples of Bihari's Inequality. See, for example, [12] which was Bihari's original paper.

provided that

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| < \delta_1 \quad \text{for all} \quad t \geq 0. \tag{2.12}$$

Later, we will show that (2.12) is satisfied for $\|\mathbf{x}_0\|$ sufficiently small. Now, multiply both sides of the inequality (2.11) by $\mathsf{e}^{-(\mu_1+\sigma)t}$ to get

$$\mathsf{e}^{-(\mu_1+\sigma)t}\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq k_1\|\mathbf{x}_0\| + k_2\int_0^t \mathsf{e}^{-(\mu_1+\sigma)s}\|\boldsymbol{\phi}_s(\mathbf{x}_0)\|^\alpha\, ds.$$

This can be manipulated, giving

$$\mathsf{e}^{-(\mu_1+\sigma)t}\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq k_1\|\mathbf{x}_0\| + k_2\int_0^t \mathsf{e}^{(\alpha-1)(\mu_1+\sigma)s}\left[\mathsf{e}^{-(\mu_1+\sigma)s}\|\boldsymbol{\phi}_s(\mathbf{x}_0)\|\right]^\alpha ds. \tag{2.13}$$

Let

$$u(t) := \mathsf{e}^{-(\mu_1+\sigma)t}\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \geq 0.$$

Then, (2.13) becomes

$$u(t) \leq k_1\|\mathbf{x}_0\| + k_2\int_0^t \mathsf{e}^{(\alpha-1)(\mu_1+\sigma)s}u(s)^\alpha\, ds. \tag{2.14}$$

Now, define

$$v(t) := k_1\|\mathbf{x}_0\| + k_2\int_0^t \mathsf{e}^{(\alpha-1)(\mu_1+\sigma)s}u(s)^\alpha\, ds > 0.$$

Note that

$$\dot{v}(t) = k_2\mathsf{e}^{(\alpha-1)(\mu_1+\sigma)t}u(t)^\alpha \geq 0 \tag{2.15}$$

and $v(0) = k_1\|\mathbf{x}_0\|$. Then, the inequality (2.14) is equivalent to

$$u(t) \leq v(t). \tag{2.16}$$

It follows from (2.15) and (2.16) that v satisfies the differential inequality

$$\dot{v}(t) \leq k_2\mathsf{e}^{(\alpha-1)(\mu_1+\sigma)t}v(t)^\alpha. \tag{2.17}$$

Dividing both sides of (2.17) by $v(t)^\alpha > 0$ and replacing t by s,

$$\frac{\dot{v}(s)}{v(s)^\alpha} \leq k_2\mathsf{e}^{(\alpha-1)(\mu_1+\sigma)s}.$$

Integrating with respect to s from 0 to t and recalling that $\alpha > 1$ and $\mu_1+\sigma < 0$,

$$\frac{1}{1-\alpha}\left[\frac{1}{v(t)^{\alpha-1}} - \frac{1}{k_1^{\alpha-1}\|\mathbf{x}_0\|^{\alpha-1}}\right] \leq \left[\frac{k_2}{(\alpha-1)(\mu_1+\sigma)}\right]\left[\mathsf{e}^{(\alpha-1)(\mu_1+\sigma)t} - 1\right].$$

Observe that

$$\left[\frac{k_2}{(\alpha-1)(\mu_1+\sigma)}\right]\left[\mathrm{e}^{(\alpha-1)(\mu_1+\sigma)t}-1\right] \leq -\frac{k_2}{(\alpha-1)(\mu_1+\sigma)}.$$

Thus, we have

$$\frac{1}{v(t)^{\alpha-1}}-\frac{1}{k_1^{\alpha-1}\|\mathbf{x}_0\|^{\alpha-1}} \geq \frac{k_2}{\mu_1+\sigma}.$$

Re-arranging,

$$\frac{1}{v(t)^{\alpha-1}} \geq \frac{1}{\|\mathbf{x}_0\|^{\alpha-1}}\left(\frac{1}{k_1^{\alpha-1}}+\frac{k_2\|\mathbf{x}_0\|^{\alpha-1}}{\mu_1+\sigma}\right). \tag{2.18}$$

Now, we want the expression in the brackets to be strictly positive, which yields the condition

$$\|\mathbf{x}_0\| < \frac{1}{k_1}\left(-\frac{\mu_1+\sigma}{k_2}\right)^{\frac{1}{\alpha-1}}.$$

Let

$$\delta := \frac{\rho}{k_1}\left(-\frac{\mu_1+\sigma}{k_2}\right)^{\frac{1}{\alpha-1}},$$

where $\rho \in (0,1)$ is arbitrary. Hence, assume that $\|\mathbf{x}_0\| < \delta$ and take

$$k := \left(\frac{1}{k_1^{\alpha-1}}+\frac{k_2\delta^{\alpha-1}}{\mu_1+\sigma}\right)^{\frac{1}{1-\alpha}} = k_1\left(1-\rho^{\alpha-1}\right)^{\frac{1}{1-\alpha}} > 0, \tag{2.19}$$

which is independent of $\|\mathbf{x}_0\|$. It follows from (2.18) that

$$\frac{1}{v(t)^{\alpha-1}} \geq \frac{1}{\|\mathbf{x}_0\|^{\alpha-1}k^{\alpha-1}}.$$

Re-arranging and recalling that $u(t) \leq v(t)$,

$$u(t) \leq k\|\mathbf{x}_0\|.$$

By definition of $u(t)$, we have

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq k\,\mathrm{e}^{(\mu_1+\sigma)t}\|\mathbf{x}_0\|.$$

All that remains is to show that (2.12) is satisfied for a particular choice of ρ. We have shown that, for a fixed $\rho \in (0,1)$,

$$\|\mathbf{x}_0\| < \delta \implies \|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq k\,\mathrm{e}^{(\mu_1+\sigma)t}\|\mathbf{x}_0\| \quad \text{for all} \quad t \geq 0.$$

This, however, is contingent on the condition $\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| < \delta_1$ for all $t \geq 0$. If $k\delta < \delta_1$ then we are finished. Using our expressions for k and δ, we see that we can choose $\rho \in (0,1)$ sufficiently close to zero to accomplish this. $\square$

Remarks 2.13:

(i) If we set $t = 0$ in (2.9) we get $\|\mathbf{x}_0\| \leq k\,\|\mathbf{x}_0\|$. It follows that $k \geq 1$.

(ii) Consider our definition (2.19) for the constant k. We chose ρ sufficiently small to satisfy certain conditions and so we expect $k \approx k_1$. Recall from the proof of the theorem that k_1 was used in the decay rate of the linear solution, that is, $\left\|\mathrm{e}^{t\mathbf{A}}\mathbf{x}_0\right\| \leq k_1 \mathrm{e}^{(\mu_1+\sigma)t}\,\|\mathbf{x}_0\|$. This strengthens our belief that the nonlinear solution behaves like the linear solution. Later, we will improve this statement.

(iii) A glance at the proof of the previous theorem shows that σ is only necessary in the basic decay rate of $\boldsymbol{\phi}_t(\mathbf{x}_0)$ if σ is necessary in the decay rate of $\mathrm{e}^{t\mathbf{A}}$. Indeed, if $\mathbf{A}$ is diagonalizable then we can take $\sigma = 0$ in (2.9).

(iv) In [28], they assume that $\|\mathbf{b}(\mathbf{x})\| = \mathsf{o}(\|\mathbf{x}\|)$ as $\|\mathbf{x}\| \to 0$. (Technically, they used $\mathbf{b}(\mathbf{x}, t)$ instead of $\mathbf{b}(\mathbf{x})$.) The proof in [28] does *not* allow one to set $\sigma = 0$ in the event that the estimate for $\mathrm{e}^{t\mathbf{A}}$ does not require σ. (Note that ε in [28] corresponds to σ in this thesis and σ in [28] is used for something related but different.)

2.3.4 Decay Rate of $\frac{\partial\boldsymbol{\phi}_t(\mathbf{x}_0)}{\partial\mathbf{x}_0}$

Proposition 2.14: *Consider the system* (2.5) *with flow* $\boldsymbol{\phi}_t(\boldsymbol{x}_0)$. *For any* $\sigma \in (0, -\mu_1)$, *there are constants* $\delta, k > 0$ *such that*

$$\left\|\frac{\partial\boldsymbol{\phi}_t(\boldsymbol{x}_0)}{\partial\boldsymbol{x}_0}\right\| \leq k\,\mathrm{e}^{(\mu_1+\sigma)t} \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta. \tag{2.20}$$

Proof: A standard result tells us that

$$\frac{d}{dt}\left(\frac{\partial\boldsymbol{\phi}_t(\mathbf{x}_0)}{\partial\mathbf{x}_0}\right) = \left[\mathbf{A} + \frac{\partial\mathbf{b}}{\partial\mathbf{x}}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right]\frac{\partial\boldsymbol{\phi}_t(\mathbf{x}_0)}{\partial\mathbf{x}_0}, \qquad \left.\frac{\partial\boldsymbol{\phi}_t(\mathbf{x}_0)}{\partial\mathbf{x}_0}\right|_{t=0} = \mathbf{I}. \tag{2.21}$$

See, for example, the corollary on page 83 of [100]. Consider $\mathbf{x}_0$ to be fixed in (2.21) and let

$$\boldsymbol{\Phi}(t) := \frac{\partial\boldsymbol{\phi}_t(\mathbf{x}_0)}{\partial\mathbf{x}_0} \quad \text{and} \quad \mathbf{B}(t) := \frac{\partial\mathbf{b}}{\partial\mathbf{x}}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right).$$

The estimates (2.4) and (2.9) tell us that there are constants $\delta, k_1 > 0$ such that

$$\|\mathbf{B}(t)\| \leq k_1 \mathrm{e}^{\beta(\mu_1+\sigma)t}\,\|\mathbf{x}_0\|^\beta \quad \text{for all} \quad (t, \mathbf{x}_0) \in \Omega_\delta. \tag{2.22}$$

Re-writing (2.21) in terms of $\mathbf{\Phi}$ and $\mathbf{B}$, we have[6]

$$\dot{\mathbf{\Phi}} = [\mathbf{A} + \mathbf{B}(t)]\,\mathbf{\Phi}, \quad \mathbf{\Phi}(0) = \mathbf{I}.$$

This initial value problem can be written as the integral equation

$$\mathbf{\Phi}(t) = \mathsf{e}^{t\mathbf{A}} + \int_0^t \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{B}(s)\mathbf{\Phi}(s)\,ds.$$

Hence, for $(t, \mathbf{x}_0) \in \Omega_\delta$ we have

$$\|\mathbf{\Phi}(t)\| \le \left\|\mathsf{e}^{t\mathbf{A}}\right\| + \int_0^t \left\|\mathsf{e}^{(t-s)\mathbf{A}}\right\| \|\mathbf{B}(s)\| \, \|\mathbf{\Phi}(s)\| \; ds.$$

Applying the estimates (2.7) and (2.22), there is a constant $k_2 > 0$ such that for each $(t, \mathbf{x}_0) \in \Omega_\delta$,

$$\begin{aligned}
\|\mathbf{\Phi}(t)\| &\le k_2 \mathsf{e}^{(\mu_1+\sigma)t} + k_1 k_2 \|\mathbf{x}_0\|^\beta \int_0^t \mathsf{e}^{(\mu_1+\sigma)(t-s)} \mathsf{e}^{\beta(\mu_1+\sigma)s} \|\mathbf{\Phi}(s)\| \; ds \\
&= \mathsf{e}^{(\mu_1+\sigma)t} \left\{ k_2 + k_1 k_2 \|\mathbf{x}_0\|^\beta \int_0^t \mathsf{e}^{(\beta-1)(\mu_1+\sigma)s} \|\mathbf{\Phi}(s)\| \; ds \right\}.
\end{aligned}$$

Re-arranging,

$$\mathsf{e}^{-(\mu_1+\sigma)t} \|\mathbf{\Phi}(t)\| \le k_2 + k_1 k_2 \|\mathbf{x}_0\|^\beta \int_0^t \mathsf{e}^{\beta(\mu_1+\sigma)s} \mathsf{e}^{-(\mu_1+\sigma)s} \|\mathbf{\Phi}(s)\| \; ds.$$

By Gronwall's Inequality, which is given in §A.6 of Appendix A on page 312,

$$\begin{aligned}
\mathsf{e}^{-(\mu_1+\sigma)t} \|\mathbf{\Phi}(t)\| &\le k_2 \exp\left(k_1 k_2 \|\mathbf{x}_0\|^\beta \int_0^t \mathsf{e}^{\beta(\mu_1+\sigma)s} \, ds \right) \\
&\le k_2 \exp\left(-\frac{k_1 k_2 \|\mathbf{x}_0\|^\beta}{\beta\,[\mu_1+\sigma]} \right) \\
&\le k_2 \exp\left(-\frac{k_1 k_2 \delta^\beta}{\beta\,[\mu_1+\sigma]} \right).
\end{aligned}$$

Taking $k := k_2 \exp\left(-\frac{k_1 k_2 \delta^\beta}{\beta[\mu_1+\sigma]}\right)$ which is independent of $\|\mathbf{x}_0\|$, gives us (2.20). $\square$

2.4 Writing One Component in terms of Another

Consider the special case $n = 2$. Suppose that we want to write one component of the solution $\mathbf{x}(t) = (x(t), y(t))$ in terms of the other, say $y(t)$ in terms of $x(t)$. For example, suppose that

$$x(t) = \mathsf{e}^{-t} + \mathcal{O}\big(\mathsf{e}^{-2t}\big) \quad \text{and} \quad y(t) = 2\,\mathsf{e}^{-t} + \mathcal{O}\big(\mathsf{e}^{-2t}\big) \quad \text{as} \quad t \to \infty.$$

[6] The differential equation is an example of an almost-constant linear differential equation since $\lim_{t\to\infty} \|\mathbf{B}(t)\| = 0$.

If we re-arrange the expression for $x(t)$ we get

$$\mathsf{e}^{-t} = x(t)\left[1 + \mathcal{O}\big(\mathsf{e}^{-t}\big)\right] = x(t)\left[1 + \mathcal{O}(x(t))\right] \quad \text{as} \quad t \to \infty.$$

Since $x(t) = \mathcal{O}\big(\mathsf{e}^{-t}\big)$ as $t \to \infty$, it follows that $\mathsf{e}^{-t} = x + \mathcal{O}\big(x^2\big)$ as $x \to 0$ and

$$y = 2x + \mathcal{O}\big(x^2\big) \quad \text{as} \quad x \to 0.$$

Let $\mathbf{x}(t) = (x(t), y(t))$ be a solution of the planar differential equation $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$. Now, the set of points $(x(t), y(t))$ defines a curve $y = y(x)$ in the xy-plane. Since the planar differential equation is autonomous, we see that $y'(x) = \frac{g_2(x,y(x))}{g_1(x,y(x))}$ where $' = \frac{d}{dx}$. Thus, writing $y(t)$ asymptotically in terms of $x(t)$ amounts to finding an asymptotic expression for $y(x)$.

The classic method of finding an asymptotic expression for a solution to a scalar differential equation $y' = f(x, y)$ is the power series method. Here, one *assumes* a solution of the form $y(x) = \sum_{i=0}^{\infty} \xi_i x^i$, substitutes into the differential equation, and arrives at recursive relationships for the coefficients which are then solved. It is possible, however, that one can perform the power series method unhindered yet the resulting power series still misses important asymptotic terms. A remedy of this problem, at least for the special case $\kappa \notin \mathbb{N}$, involves a theorem of Poincaré. This theorem, along with related concepts such as resonance and Poincaré domain, are reviewed in §A.9 of Appendix A. First, we need a result on when resonance occurs.

2.4.1 Resonance

Proposition 2.15: *Suppose that $\boldsymbol{A} \in \mathbb{R}^{2\times 2}$ has real-valued eigenvalues λ_1 and λ_2.*

(a) Suppose that $\lambda_1, \lambda_2 \neq 0$ and $\kappa := \frac{\lambda_2}{\lambda_1} > 1$. Then, there is resonance in the eigenvalues if and only if $\kappa \in \{2, 3 \ldots\}$. Moreover, the eigenvalues belong to the Poincaré domain.

(b) Suppose that $\lambda_1 = 0$ and $\lambda_2 \neq 0$. Then, resonance in the eigenvalues always occurs.

Proof: Let

$$S := \{\ (a, b) \ : \ a, b \in \mathbb{N}_0,\ a + b \geq 2\ \}.$$

Recall that, by definition, $\{\lambda_1, \lambda_2\}$ is resonant if and only if there is a $j \in \{1, 2\}$ and $(a_1, a_2) \in S$ such that $\lambda_j = a_1\lambda_1 + a_2\lambda_2$.

(a) **Case 1:** $\kappa \in \{2, 3, \ldots\}$. Since $\lambda_2 = \kappa\lambda_1$, we can take $j = 2$, $a_1 = 0$, and $a_2 = \kappa$ which yields resonance.

Case 2: $\kappa \notin \{2, 3, \ldots\}$. Assume, on the contrary, that there is resonance.

Case A. Suppose that $(a_1, a_2) \in S$ is such that $\lambda_1 = a_1\lambda_1 + a_2\lambda_2$. Then,

$$1 = a_1 + a_2\kappa \geq a_1 + a_2 \geq 2,$$

which is impossible.

Case B. Suppose that $(a_1, a_2) \in S$ is such that $\lambda_2 = a_1\lambda_1 + a_2\lambda_2$. Then,

$$\kappa = a_1 + a_2\kappa.$$

If $a_2 = 0$ then $a_1 \in \{2, 3, \ldots\}$ and $\kappa = a_1 \in \{2, 3, \ldots\}$, which is impossible. On the other hand, if $a_2 \in \mathbb{N}$ then $\kappa > \kappa$, which is impossible.

The eigenvalues are of the same sign and thus the convex hull is the closed interval with the eigenvalues as endpoints which does not contain zero. Hence, the eigenvalues belong to the Poincaré domain.

(b) Take $a_1 = 1$ and $a_2 = 1$. Then, $(a_1, a_2) \in S$ and $\lambda_2 = a_1\lambda_1 + a_2\lambda_2$.

□

2.4.2 A Theorem

Theorem 2.16: *Consider the system of ordinary differential equations*

$$\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}(\boldsymbol{x}), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0, \quad \boldsymbol{x} = \left(\begin{smallmatrix} x \\ y \end{smallmatrix}\right) \in \mathbb{R}^2, \tag{2.23}$$

where the matrix $\boldsymbol{A}$ *is Hurwitz, the vector field* $\boldsymbol{b}$ *is analytic,* $\|\boldsymbol{b}(\boldsymbol{x})\| = \mathcal{O}\left(\|\boldsymbol{x}\|^2\right)$ *as* $\|\boldsymbol{x}\| \to 0$*, and* $\|\boldsymbol{x}_0\|$ *is sufficiently small. Let the eigenvalues of* $\boldsymbol{A}$ *be*[7] λ_+ *and* λ_-*, where* $\lambda_- < \lambda_+ < 0$*, and define*

[7]In the two-dimensional case, when the eigenvalues are both distinct and negative it is common to refer to the eigenvalues as λ_+ and λ_-. The $\pm$ refers to the taking of the positive and negative root when solving the characteristic equation. Since λ_+ corresponds to the slower decay rate $\mathrm{e}^{\lambda_+ t}$ and λ_- corresponds to the faster decay rate $\mathrm{e}^{\lambda_- t}$, λ_+ is referred to as the *slow eigenvalue* (and has associated *slow eigenvector*) and λ_- is referred to as the *fast eigenvalue* (and has associated *fast eigenvector*).

the ratio $\kappa := \frac{\lambda_-}{\lambda_+} > 1$*. Suppose that* $\kappa \notin \mathbb{N}$ *(that is no resonance) and the eigenvector* $\boldsymbol{v}_+$ *satisfies* $(\boldsymbol{v}_+)_1 \neq 0$*. If* $\boldsymbol{x}(t)$ *is a solution to (2.23) which approaches the origin in the slow direction and (for simplicity) is strictly positive for sufficiently large* t*, then*

$$y(t) = \sum_{i=1}^{\lfloor \kappa \rfloor} \xi_i x(t)^i + C\, x(t)^\kappa + o(x(t)^\kappa) \quad \text{as} \quad t \to \infty \tag{2.24}$$

for some constants $\{\xi_i\}_{i=1}^{\lfloor \kappa \rfloor}$ *(which are independent of initial condition) and* C *(which depends on the initial condition).*

Proof: In order to derive the necessary asymptotic expansion for solutions $y(x)$ to (2.23) (that is $y(t)$ written in terms of $x(t)$ with t dependence dropped), we make use of the linearized problem

$$\dot{\mathbf{z}} = \mathbf{A}\mathbf{z}, \quad \mathbf{z}(0) = \mathbf{z}_0. \tag{2.25}$$

To avoid the trivial solutions, which have nothing to offer us, we will assume that $\mathbf{x}_0, \mathbf{z}_0 \neq \mathbf{0}$. Let $\mathbf{x}(t)$ and $\mathbf{z}(t)$ be, respectively, the unique solutions to (2.23) and (2.25), both of which tend to the origin as time tends to infinity. We will not consider the initial conditions $\mathbf{x}_0$ and $\mathbf{z}_0$ to be independent so that the solutions $\mathbf{x}(t)$ and $\mathbf{z}(t)$ can be related. Furthermore, we need both $\|\mathbf{x}_0\|$ and $\|\mathbf{z}_0\|$ to be small.

The solution to the linear problem $\mathbf{z}(t)$ can be written in the explicit form

$$\mathbf{z}(t) = c_+ \mathrm{e}^{\lambda_+ t} \mathbf{v}_+ + c_- \mathrm{e}^{\lambda_- t} \mathbf{v}_-,$$

where $c_+ > 0$ (since we assumed that solutions approach the origin from the right in the slow direction). In a later chapter, we will see how to calculate the coefficients (which depend on the initial condition $\mathbf{z}_0$) using right and left eigenvectors.

We know from Proposition 2.15 that there is no resonance with the eigenvalues. Moreover, the eigenvalues are in the Poincaré domain. Applying Poincaré's Theorem, there is a quadratic vector field $\mathbf{q}$ such that $\mathbf{x} = \mathbf{z} + \mathbf{q}(\mathbf{z})$. Hence, we can write[8]

$$x(t) \sim \sum_{(i,j)\in S} a_{ij} \mathrm{e}^{(i\lambda_- + j\lambda_+)t} = \sum_{(i,j)\in S} a_{ij} \mathrm{e}^{(i\kappa + j)\lambda_+ t} \quad \text{as} \quad t \to \infty, \tag{2.26a}$$

$$y(t) \sim \sum_{(i,j)\in S} b_{ij} \mathrm{e}^{(i\lambda_- + j\lambda_+)t} = \sum_{(i,j)\in S} b_{ij} \mathrm{e}^{(i\kappa + j)\lambda_+ t} \quad \text{as} \quad t \to \infty, \tag{2.26b}$$

[8] This series is not unique if $\kappa \in \mathbb{Q}$.

where

$$S := \{\ (i,j)\ :\ i,j \in \mathbb{N}_0,\ i+j \geq 1\ \}.$$

Let $\ell := \lfloor \kappa \rfloor$. Then, the first $\ell + 1$ most dominant terms in (2.26) are, in order of decreasing dominance,

$$\mathsf{e}^{\lambda_+ t}, \mathsf{e}^{2\lambda_+ t}, \ldots, \mathsf{e}^{\ell\lambda_+ t}, \mathsf{e}^{\lambda_- t}.$$

To see why this is the case, we make two observations. First, the fact that the listed exponentials are in decreasing order of dominance is obvious except maybe for the last two. Since $\kappa = \frac{\lambda_-}{\lambda_+} > \ell$, we have $\lambda_- < \ell\lambda_+ < 0$. Second, there cannot be any other exponentials of the form $\mathsf{e}^{(i\lambda_+ + j\lambda_-)t}$ in between those listed.

For our purposes, we need only the first $\ell + 1$ terms of (2.26) and hence we write

$$x(t) = \sum_{i=1}^{\ell} a_i \mathsf{e}^{i\lambda_+ t} + a_{\ell+1}\mathsf{e}^{\lambda_- t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty, \tag{2.27a}$$

$$y(t) = \sum_{i=1}^{\ell} b_i \mathsf{e}^{i\lambda_+ t} + b_{\ell+1}\mathsf{e}^{\lambda_- t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty, \tag{2.27b}$$

where $a_1 > 0$. The coefficients can be related using the differential equation. To write $y(t)$ in terms of $x(t)$, we will successively eliminate the exponentials. Manipulating (2.27a) and (2.27b),

$$y(t) - \xi_1 x(t) = \sum_{i=2}^{\ell} b_i^{(2)} \mathsf{e}^{i\lambda_+ t} + b_{\ell+1}^{(2)}\mathsf{e}^{\lambda_- t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty, \tag{2.28}$$

where $\xi_1 := \frac{b_1}{a_1}$ and $b_i^{(2)} := b_i - \xi_1 a_i$.

To go further, observe that we can write powers of $x(t)$ as

$$x(t)^j = a_1^j \mathsf{e}^{j\lambda_+ t} + \sum_{i=j+1}^{\ell} c_{ij}\mathsf{e}^{i\lambda_+ t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty,$$

where $j \in \{2, \ldots, \ell\}$. Note that there is no $\mathsf{e}^{\lambda_- t}$ term in the expansion for $x(t)^j$. Solving for the most dominant exponential,

$$\mathsf{e}^{j\lambda_+ t} = \left(\frac{1}{a_1^j}\right) x(t)^j - \sum_{i=j+1}^{\ell} \left(\frac{c_{ij}}{a_1^j}\right) \mathsf{e}^{i\lambda_+ t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty. \tag{2.29}$$

With Equation (2.29), we can successively eliminate the exponentials of (2.28)—each time introducing other exponential terms but none of order already eliminated—until we are left with an expression of the form

$$y(t) - \sum_{i=1}^{\ell} \xi_i x(t)^i = b_{\ell+1}^{(\ell+1)} \mathsf{e}^{\lambda_- t} + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty. \tag{2.30}$$

Since $x(t)^\kappa = a_1^\kappa \mathsf{e}^{\lambda_- t} + \mathsf{o}(\mathsf{e}^{\lambda_- t})$ and hence

$$\mathsf{e}^{\lambda_- t} = \left(\frac{1}{a_1^\kappa}\right) x(t)^\kappa + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty,$$

we can write (2.30) as

$$y(t) - \sum_{i=1}^{\ell} \xi_i x(t)^i = C x(t)^\kappa + \mathsf{o}\Big(\mathsf{e}^{\lambda_- t}\Big) \quad \text{as} \quad t \to \infty. \tag{2.31}$$

Using Equations (2.27) and (2.30) along with the fact that there is no $\mathsf{e}^{\lambda_- t}$ term in the expansion for $x(t)^i$ if $i \in \{2, \ldots, \ell\}$, we find

$$C := \frac{b_{\ell+1} - \xi_1 a_{\ell+1}}{a_1^\kappa}.$$

Since

$$\mathsf{e}^{\lambda_- t} = x(t)^\kappa \left[\frac{1}{a_1^\kappa} + \mathsf{o}(1)\right] = \mathcal{O}(x(t)^\kappa) \quad \text{as} \quad t \to \infty,$$

(2.31) gives the desired expression (2.24). □

Remarks 2.17:

(i) The coefficients $\{\xi_i\}_{i=1}^{\ell}$ are calculated using the power series method. That is, one assumes that the solution to the scalar version of (2.23) is $y(x) = \sum_{i=0}^{\infty} \xi_i x^i$ (where $\xi_0 = 0$ by necessity). It is easy to see why non-integral powers are missed when solving for all the coefficients $\{\xi_i\}_{i=1}^{\infty}$ even when non-integral powers are present.

(ii) The constant ξ_1 in (2.24) is the slope of the slow eigenvector $\mathbf{v}_+$.

(iii) Suppose that the elements of the sequence $\{i\kappa + j\}_{(i,j)\in S}$ are written as the strictly increasing sequence $\{r_i\}_{i=1}^{\infty}$. Then, it is easy to see (by extending the proof above) that the solution of (2.23) can be written in the form

$$y(t) \sim \sum_{i=1}^{\infty} \xi_i x(t)^{r_i} \quad \text{as} \quad t \to \infty. \tag{2.32}$$

One could (theoretically) substitute this in to the scalar differential equation and recursively calculate the coefficients. This would be much more difficult than the regular power series method. Note that, if $1 < \kappa < 2$, then $r_1 = 1$, $r_2 = \kappa$, and $r_3 = 2$.

(iv) The reader may be wondering if there are solutions $\mathbf{x}(t)$ such that there are no non-integral powers of $x(t)$ present (that is, $\xi_i = 0$ if $r_i \in \mathbb{Q}\backslash\mathbb{N}$) in the asymptotic expansion (2.32). Corollary 2.18 below establishes that this is indeed the case.

Corollary 2.18: *There exists a solution to* (2.23) *such that*

$$y(t) \sim \sum_{i=1}^{\infty} \xi_i x(t)^i \quad \textit{as} \quad t \to \infty$$

for some constants $\{\xi_i\}_{i=1}^{\infty}$.

Proof: Choose the initial condition $\mathbf{z}_0$ so that it is parallel to the slow eigenvector $\mathbf{v}_+$. Then, $\mathbf{z}(t) = c_+ \mathsf{e}^{\lambda_+ t}\mathbf{v}_+$ and hence we can write

$$x(t) \sim \sum_{i=1}^{\infty} a_i \mathsf{e}^{i\lambda_+ t} \quad \text{and} \quad y(t) \sim \sum_{i=1}^{\infty} b_i \mathsf{e}^{i\lambda_+ t} \quad \text{as} \quad t \to \infty.$$

Any positive integer power of $x(t)$ will be a series of the same form as $x(t)$ and $y(t)$. Successively eliminating exponents, just like in the proof of the theorem, gives us our desired conclusion. □

2.4.3 First Example

Consider the system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -a \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} xy \\ -xy \end{pmatrix},$$

where $a > 1$ is a constant. By inspection, $\kappa = a$. Furthermore, the power series method yields the zero series. By Theorem 2.16, if $a \notin \{2, 3, \ldots\}$ then all solutions of the corresponding scalar system

$$y' = \frac{-ay - xy}{-x + xy}$$

satisfy

$$y(x) = C\, x^a + \mathsf{o}(x^a) \quad \text{as} \quad x \to 0^+.$$

2.4.4 Second Example

Consider the system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 2 & -\frac{3}{2} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} xy \\ x^2 \end{pmatrix}.$$

The eigenvalues of the two-by-two matrix are $\lambda_+ = -1$ and $\lambda_- = -\frac{3}{2}$ and so $\kappa = \frac{3}{2}$. The eigenvectors can be taken to be

$$\mathbf{v}_+ = \begin{pmatrix} 1 \\ 4 \end{pmatrix} \quad \text{and} \quad \mathbf{v}_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Solutions approach the origin in the direction of the slow eigenvector and hence have slope 4. It follows from Theorem 2.16 that

$$y(x) = 4\,x + C\,x^{\frac{3}{2}} + \mathsf{o}\Big(x^{\frac{3}{2}}\Big) \quad \text{as} \quad x \to 0^+.$$

2.4.5 Third Example

Here is an example of resonance for which solutions are not of the form of (2.24). Consider the system

$$\dot{\mathbf{x}} = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 0 \\ x^2 \end{pmatrix},$$

where $\mathbf{x} := (x, y)^T$. This has solution $\boldsymbol{\phi}_t(\mathbf{x}_0) = (x(t), y(t))^T$ given by

$$x(t) = x_0 \mathsf{e}^{-t}, \quad y(t) = \left[y_0 + x_0^2 t\right] \mathsf{e}^{-2t}.$$

Observe that, for $x_0 \neq 0$,

$$\mathsf{e}^{-t} = \frac{x}{x_0} \quad \text{and} \quad t = -\mathsf{ln}\left(\frac{x}{x_0}\right).$$

Hence

$$y = x^2 \left[\frac{y_0}{x_0^2} - \mathsf{ln}\left(\frac{x}{x_0}\right)\right].$$

The power series method will not work in this case of resonance. If one substitutes the series $y(x) = \sum_{i=0}^{\infty} \xi_i x^i$ into the differential equation, one gets $\xi_0 = \xi_1 = 0$ but no value of ξ_2 will work. This will be the case for resonance in the Michaelis-Menten mechanism, which we will see later.

Since the differential equation for x is decoupled, we can write the differential equation for y as

$$\dot{y} = -2y + x_0 \mathsf{e}^{-2t}.$$

Thus, the forcing term is a solution of the homogeneous equation. However, if we were to replace the -2 in the original system with, say, -3 (which is still resonant), a power series would work with ξ_3 being arbitrary. In this case,

$$\dot{y} = -3y + x_0 \mathsf{e}^{-2t}$$

and the forcing term is not a solution of the homogeneous equation.

2.5 Literature Review

Some of the prominent personalities relevant to the topic of the asymptotic behaviour of solutions of differential equations are Poincaré, Hartman and Grobman, Gronwall, Bellman, and Lyapunov. In this section, we will overview some of the key results and references which are applicable to this part of the thesis.

Henri Poincaré (1854–1912) was a French Mathematician and physicist. He has been called "the last polymath" (having thorough knowledge of many subject areas) and has written many popular books on the philosophy of science and mathematics which are readily available to this day. Poincaré has also been referred to as a pioneer in the qualitative theory of ordinary differential equations and the "father of dynamical systems." There are many terms which bear his name, including Poincaré Conjecture (which is no longer a conjecture), Poincaré-Bendixson Theorem, Poincaré map, Poincaré sphere, and Lindstedt-Poincaré method. For a nice survey article on the development of the field of dynamical systems, see [60].

The two main contributions of Poincaré which are relevant to this thesis are normal forms, which originated in his Ph.D. thesis, and a result that is often referred to simply as Poincaré's Theorem, which he proved in 1879. The first volume (of eleven) of the collected works (or *Oeuvres*) of Poincaré, [101], contains these results. Interestingly, Poincaré's work in dynamical systems is related to his work on the three-body problem for which he won the King Oscar II of Sweden Prize. Poincaré's solution contained a serious error (which he later corrected) and he used the prize money to buy back all the copies of the paper with the error.

Normal form theory, loosely, involves the substitution of an analytic, near-identity transformation to simplify the nonlinear part of an ordinary differential equation. Consider, for example, the system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ where $\mathbf{b}$ is analytic in a neighbourhood of the origin and satisfies $\|\mathbf{b}(\mathbf{x})\| = \mathcal{O}\left(\|\mathbf{x}\|^2\right)$ as $\|\mathbf{x}\| \to 0$. It may be desired to find a transformation of the form $\mathbf{x} = \mathbf{y} + \mathbf{r}(\mathbf{y})$, where $\mathbf{r}$ is analytic in a neighbourhood of the origin and satisfies $\|\mathbf{r}(\mathbf{x})\| = \mathcal{O}\left(\|\mathbf{x}\|^2\right)$ as $\|\mathbf{x}\| \to 0$, that yields the system $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{c}(\mathbf{x})$ where $\mathbf{c}$ is analytic in a neighbourhood of the origin and satisfies $\|\mathbf{c}(\mathbf{x})\| = \mathcal{O}\left(\|\mathbf{x}\|^3\right)$ as $\|\mathbf{x}\| \to 0$. It is well known, however, that so-called resonant terms cannot be eliminated by such a near-identity transformation. See, for example, [16, 27, 100, 127].

Consider the two systems $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ and $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y}$, where $\mathbf{b}$ is analytic in a neighbourhood of the origin and satisfies $\|\mathbf{b}(\mathbf{x})\| = \mathcal{O}\Big(\|\mathbf{x}\|^2\Big)$ as $\|\mathbf{x}\| \to 0$. If $\mathbf{A}$ has non-resonant eigenvalues and the convex hull of the eigenvalues does not contain 0, then Poincaré's Theorem says that there is a near-identity, invertible transformation $\mathbf{h}$ with both $\mathbf{h}$ and $\mathbf{h}^{-1}$ analytic at the origin such that $\mathbf{h}(\boldsymbol{\phi}_t(\mathbf{x}_0)) = \mathsf{e}^{t\mathbf{A}}\mathbf{h}(\mathbf{x}_0)$. That is, the flows of the two systems are analytically conjugate in a neighbourhood of the origin. This aids greatly in determining qualitative properties of solutions of more complicated systems. Furthermore, if we write $\mathbf{h}(\mathbf{y}) = \mathbf{y} + \mathbf{r}(\mathbf{y})$, then the relationship $\mathbf{x}(t) = \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0 + \mathbf{r}\left(\mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right)$ can be used to extract asymptotic expansions.

The same basic principle of Poincaré's Theorem is present in the Hartman-Grobman Theorem, named after Philip Hartman and David Grobman. Consider again the systems $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ and $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y}$. The Hartman-Grobman Theorem and its variations involve the existence of an invertible map $\mathbf{h}$ such that $\mathbf{h}(\boldsymbol{\phi}_t(\mathbf{x}_0)) = \mathsf{e}^{t\mathbf{A}}\mathbf{h}(\mathbf{x}_0)$ for $\|\mathbf{x}_0\|$ sufficiently small. See, for example, [16, 26, 50, 52, 53, 54]. See also [13] which provides an answer to the question "how small is sufficiently small?"

The variations of the Hartman-Grobman Theorem, as well as Poincaré's Theorem, are distinguished by the specifics of the system: the smoothness of $\mathbf{b}$, the smoothness of $\mathbf{h}$, whether or not the eigenvalues of $\mathbf{A}$ are resonant, and whether or not the origin is a hyperbolic fixed point. For example, if $\mathbf{b} \in C^1$ and the origin is hyperbolic, then there is a homeomorphism $\mathbf{h}$; this is generally referred to as the Hartman-Grobman Theorem. If, in addition, the eigenvalues of $\mathbf{A}$ are not resonant then there exists a diffeomorphism $\mathbf{h}$; this is generally referred to as Sternberg's Theorem, after Shlomo Sternberg (see, for example, [115, 116, 117, 118]). An alternative to this is the following: if $\mathbf{b} \in C^2$ and the origin is hyperbolic, then there is a C^1-diffeomorphism $\mathbf{h}$; this is generally referred to as Hartman's Theorem. Sternberg showed that, in general, if $\mathbf{b}$ is analytic there does not exist an $\mathbf{h}$ which is C^2.

Thomas Gronwall (1877–1932) was a Swedish mathematician. The famous Gronwall Inequality, which was proven around 1919 in [51], is a fundamental result used in obtaining estimates for solutions of differential equations. A different form of Gronwall's result was proven by Richard Bellman around 1943 in [8]. A generalization of Bellman's result was proven by I. Bihari around 1956 in [12]. Further generalizations are common and frequently referred to as inequalities of the Gronwall-Bellman-Bihari type.

Norman Levinson (1912–1975) was an American mathematician. He made contributions in differential equations, complex analysis, Fourier analysis, and number theory. Two books cowritten by Levinson, namely [28, 81], are solid references for the subject matter of this part of the thesis. In particular, [28] covers general theory of ordinary differential equations with Chapter 13, "Asymptotic Behavior of Nonlinear Systems: Stability," being especially useful.

The so-called Levinson Theorem, which Levinson proved around 1946 in [79], is a well-known result. The theorem deals with the asymptotic behaviour of solutions of an almost-constant linear system. This result is given much attention in many books dealing with stability and asymptotics, for example [9, 24, 30, 36]. Actually, [36] is subtitled "Applications of the Levinson Theorem." Although we have not used the Levinson Theorem in this thesis, it is still a useful result and we could have proved Proposition 2.14 using this theorem.

Richard Bellman (1920–1984) was an American applied mathematician. He received his Ph.D. from Princeton under the supervision of another prominent American mathematician, Solomon Lefschetz (1884–1972). His doctoral work eventually led to his book [9] which is considered a classic in the field of stability theory and exemplifies his clear writing style. He spent much of his career at the RAND Corporation. Throughout his career, he published around six hundred twenty papers, forty books, and seven monographs.

There are a number of other relevant books regarding stability and asymptotics which are frequently cited and should be mentioned here. Jack Carr's book on centre manifolds, [23], is a ubiquitous reference on the subject. Centre manifolds (which are associated with non-hyperbolic fixed points), however, do not appear in this part of the thesis but they do appear in the other parts. Books useful for asymptotics in general include [19, 38, 97].

The standard methods have well-known limitations. Many results have to exclude resonance and those that do not are often limited in their practicality. Leading-order behaviour of solutions can be difficult to obtain and more detailed behaviour can be more difficult still. Finally, the standard methods often give little or no detail on the relationship between components of solutions.

2.6 Summary

In this chapter, we began our investigation of the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

where $\mathbf{A}$ is a Hurwitz matrix and $\mathbf{b}$ is a nonlinear vector field. In particular, the real parts of the eigenvalues of $\mathbf{A}$ satisfy

$$\mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1 < 0$$

and $\mathbf{b}$ is C^1 in a neighbourhood of the origin and satisfies the estimates

$$\|\mathbf{b}(\mathbf{x})\| = \mathcal{O}(\|\mathbf{x}\|^{\alpha}) \quad \text{and} \quad \|\mathbf{Db}(\mathbf{x})\| = \mathcal{O}\Big(\|\mathbf{x}\|^{\beta}\Big) \quad \text{as} \quad \|\mathbf{x}\| \to 0,$$

for some $\alpha > 1$ and $\beta > 0$. The system is equivalent to the integral equation

$$\mathbf{x}(t) = \mathsf{e}^{t\mathbf{A}}\mathbf{x}_0 + \int_0^t \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{b}(\mathbf{x}(s))\, ds.$$

The matrix exponential, as is commonly known, for any $\sigma > 0$ satisfies

$$\left\|\mathsf{e}^{t\mathbf{A}}\right\| = \mathcal{O}\Big(\mathsf{e}^{(\mu_1+\sigma)t}\Big) \quad \text{and} \quad \left\|\mathsf{e}^{-t\mathbf{A}}\right\| = \mathcal{O}\Big(\mathsf{e}^{(-\mu_n+\sigma)t}\Big) \quad \text{as} \quad t \to \infty.$$

If $\mathbf{A}$ is diagonalizable, we pointed out that we can take $\sigma = 0$ in these estimates.

An important ratio we defined is

$$\kappa = \frac{\mu_n}{\mu_1} \geq 1$$

and we showed that resonance in the eigenvalues can only occur if $\kappa \geq 2$. The techniques we will be developing in later chapters fall into two cases, closely-spaced eigenvalues where $\kappa \in [1, \alpha)$ and widely-spaced eigenvalues where $\kappa \geq \alpha$.

We showed that the solution of the initial value problem satisfies the estimate

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| = \mathcal{O}\Big(\mathsf{e}^{(\mu_1+\sigma)t}\,\|\mathbf{x}_0\|\Big) \quad \text{as} \quad \|\mathbf{x}_0\| \to 0 \quad \text{and} \quad t \to \infty$$

for any $\sigma > 0$. If $\mathbf{A}$ is diagonalizable, then we can take $\sigma = 0$. If $\mathbf{A}$ is not diagonalizable, then $\sigma > 0$ is necessary since the elements of the matrix exponential $\mathsf{e}^{t\mathbf{A}}$ contains linear combinations of terms of the form $t^i\mathsf{e}^{\lambda_j t}$, where $i \in \mathbb{N}_0$ and $j \in \{1, \ldots, n\}$.

For the two-dimensional case, that is $n = 2$, we derived a result on writing $x_2(t)$ as a function of $x_1(t)$ when $\kappa \notin \mathbb{N}$ (that is $\lambda_2 < \lambda_1 < 0$ and there is no resonance). In particular if we drop the t-dependence,

$$x_2 \sim \sum_{i=1}^{\lfloor\kappa\rfloor} \xi_i x_1^i + C\, x_1^{\kappa} \quad \text{as} \quad x_1 \to 0^+$$

for some constants $\{\xi_i\}_{i=1}^{\lfloor\kappa\rfloor}$ (which are found using the power series method and are independent of the initial condition) and C (which depends on the initial condition).

In the coming chapters, we will explore iterative techniques which will yield expressions that approximate, with arbitrary accuracy, the actual solution of the initial value problem as $t \to \infty$.

Chapter 3

The Scalar Case

3.1 Introduction

In this chapter, we will begin our exploration of iterative techniques which produce successively better asymptotic expansions as time tends to infinity of solutions of the initial value problem (2.5). The simplest case, namely the scalar case $n = 1$, will be treated carefully in this chapter to mitigate the harder cases in later chapters.

Consider the initial value problem

$$\dot{x} = ax + b(x), \quad x(0) = x_0, \tag{3.1}$$

where $a < 0$ is a constant and b is a nonlinear function which satisfies certain properties which we now specify.

3.1.1 Assumptions

Assumption 3.1: Consider the function b.

(a) There is some open interval $\mathcal{N} \subset \mathbb{R}$ with $0 \in \mathcal{N}$ and $b \in C^1(\mathcal{N}, \mathbb{R})$.

(b) There are $\delta, k > 0$ such that $B_\delta \subset \mathcal{N}$ and

$$|b(x)| \leq k\,|x|^\alpha \quad \text{for all} \quad x \in B_\delta, \tag{3.2}$$

where $\alpha > 1$ is a fixed parameter.

(c) There are $\delta, k > 0$ such that $B_\delta \subset \mathcal{N}$ and

$$\left|b'(x)\right| \leq k\,|x|^\beta \quad \text{for all} \quad x \in B_\delta, \tag{3.3}$$

where $\beta > 0$ is a fixed parameter.

Observe that the assumptions (3.2) and (3.3) imply

$$b(0) = 0 = b'(0).$$

Thus, $x = 0$ is a fixed point of the differential equation in (3.1). Our goal is to obtain the detailed asymptotic behaviour of solutions of (3.1) as $t \to \infty$ when x_0 is sufficiently small.

3.1.2 Important Estimates We Already Know

Let $\phi_t(x_0)$ be the solution to (3.1). We can specialize a few results from Chapter 2. Note that we can take $\sigma = 0$ in the estimates since the matrix $\mathbf{A} = (a)$ is, very trivially, diagonalizable.

- The flow $\phi_t(x_0)$ satisfies the integral equation

$$\phi_t(x_0) = \mathsf{e}^{at} x_0 + \int_0^t \mathsf{e}^{a(t-s)} b(\phi_s(x_0))\, ds. \tag{3.4}$$

- There are $\delta, k > 0$ such that

$$|\phi_t(x_0)| \leq k\,\mathsf{e}^{at}\,|x_0| \quad \text{for all} \quad (t, x_0) \in \Omega_\delta, \tag{3.5}$$

  where

$$\Omega_\delta := \{\ (t, x)\ :\ t \geq 0,\ \ |x| < \delta\ \}.$$

- There are $\delta, k > 0$ such that

$$\left|\frac{\partial \phi_t(x_0)}{\partial x_0}\right| \leq k\,\mathsf{e}^{at} \quad \text{for all} \quad (t, x_0) \in \Omega_\delta. \tag{3.6}$$

3.2 “Flipping the Integral” and the Initial Condition y_0

Let $\rho > 0$ be a constant. Then, trivially, we have the integrals

$$\int_0^t \mathsf{e}^{-\rho s}\, ds = \frac{1}{\rho} + \mathsf{o}(1) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \int_t^\infty \mathsf{e}^{-\rho s}\, ds = \frac{1}{\rho}\,\mathsf{e}^{-\rho t}, \tag{3.7}$$

which we will use extensively in this part of the thesis. The integrals are related to the common trick of "flipping the integral," which, if done in a careful way, allows us to extract asymptotic information about the solution of (3.1). See, for example, the proof of Theorem 4.1 (Stable Manifold Theorem) of Chapter 13 on pages 330–333 of [28] which involves the flipping of an integral in an integral equation.

3.2.1 A Useful Integral Equation

Consider the integral equation (3.4) and write

$$\phi_t(x_0) = \mathsf{e}^{at}\left[x_0 + \int_0^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\, ds\right] - \int_t^\infty \mathsf{e}^{a(t-s)} b(\phi_s(x_0))\, ds. \tag{3.8}$$

Do these improper integrals converge? The following claim establishes that they do indeed converge. Recall, first, that $\alpha > 1$.

Claim 3.2: *There are $\delta, k > 0$ such that*

$$\left|\, \mathsf{e}^{-at} b(\phi_t(x_0))\right| \leq k\, \mathsf{e}^{(\alpha-1)at}\, |x_0|^\alpha \quad \text{for all} \quad (t, x_0) \in \Omega_\delta. \tag{3.9}$$

Proof: It follows from the estimates (3.2) and (3.5). □

Looking at (3.8), it is natural to define the new "initial condition" y_0, where

$$y_0 := \psi(x_0) \quad \text{and} \quad \psi(x_0) := x_0 + \int_0^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\, ds, \quad x_0 \in B_\delta, \tag{3.10}$$

where $\delta > 0$ is as in (3.9). We have thus established the following.

Claim 3.3: *There is a $\delta > 0$ such that*

$$\phi_t(x_0) = \mathsf{e}^{at} y_0 - \int_t^\infty \mathsf{e}^{a(t-s)} b(\phi_s(x_0))\, ds \quad \text{for all} \quad (t, x_0) \in \Omega_\delta, \tag{3.11}$$

where $y_0 := \psi(x_0)$.

Claim 3.4: *There are $\delta, k > 0$ such that*

$$|x_0 - \psi(x_0)| \leq k\, |x_0|^\alpha \quad \text{for all} \quad x \in B_\delta. \tag{3.12}$$

Moreover, ψ is a near-identity transformation.

Proof: It follows from (3.7), (3.9), and (3.10) along with the fact that $\alpha > 1$. □

3.2.2 Why y_0?

Why do we bother re-writing the integral equation (3.4) in the form (3.11)? The short answer is that y_0 is a more natural choice for initial condition for the linearized differential equation $\dot{x} = ax$ than x_0. It is easy to show that

$$\left|\phi_t(x_0) - \mathsf{e}^{at}x_0\right| = \mathcal{O}\left(\mathsf{e}^{at}\,|x_0|^{\alpha}\right) \quad \text{as} \quad t \to \infty \quad \text{and} \quad |x_0| \to 0.$$

However, using y_0 instead of x_0 for the initial condition for the linear differential equation $\dot{x} = ax$ gives us the following.

Proposition 3.5: *Let $y_0 := \psi(x_0)$. Then, there are $\delta, k > 0$ such that*

$$\left|\phi_t(x_0) - \mathsf{e}^{at}y_0\right| \leq k\,\mathsf{e}^{\alpha a t}\,|x_0|^{\alpha} \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta. \tag{3.13}$$

Proof: It follows from (3.7), (3.9), and (3.11). □

3.3 Iterates of the First Type

A decent first approximation to the solution of the initial value problem (3.1) is $\mathsf{e}^{at}x_0$. However, as we have seen, a better first approximation is $\mathsf{e}^{at}y_0$, where $y_0 := \psi(x_0)$. We will use $\mathsf{e}^{at}y_0$ and the integral equation (3.11) to define an iterative scheme which will give successively better asymptotic approximations (as $t \to \infty$) to the exact solution $\phi_t(x_0)$.

3.3.1 Definition of the Iterates

We will denote the iterates by $\left\{\chi^{(m)}\left(t, y_0\right)\right\}_{m=1}^{\infty}$. Since these iterates are defined in the natural way, we refer to them as *iterates of the first type.* Later, we will define modified iterates which, in certain circumstances, may be more useful.

For y_0 sufficiently small (to ensure the relevant improper integrals converge), we will take the first iterate to be

$$\chi^{(1)}\left(t, y_0\right) := \mathsf{e}^{at}y_0 \tag{3.14a}$$

and define recursively

$$\chi^{(m+1)}\left(t, y_0\right) := \mathsf{e}^{at}y_0 - \int_t^{\infty} \mathsf{e}^{a(t-s)}b\left(\chi^{(m)}\left(s, y_0\right)\right)\,ds \quad (m \in \mathbb{N}). \tag{3.14b}$$

Observe that

$$\frac{d}{dt}\left(\chi^{(m+1)}(t,y_0)\right) = a\chi^{(m+1)}(t,y_0) + b\left(\chi^{(m)}(t,y_0)\right) \quad (m \in \mathbb{N}). \tag{3.15}$$

Remark 3.6: We have two choices for the specified initial condition in the notation for the iterates, namely $\chi^{(m)}(t,x_0)$ and $\chi^{(m)}(t,y_0)$, both of which have their advantages and disadvantages. Since, in practice, the iterates will be calculated and left in terms of y_0 which will be regarded as a parameter, we will use the $\chi^{(m)}(t,y_0)$ notation.

3.3.2 Existence and Decay Rate of the Iterates

We will be developing estimates of how close the iterates $\left\{\chi^{(m)}(t,y_0)\right\}_{m=1}^{\infty}$ are to the actual solution $\phi_t(x_0)$. First, we need the basic decay rate for the iterates. Importantly, the iterates $\left\{\chi^{(m)}(t,y_0)\right\}_{m=1}^{\infty}$ satisfy the same decay rate as $\phi_t(x_0)$ *uniformly in m*.

Remark 3.7: Since the underlying goal is to compute estimates of how close the iterates are to the actual solution (which involves x_0), we will express estimates involving the iterates in terms of x_0 (instead of y_0).

Proposition 3.8: *Consider the iterates defined by* (3.14). *Then, there is a* $\delta > 0$ *(independent of m) such that if* $|x_0| < \delta$ *then* $\chi^{(m)}(t,y_0)$ *exists for each* $m \in \mathbb{N}$. *Moreover, there is a* $k > 0$ *(independent of m) such that*

$$\left|\chi^{(m)}(t,y_0)\right| \leq k\, e^{at}\,|x_0| \quad \textit{for all} \quad (t,x_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{3.16}$$

Proof: We need to find $\delta, k > 0$ that work for each m and thus we need to be very careful with constants.

- Let $\delta_1, \ell_1 > 0$ be such that if $|x| < \delta_1$ then $|b(x)| \leq \ell_1 |x|^\alpha$. See Equation (3.2). There is no harm in taking δ_1 small enough so that
$$0 < \delta_1 < \left[\frac{(1-\alpha)\,a}{\ell_1}\right]^{\frac{1}{\alpha-1}}.$$
- Let $\delta_2 > 0$ be such that $|\phi_t(x_0)| < \delta_1$ for all $(t,x_0) \in \Omega_{\delta_2}$. See Equation (3.5). It follows that if $|x_0| < \delta_2$ then y_0 exists.
- Let $\ell_3 > 0$ be such that if $|x_0| < \delta_2$ then $|y_0| \leq \ell_3 |x_0|$. See Equation (3.12).

Take

$$k := \ell_3 \left[1 - \frac{\ell_1 \delta_1^{\alpha-1}}{(1-\alpha)\, a} \right]^{-1} > \ell_3 \quad \text{and} \quad \delta \in \left(0, \min\left\{ \frac{\delta_1}{k}, \delta_2 \right\} \right).$$

The upper bound we imposed on δ_1 ensures that k is defined and is greater than ℓ_3. Moreover, note that

$$\ell_3 + \left[\frac{\ell_1 k \delta_1^{\alpha-1}}{(1-\alpha)\, a} \right] = k. \tag{3.17}$$

The proof of the result will be by induction on m. Assume that $(t, x_0) \in \Omega_\delta$.

Consider first the base case, $m = 1$. We know y_0 exists and hence $\chi^{(1)}(t, y_0)$ exists. Furthermore,

$$\left| \chi^{(1)}(t, y_0) \right| = \mathsf{e}^{at} |y_0| \le \ell_3 \mathsf{e}^{at} |x_0| \le k\, \mathsf{e}^{at} |x_0|$$

and thus the result is true for $m = 1$.

Now, assume that the result is true for $m \in \mathbb{N}$. That is, $\chi^{(m)}(t, y_0)$ exists for $|x_0| < \delta$ and satisfies $\left|\chi^{(m)}(t, y_0)\right| \le k\, \mathsf{e}^{at} |x_0|$. Now, for $|x_0| < \delta$, we see that $\left|\chi^{(m)}(t, y_0)\right| < \delta_1$ and thus $\chi^{(m+1)}(t, y_0)$ exists. Using (3.14b),

$$\left| \chi^{(m+1)}(t, y_0) \right| \le \mathsf{e}^{at} |y_0| + \mathsf{e}^{at} \int_t^\infty \mathsf{e}^{-as} \left| b\left(\chi^{(m)}(s, y_0) \right) \right| ds.$$

By the induction hypothesis and the estimates given at the beginning of the proof,

$$\left| \chi^{(m+1)}(t, y_0) \right| \le \ell_3 \mathsf{e}^{at} |x_0| + \ell_1 k^\alpha \mathsf{e}^{at} \left[\int_t^\infty \mathsf{e}^{(\alpha-1)as}\, ds \right] |x_0|^\alpha.$$

Simplifying,

$$\begin{aligned} \left| \chi^{(m+1)}(t, y_0) \right| &\le \ell_3 \mathsf{e}^{at} |x_0| + \left[\frac{\ell_1 k^\alpha}{(1-\alpha)\, a} \right] \mathsf{e}^{\alpha a t} |x_0|^\alpha \\ &= \left\{ \ell_3 + \left[\frac{\ell_1 k^\alpha}{(1-\alpha)\, a} \right] \mathsf{e}^{(\alpha-1)at} |x_0|^{\alpha-1} \right\} \mathsf{e}^{at} |x_0|. \end{aligned}$$

Since $0 < \mathsf{e}^{(\alpha-1)at} \le 1$ and $|x_0| < \delta < \frac{\delta_1}{k}$, we have

$$\left| \chi^{(m+1)}(t, y_0) \right| \le \left\{ \ell_3 + \left[\frac{\ell_1 k^\alpha \delta^{\alpha-1}}{(1-\alpha)\, a} \right] \right\} \mathsf{e}^{at} |x_0| \le \left\{ \ell_3 + \left[\frac{\ell_1 k \delta_1^{\alpha-1}}{(1-\alpha)\, a} \right] \right\} \mathsf{e}^{at} |x_0|.$$

Using (3.17),

$$\left| \chi^{(m+1)}(t, y_0) \right| \le k\, \mathsf{e}^{at} |x_0|.$$

Hence, the result is true for $m + 1$. It follows from mathematical induction that the result is true for all $m \in \mathbb{N}$. $\square$

3.3.3 Closeness of the Iterates to the Actual Solution

Now, we establish how close each iterate $\chi^{(m)}(t, y_0)$ is to the actual solution $\phi_t(x_0)$, which is the main result of this chapter. As this theorem shows, each iteration increases the accuracy by a factor which is $\mathcal{O}\Big(\mathsf{e}^{\beta at} |x_0|^{\beta}\Big)$ as $t \to \infty$ and $x_0 \to 0$.

Theorem 3.9: *Consider the iterates defined by* (3.14). *There are constants*[1] $\delta > 0$ *and* $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ *such that*

$$\left|\phi_t(x_0) - \chi^{(m)}(t, y_0)\right| \leq k_m \mathsf{e}^{[\alpha+(m-1)\beta]at} |x_0|^{\alpha+(m-1)\beta} \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{3.18}$$

Proof: First, we need to introduce some constants and establish some estimates.

- Let $\delta_1, \ell_1 > 0$ be such that if $|x| < \delta_1$ then $|b(x)| \leq \ell_1 |x|^{\alpha}$. See Equation (3.2).
- Let $\delta_2, \ell_2 > 0$ be such that if $|x| < \delta_2$ then $|b'(x)| \leq \ell_2 |x|^{\beta}$. See Equation (3.3).
- Let $\delta_3, \ell_3 > 0$ be such that $|\phi_t(x_0)| \leq \ell_3 \mathsf{e}^{at} |x_0|$ for all $(t, x_0) \in \Omega_{\delta_3}$. See Equation (3.5).
- Let $\delta_4, \ell_4 > 0$ be such that $\left|\chi^{(m)}(t, y_0)\right| \leq \ell_4 \mathsf{e}^{at} |x_0|$ for all $(t, x_0) \in \Omega_{\delta_4}$ and $m \in \mathbb{N}$. See Equation (3.16).
- If $|x_0| < \mathsf{min}\{\delta_3, \delta_4\}$ then any number between $\phi_t(x_0)$ and $\chi^{(m)}(t, y_0)$ is bounded in absolute value by $(\ell_3 + \ell_4)\, \mathsf{e}^{at} |x_0|$ for all $t \geq 0$.

The proof of the theorem will be by induction on m. Take

$$\delta := \mathsf{min}\left\{\frac{\delta_1}{\ell_3}, \frac{\delta_1}{\ell_4}, \frac{\delta_2}{\ell_3 + \ell_4}, \delta_3, \delta_4\right\}$$

and assume that $|x_0| < \delta$ which ensures that all necessary estimates apply. The base case $m = 1$ has already been given in Equation (3.13). Assume that the result is true for $m \in \mathbb{N}$. First, for any $s \geq 0$ consider the expression

$$\left|b(\phi_s(x_0)) - b\left(\chi^{(m)}(s, y_0)\right)\right| \leq \ell_2 (\ell_3 + \ell_4)^{\beta} \mathsf{e}^{\beta as} \left|\phi_s(x_0) - \chi^{(m)}(s, y_0)\right| |x_0|^{\beta},$$

[1] In this thesis, $\mathbb{R}_+ = \{x \in \mathbb{R} \ :\ x > 0\}$. It is also common to use $\mathbb{R}_+ = \{x \in \mathbb{R} \ :\ x \geq 0\}$.

where we applied the Mean Value Theorem and estimates given at the beginning of the proof. By the induction hypothesis, for any $s \geq 0$ we know

$$\begin{aligned}\left|b(\phi_s(x_0)) - b\left(\chi^{(m)}(s, y_0)\right)\right| &\leq \ell_2 (\ell_3 + \ell_4)^\beta \mathsf{e}^{\beta a s} \left\{k_m \mathsf{e}^{[\alpha+(m-1)\beta]as} |x_0|^{\alpha+(m-1)\beta}\right\} |x_0|^\beta \\ &= k_m \ell_2 (\ell_3 + \ell_4)^\beta \mathsf{e}^{(\alpha+m\beta)as} |x_0|^{\alpha+m\beta}.\end{aligned}$$

It follows from the integral equation (3.11) for $\phi_t(x_0)$ and the definition (3.14b) of the iterate $\chi^{(m+1)}(t, y_0)$ that

$$\begin{aligned}\left|\phi_t(x_0) - \chi^{(m+1)}(t, y_0)\right| &= \mathsf{e}^{at} \left|\int_t^\infty \mathsf{e}^{-as} \left[b(\phi_s(x_0)) - b\left(\chi^{(m)}(s, y_0)\right)\right] ds\right| \\ &\leq k_m \ell_2 (\ell_3 + \ell_4)^\beta \mathsf{e}^{at} \left[\int_t^\infty \mathsf{e}^{(\alpha+m\beta-1)as} ds\right] |x_0|^{\alpha+m\beta} \\ &= \left[-\frac{k_m \ell_2 (\ell_3 + \ell_4)^\beta}{(\alpha+m\beta-1)\, a}\right] \mathsf{e}^{(\alpha+m\beta)at} |x_0|^{\alpha+m\beta} \\ &= k_{m+1} \mathsf{e}^{(\alpha+m\beta)at} |x_0|^{\alpha+m\beta},\end{aligned}$$

where $k_{m+1} > 0$ is defined in the obvious way. Hence the theorem is true for $m+1$. By induction, the theorem is true for all m. □

Remark 3.10: Suppose you have calculated a particular iterate $\chi^{(m)}(t, y_0)$. Theorem 3.9 guarantees that $\chi^{(m)}(t, y_0)$ correctly approximates $\phi_t(x_0)$ up to a certain order. A glance at the proof of the theorem indicates that we can discard the suspect terms of $\chi^{(m)}(t, y_0)$ and use the simplified iterate in the calculation of $\chi^{(m+1)}(t, y_0)$ without sacrificing the accuracy of $\chi^{(m+1)}(t, y_0)$. This potentially can simplify the calculation of iterates greatly.

3.3.4 A Simple Example

Consider the initial value problem

$$\dot{x} = -x + x^3, \quad x(0) = x_0.$$

Observe that $x = 0$ is a stable equilibrium point but $x = 1$ and $x = -1$ are both unstable equilibrium points. In particular, $\dot{x} > 0$ if $-1 < x < 0$ and $\dot{x} < 0$ if $0 < x < 1$. It follows that we need $|x_0| < 1$.

Here, we can take $a = -1$, $b(x) = x^3$, $\alpha = 3$, and $\beta = 2$. Using (3.14), we can compute the first two iterates:

$$\chi^{(1)}(t, y_0) = \mathsf{e}^{-t} y_0$$

and

$$\chi^{(2)}(t, y_0) = \mathsf{e}^{-t} y_0 - \mathsf{e}^{-t} \int_t^\infty \mathsf{e}^s \left[\mathsf{e}^{-s} y_0\right]^3 \, ds = \mathsf{e}^{-t} y_0 - \tfrac{1}{2}\, \mathsf{e}^{-3t} y_0^3.$$

It follows from Theorem 3.9 that

$$\phi_t(x_0) = \mathsf{e}^{-t} y_0 - \tfrac{1}{2}\, \mathsf{e}^{-3t} y_0^3 + \mathcal{O}\Big(\mathsf{e}^{-5t} |x_0|^5\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0.$$

Remark 3.11: Later, we will find a formula which can be used to find y_0 explicitly without actually knowing the solution $\phi_t(x_0)$. It turns out

$$y_0 = \frac{x_0}{\sqrt{1 - x_0^2}}, \quad |x_0| < 1.$$

For this example, we can find the exact solution,

$$\phi_t(x_0) = \frac{\mathsf{e}^{-t} x_0}{\sqrt{\left(1 - x_0^2\right) + x_0^2 \mathsf{e}^{-2t}}},$$

which can be used in the definition (3.10) to compute y_0. Alternatively, $\phi_t(x_0)$ can be expanded as a power series in e^{-t} and the coefficient of the e^{-t} term has to be y_0.

3.4 Iterates of the Second Type

The calculation of the iterates of the first type, $\left\{\chi^{(m)}(t, y_0)\right\}_{m=1}^\infty$ where $y := \psi(x_0)$, involves evaluating an integral. However, this integration may be difficult or impossible. In this section, we explore a way of simplifying this integration provided that $b \in C^\infty$ in some neighbourhood of 0. In particular, in calculating an iterate we require only a certain number of terms in the Taylor series for b to achieve the same exponential estimate for how close the iterate is to the actual solution.

Assume that $b \in C^\infty(\mathcal{N}, \mathbb{R})$, where $\mathcal{N} \subset \mathbb{R}$ is some open interval with $0 \in \mathcal{N}$. By Taylor's Theorem, there is an index $\ell \in \{2, 3, \ldots\}$ and constants $\{b_i\}_{i=\ell}^\infty$ such that

$$b(x) \sim \sum_{i=\ell}^\infty b_i x^i \quad \text{as} \quad x \to 0.$$

Clearly, we can take $\alpha = \ell$ and $\beta = \ell - 1$. Now, define

$$b^{(m)}(x) := \sum_{i=\ell}^m b_i x^i, \quad m \in \{\ell, \ell + 1, \ldots\}.$$

Note that

$$\left| b(x) - b^{(m)}(x) \right| = \mathcal{O}\big(x^{m+1}\big) \quad \text{as} \quad x \to 0. \tag{3.19}$$

3.4.1 Definition of the Iterates

We will denote the *iterates of the second type* by $\{\widetilde{\chi}^{(m)}(t, y_0)\}_{m=1}^{\infty}$. For y_0 sufficiently small, we will take the first iterate to be

$$\widetilde{\chi}^{(1)}(t, y_0) := \mathsf{e}^{at} y_0 \tag{3.20a}$$

and we will define the remaining iterates recursively by

$$\widetilde{\chi}^{(m+1)}(t, y_0) := \mathsf{e}^{at} y_0 - \int_t^{\infty} \mathsf{e}^{a(t-s)} b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) ds \quad (m \in \mathbb{N}). \tag{3.20b}$$

Remark 3.12: The method in this section can easily be adapted to the case in which b is C^r, where $r \in \{\ell+1, \ell+2, \ldots\}$, but not C^{r+1} in a neighbourhood of 0. In this case, we would obtain a finite number of iterates. By Taylor's Theorem,

$$b(x) = b_\ell x^\ell + \cdots + b_{r-1} x^{r-1} + \mathcal{O}(x^r) \quad \text{as} \quad x \to 0.$$

Then, $b^{(m)}$ is defined for $m \in \{\ell, \ldots, r-1\}$ and $\widetilde{\chi}^{(m)}(t, y_0)$ is defined for $m \in \left\{1, \ldots, \left\lfloor \frac{r-1}{\ell-1} \right\rfloor\right\}$.

3.4.2 Existence and Decay Rate of the Iterates

The decay rate for the iterates $\{\widetilde{\chi}^{(m)}(t, y_0)\}_{m=1}^{\infty}$ is the same as for $\phi_t(x_0)$ uniformly in m.

Proposition 3.13: *Consider the iterates defined by* (3.20)*. Then, there is a $\delta > 0$ (independent of m) such that if $|x_0| < \delta$ then $\widetilde{\chi}^{(m)}(t, y_0)$ exists for each $m \in \mathbb{N}$. Moreover, there is a $k > 0$ (independent of m) such that*

$$\left|\widetilde{\chi}^{(m)}(t, y_0)\right| \leq k\, \mathsf{e}^{at} |x_0| \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{3.21}$$

Proof: The proof is exactly the same as the proof of Proposition 3.8. □

3.4.3 Closeness of the Iterates to the Actual Solution

Now, we establish how close each iterate of the second type $\widetilde{\chi}^{(m)}(t, y_0)$ is to the actual solution $\phi_t(x_0)$. Observe that the decay rate is the same as with the iterates of the first kind (with $\alpha = \ell$ and $\beta = \ell - 1$) given in (3.18).

Theorem 3.14: *Consider the iterates defined by* (3.20)*. There are constants $\delta > 0$ and $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ such that*

$$\left|\phi_t(x_0) - \widetilde{\chi}^{(m)}(t, y_0)\right| \leq k_m \mathsf{e}^{[m(\ell-1)+1]at} |x_0|^{m(\ell-1)+1} \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta,\ m \in \mathbb{N}.$$

Proof: Let $\delta > 0$ be small enough so that all relevant estimates apply when $|x_0| < \delta$. Hence, assume that $|x_0| < \delta$. The proof will be by induction on m.

Since $\widetilde{\chi}^{(1)}(t, y_0) = \chi^{(1)}(t, y_0)$, Theorem 3.9 establishes the base case $m = 1$. Assume that the theorem is true for a given $m \in \mathbb{N}$. We will show that the theorem is true for $m+1$. First, for any $s \geq 0$ consider

$$\begin{aligned}
&\left| b\left(\phi_s(x_0)\right) - b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right| \\
&\leq \left| b\left(\phi_s(x_0)\right) - b\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right| + \left| b\left(\widetilde{\chi}^{(m)}(s, y_0)\right) - b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right|,
\end{aligned}$$

where we applied the Triangle Inequality. Now, using (3.3), (3.5), (3.21), the Mean Value Theorem, and the induction hypothesis, we know that there is a $k_m^{(1)} > 0$ such that

$$\left| b\left(\phi_s(x_0)\right) - b\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right| \leq k_m^{(1)} \mathsf{e}^{[(m+1)(\ell-1)+1]as} \left|x_0\right|^{(m+1)(\ell-1)+1}.$$

Also, we see from (3.19) and (3.21) that there is a $k_m^{(2)} > 0$ such that

$$\left| b\left(\widetilde{\chi}^{(m)}(s, y_0)\right) - b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right| \leq k_m^{(2)} \mathsf{e}^{[(m+1)(\ell-1)+1]as} \left|x_0\right|^{(m+1)(\ell-1)+1}.$$

Putting these last three estimates together,

$$\left| b\left(\phi_s(x_0)\right) - b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right| \leq \left(k_m^{(1)} + k_m^{(2)}\right) \mathsf{e}^{[(m+1)(\ell-1)+1]as} \left|x_0\right|^{(m+1)(\ell-1)+1}.$$

It follows from (3.11) and (3.20b) that

$$\begin{aligned}
\left| \phi_t(x_0) - \widetilde{\chi}^{(m)}(t, y_0) \right| &\leq \mathsf{e}^{at} \int_t^\infty \mathsf{e}^{-as} \left[b\left(\phi_s(x_0)\right) - b^{([m+1][\ell-1])}\left(\widetilde{\chi}^{(m)}(s, y_0)\right) \right] ds \\
&\leq k_{m+1} \mathsf{e}^{[(m+1)(\ell-1)+1]at} \left|x_0\right|^{(m+1)(\ell-1)+1}
\end{aligned}$$

for some $k_{m+1} > 0$. This is what we were trying to show. Therefore, by induction the theorem is true for all $m \in \mathbb{N}$. □

3.4.4 A Simple Example

Consider the initial value problem

$$\dot{x} = -x + x^2 + x^3, \quad x(0) = x_0.$$

Then, we can take

$$a = -1, \quad b(x) = x^2 + x^3, \quad \text{and} \quad \ell = 2.$$

Furthermore, take

$$b^{(2)}(x) = x^2 \quad \text{and} \quad b^{(m)}(x) = x^2 + x^3 \quad \text{for} \quad m \in \{3, 4, \ldots\}.$$

We will find the first three iterates of the second type. Using the definition (3.20) of the iterates, the first iterate is

$$\widetilde{\chi}^{(1)}(t, y_0) = \mathsf{e}^{-t} y_0,$$

the second iterate is

$$\begin{aligned}\widetilde{\chi}^{(2)}(t, y_0) &= \mathsf{e}^{-t}\left[y_0 - \int_t^\infty \mathsf{e}^s \left(\mathsf{e}^{-s} y_0\right)^2 ds\right] \\ &= \mathsf{e}^{-t} y_0 - \mathsf{e}^{-2t} y_0^2,\end{aligned}$$

and the third iterate is

$$\begin{aligned}\widetilde{\chi}^{(3)}(t, y_0) &= \mathsf{e}^{-t}\left\{y_0 - \int_t^\infty \mathsf{e}^s \left[\left(\mathsf{e}^{-s} y_0 - \mathsf{e}^{-2s} y_0^2\right)^2 + \left(\mathsf{e}^{-s} y_0 - \mathsf{e}^{-2s} y_0^2\right)^3\right] ds\right\} \\ &= \mathsf{e}^{-t} y_0 - \mathsf{e}^{-2t} y_0^2 + \tfrac{1}{2}\,\mathsf{e}^{-3t} y_0^3 + \tfrac{2}{3}\,\mathsf{e}^{-4t} y_0^4 - \tfrac{3}{4}\,\mathsf{e}^{-5t} y_0^5 + \tfrac{1}{5}\,\mathsf{e}^{-6t} y_0^6.\end{aligned}$$

It follows from Theorem 3.14 that

$$\phi_t(x_0) = \mathsf{e}^{-t} y_0 - \mathsf{e}^{-2t} y_0^2 + \tfrac{1}{2}\,\mathsf{e}^{-3t} y_0^3 + \mathcal{O}\big(\mathsf{e}^{-4t} y_0^4\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0.$$

Remark 3.15: If instead we calculated the first three iterates of the first type, we would see that $\chi^{(2)}(t, y_0)$ has terms up to $\mathsf{e}^{-3t} y_0^3$ and $\chi^{(3)}(t, y_0)$ has terms up to $\mathsf{e}^{-9t} y_0^9$. Moreover, $\chi^{(3)}(t, y_0)$ and $\widetilde{\chi}^{(3)}(t, y_0)$ agree up to the $\mathsf{e}^{-3t} y_0^3$ term but differ starting with the $\mathsf{e}^{-4t} y_0^4$ term.

3.4.5 A Curious Example

Consider the initial value problem (3.1) with

$$b(x) := \begin{cases} \exp\left(-\dfrac{1}{x^2}\right), & \text{if} \quad x \neq 0 \\ 0, \quad \text{if} \quad x = 0 \end{cases}.$$

Observe that $b \in C^\infty(\mathbb{R})$ and $b^{(m)}(0) = 0$ for all $m \in \mathbb{N}_0$. Observe also that, for *any* $\alpha > 1$ and $\beta > 0$, $|b(x)| = \mathcal{O}(|x|^\alpha)$ and $|b'(x)| = \mathcal{O}\left(|x|^\beta\right)$ as $x \to 0$. We might say that $b(x)$ is asymptotic to zero beyond all orders. It follows that the iterates of the second type are $\widetilde{\chi}^{(m)}(t, y_0) = \mathsf{e}^{at} y_0$ for any $m \in \mathbb{N}$. Moreover, Theorem 3.14 says that the actual solution $\phi_t(x_0)$ is asymptotic to $\mathsf{e}^{at} y_0$ as $t \to \infty$ and $x_0 \to 0$ beyond all orders when $y_0 = \psi(x_0)$. Finally, it follows from (3.12) that y_0 is asymptotic to x_0 as $x_0 \to 0$ beyond all orders.

3.5 The Function ψ

Let $y_0 := \psi(x_0)$, where ψ was defined earlier in (3.10). Recall that y_0, as opposed to x_0, is a more natural choice for initial condition for the linearized differential equation $\dot{x} = ax$. In this section, we will explore properties of this intriguing transformation ψ.

3.5.1 Conjugacy Condition

The Hartman-Grobman Theorem (see, for example, [50, 52] and sections §IX.7, §IX.8, and §IX.9 of [55]) says that there is a homeomorphism which maps flows of the nonlinear system onto flows of the linear system. That is,

$$h(\phi_t(x_0)) = \mathsf{e}^{at} h(x_0) \quad \text{for all} \quad t \geq 0,$$

where h is continuous with continuous inverse h^{-1} and x_0 is sufficiently small. Consequently,

$$\phi_t(x_0) = h^{-1}\left(\mathsf{e}^{at} h(x_0)\right).$$

Hence, having an expression for h and h^{-1} (or an approximation for h and h^{-1}) is useful. Techniques involving successive approximations have been used to calculate (or approximate) h. Hartman used such successive approximations in his proof of what is now known as the Hartman-Grobman Theorem.

It turns out that ψ is one such transformation which satisfies the above conjugacy condition. Later, we will find an explicit formula for $\psi(x_0)$ not involving $\phi_t(x_0)$.

Theorem 3.16: *There is a $\delta > 0$ such that*

$$\psi(\phi_t(x_0)) = \mathsf{e}^{at}\psi(x_0) \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta. \tag{3.22}$$

Proof: Let $\delta > 0$ be small enough so that all relevant estimates apply for $|x_0| < \delta$. Assume that $|x_0| < \delta$. First, replace x_0 by $\phi_t(x_0)$ in the definition (3.10) of ψ to get

$$\psi(\phi_t(x_0)) = \phi_t(x_0) + \int_0^\infty \mathsf{e}^{-a\xi} b(\phi_\xi(\phi_t(x_0)))\, d\xi.$$

Using the integral equation (3.11) and the semi-group property of the flow,

$$\begin{aligned}
\psi(\phi_t(x_0)) &= \mathsf{e}^{at}\psi(x_0) - \mathsf{e}^{at}\int_t^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\, ds + \int_0^\infty \mathsf{e}^{-a\xi} b(\phi_{\xi+t}(x_0))\, d\xi \\
&= \mathsf{e}^{at}\left[\psi(x_0) - \int_t^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\, ds + \int_0^\infty \mathsf{e}^{-a(\xi+t)} b(\phi_{\xi+t}(x_0))\, d\xi\right].
\end{aligned}$$

Using the change of variables $s = \xi + t$ in the second integral,

$$\begin{aligned}\psi\left(\phi_t(x_0)\right) &= \mathsf{e}^{at}\left[\psi(x_0) - \int_t^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\,ds + \int_t^\infty \mathsf{e}^{-as} b\left(\phi_s(x_0)\right)\,ds\right] \\ &= \mathsf{e}^{at}\psi(x_0).\end{aligned}$$

□

3.5.2 An Ordinary Differential Equation which ψ Satisfies

We can use the conjugacy relation (3.22) to derive a differential equation which $\psi(x_0)$ satisfies. In turn, we will use this differential equation to find a formula for $\psi(x_0)$ which does not involve the solution $\phi_t(x_0)$.

Proposition 3.17: *There is a $\delta > 0$ such that function ψ satisfies the non-autonomous initial value problem*

$$\left[ax_0 + b(x_0)\right]\psi' - a\psi = 0, \quad \psi(0) = 0, \quad \psi'(0) = 1 \tag{3.23}$$

for $x_0 \in B_\delta$, where $' = \frac{d}{dx_0}$.

Proof: First, we derive the differential equation. Assume that $\delta > 0$ is sufficiently small so that if $|x_0| < \delta$ then all necessary estimates apply. Now, differentiate (3.22) with respect to time and apply the differential equation in (3.1) to obtain

$$\psi'\left(\phi_t(x_0)\right)\left[a\phi_t(x_0) + b\left(\phi_t(x_0)\right)\right] = a\,\mathsf{e}^{at}\psi(x_0).$$

Setting $t = 0$ gives the differential equation. Second, to see why $\psi(0) = 0$ merely set $x_0 = 0$ in (3.12). Finally, we show that $\psi'(0) = 1$. Again using (3.12), we know $\psi(h) = h + \mathcal{O}(|h|^\alpha)$ as $h \to 0$. Since $\alpha > 1$, we have

$$\psi'(0) = \lim_{h\to 0}\frac{\psi(h) - \psi(0)}{h} = \lim_{h\to 0}\frac{\psi(h)}{h} = 1.$$

□

3.5.3 Finding ψ as a Quadrature Solution

It is possible to find a quadrature solution to (3.23) in a neighbourhood of 0. Let $\delta > 0$ be small enough so that[2] $\psi(x_0)$ is defined, (3.23) applies, $\psi(x) > 0$ for $x \in (0, \delta)$, $\psi(x) < 0$ for $x \in (-\delta, 0)$,

[2] We know that $\psi(x) = x + \mathsf{o}(x)$ and $b(x) = \mathsf{o}(x)$ as $x \to 0$. Thus, for sufficiently small $x > 0$ we can conclude $\psi(x) > 0$ and $ax + b(x) < 0$. Similarly, for sufficiently small $x < 0$ we have $\psi(x) < 0$ and $ax + b(x) > 0$.

$ax + b(x) < 0$ for $x \in (0, \delta)$, and $ax + b(x) > 0$ for $x \in (-\delta, 0)$. Furthermore, we need to assume that $\alpha \geq 2$.

For simplicity, assume that $0 < \varepsilon < x < x_0 < \delta$. Using partial fractions,

$$\frac{a}{ax + b(x)} = \frac{1}{x} - \frac{b(x)}{x\left[ax + b(x)\right]}. \tag{3.24}$$

Re-arranging the differential equation in (3.23) and applying (3.24), we have

$$\frac{\psi'(x)}{\psi(x)} = \frac{1}{x} - \frac{b(x)}{x\left[ax + b(x)\right]}.$$

Integrating with respect to x from ε to x_0, we have

$$\ln(\psi(x))\big|_{x=\varepsilon}^{x_0} = \ln(x)\big|_{x=\varepsilon}^{x_0} - \int_{\varepsilon}^{x_0} \frac{b(x)}{x\left[ax + b(x)\right]}\, dx.$$

Thus,

$$\ln\left(\frac{\psi(x_0)}{x_0}\right) = \ln\left(\frac{\psi(\varepsilon)}{\varepsilon}\right) - \int_{\varepsilon}^{x_0} \frac{b(x)}{x\left[ax + b(x)\right]}\, dx. \tag{3.25}$$

Note that we need $\alpha \geq 2$ so that the integral converges as $\varepsilon \to 0^+$. Since

$$\lim_{\varepsilon \to 0^+} \frac{\psi(\varepsilon)}{\varepsilon} = 1,$$

if we let $\varepsilon \to 0^+$ and take the exponential of both sides of (3.25), we arrive at the following.

Proposition 3.18: *Suppose that $\alpha \geq 2$. There is a $\delta > 0$ such that*

$$\psi(x_0) = x_0 \exp\left(-\int_0^{x_0} \frac{b(x)}{x\left[ax + b(x)\right]}\, dx\right) \quad \textit{for all} \quad x_0 \in B_\delta. \tag{3.26}$$

3.5.4 ψ is C^1 when b is C^1

Proposition 3.19: *There are open intervals $\mathcal{N}_1 \ni 0$ and $\mathcal{N}_2 \ni 0$ for which ψ is a C^1-diffeomorphism from $\mathcal{N}_1$ to $\mathcal{N}_2$.*

Proof: First, we will show that the integrand, namely $\mathsf{e}^{-as} b\left(\phi_s(x_0)\right)$, of the improper integral in the definition (3.10) of $\psi(x_0)$ is C^1 in a neighbourhood of 0. Since b is C^1 in a neighbourhood of 0, the right-hand side of the differential equation $\dot{x} = ax + b(x)$ is C^1 in a neighbourhood of 0. Thus, $\phi_t(x_0)$ is C^1 in both t and x_0 for sufficiently small x_0. Thus, $\mathsf{e}^{-as} b\left(\phi_s(x_0)\right)$ is C^1 in x_0 for sufficiently small x_0.

To ensure convergence of the relevant improper integrals we need estimates for $\mathsf{e}^{-as}b\left(\phi_s(x_0)\right)$ and $\frac{d}{ds}\left(\mathsf{e}^{-as}b\left(\phi_s(x_0)\right)\right)$. We know from (3.2), (3.3), (3.5), and (3.6) that there are $\delta, k_1, k_2 > 0$ such that

$$\left|\mathsf{e}^{-as}b\left(\phi_s(x_0)\right)\right| \le k_1\mathsf{e}^{(\alpha-1)as}\left|x_0\right|^\alpha \quad \text{for all} \quad (s, x_0) \in \Omega_\delta$$

and

$$\left|\mathsf{e}^{-as}b'\left(\phi_s(x_0)\right)\frac{\partial\phi_s(x_0)}{\partial x_0}\right| \le k_2\mathsf{e}^{\beta as}\left|x_0\right|^\beta \quad \text{for all} \quad (s, x_0) \in \Omega_\delta.$$

Thus, ψ is continuously differentiable for $|x_0| < \delta$ and we can differentiate (3.10) with respect to x_0 under the integral sign:

$$\psi'(x_0) = 1 + \int_0^\infty \mathsf{e}^{-as}b'(\phi_s(x_0))\frac{\partial\phi_s(x_0)}{\partial x_0}\,ds.$$

Let $\mathcal{N}_1$ be an open interval, with $0 \in \mathcal{N}_1$ and $\mathcal{N}_1 \subset B_\delta$, such that $\psi'(x_0) > 0$ for all $x_0 \in \mathcal{N}_1$. Now, take $\mathcal{N}_2 := \psi\left(\mathcal{N}_1\right)$, which is an open interval containing 0, and so we can write $\psi \in C^1(\mathcal{N}_1, \mathcal{N}_2)$. By the Inverse Function Theorem, ψ is invertible with inverse $\psi^{-1} \in C^1(\mathcal{N}_2, \mathcal{N}_1)$. $\square$

3.5.5 Analyticity of ψ when b is Analytic

Proposition 3.20: *If b is analytic at zero, then ψ is analytic at zero. Furthermore, ψ is invertible and ψ^{-1} is analytic at zero.*

Proof: First, we need to show that the integral

$$\int_0^\infty \mathsf{e}^{-as}b\left(\phi_s(x_0)\right)\,ds,$$

which is equal to $\psi(x_0) - x_0$, is an analytic function of x_0 at 0. Let $F(z,t) := \mathsf{e}^{-at}b\left(\phi_t(z)\right)$ where we consider $z \in \mathbb{C}$ and $t \ge 0$. See, for example, [59] and §1.8 of [28] for a discussion of how we can regard x and x_0 as complex numbers in (3.1). We know that there is a domain $\Omega \subset \mathbb{C}$ containing $z = 0$ such that $F(z,t)$ is complex analytic in z over Ω and continuous in t. Furthermore, we assume that Ω is small enough so that

$$|F(z,t)| \le k\,\mathsf{e}^{(\alpha-1)at}\,|z|^\alpha \quad \text{for all} \quad z \in \Omega \quad \text{and} \quad t \ge 0$$

for some $k > 0$. We know we can do this because of the estimate (3.9). Let $r > 0$ be large enough so that $\Omega \subset B_r$. Then,

$$|F(z,t)| \le k\,\mathsf{e}^{(\alpha-1)at}r^\alpha \quad \text{and} \quad \int_0^\infty \left(k\,\mathsf{e}^{(\alpha-1)as}r^\alpha\right)\,ds = \frac{kr^\alpha}{(1-\alpha)\,a} < \infty.$$

It follows that the integral $\int_0^\infty F(z,s)\,ds$ is complex analytic in z. (See §2.2 on page 18.) Hence, $\psi(z)$ is a complex analytic function of z in Ω. Therefore, $\psi(x_0)$ is (real) analytic in x_0 at 0.

The fact that ψ is invertible with ψ^{-1} being analytic at zero follows from the fact that $\psi'(0) = 1$ and the Real Analytic Inverse Function Theorem (see, for example, page 47 of [73]). $\square$

3.5.6 Taylor Series for ψ if b has a Taylor Series

Assume that both b and ψ can be written as Taylor series at 0,

$$b(x) = \sum_{i=0}^{\infty} b_i x^i \quad \text{and} \quad \psi(x_0) = \sum_{i=0}^{\infty} \sigma_i x_0^i.$$

Based on our knowledge of b and ψ, we can conclude

$$b_0 = 0, \quad b_1 = 0, \quad \sigma_0 = 0, \quad \text{and} \quad \sigma_1 = 1.$$

We will derive a recursive expression for the coefficients $\{\sigma_i\}_{i=0}^{\infty}$ in terms of $\{b_i\}_{i=0}^{\infty}$.

For simplicity we will refer to x as opposed to x_0. Substitute the series for b and ψ into the differential equation (3.23) to obtain

$$\left[ax + \sum_{i=0}^{\infty} b_i x^i\right]\left[\sum_{i=0}^{\infty} (i+1)\,\sigma_{i+1} x^i\right] - a\left[\sum_{i=0}^{\infty} \sigma_i x^i\right] = 0.$$

Expanding the products and adjusting the indices,

$$a\left[\sum_{i=0}^{\infty} i\sigma_i x^i\right] + \sum_{i=0}^{\infty}\left[\sum_{j=0}^{i} b_{i-j}\,(j+1)\,\sigma_{j+1}\right] x^i - a\left[\sum_{i=0}^{\infty} \sigma_i x^i\right] = 0.$$

The reader may wish to consult §A.13 of Appendix A which covers the Cauchy product of series. Recalling that $b_0 = b_1 = 0$, it follows that

$$\sigma_0 = 0, \quad \sigma_1 = 1, \quad \sigma_i = \left[\frac{1}{a(1-i)}\right] \sum_{j=0}^{i-2} (j+1)\, b_{i-j}\sigma_{j+1} \quad (i \geq 2).$$

The second and third terms are, respectively,

$$\sigma_2 = -\frac{b_2}{a} \quad \text{and} \quad \sigma_3 = \frac{2b_2^2 - ab_3}{2a^2}.$$

3.5.7 Optimality of the Linearized Solution $\mathsf{e}^{at}y_0$

The following theorem shows that the initial condition y_0 yields the linear solution $\mathsf{e}^{at}y_0$ that is closest to the actual solution $\phi_t(x_0)$. Note that, as can be deduced from (3.13) and Remark 2.8,

$$\limsup_{t\to\infty} \frac{\ln\left|\phi_t(x_0) - \mathsf{e}^{at}\psi(x_0)\right|}{t} \leq \alpha a.$$

We claim that this inequality is not preserved if we replace $\psi(x_0)$ with $z_0 \neq \psi(x_0)$. In other words, $\left|\phi_t(x_0) - \mathsf{e}^{at}\psi(x_0)\right|$ has a faster exponential decay rate than $\left|\phi_t(x_0) - \mathsf{e}^{at}z_0\right|$ for any $z_0 \neq \psi(x_0)$.

Theorem 3.21: *There are neighbourhoods $\mathcal{N}_1$ and $\mathcal{N}_2$ of zero such that for any $y_0 \in \mathcal{N}_2$ there exists a unique $x_0 \in \mathcal{N}_1$ such that*[3]

$$\limsup_{t\to\infty} \frac{\ln\left|\phi_t(x_0) - \mathsf{e}^{at}y_0\right|}{t} \leq \alpha a.$$

Proof: Let $\delta > 0$ be sufficiently small so that if $x_0 \in \mathcal{N}_1 := B_\delta$ then all appropriate estimates apply and ψ is a bijection from $\mathcal{N}_1$ to $\mathcal{N}_2 := \psi(\mathcal{N}_1)$. Let $y_0 \in \mathcal{N}_2$ be fixed.

To show existence, take $x_0 := \psi^{-1}(y_0)$. The estimate is satisfied by virtue of (3.13). To show uniqueness, suppose that $\widehat{x}_0 \in \mathcal{N}_1$ has $\phi_t(\widehat{x}_0)$ also satisfying the given estimate. Let $\widehat{y}_0 := \psi(\widehat{x}_0)$. Using the integral equation (3.11),

$$\phi_t(\widehat{x}_0) = \mathsf{e}^{at}\widehat{y}_0 - \int_t^\infty \mathsf{e}^{a(t-s)} b\left(\phi_s(\widehat{x}_0)\right)\, ds.$$

Subtracting $\mathsf{e}^{at}y_0$ from both sides and re-arranging,

$$\mathsf{e}^{at}\left(\widehat{y}_0 - y_0\right) = \phi_t(\widehat{x}_0) - \mathsf{e}^{at}y_0 + \int_t^\infty \mathsf{e}^{a(t-s)} b\left(\phi_s(\widehat{x}_0)\right)\, ds.$$

Taking the absolute value of both sides and applying the Triangle Inequality,

$$\mathsf{e}^{at}\left|\widehat{y}_0 - y_0\right| \leq \left|\phi_t(\widehat{x}_0) - \mathsf{e}^{at}y_0\right| + \mathsf{e}^{at}\left|\int_t^\infty \mathsf{e}^{-as} b\left(\phi_s(\widehat{x}_0)\right)\, ds\right|.$$

Using the estimate (3.9) along with the estimate that $\phi_t(\widehat{x}_0)$ is assumed to satisfy, we see that there is a $k > 0$ such that

$$\mathsf{e}^{at}\left|\widehat{y}_0 - y_0\right| \leq k\,\mathsf{e}^{\alpha at} \quad \text{for all} \quad t \geq 0.$$

Thus,

$$\left|\widehat{y}_0 - y_0\right| \leq k\,\mathsf{e}^{(\alpha-1)at} \quad \text{for all} \quad t \geq 0.$$

Letting $t \to \infty$, we see that $\widehat{y}_0 = y_0$. Since ψ is a bijection from $\mathcal{N}_1$ to $\mathcal{N}_2$, $\widehat{x}_0 = x_0$. □

[3] If $\left|\phi_t(x_0) - \mathsf{e}^{at}y_0\right| = 0$ then we take the natural logarithm to be $-\infty$.

Corollary 3.22: *There are neighbourhoods $\mathcal{N}_1$ and $\mathcal{N}_2$ of 0 such that if $x_0 \in \mathcal{N}_1$ and $y_0 \in \mathcal{N}_2 \setminus \{\psi(x_0)\}$ then*

$$\limsup_{t\to\infty} \frac{\ln\left|\phi_t(x_0) - \mathrm{e}^{at} y_0\right|}{t} > \alpha a.$$

3.5.8 A Simple Example

We will conclude this section with two simple examples of using (3.26) to find $\psi(x_0)$. First, consider the initial value problem

$$\dot{x} = ax + \varepsilon x^r, \quad x(0) = x_0,$$

where $a < 0$, $r \geq 2$, and $\varepsilon > 0$. Then,

$$\begin{aligned}
\psi(x_0) &= x_0 \exp\left(-\int_0^{x_0} \frac{\varepsilon x^r}{x\,[ax + \varepsilon x^r]}\,dx\right) \\
&= x_0 \exp\left(\ln\left(\frac{a}{a + \varepsilon x_0^{r-1}}\right)^{\frac{1}{r-1}}\right) \\
&= x_0 \left(\frac{a}{a + \varepsilon x_0^{r-1}}\right)^{\frac{1}{r-1}}.
\end{aligned}$$

From this, we see that we should restrict x_0 by requiring

$$|x_0| < \left(-\frac{a}{\varepsilon}\right)^{\frac{1}{r-1}}.$$

3.5.9 Another Simple Example

Now consider the initial value problem

$$\dot{x} = -\sin(x)\,, \quad x(0) = x_0,$$

where $|x_0| < \pi$. Clearly, we can take $a = -1$, $b(x) = x - \sin(x)$, $\alpha = 3$, and $\beta = 2$. Using (3.26),

$$\psi(x_0) = x_0 \exp\left(\int_0^{x_0} \frac{x - \sin(x)}{x\sin(x)}\,dx\right) = \frac{2\,[1 - \cos(x_0)]}{\sin(x_0)}.$$

Observe that

$$\psi(x_0) = x_0 + \tfrac{1}{12}\,x_0^3 + \mathcal{O}\big(x_0^5\big) \quad \text{as} \quad x_0 \to 0.$$

By Theorem 3.9, the solution $\phi_t(x_0)$ of the initial value problem satisfies

$$\phi_t(x_0) = \frac{2\,[1 - \cos(x_0)]}{\sin(x_0)}\,\mathrm{e}^{-t} + \mathcal{O}\big(\mathrm{e}^{-3t} x_0^3\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0.$$

3.6 Iterates of the Third Type (which are Flows)

The iterates $\left\{\chi^{(m)}(t, y_0)\right\}_{m=1}^{\infty}$, where $y_0 := \psi(x_0)$ and x_0 is sufficiently small, have an undesired feature, namely that they are not themselves flows. To see why the iterates are not flows, we need not look any further than the example in §3.3.4 on page 46. We calculated

$$\chi^{(2)}(t, y_0) = \mathsf{e}^{-t} y_0 - \tfrac{1}{2}\,\mathsf{e}^{-3t} y_0^3.$$

It is easy to see that

$$\chi^{(2)}(0, y_0) \neq y_0 \quad \text{and} \quad \chi^{(2)}\left(s, \chi^{(2)}(t, y_0)\right) \neq \chi^{(2)}(s+t, y_0).$$

The problem is in how we set up the iterates of the first type. Fortunately, we can construct new iterates from the old iterates which are in fact flows.

3.6.1 A Lemma

In order to construct iterates that are flows, first we need to establish an interesting property of the iterates of the first type. This property resembles the semi-group property of flows.

Lemma 3.23: *There exists a $\delta > 0$ such that*

$$\chi^{(m)}(s, \psi(\phi_t(x_0))) = \chi^{(m)}(s+t, \psi(x_0)) \quad \textit{for all} \quad s, t \geq 0,\ x_0 \in B_\delta,\ m \in \mathbb{N}. \tag{3.27}$$

Proof: There is a $\delta > 0$ (independent of m) such that if $|x_0| < \delta$ then all relevant improper integrals converge and all relevant estimates apply. Hence, we will assume that $|x_0| < \delta$. The proof will be by induction on m. Consider first the base case $m = 1$, which involves the iterate $\chi^{(1)}(t, y_0) = \mathsf{e}^{at} y_0$. Using the conjugacy condition (3.22), we easily see that the first iterate satisfies the lemma:

$$\chi^{(1)}(s, \psi(\phi_t(x_0))) = \mathsf{e}^{as}\psi(\phi_t(x_0)) = \mathsf{e}^{as}\mathsf{e}^{at}\psi(x_0) = \mathsf{e}^{a(s+t)}\psi(x_0) = \chi^{(1)}(s+t, \psi(x_0)).$$

Now, assume the lemma is true for $m \in \mathbb{N}$. Using the definition (3.14b) of the iterate $\chi^{(m+1)}(t, y_0)$, the conjugacy condition (3.22), and the induction hypothesis, we have

$$\begin{aligned}
\chi^{(m+1)}(s, \psi(\phi_t(x_0))) &= \mathsf{e}^{as}\psi(\phi_t(x_0)) - \int_s^\infty \mathsf{e}^{a(s-r)} b\left(\chi^{(m)}(r, \psi(\phi_t(x_0)))\right) dr \\
&= \mathsf{e}^{as}\mathsf{e}^{at}\psi(x_0) - \int_s^\infty \mathsf{e}^{a(s-r)} b\left(\chi^{(m)}(r+t, \psi(x_0))\right) dr.
\end{aligned}$$

Using the change of variables $\xi = r + t$ in the integral, we get

$$\begin{aligned}\chi^{(m+1)}\left(s, \psi\left(\phi_t(x_0)\right)\right) &= \mathrm{e}^{a(s+t)}\psi(x_0) - \int_{s+t}^{\infty} \mathrm{e}^{a(s+t-\xi)} b\left(\chi^{(m)}\left(\xi, \psi\left(x_0\right)\right)\right) d\xi \\ &= \chi^{(m+1)}\left(s+t, \psi\left(x_0\right)\right).\end{aligned}$$

Hence the lemma is true for $m+1$. By induction, the lemma is true for all $m \in \mathbb{N}$. □

Corollary 3.24: *There is a $\delta > 0$ such that*

$$\chi^{(m)}\left(s, \mathrm{e}^{at}\psi(x_0)\right) = \chi^{(m)}\left(s+t, \psi(x_0)\right) \quad \textit{for all} \quad s, t \geq 0,\ x_0 \in B_\delta,\ m \in \mathbb{N}. \tag{3.28}$$

Proof: It follows from (3.22) and (3.27). □

3.6.2 Definition of the Iterates

Now, we are in a position to define the *iterates of the third type*, $\left\{\varphi_t^{(m)}\left(z_0\right)\right\}_{m=1}^{\infty}$, which are indeed flows. Generally, $\chi^{(m)}\left(0, y_0\right) \neq y_0$. The new iterates will be constructed with $\chi^{(m)}\left(0, y_0\right)$ (for a given m) as the initial point. Hence, take

$$z_0^{(m)} := \chi^{(m)}\left(0, y_0\right) \quad \left(m \in \mathbb{N}\right).$$

The estimate (3.16) implies that there are $\delta, k > 0$ (independent of m) such that

$$\left|z_0^{(m)}\right| \leq k\left|x_0\right| \quad \text{for all} \quad x_0 \in B_\delta,\ m \in \mathbb{N}.$$

Define

$$\varphi_t^{(m)}\left(z_0\right) := \chi^{(m)}\left(t, \left[\chi^{(m)}\left(0, \cdot\right)\right]^{-1}\left(z_0\right)\right) \quad \left(m \in \mathbb{N}\right), \tag{3.29}$$

where z_0 is sufficiently small. (Note that there is no problem using z_0 in the definition (3.29) instead of $z_0^{(m)}$.) That is,

$$\varphi_t^{(m)}\left(z_0^{(m)}\right) = \chi^{(m)}\left(t, y_0\right) \quad \left(m \in \mathbb{N}\right). \tag{3.30}$$

Proposition 3.25: *There is a $\delta > 0$ such that if $|z_0| < \delta$ then, for each $m \in \mathbb{N}$, $\varphi_t^{(m)}\left(z_0\right)$ is a flow.*

Proof: There is a $\delta > 0$ (independent of m) such that if $|z_0| < \delta$ then all relevant improper integrals converge and all relevant estimates apply. Assume that $|z_0| < \delta$. Note that $\chi^{(m)}\left(0, \cdot\right)$ is indeed invertible since it is a near-identity transformation. Now, for $\varphi_t^{(m)}\left(z_0\right)$ to be a flow, we need

$$\varphi_0^{(m)}\left(z_0\right) = z_0 \quad \text{and} \quad \varphi_s^{(m)}\left(\varphi_t^{(m)}\left(z_0\right)\right) = \varphi_{s+t}^{(m)}\left(z_0\right).$$

The first condition is obtained by setting $t = 0$ in the definition (3.29). To obtain the second condition, first use the definition of $\varphi_t^{(m)}(z_0)$, which tells us

$$\begin{aligned}\varphi_s^{(m)}\left(\varphi_t^{(m)}(z_0)\right) &= \chi^{(m)}\left(s, \left[\chi^{(m)}(0,\cdot)\right]^{-1}\left(\varphi_t^{(m)}(z_0)\right)\right)\\ &= \chi^{(m)}\left(s, \left[\chi^{(m)}(0,\cdot)\right]^{-1}\left(\chi^{(m)}\left(t, \left[\chi^{(m)}(0,\cdot)\right]^{-1}(z_0)\right)\right)\right).\end{aligned}$$

Using (3.28) with $s = 0$ and canceling inverse functions,

$$\begin{aligned}\varphi_s^{(m)}\left(\varphi_t^{(m)}(z_0)\right) &= \chi^{(m)}\left(s, \left[\chi^{(m)}(0,\cdot)\right]^{-1}\left(\chi^{(m)}\left(0, \mathsf{e}^{at}\left[\chi^{(m)}(0,\cdot)\right]^{-1}(z_0)\right)\right)\right)\\ &= \chi^{(m)}\left(s, \mathsf{e}^{at}\left[\chi^{(m)}(0,\cdot)\right]^{-1}(z_0)\right).\end{aligned}$$

Using (3.28) again,

$$\varphi_s^{(m)}\left(\varphi_t^{(m)}(z_0)\right) = \chi^{(m)}\left(s+t, \left[\chi^{(m)}(0,\cdot)\right]^{-1}(z_0)\right) = \varphi_{s+t}^{(m)}(z_0).$$

□

3.6.3 Differential Equation which the Iterates Satisfy

The solution of an autonomous differential equation defines a flow as a solution. In fact, a flow defines an autonomous differential equation. The standard argument, for the scalar case, is as follows. Consider $\varphi_t^{(m)}(z_0)$, which we know is a flow, and define

$$g^{(m)}(z) := \frac{d}{dt}\left(\varphi_t^{(m)}(z)\right)\Big|_{t=0} = \lim_{h\to 0}\frac{\varphi_h^{(m)}(z) - z}{h}.$$

We know that $\varphi_0^{(m)}(z_0) = z_0$. Calculate

$$\frac{d}{dt}\left(\varphi_t^{(m)}(z_0)\right) = \lim_{h\to 0}\frac{\varphi_{t+h}^{(m)}(z_0) - \varphi_t^{(m)}(z_0)}{h} = \lim_{h\to 0}\frac{\varphi_h^{(m)}\left(\varphi_t^{(m)}(z_0)\right) - \varphi_t^{(m)}(z_0)}{h} = g^{(m)}\left(\varphi_t^{(m)}(z_0)\right).$$

Hence, $\varphi_t^{(m)}(z_0)$ is the solution of the initial value problem

$$\dot{z} = g^{(m)}(z), \quad z(0) = z_0.$$

Consider the sequence $\left\{g^{(m)}\right\}_{m=1}^{\infty}$. We can actually write down an expression for $g^{(m)}(z)$. Trivially,

$$g^{(1)}(z) = az.$$

To specify $g^{(m+1)}(z)$, we need $\chi^{(m)}(0,\cdot)$ and $\left[\chi^{(m+1)}(0,\cdot)\right]^{-1}$. Now, for a fixed $m \in \mathbb{N}$ substitute

$$y_0 = \left[\chi^{(m+1)}(0,\cdot)\right]^{-1}(z)$$

into (3.15) and use the definition (3.29) of the iterates of the third type to obtain

$$\frac{d}{dt}\left(\varphi_t^{(m+1)}(z)\right) = a\,\varphi_t^{(m+1)}(z) + b\left(\chi^{(m)}\left(t, \left[\chi^{(m+1)}(0,\cdot)\right]^{-1}(z)\right)\right).$$

Setting $t = 0$ gives

$$g^{(m+1)}(z) = az + b\left(\chi^{(m)}\left(0, \left[\chi^{(m+1)}(0,\cdot)\right]^{-1}(z)\right)\right) \quad (m \in \mathbb{N}).$$

We have thus shown the following.

Claim 3.26: *Let z_0 be sufficiently small. The iterate $\varphi_t^{(m)}(z_0)$ is the solution of*

$$\dot{z} = g^{(m)}(z), \quad z(0) = z_0,$$

where

$$g^{(m)}(z) := \begin{cases} az, & \text{if} \quad m = 1 \\ az + b\left(\chi^{(m-1)}\left(0, \left[\chi^{(m)}(0,\cdot)\right]^{-1}(z)\right)\right), & \text{if} \quad m > 1 \end{cases}.$$

Recall that the right-hand side of the differential equation in (3.1) is $ax + b(x)$. How close is $g^{(m)}(z)$ to $az + b(z)$? First, observe that if we set $t = 0$ in (3.18) we obtain

$$\chi^{(m)}(0, \psi(x_0)) = x_0 + \mathcal{O}\left(|x_0|^{\alpha+(m-1)\beta}\right) \quad \text{as} \quad x_0 \to 0.$$

For $m > 1$, it can be shown that[4]

$$\chi^{(m-1)}\left(0, \left[\chi^{(m)}(0,\cdot)\right]^{-1}(z)\right) = z + \mathcal{O}\left(|z|^{\alpha+(m-2)\beta}\right) \quad \text{as} \quad z \to 0.$$

Using this in conjunction with the definition of $g^{(m)}(z)$ (given in the claim) and the Mean Value Theorem gives us the following.

Claim 3.27: *The function $g^{(m)}(z)$ satisfies*

$$\left|az + b(z) - g^{(m)}(z)\right| = \mathcal{O}\left(|z|^{\alpha+(m-1)\beta}\right) \quad \text{as} \quad z \to 0.$$

[4]The following fact will come in handy. If f is a function which satisfies, for some $r > 1$,

$$f(u) = u + \mathcal{O}(|u|^r) \quad \text{as} \quad u \to 0$$

then f is invertible in a neighbourhood of $u = 0$ with

$$f^{-1}(v) = v + \mathcal{O}(|v|^r) \quad \text{as} \quad v \to 0.$$

3.6.4 A Conjugacy Condition for the Iterates

Define, for sufficiently small x_0,

$$\widehat{\psi}^{(m)}(x_0) := \chi^{(m)}\left(0, \psi(x_0)\right) \quad (m \in \mathbb{N}). \tag{3.31}$$

The initial condition $z_0^{(m)}$ above thus can be written

$$z_0^{(m)} = \widehat{\psi}^{(m)}(x_0).$$

Observe that

$$\varphi_t^{(m)}\left(\widehat{\psi}^{(m)}(x_0)\right) = \chi^{(m)}\left(t, \psi(x_0)\right), \tag{3.32}$$

which follows from (3.30). Observe also that $\widehat{\psi}^{(1)} = \psi$.

Recall that the function ψ, which maps the initial condition x_0 to the initial condition y_0, satisfies the conjugacy condition $\psi\left(\phi_t(x_0)\right) = \mathsf{e}^{at}\psi(x_0)$. That is, ψ maps flows of the nonlinear differential equation onto flows of the linear differential equation. It turns out that the function $\widehat{\psi}^{(m)}$, which maps the initial condition x_0 to $z_0^{(m)}$, satisfies its own conjugacy condition. In particular, $\widehat{\psi}^{(m)}$ maps flows of the original nonlinear differential equation onto flows of the (generally nonlinear) differential equation which $\varphi_t^{(m)}(z_0)$ satisfies.

Theorem 3.28: *Consider the function $\widehat{\psi}^{(m)}$. There is a $\delta > 0$ such that*

$$\widehat{\psi}^{(m)}\left(\phi_t(x_0)\right) = \varphi_t^{(m)}\left(\widehat{\psi}^{(m)}(x_0)\right) \quad \textit{for all} \quad (t, x_0) \in \Omega_\delta,\ m \in \mathbb{N}.$$

Proof: Let x_0 be sufficiently small, say $|x_0| < \delta$ where $\delta > 0$. Consider

$$\begin{aligned}\widehat{\psi}^{(m)}\left(\phi_t(x_0)\right) &= \chi^{(m)}\left(0, \psi\left(\phi_t(x_0)\right)\right) \quad \text{(using (3.31))}\\ &= \chi^{(m)}\left(t, \psi(x_0)\right) \quad \text{(using (3.27) with } s = 0\text{)}\\ &= \varphi_t^{(m)}\left(\widehat{\psi}^{(m)}(x_0)\right) \quad \text{(using (3.32)).}\end{aligned}$$

□

Proposition 3.29: *There is a $\delta > 0$ and $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ such that*

$$\left|\widehat{\psi}^{(m)}(x_0) - x_0\right| \leq k_m\,|x_0|^{\alpha+(m-1)\beta} \quad \textit{for all} \quad x_0 \in B_\delta,\ m \in \mathbb{N}.$$

Proof: Set $t = 0$ in (3.18) and apply (3.31). □

3.6.5 A Simple Example

Consider the initial value problem

$$\dot{x} = -x + x^2, \quad x(0) = x_0.$$

We will find the first two iterates of the first type and the first two iterates of the third type. We will also find the autonomous differential equation which the second iterate of the third type satisfies. First, note that using (3.26) we can calculate

$$y_0 = \frac{x_0}{1 - x_0}, \quad |x_0| < 1.$$

Using (3.14), we can calculate the first two iterates of the first type, which are

$$\chi^{(1)}(t, y_0) = \mathsf{e}^{-t} y_0 \quad \text{and} \quad \chi^{(2)}(t, y_0) = \mathsf{e}^{-t} y_0 - \mathsf{e}^{-2t} y_0^2.$$

In order to find the first two iterates of the third type, we need to invert

$$z_0^{(1)} = \chi^{(1)}(0, y_0) = y_0 \quad \text{and} \quad z_0^{(2)} = \chi^{(2)}(0, y_0) = y_0 - y_0^2.$$

Thus,

$$\left[\chi^{(1)}(0, \cdot)\right]^{-1}(z_0) = z_0 \quad \text{and} \quad \left[\chi^{(2)}(0, \cdot)\right]^{-1}(z_0) = \tfrac{1}{2}\left(1 - \sqrt{1 - 4z_0}\right), \quad |z_0| < \tfrac{1}{4}.$$

(Note that in finding $\left[\chi^{(2)}(0, \cdot)\right]^{-1}(z_0)$, we take the negative root so that the resulting expression is near-identity.) Hence,

$$\varphi_t^{(1)}(z_0) = \chi^{(1)}(t, z_0) = \mathsf{e}^{-t} z_0$$

and

$$\varphi_t^{(2)}(z_0) = \chi^{(2)}\left(t, \tfrac{1}{2}\left[1 - \sqrt{1 - 4z_0}\right]\right) = \mathsf{e}^{-t}\left(\tfrac{1}{2}\left[1 - \sqrt{1 - 4z_0}\right]\right) - \mathsf{e}^{-2t}\left(\tfrac{1}{2}\left[1 - \sqrt{1 - 4z_0}\right]\right)^2.$$

We will use the material in §3.6.3 on page 60 to find the autonomous differential equation which $\varphi_t^{(2)}(z_0)$ satisfies. Here, $a = -1$ and $b(x) = x^2$. Calculate

$$\chi^{(1)}\left(0, \left[\chi^{(2)}(0, \cdot)\right]^{-1}(z)\right) = \tfrac{1}{2}\left(1 - \sqrt{1 - 4z}\right).$$

Thus, $\varphi_t^{(2)}(z_0)$ is the solution of

$$\dot{z} = -z + \tfrac{1}{4}\left(1 - \sqrt{1 - 4z}\right)^2, \quad z(0) = z_0.$$

3.7 Summary

The topic of this chapter was the nonlinear initial value problem

$$\dot{x} = ax + b(x), \quad x(0) = x_0$$

and an iteration procedure to find the asymptotic behaviour of the solution $\phi_t(x_0)$ as $t \to \infty$. In particular, $a < 0$ is a constant and the function b is C^1 in a neighbourhood of 0 with

$$|b(x)| = \mathcal{O}(|x|^\alpha) \quad \text{and} \quad \left|b'(x)\right| = \mathcal{O}\Big(|x|^\beta\Big) \quad \text{as} \quad x \to 0$$

for constants $\alpha > 1$ and $\beta > 0$. The flow $\phi_t(x_0)$ satisfies the estimate

$$|\phi_t(x_0)| = \mathcal{O}\big(\mathsf{e}^{at}\,|x_0|\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0.$$

We re-wrote the standard integral equation for the flow $\phi_t(x_0)$ as

$$\phi_t(x_0) = \mathsf{e}^{at} y_0 - \int_t^\infty \mathsf{e}^{a(t-s)} b(\phi_s(x_0))\, ds,$$

where

$$y_0 = \psi(x_0) = x_0 + \int_0^\infty \mathsf{e}^{-as} b(\phi_s(x_0))\, ds$$

is a useful, related initial condition. Note that our assumptions on a and $b(x)$ as well as our exponential estimate for the flow guarantee that the above improper integrals converge for sufficiently small x_0. Interestingly, the function ψ is near-identity and y_0 is the unique point such that

$$\lim_{t\to\infty} \frac{\ln\left|\phi_t(x_0) - \mathsf{e}^{at} y_0\right|}{t} \le \alpha a.$$

In other words, y_0 is the optimal initial condition for the linearized initial value problem.

This chapter introduced iterates of the first type $\left\{\chi^{(m)}\,(t, y_0)\right\}_{m=1}^\infty$, given by

$$\chi^{(1)}\,(t, y_0) = \mathsf{e}^{at} y_0, \quad \chi^{(m+1)}\,(t, y_0) = \mathsf{e}^{at} y_0 - \int_t^\infty \mathsf{e}^{a(t-s)} b\left(\chi^{(m)}\,(s, y_0)\right)\, ds \quad (m \in \mathbb{N}).$$

In practice, y_0 is left as a parameter so that is why we regard y_0 as a variable instead of x_0. These iterates satisfy the decay rate

$$\left|\chi^{(m)}\,(t, y_0)\right| = \mathcal{O}\big(\mathsf{e}^{at}\,|x_0|\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0 \quad \text{uniformly in} \quad m.$$

Furthermore, the iterates are successively better asymptotic approximations to the actual solution as $t \to \infty$, satisfying

$$\left|\phi_t(x_0) - \chi^{(m)}(t, y_0)\right| = \mathcal{O}\Big(\mathrm{e}^{[\alpha+(m-1)\beta]at}\,|x_0|^{\alpha+(m-1)\beta}\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad x_0 \to 0.$$

If we can approximate $b(x)$ by a Taylor series, then we can construct the iterates of the second type $\{\widetilde{\chi}^{(m)}(t, y_0)\}_{m=1}^{\infty}$ similar to the iterates of the first type by truncating $b(x)$ to a certain order. If we only have a Taylor polynomial for $b(x)$, we can only define a certain number of iterates.

The function ψ satisfies the conjugacy condition

$$\psi(\phi_t(x_0)) = \mathrm{e}^{at}\psi(x_0),$$

which is reminiscent of the Hartman-Grobman Theorem. Also, ψ satisfies the initial value problem

$$[ax_0 + b(x_0)]\,\psi' - a\psi = 0, \quad \psi(0) = 0, \quad \psi'(0) = 1.$$

If $\alpha \geq 2$, we can express $\psi(x)$ as the quadrature solution

$$\psi(x_0) = x_0 \exp\left(-\int_0^{x_0} \frac{b(x)}{x\,[ax + b(x)]}\,dx\right).$$

Finally, we know that if $b(x)$ is analytic then $\psi(x_0)$ is analytic.

The iterates of the first type have a natural definition but have an aesthetically-unpleasing feature: the iterates are not flows. Hence, we defined the iterates of the third type $\left\{\varphi_t^{(m)}(z_0)\right\}_{m=1}^{\infty}$, given by

$$\varphi_t^{(m)}(z_0) = \chi^{(m)}\left(t, \left[\chi^{(m)}(0, \cdot)\right]^{-1}(z_0)\right) \quad (m \in \mathbb{N})$$

which are indeed flows. That is,

$$\varphi_0^{(m)}(z_0) = z_0 \quad \text{and} \quad \varphi_s^{(m)}\left(\varphi_t^{(m)}(z_0)\right) = \varphi_{s+t}^{(m)}(z_0).$$

The initial point z_0 for the iterate $\varphi_t^{(m)}(z_0)$ is $z_0 = \chi^{(m)}(0, y_0)$. Furthermore, these iterates satisfy the conjugacy condition

$$\widehat{\psi}^{(m)}(\phi_t(x_0)) = \varphi_t^{(m)}\left(\widehat{\psi}^{(m)}(x_0)\right), \quad \text{where} \quad \widehat{\psi}^{(m)}(x_0) = \chi^{(m)}(0, \psi(x_0)).$$

That is, $\widehat{\psi}^{(m)}$ (which gives z_0 as a function of x_0 for a given m) maps flows of the nonlinear differential equation onto flows of the differential equation which $\varphi_t^{(m)}(z_0)$ satisfies.

Chapter 4

Closely-Spaced Eigenvalues ($\kappa < \alpha$)

4.1 Introduction

In the previous chapter, we explored an iterative procedure which yielded successively better asymptotic approximations $\left\{\chi^{(m)}\left(t, y_0\right)\right\}_{m=1}^{\infty}$ to solutions $\phi_t(x_0)$ of the scalar version of (2.5) as $t \to \infty$ when x_0 is sufficiently small. Here, we will extend the results of Chapter 3 to the multi-dimensional case where the eigenvalues of $\mathbf{A}$ are closely-spaced relative to the nonlinear part $\mathbf{b}(\mathbf{x})$. Consider once again the system

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0. \tag{4.1}$$

We will restate the important general assumptions about this system and then specify the special assumption for this chapter.

4.1.1 Assumptions

Assumption 4.1: The real parts of the eigenvalues of the matrix $\mathbf{A}$ satisfy

$$\mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1 < 0.$$

Assumption 4.2: Consider the vector field $\mathbf{b}$.

(a) There is some neighbourhood $\mathcal{N} \subset \mathbb{R}^n$ with $\mathbf{0} \in \mathcal{N}$ and $\mathbf{b} \in C^1(\mathcal{N}, \mathbb{R}^n)$.

(b) There are $\delta, k > 0$ such that

$$\|\mathbf{b}(\mathbf{x})\| \leq k \, \|\mathbf{x}\|^{\alpha} \quad \text{for all} \quad \mathbf{x} \in B_{\delta}, \tag{4.2}$$

where $\alpha > 1$ is a fixed parameter.

(c) There are $\delta, k > 0$ such that

$$\|\mathbf{Db}(\mathbf{x})\| \leq k \|\mathbf{x}\|^{\beta} \quad \text{for all} \quad \mathbf{x} \in B_{\delta}, \tag{4.3}$$

where $\beta > 0$ is a fixed parameter.

Assumption 4.3: Recall the ratio

$$\kappa = \frac{\mu_n}{\mu_1}$$

which quantifies the spacing of the eigenvalues and satisfies $\kappa \geq 1$. In this chapter, we will consider only the case where the eigenvalues are closely-spaced. That is, we will assume $\kappa < \alpha$. Equivalently,

$$\alpha\mu_1 < \mu_n. \tag{4.4}$$

Remark 4.4: Observe that the scalar case, which we covered in Chapter 3, has $\kappa = 1$ and is a special case of closely-spaced eigenvalues. Consequently, this chapter will very much echo Chapter 3. However, there are many complications introduced by switching to multiple dimensions.

4.1.2 Martin Wainwright

Martin Wainwright, who is the son of the cosmologist John Wainwright, once worked as a summer undergraduate research assistant with David Siegel. The content of this part of the thesis was born out of the work done during that summer. In particular, the exploration of (what we now call) iterates of the first type for the case of closely-spaced eigenvalues was initiated. Moreover, the assumptions on the vector field $\mathbf{b}$ were different and special cases of Theorems 2.12, 4.9, and 4.20 were proved.

4.1.3 Important Estimates We Already Know

Define, for any $\delta > 0$, the set

$$\Omega_{\delta} := \{\ (t, \mathbf{x}) \ : \ t \geq 0,\ \mathbf{x} \in \mathbb{R}^n,\ \ \|\mathbf{x}\| < \delta\ \}.$$

The basic estimates, which we saw in Chapter 2, that we will use frequently in this chapter are restated below. Recall that if $\mathbf{A}$ is diagonalizable, then we may take $\sigma = 0$ in (4.5), (4.6), and (4.7) below.

- For any $\sigma > 0$ there is a $k > 0$ such that

$$\left\|\mathsf{e}^{t\mathbf{A}}\right\| \le k\,\mathsf{e}^{(\mu_1+\sigma)t} \quad \text{for all} \quad t \ge 0. \tag{4.5}$$

- For any $\sigma > 0$ there is a $k > 0$ such that

$$\left\|\mathsf{e}^{-t\mathbf{A}}\right\| \le k\,\mathsf{e}^{(-\mu_n+\sigma)t} \quad \text{for all} \quad t \ge 0. \tag{4.6}$$

- For any $\sigma > 0$ there are $\delta, k > 0$ such that

$$\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \le k\,\mathsf{e}^{(\mu_1+\sigma)t}\,\|\mathbf{x}_0\| \quad \text{for all} \quad (t, \mathbf{x}_0) \in \Omega_\delta. \tag{4.7}$$

4.2 "Flipping the Integral" and the Initial Condition $\mathbf{y}_0$

Consider the system (4.1) and the corresponding integral equation (2.6). As in Chapter 3, we will "flip the integral" and re-write the integral equation in a different, more useful form. First, we need the following estimate to justify this action.

Claim 4.5: *For any $\sigma > 0$ there are $\delta, k > 0$ such that*

$$\left\|\mathsf{e}^{-t\boldsymbol{A}}\boldsymbol{b}(\boldsymbol{\phi}_t(\boldsymbol{x}_0))\right\| \le k\,\mathsf{e}^{[(\alpha\mu_1-\mu_n)+\sigma]t}\,\|\boldsymbol{x}_0\|^\alpha \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta. \tag{4.8}$$

Proof: It follows from (4.2), (4.6), and (4.7). Note that when applying (4.6) and (4.7), you use $\frac{\sigma}{\alpha+1}$ instead of σ. □

Using the integral equation (2.6) along with (4.4) and (4.8), for sufficiently small $\|\mathbf{x}_0\|$ we know we can write

$$\boldsymbol{\phi}_t(\mathbf{x}_0) = \mathsf{e}^{t\mathbf{A}}\left[\mathbf{x}_0 + \int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds\right] - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds. \tag{4.9}$$

Now, there is a $\delta > 0$ (the one in (4.8) will work) such that we can define the function

$$\boldsymbol{\psi}(\mathbf{x}_0) := \mathbf{x}_0 + \int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0))\,ds, \quad \mathbf{x}_0 \in B_\delta. \tag{4.10}$$

Using (4.9), we have thus proven the following.

Claim 4.6: *There is a $\delta > 0$ such that*

$$\boldsymbol{\phi}_t(\boldsymbol{x}_0) = \mathsf{e}^{t\boldsymbol{A}}\boldsymbol{y}_0 - \int_t^\infty \mathsf{e}^{(t-s)\boldsymbol{A}}\boldsymbol{b}(\boldsymbol{\phi}_s(\boldsymbol{x}_0))\,ds \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta, \tag{4.11}$$

where $\boldsymbol{y}_0 := \boldsymbol{\psi}(\boldsymbol{x}_0)$.

Claim 4.7: *There are $\delta, k > 0$ such that*

$$\|\boldsymbol{x}_0 - \boldsymbol{\psi}(\boldsymbol{x}_0)\| \leq k\,\|\boldsymbol{x}_0\|^{\alpha} \quad \text{for all} \quad \boldsymbol{x}_0 \in B_\delta. \tag{4.12}$$

Moreover, $\boldsymbol{\psi}$ is a near-identity transformation.

Proof: It follows from (4.8) and (4.10). □

4.3 Iterates of the First Type

Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$. This new "initial condition" is a more appropriate initial condition for the linearized system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$. We will now define an iterative scheme that will produce successively better asymptotic approximations as $t \to \infty$ to the solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$ of the initial value problem (4.1). These iterates are inspired by the integral equation (4.11).

4.3.1 Definition of the Iterates

Let $\|\mathbf{x}_0\|$ be sufficiently small. The iterates we are about to define will be denoted by $\left\{\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right\}_{m=1}^{\infty}$. Since these iterates are defined in the natural way using the integral equation (4.11) and other types of iterates will appear later in this chapter, we will refer to these "natural" iterates as the *iterates of the first type*. Take the best linear approximation (for large t) as the first iterate,

$$\boldsymbol{\chi}^{(1)}\left(t, \mathbf{y}_0\right) := \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0, \tag{4.13a}$$

and define the remainder recursively via

$$\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right) := \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0 - \int_t^{\infty} \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(s, \mathbf{y}_0\right)\right) ds \quad (m \in \mathbb{N})\,. \tag{4.13b}$$

Observe that

$$\frac{d}{dt}\left(\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right)\right) = \mathbf{A}\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right) + \mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right) \quad (m \in \mathbb{N})\,. \tag{4.14}$$

4.3.2 Existence and Decay Rate of the Iterates

The main result of this chapter will describe how close the iterate $\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)$ is to the actual solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$. First, we need to establish the existence and basic decay rate of $\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)$.

Proposition 4.8: *Consider the iterates defined by* (4.13) *and let* $\sigma \in \left(0, \frac{\mu_n - \alpha\mu_1}{\alpha+1}\right)$. *Then, there is a* $\delta > 0$ *(independent of* m*) such that if* $\|\boldsymbol{x}_0\| < \delta$ *then* $\boldsymbol{\chi}^{(m)}(t, \boldsymbol{y}_0)$ *exists for each* $m \in \mathbb{N}$. *Moreover, there is a* $k > 0$ *(independent of* m*) such that*

$$\left\|\boldsymbol{\chi}^{(m)}(t, \boldsymbol{y}_0)\right\| \le k\, \mathsf{e}^{(\mu_1+\sigma)t} \|\boldsymbol{x}_0\| \quad \text{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{4.15}$$

Proof: We need to find $\delta, k > 0$ that work for each m and thus we need to be very careful with constants.

- Let $\delta_1, \ell_1 > 0$ be such that $\|\mathbf{b}(\mathbf{x})\| \le \ell_1 \|\mathbf{x}\|^\alpha$ for all $\mathbf{x} \in B_{\delta_1}$. See Equation (4.2).
- Let $\delta_2 > 0$ be such that $\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| < \delta_1$ for all $(t, \mathbf{x}_0) \in \Omega_{\delta_2}$. See Equation (4.7). It follows that if $\|\mathbf{x}_0\| < \delta_2$ then $\mathbf{y}_0$ exists.
- Let $\ell_3 > 0$ be such that $\|\mathbf{y}_0\| \le \ell_3 \|\mathbf{x}_0\|$ for all $\mathbf{x}_0 \in B_{\delta_2}$. See Equation (4.12).
- Let $\ell_4 > 0$ be such that $\left\|\mathsf{e}^{t\mathbf{A}}\right\| \le \ell_4 \mathsf{e}^{(\mu_1+\sigma)t}$ for all $t \ge 0$. See Equation (4.5).
- Let $\ell_5 > 0$ be such that $\left\|\mathsf{e}^{-t\mathbf{A}}\right\| \le \ell_5 \mathsf{e}^{(-\mu_n+\sigma)t}$ for all $t \ge 0$. See Equation (4.6).

There is no harm in taking δ_1 small enough so that

$$0 < \delta_1 < \left[\frac{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}{\ell_1 \ell_5}\right]^{\frac{1}{\alpha-1}}.$$

Note that the restriction on σ implies

$$\mu_1 < \mu_1 + \sigma < 0 \quad \text{and} \quad (\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma > 0.$$

Take

$$k := \ell_3 \ell_4 \left[1 - \frac{\ell_1 \ell_5 \delta_1^{\alpha-1}}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}\right]^{-1} > \ell_3\ell_4 \quad \text{and} \quad \delta \in \left(0, \min\left\{\frac{\delta_1}{k}, \delta_2\right\}\right).$$

The upper bound we imposed on δ_1 ensures that k is defined and is greater than $\ell_3\ell_4$. Observe that

$$\ell_3\ell_4 + \left[\frac{\ell_1 \ell_5 k \delta_1^{\alpha-1}}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}\right] = k. \tag{4.16}$$

The proof of the result will be by induction on m. Assume that $(t, \mathbf{x}_0) \in \Omega_\delta$.

Consider first the base case $m = 1$. We know $\mathbf{y}_0$ exists and hence $\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)$ exists. Furthermore,

$$\left\|\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)\right\| = \left\|\mathsf{e}^{t\mathbf{A}} \mathbf{y}_0\right\| \le \ell_4 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{y}_0\| \le \ell_3\ell_4 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\| \le k\, \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|.$$

Thus, the result is true for $m = 1$.

Now, assume that the result is true for $m \in \mathbb{N}$. That is, $\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)$ exists for $\mathbf{x}_0 \in B_\delta$ and satisfies $\left\|\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\| \leq k\, \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|$. Since $\|\mathbf{x}_0\| < \delta$, we see that $\left\|\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\| < \delta_1$ and thus $\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)$ exists. Using (4.13b),

$$\left\|\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)\right\| \leq \left\|\mathsf{e}^{t\mathbf{A}}\right\| \|\mathbf{y}_0\| + \int_t^\infty \left\|\mathsf{e}^{(t-s)\mathbf{A}}\right\| \left\|\mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right)\right\| ds.$$

By the induction hypothesis and the estimates given at the beginning of the proof,

$$\left\|\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)\right\| \leq \ell_3 \ell_4 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\| + \ell_1 \ell_5 k^\alpha \mathsf{e}^{(\mu_n-\sigma)t} \left[\int_t^\infty \mathsf{e}^{[(\alpha\mu_1-\mu_n)+(\alpha+1)\sigma]s}\, ds\right] \|\mathbf{x}_0\|^\alpha.$$

Simplifying,

$$\begin{aligned}
\left\|\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)\right\| &\leq \ell_3 \ell_4 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\| + \left[\frac{\ell_1 \ell_5 k^\alpha}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}\right] \mathsf{e}^{\alpha(\mu_1+\sigma)t} \|\mathbf{x}_0\|^\alpha \\
&= \left\{\ell_3 \ell_4 + \left[\frac{\ell_1 \ell_5 k^\alpha}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}\right] \mathsf{e}^{(\alpha-1)(\mu_1+\sigma)t} \|\mathbf{x}_0\|^{\alpha-1}\right\} \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|.
\end{aligned}$$

Since $0 < \mathsf{e}^{(\alpha-1)(\mu_1+\sigma)t} \leq 1$ and $\|\mathbf{x}_0\| < \delta < \frac{\delta_1}{k}$, we have

$$\left\|\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)\right\| \leq \left\{\ell_3 \ell_4 + \left[\frac{\ell_1 \ell_5 k \delta_1^{\alpha-1}}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}\right]\right\} \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|.$$

Using (4.16),

$$\left\|\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)\right\| \leq k\, \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|.$$

Hence, the result is true for $m + 1$. By mathematical induction, the result is true for each $m \in \mathbb{N}$.

$\square$

4.3.3 Closeness of the Iterates to the Actual Solution

Now, we establish how close each iterate $\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)$ is to the actual solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$. As this theorem shows, each iteration increases the accuracy by a factor which is, for any sufficiently small $\sigma > 0$, $\mathcal{O}\left(\mathsf{e}^{\beta(\mu_1+\sigma)t} \|\mathbf{x}_0\|^\beta\right)$ as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$.

Theorem 4.9: *Consider the iterates defined by* (4.13) *and let* $\sigma \in \left(0, \frac{\mu_n - \alpha\mu_1}{\alpha+1}\right)$. *There are constants* $\delta > 0$ *and* $\{k_m\}_{m=1}^\infty \subset \mathbb{R}_+$ *such that*

$$\left\|\boldsymbol{\phi}_t(\boldsymbol{x}_0) - \boldsymbol{\chi}^{(m)}(t, \boldsymbol{y}_0)\right\| \leq k_m \mathsf{e}^{[\alpha+(m-1)\beta][\mu_1+\sigma]t} \|\boldsymbol{x}_0\|^{\alpha+(m-1)\beta} \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{4.17}$$

Proof: Since we want to find $\delta > 0$ that works for each $m \in \mathbb{N}$, we need to be very careful with the constants.

- Let $\delta_1, \ell_1 > 0$ be such that $\|\mathbf{b}(\mathbf{x})\| \leq \ell_1 \|\mathbf{x}\|^\alpha$ for all $\mathbf{x} \in B_{\delta_1}$. See Equation (4.2).
- Let $\delta_2, \ell_2 > 0$ be such that $\|\mathbf{Db}(\mathbf{x})\| \leq \ell_2 \|\mathbf{x}\|^\beta$ for all $\mathbf{x} \in B_{\delta_2}$. See Equation (4.3).
- Let $\delta_3, \ell_3 > 0$ be such that $\|\boldsymbol{\phi}_t(\mathbf{x}_0)\| \leq \ell_3 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|$ for all $(t, \mathbf{x}_0) \in \Omega_{\delta_3}$. See Equation (4.7).
- Let $\delta_4, \ell_4 > 0$ be such that $\left\|\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\| \leq \ell_4 \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|$ for all $(t, \mathbf{x}_0) \in \Omega_{\delta_4}$ and $m \in \mathbb{N}$. See Equation (4.15).
- Let $\ell_5 > 0$ be such that $\left\|\mathsf{e}^{-t\mathbf{A}}\right\| \leq \ell_5 \mathsf{e}^{(-\mu_n+\sigma)t}$ for all $t \geq 0$. See Equation (4.6).
- If $\|\mathbf{x}_0\| < \mathsf{min}\{\delta_3, \delta_4\}$ then any point between $\boldsymbol{\phi}_t(\mathbf{x}_0)$ and $\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)$ is bounded in norm by $(\ell_3 + \ell_4)\, \mathsf{e}^{(\mu_1+\sigma)t} \|\mathbf{x}_0\|$ for all $t \geq 0$.

The proof of the theorem will be by induction on m. Take

$$\delta := \mathsf{min}\left\{\frac{\delta_1}{\ell_3}, \frac{\delta_1}{\ell_4}, \frac{\delta_2}{\ell_3+\ell_4}, \delta_3, \delta_4\right\}.$$

Hence assume $(t, \mathbf{x}_0) \in \Omega_\delta$, which guarantees that all necessary estimates apply. Note that the restriction on σ implies

$$\mu_1 < \mu_1 + \sigma < 0 \quad \text{and} \quad (\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma > 0.$$

Consider first the base case, $m = 1$. Using (4.11) and (4.13a),

$$\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)\right\| = \left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right\| \leq \int_t^\infty \left\|\mathsf{e}^{(t-s)\mathbf{A}}\right\| \|\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0))\|\, ds.$$

Using the estimates at the beginning of the proof and simplifying,

$$\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)\right\| \leq k_1 \mathsf{e}^{\alpha(\mu_1+\sigma)t} \|\mathbf{x}_0\|^\alpha, \quad \text{where} \quad k_1 := \frac{\ell_1 \ell_3^\alpha \ell_5}{(\mu_n - \alpha\mu_1) - (\alpha+1)\,\sigma}.$$

Note that k_1 is defined and strictly positive due to the restrictions we placed on σ. Thus, the theorem is true for $m = 1$.

Now, assume that the theorem is true for a fixed $m \in \mathbb{N}$. First, for any $s \geq 0$ consider the expression

$$\left\|\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0)) - \mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right)\right\| \leq \ell_2 (\ell_3+\ell_4)^\beta \mathsf{e}^{\beta(\mu_1+\sigma)s} \left\|\boldsymbol{\phi}_s(\mathbf{x}_0) - \boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right\| \|\mathbf{x}_0\|^\beta,$$

where we applied the Mean Value Theorem and estimates given at the beginning of the proof. By the induction hypothesis, we know

$$\begin{aligned}
&\left\|\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(s, \mathbf{y}_0\right)\right)\right\| \\
&\leq \ell_2\left(\ell_3 + \ell_4\right)^{\beta} \mathrm{e}^{\beta(\mu_1+\sigma)s}\left[k_m \mathrm{e}^{[\alpha+(m-1)\beta][\mu_1+\sigma]s}\left\|\mathbf{x}_0\right\|^{\alpha+(m-1)\beta}\right]\left\|\mathbf{x}_0\right\|^{\beta} \\
&= k_m \ell_2\left(\ell_3 + \ell_4\right)^{\beta} \mathrm{e}^{[\alpha+m\beta][\mu_1+\sigma]s}\left\|\mathbf{x}_0\right\|^{\alpha+m\beta}.
\end{aligned}$$

It follows from the integral equation (4.11) for $\boldsymbol{\phi}_t(\mathbf{x}_0)$ and the definition (4.13b) for $\boldsymbol{\chi}^{(m+1)}\left(s, \mathbf{y}_0\right)$ that

$$\begin{aligned}
&\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right)\right\| \\
&\leq \int_t^{\infty}\left\|\mathrm{e}^{(t-s)\mathbf{A}}\right\|\left\|\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(s, \mathbf{y}_0\right)\right)\right\| ds \\
&\leq k_m \ell_2\left(\ell_3 + \ell_4\right)^{\beta} \ell_5\left\{\int_t^{\infty} \mathrm{e}^{(\mu_n-\sigma)(t-s)} \mathrm{e}^{[\alpha+m\beta][\mu_1+\sigma]s}\, ds\right\}\left\|\mathbf{x}_0\right\|^{\alpha+m\beta} \\
&\leq k_m \ell_2\left(\ell_3 + \ell_4\right)^{\beta} \ell_5 \mathrm{e}^{(\mu_n-\sigma)t}\left\{\int_t^{\infty} \mathrm{e}^{[(\alpha\mu_1-\mu_n)+m\beta\mu_1+(\alpha+m\beta+1)\sigma]s}\, ds\right\}\left\|\mathbf{x}_0\right\|^{\alpha+m\beta} \\
&= \left[\frac{k_m \ell_2\left(\ell_3 + \ell_4\right)^{\beta} \ell_5}{(\mu_n-\alpha\mu_1)-m\beta\mu_1-(\alpha+m\beta+1)\,\sigma}\right] \mathrm{e}^{[\alpha+m\beta][\mu_1+\sigma]}\left\|\mathbf{x}_0\right\|^{\alpha+m\beta},
\end{aligned}$$

where $k_{m+1} > 0$ is defined in the obvious way. Note that $k_{m+1} > 0$ is indeed defined and strictly positive since

$$\begin{aligned}
(\mu_n-\alpha\mu_1)-m\beta\mu_1-(\alpha+m\beta+1)\,\sigma &= (\mu_n-\alpha\mu_1)-m\beta\,(\mu_1+\sigma)-(\alpha+1)\,\sigma \\
&> (\mu_n-\alpha\mu_1)-(\alpha+1)\,\sigma \\
&> 0.
\end{aligned}$$

Hence, the theorem is true for $m+1$ and therefore by induction the theorem is true for all $m \in \mathbb{N}$.

$\square$

Remark 4.10: Theorem 4.9 guarantees that $\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)$ correctly approximates $\boldsymbol{\phi}_t(\mathbf{x}_0)$ up to a certain order. However, $\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)$ may contain higher-order terms. Fortunately, as is evident from the proof of the theorem, we can discard the terms of $\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)$ which are not guaranteed to be correct by the theorem. If we use this simplified iterate in the calculation of $\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right)$ we will not sacrifice accuracy. This potentially can simplify the calculation of iterates greatly.

4.3.4 A Simple Example

Consider the system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$, where

$$\mathbf{A} := \begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad \mathbf{b}(\mathbf{x}) := \begin{pmatrix} 0 \\ r x_1 x_2 \end{pmatrix}$$

with $r \in \mathbb{R} \backslash \{0\}$ being a constant. Then,

$$\mathsf{e}^{t\mathbf{A}} = \mathsf{e}^{-t} \begin{pmatrix} 1 & 0 \\ t & 1 \end{pmatrix}, \quad \mu_1 = -1 = \mu_2, \quad \text{and} \quad \kappa = 1.$$

Furthermore, we can take $\alpha = 2$ and $\beta = 1$. Thus, $\kappa < \alpha$ and the eigenvalues are closely-spaced. Observe that the origin is a Jordan node. (See §A.8 of Appendix A for an overview of some different types of equilibria.)

Denote $\mathbf{x}(t) := \boldsymbol{\phi}_t(\mathbf{x}_0)$ and define, as always, $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$. Using (4.13), the first two iterates are given by

$$\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0) = \mathsf{e}^{-t} \begin{pmatrix} y_{01} \\ y_{02} + y_{01} t \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0) = \boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0) - r y_{01} \mathsf{e}^{-2t} \begin{pmatrix} 0 \\ y_{01} + y_{02} + y_{01} t \end{pmatrix}.$$

It follows from Theorem 4.9 that, for any $\sigma \in (0, 1)$,

$$\left\| \mathbf{x}(t) - \boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0) \right\| = \mathcal{O}\left(\mathsf{e}^{(-3+\sigma)t} \left\| \mathbf{x}_0 \right\|^3 \right) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \left\| \mathbf{x}_0 \right\| \to 0.$$

Moreover, it can be easily shown that we can write $x_2(t)$ in terms of $x_1(t)$ as

$$x_2 = -x_1 \ln|x_1| + \left(\frac{y_{02}}{y_{01}} + \ln|y_{01}| \right) x_1 + r\, x_1^2 \ln|x_1| + \mathcal{O}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0.$$

Depending on the size of r, the term $r\, x_1^2 \ln|x_1|$, which we only know about because of $\boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0)$, may make the phase portrait near the origin of the nonlinear system significantly different from the phase portrait of the linearized system.

4.3.5 A Complicated Example

Take

$$\mathbf{A} := \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \quad \text{and} \quad \mathbf{b}(\mathbf{x}) := \begin{pmatrix} b_{111} x_1^2 + b_{112} x_1 x_2 + b_{122} x_2^2 \\ b_{211} x_1^2 + b_{212} x_1 x_2 + b_{222} x_2^2 \end{pmatrix},$$

where $a < 0$ and $\{b_{ijk}\}_{i,j,k=1}^{2} \subset \mathbb{R}$ are constants. Assume that at least one b_{ijk} is non-zero and consider the system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$. The origin, as we see, is a star node. Now,

$$\mathsf{e}^{t\mathbf{A}} = \mathsf{e}^{at}\mathbf{I}, \quad \mu_1 = a = \mu_2, \quad \text{and} \quad \kappa = 1.$$

Also, we can take $\alpha = 2$ and $\beta = 1$. Thus, $\kappa < \alpha$ and the eigenvalues are closely-spaced.

Define $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$ and $\mathbf{x}(t) := \boldsymbol{\phi}_t(\mathbf{x}_0)$. The first iterate, which gives us the linearization, is

$$\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0) = \mathsf{e}^{at}\mathbf{y}_0.$$

Standard reasoning (as does Theorem 4.9) tells us that

$$x_1(t) \sim \mathsf{e}^{at} y_{01} \quad \text{and} \quad x_2(t) \sim \mathsf{e}^{at} y_{02} \quad \text{as} \quad t \to \infty.$$

Provided that $y_{01} \neq 0$, we have

$$x_2(t) \sim \left(\frac{y_{02}}{y_{01}}\right) x_1(t) \quad \text{as} \quad t \to \infty.$$

We will use the second iterate, $\boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0)$, to obtain a more detailed relationship between $x_1(t)$ and $x_2(t)$. Using (4.13b) and the fact that $\mathbf{b}\left(\mathsf{e}^{at}\mathbf{y}_0\right) = \mathsf{e}^{2at}\mathbf{b}\left(\mathbf{y}_0\right)$, we can calculate

$$\boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0) = \mathsf{e}^{at}\mathbf{y}_0 + \left(\frac{1}{a}\right) \mathsf{e}^{2at}\mathbf{b}\left(\mathbf{y}_0\right). \tag{4.18}$$

For notational simplicity, let $\boldsymbol{\xi} := \left(\frac{1}{a}\right) \mathbf{b}(\mathbf{y}_0)$.

Case 1: $y_{01} = y_{02} = 0$**.** If $\mathbf{y}_0 = \mathbf{0}$ then $\mathbf{x}_0 = \mathbf{0}$ and $\mathbf{x}(t) \equiv \mathbf{0}$.

Case 2: $y_{01} \neq 0$**.** It follows from (4.18) and Theorem 4.9 that

$$x_1(t) = \mathsf{e}^{at} y_{01} + \xi_1 \mathsf{e}^{2at} + \mathcal{O}\left(\mathsf{e}^{3at}\right) \quad \text{as} \quad t \to \infty \tag{4.19a}$$

and

$$x_2(t) = \mathsf{e}^{at} y_{02} + \xi_2 \mathsf{e}^{2at} + \mathcal{O}\left(\mathsf{e}^{3at}\right) \quad \text{as} \quad t \to \infty. \tag{4.19b}$$

Using (4.19a), we see $x_1 = \mathcal{O}\left(\mathsf{e}^{at}\right)$ as $t \to \infty$ and $\mathsf{e}^{at} = \mathcal{O}(x_1)$ as $x_1 \to 0$. Also, we can solve for e^{at} and back substitute to obtain an asymptotic expression for e^{at} in terms of x_1 only.

This gives

$$\begin{aligned}
\mathrm{e}^{at} &= \left(\frac{x_1}{y_{01}}\right)\left[1 - \left(\frac{\xi_1}{y_{01}}\right)\mathrm{e}^{at} + \mathcal{O}\big(\mathrm{e}^{2at}\big)\right] \quad \text{as} \quad t \to \infty \\
&= \left(\frac{1}{y_{01}}\right)x_1 - \left(\frac{\xi_1}{y_{01}^2}\right)\mathrm{e}^{at}x_1 + \mathcal{O}\big(\mathrm{e}^{3at}\big) \quad \text{as} \quad t \to \infty \\
&= \left(\frac{1}{y_{01}}\right)x_1 - \left(\frac{\xi_1}{y_{01}^3}\right)x_1^2 + \mathcal{O}\big(\mathrm{e}^{3at}\big) \quad \text{as} \quad t \to \infty \\
&= \left(\frac{1}{y_{01}}\right)x_1 - \left(\frac{\xi_1}{y_{01}^3}\right)x_1^2 + \mathcal{O}\big(x_1^3\big) \quad \text{as} \quad x_1 \to 0.
\end{aligned}$$

It follows from (4.19b) that

$$x_2 = \left(\frac{y_{02}}{y_{01}}\right)x_1 + \left(\frac{\xi_2}{y_{01}^2} - \frac{y_{02}\xi_1}{y_{01}^3}\right)x_1^2 + \mathcal{O}\big(x_1^3\big) \quad \text{as} \quad x_1 \to 0. \tag{4.20}$$

Case 3: $y_{02} \neq 0$. Similar to the case above, we get

$$x_1 = \left(\frac{y_{01}}{y_{02}}\right)x_2 + \left(\frac{\xi_1}{y_{02}^2} - \frac{y_{01}\xi_2}{y_{02}^3}\right)x_2^2 + \mathcal{O}\big(x_2^3\big) \quad \text{as} \quad x_2 \to 0. \tag{4.21}$$

Claim 4.11:

(a) If $y_{01} = 0$ and $b_{122} = 0$ then $x_1(t) \equiv 0$. If $y_{01} = 0$ and $b_{122} \neq 0$ then

$$x_1 = \left(\frac{b_{122}}{a}\right)x_2^2 + \mathcal{O}\big(x_2^3\big) \quad \textit{as} \quad x_2 \to 0.$$

(b) If $y_{02} = 0$ and $b_{211} = 0$ then $x_2(t) \equiv 0$. If $y_{02} = 0$ and $b_{211} \neq 0$ then

$$x_2 = \left(\frac{b_{211}}{a}\right)x_1^2 + \mathcal{O}\big(x_1^3\big) \quad \textit{as} \quad x_1 \to 0.$$

Proof:

(a) To prove the first statement, observe that if $x_1 = 0$ and $b_{122} = 0$ then $[\mathbf{b}(\mathbf{x})]_1 = 0$. Since $y_{01} = 0$, $\big[\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)\big]_1 = 0$. A simple inductive argument shows that $\big[\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\big]_1 = 0$ for each $m \in \mathbb{N}$. It follows from Theorem 4.9 that $x_1(t) \equiv 0$.

To prove the second statement, set $y_{01} = 0$ in (4.21). Note that $\xi_1 = \frac{b_{122}y_{02}^2}{a}$ when $y_{01} = 0$.

(b) The first statement is proven exactly the same way as the first statement in the first part of the claim. To prove the second statement, set $y_{02} = 0$ in (4.20). Note that $\xi_2 = \frac{b_{211}y_{01}^2}{a}$ when $y_{02} = 0$.

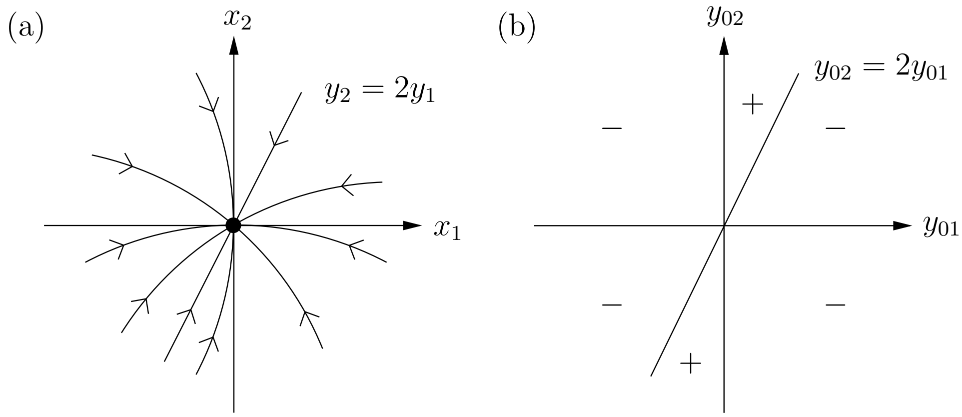

Figure 4.1: (a) The phase portrait near the origin for the example system (4.22). (b) The sign of $\left(\frac{y_{02}}{y_{01}}\right)^3 - 8$ in different regions of the $y_{01}y_{02}$-plane. This tells us the sign of the coefficient in front of the x_1^2 term in the expression for x_2.

$\square$

For a more concrete example, consider the system

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} x_1^2 + 8\,x_1x_2 + x_2^2 \\ 8\,x_1^2 + x_1x_2 + 8\,x_2^2 \end{pmatrix}. \tag{4.22}$$

Using (4.20), for $y_{01} \neq 0$ we know

$$x_2 = \left(\frac{y_{02}}{y_{01}}\right) x_1 + \left[\left(\frac{y_{02}}{y_{01}}\right)^3 - 8\right] x_1^2 + \mathcal{O}\big(x_1^3\big) \quad \text{as} \quad x_1 \to 0.$$

Moreover, using (4.21), for $y_{02} \neq 0$ we know

$$x_1 = \left(\frac{y_{01}}{y_{02}}\right) x_2 + \left[8\left(\frac{y_{01}}{y_{02}}\right)^3 - 1\right] x_2^2 + \mathcal{O}\big(x_2^3\big) \quad \text{as} \quad x_2 \to 0.$$

Observe that we can use the sign of the coefficient $\left(\frac{y_{02}}{y_{01}}\right)^3 - 8$ in front of the x_1^2 term in the expression for x_2 to deduce concavity. A phase portrait of the system (4.22) is sketched in Figure 4.1.

4.4 Iterates of the Second Type

The calculation of the iterates of the first type $\left\{\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right\}_{m=1}^{\infty}$, where $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, may be very difficult or possibly impossible. However, if $\mathbf{b} \in C^\infty$ in a neighbourhood of $\mathbf{0}$ then we can (ideally) simplify the integration by using the Taylor series for $\mathbf{b}(\mathbf{x})$. Moreover, for a given iterate we only need to use a Taylor polynomial of a certain order to obtain the same precision as if we used the full function $\mathbf{b}(\mathbf{x})$.

Assume that $\mathbf{b} \in C^\infty(\mathcal{N}, \mathbb{R}^n)$, where $\mathcal{N} \subset \mathbb{R}^n$ is a neighbourhood with $\mathbf{0} \in \mathcal{N}$. By Taylor's Theorem, we can write

$$\mathbf{b}(\mathbf{x}) \sim \sum_{i=\ell}^{\infty} \mathbf{b}_i(\mathbf{x}) \quad \text{as} \quad \|\mathbf{x}\| \to 0$$

for some index $\ell \in \{2, 3, \ldots\}$, where each $\mathbf{b}_i(\mathbf{x})$ has components which are homogeneous polynomials of degree i. Note that we can take $\alpha = \ell$ and $\beta = \ell - 1$. Define

$$\mathbf{b}^{(m)}(\mathbf{x}) := \sum_{i=\ell}^{m} \mathbf{b}_i(\mathbf{x}), \quad m \in \{\ell, \ell+1, \ldots\},$$

which is the Taylor polynomial of $\mathbf{b}(\mathbf{x})$ of order m. Observe that

$$\left\| \mathbf{b}(\mathbf{x}) - \mathbf{b}^{(m)}(\mathbf{x}) \right\| = \mathcal{O}\Big(\|\mathbf{x}\|^{m+1} \Big) \quad \text{as} \quad \|\mathbf{x}\| \to 0. \tag{4.23}$$

4.4.1 Definition of the Iterates

The *iterates of the second type* will be denoted by $\{\widetilde{\boldsymbol{\chi}}^{(m)}(t, \mathbf{y}_0)\}_{m=1}^{\infty}$. The first iterate $\widetilde{\boldsymbol{\chi}}^{(1)}(t, \mathbf{y}_0)$ is the same as $\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)$ and, for $m \in \mathbb{N}$, $\widetilde{\boldsymbol{\chi}}^{(m+1)}(t, \mathbf{y}_0)$ is defined exactly as $\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)$ (see Equation (4.13b)) except $\mathbf{b}$ inside the integral is replaced by $\mathbf{b}^{([m+1][\ell-1])}$. We use $\mathbf{b}^{([m+1][\ell-1])}$ because, with this choice, the iterates of the second type achieve exactly the same closeness to the exact solution as the iterates of the first type.

Assuming $\|\mathbf{x}_0\|$ is sufficiently small, hence define the first iterate as

$$\widetilde{\boldsymbol{\chi}}^{(1)}(t, \mathbf{y}_0) := \mathsf{e}^{t\mathbf{A}} \mathbf{y}_0 \tag{4.24a}$$

and define the successive iterates recursively by

$$\widetilde{\boldsymbol{\chi}}^{(m+1)}(t, \mathbf{y}_0) := \mathsf{e}^{t\mathbf{A}} \mathbf{y}_0 - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}} \mathbf{b}^{([m+1][\ell-1])} \Big(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0) \Big) \, ds \quad (m \in \mathbb{N}). \tag{4.24b}$$

Remark 4.12: Alternatively, suppose instead that $\mathbf{b} \in C^r(\mathcal{N}, \mathbb{R}^n)$ but $\mathbf{b} \notin C^{r+1}(\mathcal{N}, \mathbb{R}^n)$ for some $r \in \{\ell+1, \ell+2, \ldots\}$. Then, $\mathbf{b}^{(m)}$ is defined only for $m \in \{\ell, \ldots, r-1\}$ and $\widetilde{\boldsymbol{\chi}}^{(m)}(t, \mathbf{y}_0)$ is defined for $m \in \left\{1, \ldots, \left\lfloor \frac{r-1}{\ell-1} \right\rfloor \right\}$.

4.4.2 Existence and Decay Rate of the Iterates

The decay rate for the iterates of the second type is the same as for the iterates of the first type.

Proposition 4.13: *Consider the iterates defined by* (4.24) *and let* $\sigma \in \left(0, \frac{\mu_n - \alpha\mu_1}{\ell+1}\right)$. *Then, there is a* $\delta > 0$ *(independent of* m*) such that if* $\|\boldsymbol{x}_0\| < \delta$ *then* $\widetilde{\boldsymbol{\chi}}^{(m)}(t, \boldsymbol{y}_0)$ *exists for each* $m \in \mathbb{N}$*. Moreover, there is a* $k > 0$ *(independent of* m*) such that*

$$\left\|\widetilde{\boldsymbol{\chi}}^{(m)}(t, \boldsymbol{y}_0)\right\| \leq k\, \mathsf{e}^{(\mu_1+\sigma)t} \|\boldsymbol{x}_0\| \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \mathbb{N}. \tag{4.25}$$

Proof: The proof is exactly the same as the proof for Proposition 4.8, which establishes the decay rate for the iterates of the first type. □

4.4.3 Closeness of the Iterates to the Actual Solution

Now, we establish how close each iterate of the second type $\widetilde{\boldsymbol{\chi}}^{(m)}(t, \mathbf{y}_0)$ is to the actual solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$. Observe that the decay rate is the same as with the iterates of the first kind (with $\alpha = \ell$ and $\beta = \ell - 1$) given in (4.17).

Theorem 4.14: *Consider the iterates defined by* (4.24) *and let* $\sigma \in \left(0, \frac{\mu_n - \ell\mu_1}{\ell+1}\right)$. *There are constants* $\delta > 0$ *and* $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ *such that*

$$\left\|\boldsymbol{\phi}_t(\boldsymbol{x}_0) - \widetilde{\boldsymbol{\chi}}^{(m)}(t, \boldsymbol{y}_0)\right\| \leq k_m \mathsf{e}^{[m(\ell-1)+1][\mu_1+\sigma]t} \|\boldsymbol{x}_0\|^{m(\ell-1)+1} \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \mathbb{N}.$$

Proof: Let $\delta > 0$ be small enough so that all necessary estimates apply when $\mathbf{x}_0 \in B_\delta$. Hence, we will assume that $\mathbf{x}_0 \in B_\delta$. The proof will be by induction on m.

Since $\widetilde{\boldsymbol{\chi}}^{(1)}(t, \mathbf{y}_0) = \boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0)$, the base case $m = 1$ was already proven in Theorem 4.9. Assume now that the theorem is true for a fixed $m \in \mathbb{N}$ and we will proceed to show that the theorem is true for $m + 1$.

For $s \geq 0$, consider first the expression

$$\begin{aligned}
&\left\|\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}^{([m+1][\ell-1])}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s, \mathbf{y}_0)\right)\right\| \\
&\leq \left\|\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s, \mathbf{y}_0)\right)\right\| + \left\|\mathbf{b}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s, \mathbf{y}_0)\right) - \mathbf{b}^{([m+1][\ell-1])}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s, \mathbf{y}_0)\right)\right\|,
\end{aligned}$$

where we applied the Triangle Inequality. Now, using (4.3), (4.7), (4.25), the Mean Value Theorem, and the induction hypothesis, we know there is some $k_m^{(1)} > 0$ such that

$$\left\|\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s, \mathbf{y}_0)\right)\right\| \leq k_m^{(1)} \mathsf{e}^{[(m+1)(\ell-1)+1][\mu_1+\sigma]s} \|\mathbf{x}_0\|^{(m+1)(\ell-1)+1}.$$

Furthermore, using (4.25) and (4.23), we know there is some $k_m^{(2)} > 0$ such that

$$\left\| \mathbf{b}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s,\mathbf{y}_0)\right) - \mathbf{b}^{([m+1][\ell-1])}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s,\mathbf{y}_0)\right) \right\| \le k_m^{(2)} \mathsf{e}^{[(m+1)(\ell-1)+1][\mu_1+\sigma]s} \left\|\mathbf{x}_0\right\|^{(m+1)(\ell-1)+1}.$$

These last three estimate together imply

$$\left\| \mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right) - \mathbf{b}^{([m+1][\ell-1])}\left(\widetilde{\boldsymbol{\chi}}^{(m)}(s,\mathbf{y}_0)\right) \right\| \le \left(k_m^{(1)} + k_m^{(2)}\right) \mathsf{e}^{[(m+1)(\ell-1)+1][\mu_1+\sigma]s} \left\|\mathbf{x}_0\right\|^{(m+1)(\ell-1)+1}. \tag{4.26}$$

It follows from (4.6), (4.11), (4.24b), and (4.26) that there is a $k_{m+1} > 0$ such that

$$\left\| \boldsymbol{\phi}_t(\mathbf{x}_0) - \widetilde{\boldsymbol{\chi}}^{(m+1)}(t,\mathbf{y}_0) \right\| \le k_{m+1} \mathsf{e}^{[(m+1)(\ell-1)+1][\mu_1+\sigma]s} \left\|\mathbf{x}_0\right\|^{(m+1)(\ell-1)+1}.$$

Note that the restriction on σ given in the statement of the theorem ensures that the improper integral in the expression for $\boldsymbol{\phi}_t(\mathbf{x}_0) - \widetilde{\boldsymbol{\chi}}^{(m+1)}(t,\mathbf{y}_0)$ converges and also that k_{m+1} indeed exists and is positive. Hence, the theorem is true for $m+1$. By induction, the theorem is true for all $m \in \mathbb{N}$.

□

4.5 The Function $\boldsymbol{\psi}$

Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, where $\boldsymbol{\psi}$ was given in (4.10). This new "initial condition," as we have seen is in some sense more natural than the original initial condition $\mathbf{x}_0$. In this section, we explore properties of the transformation $\boldsymbol{\psi}$.

4.5.1 Conjugacy Condition

The Hartman-Grobman Theorem asserts that there is a homeomorphism $\mathbf{h}$ which maps flows of the nonlinear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ onto flows of the linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$. That is, there is a $\delta > 0$ such that

$$\mathbf{h}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \mathsf{e}^{t\mathbf{A}}\mathbf{h}(\mathbf{x}_0) \quad \text{for all} \quad (t,\mathbf{x}_0) \in \Omega_\delta.$$

See Figure 4.2. As we will now show, $\boldsymbol{\psi}$ is one such homeomorphism.

Theorem 4.15: *There is a $\delta > 0$ such that*

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\boldsymbol{x}_0)\right) = \mathsf{e}^{t\boldsymbol{A}}\boldsymbol{\psi}(\boldsymbol{x}_0) \quad \textit{for all} \quad (t,\boldsymbol{x}_0) \in \Omega_\delta. \tag{4.27}$$

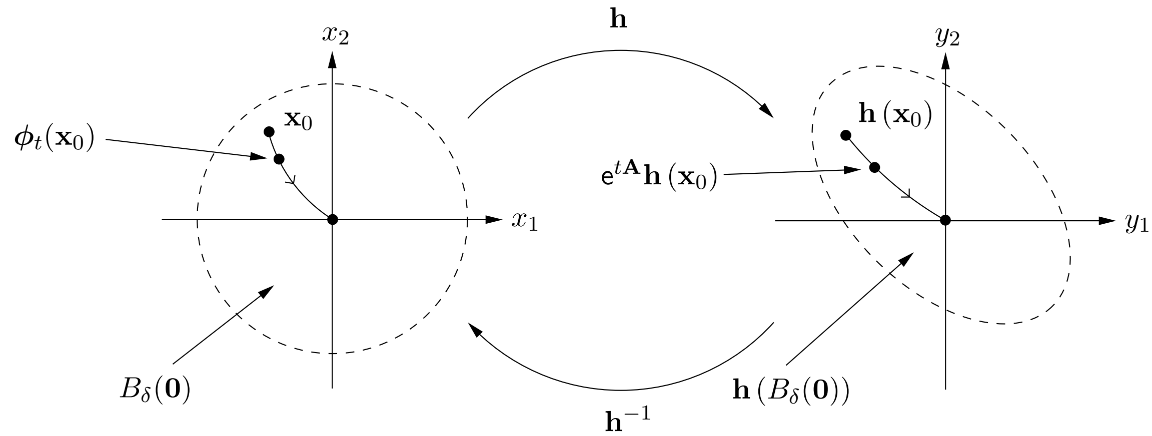

Figure 4.2: The nonlinear flow $\boldsymbol{\phi}_t(\mathbf{x}_0)$ is mapped onto the linear flow $\mathsf{e}^{t\mathbf{A}}\mathbf{y}_0$ by the homeomorphism $\mathbf{h}$.

Proof: Let $\delta > 0$ be small enough so that if $\mathbf{x}_0 \in B_\delta$ then all relevant estimates apply. Hence, assume that $\mathbf{x}_0 \in B_\delta$.

If we replace $\mathbf{x}_0$ in (4.10) with $\boldsymbol{\phi}_t(\mathbf{x}_0)$, we have

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \boldsymbol{\phi}_t(\mathbf{x}_0) + \int_0^\infty \mathsf{e}^{-\xi\mathbf{A}}\mathbf{b}(\boldsymbol{\phi}_\xi(\boldsymbol{\phi}_t(\mathbf{x}_0)))\,d\xi.$$

Using the integral equation (4.11) and the semi-group property of flows,

$$\begin{aligned}\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) &= \mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds + \int_0^\infty \mathsf{e}^{-\xi\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_{\xi+t}(\mathbf{x}_0)\right)\,d\xi \\ &= \mathsf{e}^{t\mathbf{A}}\left[\boldsymbol{\psi}(\mathbf{x}_0) - \int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds + \int_0^\infty \mathsf{e}^{-(\xi+t)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_{\xi+t}(\mathbf{x}_0)\right)\,d\xi\right].\end{aligned}$$

With the change of variables $s = \xi + t$ in the second integral, we see that

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \mathsf{e}^{t\mathbf{A}}\left[\boldsymbol{\psi}(\mathbf{x}_0) - \int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds + \int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds\right] = \mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0).$$

□

4.5.2 A Partial Differential Equation which ψ Satisfies

The conjugacy condition (4.27) allows us to specify a partial differential equation which $\boldsymbol{\psi}$ satisfies.

Proposition 4.16: *There is a $\delta > 0$ such that the function $\boldsymbol{\psi}$ satisfies*

$$[\boldsymbol{D}\boldsymbol{\psi}(\boldsymbol{x}_0)]\,[\boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{b}(\boldsymbol{x}_0)] - \boldsymbol{A}\boldsymbol{\psi}(\boldsymbol{x}_0) = \boldsymbol{0}, \quad \boldsymbol{\psi}(\boldsymbol{0}) = \boldsymbol{0}, \quad \boldsymbol{D}\boldsymbol{\psi}(\boldsymbol{0}) = \boldsymbol{I}, \tag{4.28}$$

for $\boldsymbol{x}_0 \in B_\delta$, where $\boldsymbol{D}$ denotes the operator for differentiation with respect to spatial variables.

Proof: First, we will establish the partial differential equations. Assume $\delta > 0$ is sufficiently small so that all necessary estimates apply when $\|\mathbf{x}_0\| < \delta$. If we differentiate the conjugacy relation (4.27) with respect to t and apply the differential equation which $\boldsymbol{\phi}_t(\mathbf{x}_0)$ satisfies, we obtain

$$[\mathbf{D}\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)]\left[\mathbf{A}\boldsymbol{\phi}_t(\mathbf{x}_0) + \mathbf{b}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right] = \mathbf{A}\mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0).$$

Setting $t = 0$ gives what we needed to show. Second, we show that $\boldsymbol{\psi}(\mathbf{0}) = \mathbf{0}$. This can be obtained by setting $\mathbf{x}_0 = \mathbf{0}$ in (4.12). Finally, we show that $\mathbf{D}\boldsymbol{\psi}(\mathbf{0}) = \mathbf{I}$. Observe that

$$\lim_{\|\mathbf{h}\|\to 0} \frac{\|\boldsymbol{\psi}(\mathbf{h}) - \boldsymbol{\psi}(\mathbf{0}) - \mathbf{I}\mathbf{h}\|}{\|\mathbf{h}\|} = \lim_{\|\mathbf{h}\|\to 0} \frac{\|\boldsymbol{\psi}(\mathbf{h}) - \mathbf{h}\|}{\|\mathbf{h}\|} = 0,$$

where we again applied (4.12) and used the fact that $\alpha > 1$. It follows that $\boldsymbol{\psi}$ is differentiable at $\mathbf{0}$ with $\mathbf{D}\boldsymbol{\psi}(\mathbf{0}) = \mathbf{I}$. $\square$

In Chapter 3, where we explored the scalar case, we were able to derive a quadrature solution for $\psi(x_0)$. Here, however, we cannot find such a simple expression. If one is interested in approximating $\boldsymbol{\psi}(\mathbf{x}_0)$, a power series approximation can be obtained. See, for example, [5, 65], both of which appear in the proceedings of the 2003 International Symposium on Symbolic and Algebraic Computation (ISSAC 2003).

4.5.3 $\boldsymbol{\psi}$ is C^1 when $\mathbf{b}$ is C^1 and $\kappa < \beta + 1$

Proposition 4.17: *Consider the function $\boldsymbol{\psi}$. If we assume that $\kappa < \beta + 1$, then there are neighbourhoods $\mathcal{N}_1 \ni \mathbf{0}$ and $\mathcal{N}_2 \ni \mathbf{0}$ for which $\boldsymbol{\psi}$ is a C^1-diffeomorphism from $\mathcal{N}_1$ to $\mathcal{N}_2$.*

Proof: We know that $\mathbf{b}$ is C^1 in a neighbourhood of the origin and thus so is the right-hand side of the differential equation, $\mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$. It follows that $\boldsymbol{\phi}_t(\mathbf{x}_0)$ is C^1 in both t and $\mathbf{x}_0$ for sufficiently small $\|\mathbf{x}_0\|$. Thus, for sufficiently small $\|\mathbf{x}_0\|$, we can conclude that the integrand of the improper integral in the definition (4.10) of $\boldsymbol{\psi}(\mathbf{x}_0)$, namely $\mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)$, is C^1 in $\mathbf{x}_0$.

Using (2.20), (4.2), (4.3), (4.6), (4.7), for any sufficiently small $\sigma > 0$ we know that there are $\delta, k_1, k_2 > 0$ such that

$$\left\|\mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\right\| \le k_1 \mathsf{e}^{(\alpha\mu_1 - \mu_n + \sigma)s}\|\mathbf{x}_0\|^{\alpha} \quad \text{for all} \quad (s, \mathbf{x}_0) \in \Omega_\delta$$

and

$$\left\|\mathsf{e}^{-s\mathbf{A}}\mathbf{D}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\mathbf{D}\boldsymbol{\phi}_s(\mathbf{x}_0)\right\| \le k_2 \mathsf{e}^{[(\beta+1)\mu_1 - \mu_n + \sigma]s}\|\mathbf{x}_0\|^{\beta} \quad \text{for all} \quad (s, \mathbf{x}_0) \in \Omega_\delta.$$

Since $\alpha\mu_1 - \mu_n < 0$ and $(\beta+1)\,\mu_1 - \mu_n < 0$, we know that both of these exponentials decay as $s \to \infty$. It follows that

$$\int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds \quad \text{and} \quad \int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{D}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\mathbf{D}\boldsymbol{\phi}_s(\mathbf{x}_0)\,ds$$

are continuous in $\mathbf{x}_0$ for $\mathbf{x}_0 \in B_\delta$. Observe that the second integral is obtained from the first by differentiating under the integral sign. Observe also that these two integrals equal, respectively, $\boldsymbol{\psi}(\mathbf{x}_0) - \mathbf{x}_0$ and $\mathbf{D}\boldsymbol{\psi}(\mathbf{x}_0) - \mathbf{I}$.

Since $\boldsymbol{\psi}$ is continuously differentiable in a neighbourhood of the origin and $\mathbf{D}\boldsymbol{\psi}(\mathbf{0}) = \mathbf{I}$, by virtue of the Inverse Function Theorem we know that there is a neighbourhood $\mathcal{N}_1$ of the origin such that $\mathcal{N}_1 \subset B_\delta$ and $\boldsymbol{\psi}$ is invertible in $\mathcal{N}_1$. If we take $\mathcal{N}_2 := \boldsymbol{\psi}\left(\mathcal{N}_1\right)$, which is a neighbourhood of the origin, we can write $\boldsymbol{\psi} \in C^1(\mathcal{N}_1, \mathcal{N}_2)$ and $\boldsymbol{\psi}^{-1} \in C^1(\mathcal{N}_2, \mathcal{N}_1)$. □

Remark 4.18: It is interesting to compare, for a special case, Proposition 4.17 and Theorem 3.4 of Chapter II in [16]. Now, the vector fields $\boldsymbol{\xi}(\mathbf{x}) := \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ and $\boldsymbol{\eta}(\mathbf{x}) := \mathbf{A}\mathbf{x}$ are C^k-conjugate near the origin if there exists a C^k-diffeomorphism $\mathbf{h}$ and a $\delta > 0$ such that $\mathbf{h}(\boldsymbol{\phi}_t(\mathbf{x}_0)) = \mathsf{e}^{t\mathbf{A}}\mathbf{h}(\mathbf{x}_0)$ for all $(t, \mathbf{x}_0) \in \Omega_\delta$. Suppose that $\mathbf{b} \in C^1$ in a neighbourhood of the origin with $\alpha = 2$ and $\beta = 1$. Assume that $\kappa < \alpha$. With these assumptions, Proposition 4.17 can be used to conclude $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ are C^1-conjugate (with $\boldsymbol{\psi}$ being one such homeomorphism). On the other hand, the theorem in [16] requires the stronger conditions $\|\mathbf{b}(\mathbf{x})\| = \mathsf{o}\left(\|\mathbf{x}\|^2\right)$ and $\|\mathbf{D}\mathbf{b}(\mathbf{x})\| = \mathsf{o}(\|\mathbf{x}\|)$ as $\|\mathbf{x}\| \to 0$ in order to conclude that $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ are C^1-conjugate.

4.5.4 Analyticity of ψ when b is Analytic

Proposition 4.19: *If $\boldsymbol{b}$ is analytic at the origin, then $\boldsymbol{\psi}$ is analytic at the origin. Furthermore, $\boldsymbol{\psi}$ is invertible and $\boldsymbol{\psi}^{-1}$ is analytic at the origin.*

Proof: First, we will show that the improper integral

$$\int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\mathbf{x}_0)\right)\,ds$$

is analytic (in $\mathbf{x}_0$) at the origin. Note that this integral equals $\boldsymbol{\psi}(\mathbf{x}_0) - \mathbf{x}_0$. Let $\sigma > 0$ be sufficiently small. We know that there are $\delta, k > 0$ such that

$$\left\|\mathsf{e}^{-t\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right\| \le k\,\mathsf{e}^{(\alpha\mu_1 - \mu_n + \sigma)t}\,\|\mathbf{x}_0\|^\alpha \quad \text{for all} \quad (t, \mathbf{x}_0) \in \Omega_\delta.$$

Let

$$\mathbf{F}(\mathbf{z}, t) := \mathsf{e}^{-t\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_t(\mathbf{z})\right) \quad \text{for} \quad (t, \mathbf{z}) \in \Omega_\delta,$$

where $\boldsymbol{\phi}_t(\mathbf{x}_0)$ and Ω_δ are extended in the natural way for complex vectors. Thus,

$$\|\mathbf{F}(\mathbf{z}, t)\| \leq k\,\mathsf{e}^{(\alpha\mu_1 - \mu_n + \sigma)t}\,\|\mathbf{z}\|^\alpha \quad \text{for all} \quad (t, \mathbf{z}) \in \Omega_\delta.$$

Since the right-hand side of the differential equation $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ is real analytic (in $\mathbf{x}$) at the origin, we know that $\boldsymbol{\phi}_t(\mathbf{x}_0)$ is real analytic (in $\mathbf{x}_0$) at the origin. It follows that $\mathbf{F}(\mathbf{z}, t)$ is complex analytic in $\mathbf{z}$ at the origin. Hence, $\int_0^\infty \mathbf{F}(\mathbf{z}, s)\,ds$ is complex analytic in $\mathbf{z}$ at the origin. Therefore, $\boldsymbol{\psi}(\mathbf{x}_0)$ is real analytic in $\mathbf{x}_0$ at the origin.

The fact that $\boldsymbol{\psi}$ is invertible with $\boldsymbol{\psi}^{-1}$ being analytic at the origin follows from the fact that $\mathbf{D}\boldsymbol{\psi}(\mathbf{0}) = \mathbf{I}$ and the Real Analytic Inverse Function Theorem. □

4.5.5 Optimality of the Linearized Solution $\mathbf{e}^{t\mathbf{A}}\mathbf{y}_0$

We have seen that $\mathbf{y}_0$, where $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, gives a more natural "initial condition" for the linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$. As we will now show, the choice of initial condition $\mathbf{y}_0$ is in fact optimal in the sense that $\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0)\right\|$ has a faster exponential decay rate than $\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{z}_0\right\|$ for any $\mathbf{z}_0 \neq \boldsymbol{\psi}(\mathbf{x}_0)$.

Theorem 4.20: *There are neighbourhoods $\mathcal{N}_1$ and $\mathcal{N}_2$ of the origin such that for any $\boldsymbol{y}_0 \in \mathcal{N}_2$ there exists a unique $\boldsymbol{x}_0 \in \mathcal{N}_1$ such that*[1]

$$\limsup_{t\to\infty} \frac{\ln\left\|\boldsymbol{\phi}_t(\boldsymbol{x}_0) - e^{t\boldsymbol{A}}\boldsymbol{y}_0\right\|}{t} \leq \alpha\mu_1. \tag{4.29}$$

Proof: Let $\delta > 0$ be sufficiently small so that if $\mathbf{x}_0 \in \mathcal{N}_1 := B_\delta$ then all appropriate estimates apply and $\boldsymbol{\psi}$ is a bijection from $\mathcal{N}_1$ to $\mathcal{N}_2 := \boldsymbol{\psi}\left(\mathcal{N}_1\right)$. Let $\mathbf{y}_0 \in \mathcal{N}_2$ be fixed.

Existence follows by taking $\mathbf{x}_0 := \boldsymbol{\psi}^{-1}(\mathbf{y}_0)$ and using (4.17) with $m = 1$ and the definition (4.13a) of $\boldsymbol{\chi}^{(1)}\left(t, \mathbf{y}_0\right)$. To show uniqueness, suppose that $\widehat{\mathbf{x}}_0 \in \mathcal{N}_1$ has $\boldsymbol{\phi}_t(\widehat{\mathbf{x}}_0)$ satisfying the given estimate (4.29) and let $\widehat{\mathbf{y}}_0 := \boldsymbol{\psi}(\widehat{\mathbf{x}}_0)$. Using the integral equation (4.11) with $\widehat{\mathbf{x}}_0$ instead of $\mathbf{x}_0$,

$$\boldsymbol{\phi}_t(\widehat{\mathbf{x}}_0) = \mathsf{e}^{t\mathbf{A}}\widehat{\mathbf{y}}_0 - \mathsf{e}^{t\mathbf{A}}\int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\widehat{\mathbf{x}}_0)\right)\,ds.$$

[1] If $\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right\| = 0$ then we take the natural logarithm to be $-\infty$.

Subtracting $\mathsf{e}^{t\mathbf{A}}\mathbf{y}_0$ from both sides,

$$\boldsymbol{\phi}_t(\widehat{\mathbf{x}}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0 = \mathsf{e}^{t\mathbf{A}}\left[\widehat{\mathbf{y}}_0 - \mathbf{y}_0\right] - \mathsf{e}^{t\mathbf{A}}\int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\widehat{\mathbf{x}}_0)\right)\,ds.$$

Thus,

$$\widehat{\mathbf{y}}_0 - \mathbf{y}_0 = \mathsf{e}^{-t\mathbf{A}}\left[\boldsymbol{\phi}_t(\widehat{\mathbf{x}}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right] + \int_t^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\widehat{\mathbf{x}}_0)\right)\,ds.$$

It follows that

$$\|\widehat{\mathbf{y}}_0 - \mathbf{y}_0\| \le \left\|\mathsf{e}^{-t\mathbf{A}}\right\|\left\|\boldsymbol{\phi}_t(\widehat{\mathbf{x}}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right\| + \int_t^\infty \left\|\mathsf{e}^{-s\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}_s(\widehat{\mathbf{x}}_0)\right)\right\|\,ds.$$

Let $\sigma > 0$ be sufficiently small. Using (4.6), (4.8), and (4.29), we know there is a $k > 0$ such that

$$\|\widehat{\mathbf{y}}_0 - \mathbf{y}_0\| \le k\,\mathsf{e}^{(\alpha\mu_1 - \mu_n + \sigma)t} \quad \text{for all} \quad t \ge 0.$$

Letting $t \to \infty$, we see that $\widehat{\mathbf{y}}_0 = \mathbf{y}_0$. Since $\boldsymbol{\psi}$ is a bijection from $\mathcal{N}_1$ to $\mathcal{N}_2$, we conclude $\widehat{\mathbf{x}}_0 = \mathbf{x}_0$.

$\square$

Corollary 4.21: *There are neighbourhoods $\mathcal{N}_1$ and $\mathcal{N}_2$ of the origin such that if $\boldsymbol{x}_0 \in \mathcal{N}_1$ and $\boldsymbol{y}_0 \in \mathcal{N}_2 \setminus \{\boldsymbol{\psi}(\boldsymbol{x}_0)\}$ then*

$$\limsup_{t\to\infty} \frac{\ln\left\|\boldsymbol{\phi}_t(\boldsymbol{x}_0) - e^{t\boldsymbol{A}}\boldsymbol{y}_0\right\|}{t} > \alpha\mu_1.$$

4.5.6 A Simple Example

Let

$$\mathbf{A} := \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \quad \text{and} \quad \mathbf{b}(\mathbf{x}) := \begin{pmatrix} 0 \\ x_1^3 \end{pmatrix}$$

and consider the system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$. We will use the partial differential equation in (4.28) to find $\boldsymbol{\psi}(\mathbf{x})$. Note that the eigenvalues are closely spaced and there is resonance in the eigenvalues.

Since the differential equation for x_1 is decoupled from x_2, we will use the ansatz

$$\boldsymbol{\psi}(\mathbf{x}) := \begin{pmatrix} x_1 \\ x_2 + \xi(x_1) \end{pmatrix},$$

where $\xi(0) = 0 = \xi'(0)$ and $' = \frac{d}{dx_1}$. Using the partial differential equation,

$$\begin{pmatrix} 1 & 0 \\ \xi'(x_1) & 1 \end{pmatrix}\begin{pmatrix} -x_1 \\ -2x_2 + x_1^3 \end{pmatrix} - \begin{pmatrix} -x_1 \\ -2x_2 - 2\xi(x_1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The first component is already satisfied and thus we have the ordinary differential equation

$$\xi'(x_1) = x_1^2 + \frac{2\xi(x_1)}{x_1}.$$

Solving this using an integrating factor,

$$\xi(x_1) = (x_1 + C)\, x_1^2,$$

where $C \in \mathbb{R}$ is an arbitrary constant. Note that $\xi(0) = \xi'(0) = 0$ for all choices of C. Appealing to (4.12), we know $\|\mathbf{x} - \boldsymbol{\psi}(\mathbf{x})\| = \mathcal{O}\Big(\|\mathbf{x}\|^3\Big)$ as $\|\mathbf{x}\| \to 0$ and so it must be that $C = 0$. Thus,

$$\boldsymbol{\psi}(\mathbf{x}) = \begin{pmatrix} x_1 \\ x_2 + x_1^3 \end{pmatrix}.$$

The exact solution, which can be found easily, is given by

$$\boldsymbol{\phi}_t(\mathbf{x}_0) = \begin{pmatrix} \mathsf{e}^{-t} x_{01} \\ \mathsf{e}^{-2t}\left[x_{02} + x_{01}^3\right] - \mathsf{e}^{-3t} x_{01}^3 \end{pmatrix}.$$

Observe that

$$\boldsymbol{\phi}_t(\mathbf{x}_0) = \mathsf{e}^{t\mathbf{A}} \boldsymbol{\psi}(\mathbf{x}_0) + \begin{pmatrix} 0 \\ -\mathsf{e}^{-3t} x_{01}^3 \end{pmatrix}.$$

Thus,

$$\limsup_{t\to\infty} \frac{\ln \left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0)\right\|}{t} \leq -3.$$

(The limit is -3 if $x_{01} \neq 0$ and $-\infty$ if $x_{01} = 0$.) However, if $\mathbf{y}_0 \neq \boldsymbol{\psi}(\mathbf{x}_0)$ we see

$$\limsup_{t\to\infty} \frac{\ln \left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0\right\|}{t} \geq -2.$$

(The limit is either -1 or -2.) These results are consistent with Theorem 4.20 and Corollary 4.21.

4.6 Iterates of the Third Type (which are Flows)

The iterates of the first type $\left\{\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\}_{m=1}^{\infty}$, where $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, are defined in the natural way using the integral equation (4.11) which the actual solution $\boldsymbol{\phi}_t(\mathbf{x}_0)$ satisfies. However, the iterates of the first type are, generally, not flows. We will specify adjustments to the iterates which make them flows.

4.6.1 A Lemma

The following lemma resembles the semi-group property of flows. We will use this to construct the iterates of the third type.

Lemma 4.22: *There exists a $\delta > 0$ such that*

$$\boldsymbol{\chi}^{(m)}\left(s, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\boldsymbol{x}_0)\right)\right) = \boldsymbol{\chi}^{(m)}\left(s+t, \boldsymbol{\psi}\left(\boldsymbol{x}_0\right)\right) \quad \textit{for all} \quad s,t \geq 0,\ \boldsymbol{x}_0 \in B_\delta,\ m \in \mathbb{N}. \tag{4.30}$$

Proof: Let $\delta > 0$ be small enough so that all relevant estimates apply if $\|\mathbf{x}_0\| < \delta$. Hence, let $\mathbf{x}_0 \in B_\delta$. The proof will be by induction on m.

Consider first the base case $m = 1$. The iterate in question is $\boldsymbol{\chi}^{(1)}(t, \mathbf{y}_0) = \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0$. Using the conjugacy condition (4.27),

$$\boldsymbol{\chi}^{(1)}\left(s, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right) = \mathsf{e}^{s\mathbf{A}}\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \mathsf{e}^{s\mathbf{A}}\mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0) = \mathsf{e}^{(s+t)\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0) = \boldsymbol{\chi}^{(1)}\left(s+t, \boldsymbol{\psi}\left(\mathbf{x}_0\right)\right).$$

Thus, the lemma is true for $m = 1$.

Now, assume that the lemma is true for a fixed $m \in \mathbb{N}$. Using the definition (4.13b) for the iterate $\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0)$, the conjugacy condition (4.27), and the induction hypothesis, we have

$$\begin{aligned}\boldsymbol{\chi}^{(m+1)}\left(s, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right) &= \mathsf{e}^{s\mathbf{A}}\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) - \int_s^\infty \mathsf{e}^{(s-r)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(r, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right)\right) dr \\ &= \mathsf{e}^{s\mathbf{A}}\mathsf{e}^{t\mathbf{A}}\boldsymbol{\psi}\left(\mathbf{x}_0\right) - \int_s^\infty \mathsf{e}^{(s-r)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(r+t, \boldsymbol{\psi}\left(\mathbf{x}_0\right)\right)\right) dr.\end{aligned}$$

Using the change of variables $\xi = r + t$ in the integral, we get

$$\begin{aligned}\boldsymbol{\chi}^{(m+1)}\left(s, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right) &= \mathsf{e}^{(s+t)\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0) - \int_{s+t}^\infty \mathsf{e}^{(s+t-\xi)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(\xi, \boldsymbol{\psi}\left(\mathbf{x}_0\right)\right)\right) d\xi \\ &= \boldsymbol{\chi}^{(m+1)}\left(s+t, \boldsymbol{\psi}\left(\mathbf{x}_0\right)\right).\end{aligned}$$

Hence the lemma is true for $m + 1$. By induction, the lemma is true for all $m \in \mathbb{N}$. □

Corollary 4.23: *There is a $\delta > 0$ such that*

$$\boldsymbol{\chi}^{(m)}\left(s, \mathsf{e}^{t\boldsymbol{A}}\boldsymbol{\psi}(\boldsymbol{x}_0)\right) = \boldsymbol{\chi}^{(m)}\left(s+t, \boldsymbol{\psi}(\boldsymbol{x}_0)\right) \quad \textit{for all} \quad s,t \geq 0,\ \boldsymbol{x}_0 \in B_\delta,\ m \in \mathbb{N}. \tag{4.31}$$

Proof: It follows from (4.27) and (4.30). □

4.6.2 Definition of the Iterates

We will denote the *iterates of the third type* by $\left\{\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right\}_{m=1}^{\infty}$. For the initial point for these iterates, we will take

$$\mathbf{z}_0^{(m)} := \boldsymbol{\chi}^{(m)}(0, \mathbf{y}_0) \quad (m \in \mathbb{N}).$$

The estimate (4.15) implies there are $\delta, k > 0$ (independent of m) such that

$$\left\|\mathbf{z}_0^{(m)}\right\| \le k \|\mathbf{x}_0\| \quad \text{for all} \quad \mathbf{x}_0 \in B_\delta,\ m \in \mathbb{N}.$$

Define

$$\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0) := \boldsymbol{\chi}^{(m)}\left(t, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right) \quad (m \in \mathbb{N}), \tag{4.32}$$

where $\|\mathbf{z}_0\|$ is sufficiently small. (Note that there is no problem using $\mathbf{z}_0$ in the definition (4.32) instead of $\mathbf{z}_0^{(m)}$.) That is,

$$\boldsymbol{\varphi}_t^{(m)}\left(\mathbf{z}_0^{(m)}\right) = \boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0) \quad (m \in \mathbb{N}). \tag{4.33}$$

Proposition 4.24: *There is a $\delta > 0$ such that if $\|\mathbf{z}_0\| < \delta$ then, for each $m \in \mathbb{N}$, $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$ is a flow.*

Proof: There is a $\delta > 0$ (independent of m) such that if $\|\mathbf{z}_0\| < \delta$ then all relevant improper integrals converge and all relevant estimates apply. Hence, we will assume that $\|\mathbf{z}_0\| < \delta$. Note that $\boldsymbol{\chi}^{(m)}(0,\cdot)$ is indeed invertible since it is a near-identity transformation. Now, for $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$ to be a flow, we need

$$\boldsymbol{\varphi}_0^{(m)}(\mathbf{z}_0) = \mathbf{z}_0 \quad \text{and} \quad \boldsymbol{\varphi}_s^{(m)}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right) = \boldsymbol{\varphi}_{s+t}^{(m)}(\mathbf{z}_0).$$

The first condition is obtained by setting $t = 0$ in the definition (4.32) and canceling inverse functions. To obtain the second condition, first use the definition of $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$, which tells us

$$\begin{aligned}\boldsymbol{\varphi}_s^{(m)}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right) &= \boldsymbol{\chi}^{(m)}\left(s, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right)\right) \\ &= \boldsymbol{\chi}^{(m)}\left(s, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}\left(\boldsymbol{\chi}^{(m)}\left(t, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right)\right)\right).\end{aligned}$$

Using (4.31) with $s = 0$ and canceling inverse functions,

$$\begin{aligned}\boldsymbol{\varphi}_s^{(m)}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right) &= \boldsymbol{\chi}^{(m)}\left(s, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}\left(\boldsymbol{\chi}^{(m)}\left(0, \mathsf{e}^{t\mathbf{A}}\left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right)\right)\right) \\ &= \boldsymbol{\chi}^{(m)}\left(s, \mathsf{e}^{t\mathbf{A}}\left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right).\end{aligned}$$

Using (4.31) again,

$$\boldsymbol{\varphi}_s^{(m)}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right) = \boldsymbol{\chi}^{(m)}\left(s+t, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right) = \boldsymbol{\varphi}_{s+t}^{(m)}(\mathbf{z}_0)\,.$$

□

4.6.3 Differential Equation which the Iterates Satisfy

Since the iterates of the third type, $\left\{\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right\}_{m=1}^{\infty}$, are flows, we know that they must be the solution of an autonomous ordinary differential equation. We can use the iterates of the first type along with (4.14) to specify this differential equation. The following results can be shown in exactly the same manner as the corresponding results in §3.6.3.

Claim 4.25:

(a) Let $\|\boldsymbol{z}_0\|$ be sufficiently small. The iterate $\boldsymbol{\varphi}_t^{(m)}(\boldsymbol{z}_0)$ is the solution of

$$\dot{\boldsymbol{z}} = \boldsymbol{g}^{(m)}(\boldsymbol{z}), \quad \boldsymbol{z}(0) = \boldsymbol{z}_0,$$

where

$$\boldsymbol{g}^{(m)}(\boldsymbol{z}) := \begin{cases} \boldsymbol{A}\boldsymbol{z}, & \text{if} \quad m=1 \\ \boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}\left(\boldsymbol{\chi}^{(m-1)}\left(0, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\boldsymbol{z})\right)\right), & \text{if} \quad m>1 \end{cases}.$$

(b) The function $\boldsymbol{g}^{(m)}(\boldsymbol{z})$ satisfies

$$\left\|\boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}(\boldsymbol{z}) - \boldsymbol{g}^{(m)}(\boldsymbol{z})\right\| = \mathcal{O}\left(\|\boldsymbol{z}\|^{\alpha+(m-1)\beta}\right) \quad \text{as} \quad \|\boldsymbol{z}\| \to 0.$$

4.6.4 A Conjugacy Condition for the Iterates

Define, for sufficiently small $\|\mathbf{x}_0\|$,

$$\widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0) := \boldsymbol{\chi}^{(m)}(0, \boldsymbol{\psi}(\mathbf{x}_0)) \quad (m \in \mathbb{N})\,. \tag{4.34}$$

The initial condition $\mathbf{z}_0^{(m)}$ above, which we use for the iterates of the third type, thus can be written

$$\mathbf{z}_0^{(m)} = \widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0).$$

Observe that

$$\boldsymbol{\varphi}_t^{(m)}\left(\widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0)\right) = \boldsymbol{\chi}^{(m)}(t, \boldsymbol{\psi}(\mathbf{x}_0))\,, \tag{4.35}$$

which follows from (4.33). Observe also that $\widehat{\boldsymbol{\psi}}^{(1)} = \boldsymbol{\psi}$.

Recall that the function $\boldsymbol{\psi}$, which maps the initial condition $\mathbf{x}_0$ to the initial condition $\mathbf{y}_0$, satisfies the conjugacy condition $\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \mathrm{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0)$. That is, $\boldsymbol{\psi}$ maps flows of the nonlinear differential equation onto flows of the linear differential equation. It turns out that the function $\widehat{\boldsymbol{\psi}}^{(m)}$, which maps the initial condition $\mathbf{x}_0$ to $\mathbf{z}_0^{(m)}$, satisfies its own conjugacy condition. In particular, $\widehat{\boldsymbol{\psi}}^{(m)}$ maps flows of the original nonlinear differential equation onto flows of the (generally nonlinear) differential equation which $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$ satisfies.

Theorem 4.26: *Consider the function $\widehat{\boldsymbol{\psi}}^{(m)}$. There is a $\delta > 0$ such that*

$$\widehat{\boldsymbol{\psi}}^{(m)}\left(\boldsymbol{\phi}_t(\boldsymbol{x}_0)\right) = \boldsymbol{\varphi}_t^{(m)}\left(\widehat{\boldsymbol{\psi}}^{(m)}(\boldsymbol{x}_0)\right) \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \mathbb{N}.$$

Proof: Let $\mathbf{x}_0$ be sufficiently small, say $\|\mathbf{x}_0\| < \delta$ where $\delta > 0$. Consider

$$\begin{aligned}
\widehat{\boldsymbol{\psi}}^{(m)}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) &= \boldsymbol{\chi}^{(m)}\left(0, \boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right)\right) \quad \text{(using (4.34))} \\
&= \boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}(\mathbf{x}_0)\right) \quad \text{(using (4.30) with } s = 0\text{)} \\
&= \boldsymbol{\varphi}_t^{(m)}\left(\widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0)\right) \quad \text{(using (4.35))}.
\end{aligned}$$

□

Proposition 4.27: *There is a $\delta > 0$ and $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ such that*

$$\left\|\widehat{\boldsymbol{\psi}}^{(m)}(\boldsymbol{x}_0) - \boldsymbol{x}_0\right\| \leq k_m \left\|\boldsymbol{x}_0\right\|^{\alpha+(m-1)\beta} \quad \textit{for all} \quad \boldsymbol{x}_0 \in B_\delta,\ m \in \mathbb{N}.$$

Proof: Set $t = 0$ in (4.17) and apply (4.34). □

4.6.5 A Simple Example

Consider the system in §4.3.4 along with the first two iterates of the first type. We will calculate the first two iterates of the third type. Setting $t = 0$ in the first two iterates, we see

$$\boldsymbol{\chi}^{(1)}\left(0, \mathbf{y}_0\right) = \begin{pmatrix} y_{01} \\ y_{02} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}\left(0, \mathbf{y}_0\right) = \begin{pmatrix} y_{01} \\ y_{02}\left[1 - r y_{01}\right] - r y_{01}^2 \end{pmatrix}.$$

It follows that

$$\left[\boldsymbol{\chi}^{(1)}\left(0, \cdot\right)\right]^{-1}(\mathbf{z}_0) = \begin{pmatrix} z_{01} \\ z_{02} \end{pmatrix} \quad \text{and} \quad \left[\boldsymbol{\chi}^{(2)}\left(0, \cdot\right)\right]^{-1}(\mathbf{z}_0) = \begin{pmatrix} z_{01} \\ \xi(\mathbf{z}_0) \end{pmatrix}, \quad \|\mathbf{z}_0\| < \frac{1}{|r|},$$

where

$$\xi(\mathbf{z}) := \frac{z_2 + r z_1^2}{1 - r z_1}.$$

Therefore, we have

$$\boldsymbol{\varphi}_t^{(1)}(\mathbf{z}_0) = \mathsf{e}^{-t}\begin{pmatrix} z_{01} \\ z_{02} + z_{01}t \end{pmatrix} \quad \text{and} \quad \boldsymbol{\varphi}_t^{(2)}(\mathbf{z}_0) = \mathsf{e}^{-t}\begin{pmatrix} z_{01} \\ \xi(\mathbf{z}_0) + z_{01}t \end{pmatrix} - r z_{01}\mathsf{e}^{-2t}\begin{pmatrix} 0 \\ z_{01} + \xi(\mathbf{z}_0) + z_{01}t \end{pmatrix}.$$

Furthermore, using Claim 4.25 we know that the iterate $\boldsymbol{\varphi}_t^{(2)}(\mathbf{z}_0)$ is the solution of

$$\dot{\mathbf{z}} = \begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix}\mathbf{z} + \begin{pmatrix} 0 \\ r z_1 \xi(\mathbf{z}) \end{pmatrix}, \quad \mathbf{z}(0) = \mathbf{z}_0,$$

where $\|\mathbf{z}_0\| < |r|^{-1}$. Note that

$$\xi(\mathbf{z}) = z_2 + \mathcal{O}\Big(\|\mathbf{z}\|^2\Big) \quad \text{as} \quad \|\mathbf{z}\| \to 0.$$

4.7 Transforming Widely-Spaced to Closely-Spaced Eigenvalues

This chapter deals with the case where the eigenvalues are closely-spaced relative to the nonlinear part of the differential equation. That is, $\kappa < \alpha$. In Chapter 5, we will deal with the case where the eigenvalues are widely-spaced relative to the nonlinear part of the differential equation. That is, $\kappa \geq \alpha$. However, the techniques for widely-spaced eigenvalues are decidedly more complicated. Fortunately, in practice it is sometimes possible to transform a system with widely-spaced eigenvalues to a system with closely-spaced eigenvalues.

4.7.1 Linearization Transformation

Suppose that $\boldsymbol{\zeta} \in C^1(\mathcal{N}, \mathbb{R}^n)$, where $\mathcal{N} \subset \mathbb{R}^n$ is some neighbourhood of the origin, satisfies

$$\mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\left[\mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})\right] - \mathbf{A}\boldsymbol{\zeta}(\mathbf{x}) = \mathbf{0}, \quad \boldsymbol{\zeta}(\mathbf{0}) = \mathbf{0}, \quad \mathbf{D}\boldsymbol{\zeta}(\mathbf{0}) = \mathbf{I}. \tag{4.36}$$

The matrix $\mathbf{A}$ and vector field $\mathbf{b}$ still satisfy the same assumptions as before but we no longer assume that the eigenvalues are closely-spaced relative to $\mathbf{b}$. By Taylor's Theorem,

$$\|\boldsymbol{\zeta}(\mathbf{x}) - \mathbf{x}\| = \mathsf{o}(\|\mathbf{x}\|) \quad \text{and} \quad \|\mathbf{D}\boldsymbol{\zeta}(\mathbf{x}) - \mathbf{I}\| = \mathsf{o}(1) \quad \text{as} \quad \|\mathbf{x}\| \to 0. \tag{4.37}$$

Observe that $\boldsymbol{\zeta}$ is a near-identity transformation which is invertible in a neighbourhood of the origin. The inverse of $\boldsymbol{\zeta}$ satisfies

$$\left\|\boldsymbol{\zeta}^{-1}(\mathbf{y})-\mathbf{y}\right\|=\mathsf{o}(\|\mathbf{y}\|) \quad \text{as} \quad \|\mathbf{y}\|\to 0. \tag{4.38}$$

We know that $\boldsymbol{\psi}$ is one such transformation (when the eigenvalues are closely-spaced relative to $\mathbf{b}$).

Proposition 4.28: *The change of variables $\boldsymbol{y}:=\boldsymbol{\zeta}(\boldsymbol{x})$ transforms the initial value problem*

$$\dot{\boldsymbol{x}}=\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b}(\boldsymbol{x}), \quad \boldsymbol{x}(0)=\boldsymbol{x}_0$$

into the initial value problem

$$\dot{\boldsymbol{y}}=\boldsymbol{A}\boldsymbol{y}, \quad \boldsymbol{y}(0)=\boldsymbol{\zeta}(\boldsymbol{x}_0).$$

Proof: Obviously, $\mathbf{y}(0)=\boldsymbol{\zeta}(\mathbf{x}_0)$. Now, calculate

$$\dot{\mathbf{y}}=\mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\dot{\mathbf{x}}=\mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\left[\mathbf{A}\mathbf{x}+\mathbf{b}(\mathbf{x})\right]=\mathbf{A}\boldsymbol{\zeta}(\mathbf{x})=\mathbf{A}\mathbf{y},$$

□

Remark 4.29: The fact that a linearization transformation satisfies a partial differential equation has been explored by others. See, for example, [37].

We will use the fact that $\boldsymbol{\zeta}$ converts the nonlinear system into a linear one to simplify more complicated systems. In particular, $\boldsymbol{\zeta}$ will annihilate lower-order terms so that the resulting system has closely-spaced eigenvalues.

Proposition 4.30: *Suppose that $\widehat{\boldsymbol{b}}\in C^1(\mathcal{N},\mathbb{R}^n)$ satisfies*

$$\left\|\widehat{\boldsymbol{b}}(\boldsymbol{x})\right\|=\mathcal{O}\left(\|\boldsymbol{x}\|^{\widehat{\alpha}}\right) \quad \textit{as} \quad \|\boldsymbol{x}\|\to 0,$$

where $\widehat{\alpha}>1$ is a parameter. Then, the change of variables $\boldsymbol{y}:=\boldsymbol{\zeta}(\boldsymbol{x})$ transforms the initial value problem

$$\dot{\boldsymbol{x}}=\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b}(\boldsymbol{x})+\widehat{\boldsymbol{b}}(\boldsymbol{x}), \quad \boldsymbol{x}(0)=\boldsymbol{x}_0$$

into the initial value problem

$$\dot{\boldsymbol{y}}=\boldsymbol{A}\boldsymbol{y}+\overline{\boldsymbol{b}}(\boldsymbol{y}), \quad \boldsymbol{y}(0)=\boldsymbol{\zeta}(\boldsymbol{x}_0),$$

where

$$\overline{\boldsymbol{b}}(\boldsymbol{y}):=\boldsymbol{D}\boldsymbol{\zeta}\left(\boldsymbol{\zeta}^{-1}(\boldsymbol{y})\right)\widehat{\boldsymbol{b}}\left(\boldsymbol{\zeta}^{-1}(\boldsymbol{y})\right) \quad \textit{and} \quad \left\|\overline{\boldsymbol{b}}(\boldsymbol{y})\right\|=\mathcal{O}\left(\|\boldsymbol{y}\|^{\widehat{\alpha}}\right) \quad \textit{as} \quad \|\boldsymbol{y}\|\to 0.$$

Proof: Calculate

$$\begin{aligned}
\dot{\mathbf{y}} &= \mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\dot{\mathbf{x}} \\
&= \mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\left[\mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}) + \widehat{\mathbf{b}}(\mathbf{x})\right] \quad \text{(by the DE)} \\
&= \mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\left[\mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})\right] + \mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\widehat{\mathbf{b}}(\mathbf{x}) \\
&= \mathbf{A}\boldsymbol{\zeta}(\mathbf{x}) + \mathbf{D}\boldsymbol{\zeta}(\mathbf{x})\widehat{\mathbf{b}}(\mathbf{x}) \quad \text{(applying (4.36))} \\
&= \mathbf{A}\mathbf{y} + \mathbf{D}\boldsymbol{\zeta}\left(\boldsymbol{\zeta}^{-1}(\mathbf{y})\right)\widehat{\mathbf{b}}\left(\boldsymbol{\zeta}^{-1}(\mathbf{y})\right).
\end{aligned}$$

Moreover, the decay rate of $\overline{\mathbf{b}}(\mathbf{y})$ follows from (4.37), (4.38) and the decay rate of $\widehat{\mathbf{b}}(\mathbf{x})$. □

Remark 4.31: Suppose you have a system with widely-spaced eigenvalues. Assume that the nonlinear part has been split into the form $\mathbf{b}(\mathbf{x}) + \widehat{\mathbf{b}}(\mathbf{x})$. Unfortunately, it is not always possible to solve (4.36) for $\boldsymbol{\zeta}(\mathbf{x})$. The following example is one in which there is resonance in the eigenvalues and $\boldsymbol{\zeta}(\mathbf{x})$ can be found.

4.7.2 A Simple Example

Let

$$\mathbf{A} := \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) := \begin{pmatrix} 0 \\ x_1^2 \end{pmatrix}, \quad \text{and} \quad \widehat{\mathbf{b}}(\mathbf{x}) := \begin{pmatrix} 0 \\ x_1^3 \end{pmatrix}.$$

Hence, consider the system

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}) + \widehat{\mathbf{b}}(\mathbf{x}). \tag{4.39}$$

Observe that there is resonance in the eigenvalues of $\mathbf{A}$ and that the eigenvalues are widely-spaced relative to the nonlinear part. Ultimately, our goal is to find asymptotic approximations for solutions $\mathbf{x}(t)$ of (4.39) as $t \to \infty$.

Finding $\boldsymbol{\zeta}$

We will find a near-identity transformation $\boldsymbol{\zeta}$ such that the change of variables $\mathbf{y} := \boldsymbol{\zeta}(\mathbf{x})$ converts the system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ into the system $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y}$. Since the differential equation for x_1 is decoupled from x_2, we will use the ansatz

$$\boldsymbol{\zeta}(\mathbf{x}) := \begin{pmatrix} x_1 \\ x_2 + \xi(x_1) \end{pmatrix},$$

where $\xi(0) = 0 = \xi'(0)$ and $' = \frac{d}{dx_1}$. Using (4.36),

$$\begin{pmatrix} 1 & 0 \\ \xi'(x_1) & 1 \end{pmatrix} \begin{pmatrix} -x_1 \\ -2x_2 + x_1^2 \end{pmatrix} - \begin{pmatrix} -x_1 \\ -2x_2 - 2\xi(x_1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The first component is satisfied trivially and the second component yields the ordinary differential equation

$$\xi'(x_1) = \frac{2\xi(x_1)}{x_1} + x_1.$$

Solving with an integrating factor,

$$\xi(x_1) = (\ln|x_1| + C)\, x_1^2,$$

where $C \in \mathbb{R}$ is an arbitrary constant. We will take[2]

$$\boldsymbol{\zeta}(\mathbf{x}) = \begin{pmatrix} x_1 \\ x_2 + x_1^2 \ln|x_1| \end{pmatrix}.$$

Note that $\boldsymbol{\zeta} \in C^1$ but $\boldsymbol{\zeta} \notin C^2$ with

$$\mathbf{D}\boldsymbol{\zeta}(\mathbf{x}) = \begin{pmatrix} 1 & 0 \\ x_1\,[2\ln|x_1| + 1] & 1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\zeta}^{-1}(\mathbf{y}) = \begin{pmatrix} y_1 \\ y_2 - y_1^2 \ln|y_1| \end{pmatrix}.$$

Finding the Transformed System

Calculate

$$\overline{\mathbf{b}}(\mathbf{y}) = \mathbf{D}\boldsymbol{\zeta}\left(\boldsymbol{\zeta}^{-1}(\mathbf{y})\right) \widehat{\mathbf{b}}\left(\boldsymbol{\zeta}^{-1}(\mathbf{y})\right) = \begin{pmatrix} 0 \\ y_1^3 \end{pmatrix}.$$

By Proposition 4.30, under the change of variables $\mathbf{y} := \boldsymbol{\zeta}(\mathbf{x})$ the system (4.39) is converted to the system

$$\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \overline{\mathbf{b}}(\mathbf{y}). \tag{4.40}$$

Importantly, this system has eigenvalues which are closely-spaced relative to the nonlinear part.

[2] Sometimes, you may want to choose the arbitrary constant to be something other than zero to simplify the resulting system.

Finding Iterates for the Transformed System

For the transformed system (4.40), the first two iterates are

$$\boldsymbol{\chi}^{(1)}(t,\mathbf{c}) = \begin{pmatrix} \mathsf{e}^{-t}c_1 \\ \mathsf{e}^{-2t}c_2 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}(t,\mathbf{c}) = \begin{pmatrix} \mathsf{e}^{-t}c_1 \\ \mathsf{e}^{-2t}c_2 - \mathsf{e}^{-3t}c_1^3 \end{pmatrix},$$

where $\mathbf{c} := \boldsymbol{\psi}(\mathbf{y}_0)$ and $\boldsymbol{\psi}$ is defined with respect to the system (4.40). By Theorem 4.9,

$$\mathbf{y}(t) = \begin{pmatrix} \mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \\ \mathsf{e}^{-2t}c_2 - \mathsf{e}^{-3t}c_1^3 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \end{pmatrix} \quad \text{as} \quad t \to \infty,$$

where $\mathbf{y}(t)$ is the solution of (4.40) with $\mathbf{y}(0) = \mathbf{y}_0$.

Finding Associated Iterates for the Original System

Let $\mathbf{x}(t)$ be the solution of the original system (4.39). Since $\mathbf{y} = \boldsymbol{\zeta}(\mathbf{x})$, we have

$$\begin{aligned} \mathbf{x}(t) &= \boldsymbol{\zeta}^{-1}\left(\mathbf{y}(t)\right) \\ &= \begin{pmatrix} \mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \\ \big[\mathsf{e}^{-2t}c_2 - \mathsf{e}^{-3t}c_1^3 + \mathcal{O}\big(\mathsf{e}^{-5t}\big)\big] - \big[\mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big)\big]^2 \ln\left|\mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big)\right| \end{pmatrix}. \end{aligned}$$

Since $\ln(1+u) = \mathcal{O}(u)$ as $u \to 0$, we can write

$$\begin{aligned} \ln\left|\mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big)\right| &= \ln\left|\mathsf{e}^{-t}\right| |c_1| \left|1 + \mathcal{O}\big(\mathsf{e}^{-4t}\big)\right| \\ &= \ln\left|\mathsf{e}^{-t}\right| + \ln|c_1| + \ln\left|1 + \mathcal{O}\big(\mathsf{e}^{-4t}\big)\right| \\ &= -t + \ln|c_1| + \mathcal{O}\big(\mathsf{e}^{-4t}\big) \quad \text{as} \quad t \to \infty. \end{aligned}$$

Thus,

$$\begin{aligned} \mathbf{x}(t) &= \begin{pmatrix} \mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \\ \big[\mathsf{e}^{-2t}c_2 - \mathsf{e}^{-3t}c_1^3 + \mathcal{O}\big(\mathsf{e}^{-5t}\big)\big] - \big[\mathsf{e}^{-2t}c_1^2 + \mathcal{O}\big(\mathsf{e}^{-6t}\big)\big]\big[-t + \ln|c_1| + \mathcal{O}\big(\mathsf{e}^{-4t}\big)\big] \end{pmatrix} \\ &= \begin{pmatrix} \mathsf{e}^{-t}c_1 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \\ \mathsf{e}^{-2t}\left[c_2 - c_1^2\ln|c_1| + c_1^2 t\right] - \mathsf{e}^{-3t}c_1^3 + \mathcal{O}\big(\mathsf{e}^{-5t}\big) \end{pmatrix}. \end{aligned}$$

Remark 4.32: It turns out that $\boldsymbol{\chi}^{(3)}(t,\mathbf{c}) = \boldsymbol{\chi}^{(2)}(t,\mathbf{c})$. Consequently, $\boldsymbol{\chi}^{(m)}(t,\mathbf{c}) = \boldsymbol{\chi}^{(2)}(t,\mathbf{c})$ for any $m \in \{2,3,\ldots\}$ and $\mathbf{y}(t) = \boldsymbol{\chi}^{(2)}(t,\mathbf{c})$. Hence, we can drop the error terms in our expression for $\mathbf{x}(t)$. In terms of the initial condition $\mathbf{x}(0) = \mathbf{x}_0$, the actual solution is

$$\mathbf{x}(t) = \begin{pmatrix} \mathsf{e}^{-t}x_{01} \\ \mathsf{e}^{-2t}\left[x_{01}^3 + x_{02} + x_{01}^2 t\right] - \mathsf{e}^{-3t}x_{01}^3 \end{pmatrix}.$$

4.7.3 Normal Forms

The concept of reducing the case of widely-spaced eigenvalues to the case of closely-spaced eigenvalues is related to the theory of normal forms. Suppose that the nonlinear vector field $\mathbf{b}$ is analytic (or sufficiently smooth) at the origin and the eigenvalues of $\mathbf{A}$ are widely-spaced relative to $\mathbf{b}$. By means of a near-identity, analytic transformation, it is sometimes possible to convert the system to a new system with closely-spaced eigenvalues.

Suppose that there is no resonance in the eigenvalues of $\mathbf{A}$. For a given $m > \kappa$, by the Normal Form Theorem there exists a sequence of near-identity, analytic transformations such that the differential equation $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ is converted to a differential equation of the form $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{c}(\mathbf{y})$ where $\|\mathbf{c}(\mathbf{y})\| = \mathcal{O}(\|\mathbf{y}\|^m)$ as $\|\mathbf{y}\| \to 0$. The new system, of course, has eigenvalues which are closely-spaced relative to the nonlinear part. See §A.11 in Appendix A which covers normal forms.

Suppose now that there is resonance in the eigenvalues of $\mathbf{A}$, say with lowest order m (see §A.9). The best we can do is find a sequence of near-identity, analytic transformations to convert $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x})$ to $\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{c}(\mathbf{y})$ where $\|\mathbf{c}(\mathbf{y})\| = \mathcal{O}(\|\mathbf{y}\|^m)$ as $\|\mathbf{y}\| \to 0$. Hopefully $m > \kappa$.

4.8 Summary

In this chapter, we explored the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

where the eigenvalues of $\mathbf{A}$ are closely-spaced relative to the vector field $\mathbf{b}$. In particular, the real parts $\{\mu_i\}_{i=1}^n$ of the eigenvalues of $\mathbf{A}$ and the parameters α and β are as in Chapter 2 and, in this chapter, we assumed $\alpha\mu_1 - \mu_n < 0$.

We re-wrote the standard integral equation for the flow $\boldsymbol{\phi}_t(\mathbf{x}_0)$ as

$$\boldsymbol{\phi}_t(\mathbf{x}_0) = \mathsf{e}^{t\mathbf{A}}\mathbf{y}_0 - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}}\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0))\,ds,$$

where

$$\mathbf{y}_0 = \boldsymbol{\psi}(\mathbf{x}_0) = \mathbf{x}_0 + \int_0^\infty \mathsf{e}^{-s\mathbf{A}}\mathbf{b}(\boldsymbol{\phi}_s(\mathbf{x}_0))\,ds$$

is a useful, related initial condition. Note that our assumptions on $\mathbf{A}$ and $\mathbf{b}(\mathbf{x})$ as well as our exponential estimate for the flow guarantee that the above improper integrals converge for sufficiently small $\|\mathbf{x}_0\|$. Interestingly, the function $\boldsymbol{\psi}$ is near-identity and $\mathbf{y}_0$ is the unique point such that

$$\limsup_{t\to\infty} \frac{\ln\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \mathrm{e}^{t\mathbf{A}}\mathbf{y}_0\right\|}{t} \le \alpha\mu_1.$$

In other words, $\mathbf{y}_0$ is the optimal initial condition for the linearized initial value problem.

This chapter introduced iterates of the first type $\left\{\boldsymbol{\chi}^{(m)}(t,\mathbf{y}_0)\right\}_{m=1}^{\infty}$, given by

$$\boldsymbol{\chi}^{(1)}(t,\mathbf{y}_0) = \mathrm{e}^{t\mathbf{A}}\mathbf{y}_0, \quad \boldsymbol{\chi}^{(m+1)}(t,\mathbf{y}_0) = \mathrm{e}^{t\mathbf{A}}\mathbf{y}_0 - \int_t^{\infty} \mathrm{e}^{(t-s)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s,\mathbf{y}_0)\right) ds \quad (m \in \mathbb{N}).$$

In practice, $\mathbf{y}_0$ is left as a parameter so that is why we regard $\mathbf{y}_0$ as a variable instead of $\mathbf{x}_0$. These iterates satisfy, for any sufficiently small $\sigma > 0$, the decay rate

$$\left\|\boldsymbol{\chi}^{(m)}(t,\mathbf{y}_0)\right\| = \mathcal{O}\left(\mathrm{e}^{(\mu_1+\sigma)t}\|\mathbf{x}_0\|\right) \quad \text{as} \quad t\to\infty \quad \text{and} \quad \|\mathbf{x}_0\|\to 0 \quad \text{uniformly in} \quad m.$$

Furthermore, the iterates are successively better asymptotic approximations to the actual solution as $t\to\infty$, satisfying

$$\left\|\boldsymbol{\phi}_t(\mathbf{x}_0) - \boldsymbol{\chi}^{(m)}(t,\mathbf{y}_0)\right\| = \mathcal{O}\left(\mathrm{e}^{[\alpha+(m-1)\beta][\mu_1+\sigma]t}\|\mathbf{x}_0\|^{\alpha+(m-1)\beta}\right) \quad \text{as} \quad t\to\infty \quad \text{and} \quad \|\mathbf{x}_0\|\to 0,$$

where $\sigma > 0$ is sufficiently small. Note that if $\mathbf{A}$ is diagonalizable, we can take $\sigma = 0$ for these estimates.

If we can approximate $\mathbf{b}(\mathbf{x})$ by a Taylor series, then we can construct the iterates of the second type $\left\{\widetilde{\boldsymbol{\chi}}^{(m)}(t,\mathbf{y}_0)\right\}_{m=1}^{\infty}$ similar to the iterates of the first type by truncating $\mathbf{b}(\mathbf{x})$ to a certain order. If we only have a Taylor polynomial for $\mathbf{b}(\mathbf{x})$, we can only define a certain number of iterates.

The function $\boldsymbol{\psi}$ satisfies the conjugacy condition

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\mathbf{x}_0)\right) = \mathrm{e}^{t\mathbf{A}}\boldsymbol{\psi}(\mathbf{x}_0),$$

which is the same conjugacy condition in the Hartman-Grobman Theorem. Also, $\boldsymbol{\psi}$ satisfies the initial value problem

$$\left[\mathbf{D}\boldsymbol{\psi}(\mathbf{x}_0)\right]\left[\mathbf{A}\mathbf{x}_0 + \mathbf{b}(\mathbf{x}_0)\right] - \mathbf{A}\boldsymbol{\psi}(\mathbf{x}_0) = \mathbf{0}, \quad \boldsymbol{\psi}(\mathbf{0}) = \mathbf{0}, \quad \mathbf{D}\boldsymbol{\psi}(\mathbf{0}) = \mathbf{I}.$$

Finally, we know that if $\mathbf{b}(\mathbf{x})$ is analytic then $\boldsymbol{\psi}(\mathbf{x}_0)$ is analytic.

The iterates of the first type have a natural definition but unfortunately these iterates are not flows. Hence, we defined the iterates of the third type $\left\{\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right\}_{m=1}^{\infty}$, given by

$$\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0) = \boldsymbol{\chi}^{(m)}\left(t, \left[\boldsymbol{\chi}^{(m)}(0,\cdot)\right]^{-1}(\mathbf{z}_0)\right) \quad (m \in \mathbb{N})$$

which are indeed flows. That is,

$$\boldsymbol{\varphi}_0^{(m)}(\mathbf{z}_0) = \mathbf{z}_0 \quad \text{and} \quad \boldsymbol{\varphi}_s^{(m)}\left(\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)\right) = \boldsymbol{\varphi}_{s+t}^{(m)}(\mathbf{z}_0).$$

The initial point $\mathbf{z}_0$ for the iterate $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$ is $\mathbf{z}_0 = \boldsymbol{\chi}^{(m)}(0, \mathbf{y}_0)$. Furthermore, these iterates satisfy the conjugacy condition

$$\widehat{\boldsymbol{\psi}}^{(m)}(\boldsymbol{\phi}_t(\mathbf{x}_0)) = \boldsymbol{\varphi}_t^{(m)}\left(\widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0)\right), \quad \text{where} \quad \widehat{\boldsymbol{\psi}}^{(m)}(\mathbf{x}_0) = \boldsymbol{\chi}^{(m)}(0, \boldsymbol{\psi}(\mathbf{x}_0)).$$

That is, $\widehat{\boldsymbol{\psi}}^{(m)}$ (which gives $\mathbf{z}_0$ as a function of $\mathbf{x}_0$ for a given m) maps flows of the nonlinear differential equation onto flows of the differential equation which $\boldsymbol{\varphi}_t^{(m)}(\mathbf{z}_0)$ satisfies.

We concluded this chapter with a brief discussion on how it is sometimes possible to convert a system with widely-spaced eigenvalues into a system with closely-spaced eigenvalues. In the next chapter, we explore separately the case of widely-spaced eigenvalues.

Chapter 5

Widely-Spaced Eigenvalues ($\kappa \geq \alpha$)

5.1 Introduction

Recall the initial value problem (2.5). Our goal in this part of the thesis is to use an iterative scheme to obtain asymptotic information about the solution $\mathbf{x}(t)$ as $t \to \infty$ when $\|\mathbf{x}_0\|$ is sufficiently small. In Chapter 3 we explored the scalar case and in Chapter 4 we explored the multi-dimensional case in which the eigenvalues of the matrix $\mathbf{A}$ are closely-spaced relative to the nonlinear part $\mathbf{b}(\mathbf{x})$. In this chapter, we will explore the multi-dimensional case in which the eigenvalues are widely-spaced relative to the nonlinear part. For simplicity, we will restrict our attention to a special case (namely the planar, diagonal case) which is most applicable to us.

5.1.1 The Problem

Consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{5.1}$$

where

$$\mathbf{A} := \begin{pmatrix} a & 0 \\ 0 & \kappa a \end{pmatrix} \quad \text{and} \quad \mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_1(\mathbf{x}) \\ b_2(\mathbf{x}) \end{pmatrix}.$$

Denote the solution of (5.1) by

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \begin{pmatrix} \phi_1(t, \mathbf{x}_0) \\ \phi_2(t, \mathbf{x}_0) \end{pmatrix}.$$

We need to alter the notation for the flow from previous chapters since we will have to frequently refer to the components.

Assumption 5.1: Consider the matrix $\mathbf{A}$ and vector field $\mathbf{b}$.

(a) There is some neighbourhood $\mathcal{N} \subset \mathbb{R}^2$ with $\mathbf{0} \in \mathcal{N}$ and $\mathbf{b} \in C^1(\mathcal{N}, \mathbb{R}^2)$.

(b) There are $\delta, k > 0$ such that

$$\|\mathbf{b}(\mathbf{x})\| \leq k \|\mathbf{x}\|^{\alpha} \quad \text{for all} \quad \mathbf{x} \in B_\delta, \tag{5.2}$$

where $\alpha > 1$ is a fixed parameter.

(c) There are $\delta, k > 0$ such that

$$\|\mathbf{Db}(\mathbf{x})\| \leq k \|\mathbf{x}\|^{\beta} \quad \text{for all} \quad \mathbf{x} \in B_\delta, \tag{5.3}$$

where $\beta > 0$ is a fixed parameter.

(d) It is assumed that $a < 0$ and $\kappa \geq \alpha$. Thus,

$$\kappa a \leq \alpha a < a < 0. \tag{5.4}$$

5.1.2 Integral Equation

The initial value problem (5.1) can be written as the integral equation

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \mathrm{e}^{t\mathbf{A}}\mathbf{x}_0 + \int_0^t \mathrm{e}^{(t-s)\mathbf{A}}\mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds. \tag{5.5}$$

Due to the form of the matrix $\mathbf{A}$ and vector field $\mathbf{b}$, we can write the integral equation (5.5) as

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \begin{pmatrix} \mathrm{e}^{at}x_{01} + \int_0^t \mathrm{e}^{a(t-s)}b_1\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds \\ \mathrm{e}^{\kappa at}x_{02} + \int_0^t \mathrm{e}^{\kappa a(t-s)}b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds \end{pmatrix}, \tag{5.6}$$

where $\mathbf{x}_0 = (x_{01}, x_{02})^T$.

5.1.3 Important Estimates We Already Know

Define, for any $\delta > 0$, the set

$$\Omega_\delta := \left\{ \ (t, \mathbf{x}) \ : \ t \geq 0, \ \mathbf{x} \in \mathbb{R}^2, \ \|\mathbf{x}\| < \delta \ \right\}.$$

The basic estimates, which we saw in Chapter 2, that we will make extensive use of in this chapter are restated below.

- We know from Claim 2.9 that

$$\mathsf{e}^{\kappa a t} \leq \left\| \mathsf{e}^{t\mathbf{A}} \right\| \leq \mathsf{e}^{a t} \quad \text{for all} \quad t \geq 0.$$

- We also know from Claim 2.9 that

$$\mathsf{e}^{-a t} \leq \left\| \mathsf{e}^{-t\mathbf{A}} \right\| \leq \mathsf{e}^{-\kappa a t} \quad \text{for all} \quad t \geq 0. \tag{5.7}$$

- Since $\mathbf{A}$ is diagonal, we know from (2.9) that there are $\delta, k > 0$ such that

$$\|\boldsymbol{\phi}(t, \mathbf{x}_0)\| \leq k\, \mathsf{e}^{a t}\, \|\mathbf{x}_0\| \quad \text{for all} \quad (t, \mathbf{x}_0) \in \Omega_\delta. \tag{5.8}$$

5.1.4 Decay Rate of $\phi_2(t, \mathbf{x}_0)$

Consider the decay rate (5.8). We cannot improve, in general, the decay rate for the first component $\phi_1(t, \mathbf{x}_0)$ but we can improve the decay rate of the second component $\phi_2(t, \mathbf{x}_0)$.

Claim 5.2: *For any $\sigma > 0$ there are $\delta, k > 0$ such that*

$$|\phi_2(t, \boldsymbol{x}_0)| \leq k\, \mathsf{e}^{(\alpha a + \sigma) t}\, \|\boldsymbol{x}_0\| \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta. \tag{5.9}$$

Proof: Using (5.6), we see that

$$\phi_2(t, \mathbf{x}_0) = \mathsf{e}^{\kappa a t} x_{02} + \mathsf{e}^{\kappa a t} \int_0^t \mathsf{e}^{-\kappa a s} b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right)\, ds.$$

Applying the estimates (5.2) and (5.8), we know that there are $\delta, k_1, k_2 > 0$ such that if $(t, \mathbf{x}_0) \in \Omega_\delta$ then

$$\begin{aligned} |\phi_2(t, \mathbf{x}_0)| &\leq \mathsf{e}^{\kappa a t} |x_{02}| + \mathsf{e}^{\kappa a t} \int_0^t \mathsf{e}^{-\kappa a s} \left| b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \right|\, ds \\ &\leq k_1 \mathsf{e}^{\kappa a t} \|\mathbf{x}_0\| + k_2 \mathsf{e}^{\kappa a t} \left[\int_0^t \mathsf{e}^{-(\kappa - \alpha) a s}\, ds \right] \|\mathbf{x}_0\|^\alpha. \end{aligned}$$

In order to simplify the integral, we need to account for the case where $\kappa = \alpha$. To accomplish this, let $\sigma > 0$. Thus,

$$\sigma - (\kappa - \alpha)\, a > 0 \quad \text{and} \quad \mathsf{e}^{-(\kappa - \alpha) a s} \leq \mathsf{e}^{[\sigma - (\kappa - \alpha) a] s} \quad \text{for all} \quad s \geq 0$$

and hence

$$\begin{aligned} |\phi_2(t, \mathbf{x}_0)| &\leq k_1 \mathsf{e}^{\kappa a t} \|\mathbf{x}_0\| + \left[\frac{k_2}{\sigma - (\kappa - \alpha)\, a} \right] \left[\mathsf{e}^{(\alpha a + \sigma) t} - \mathsf{e}^{\kappa a t} \right] \|\mathbf{x}_0\|^\alpha \\ &\leq k_1 \mathsf{e}^{\kappa a t} \|\mathbf{x}_0\| + \left[\frac{k_2}{\sigma - (\kappa - \alpha)\, a} \right] \mathsf{e}^{(\alpha a + \sigma) t} \|\mathbf{x}_0\|^\alpha. \end{aligned}$$

Let

$$k_3 := \frac{k_2}{\sigma - (\kappa - \alpha)\, a} \quad \text{and} \quad k := k_1 + k_3 \delta^{\alpha-1}.$$

Since $\alpha > 1$ and $\kappa \geq \alpha$, we have

$$\begin{aligned} |\phi_2(t, \mathbf{x}_0)| &\leq \left\{ k_1 \mathsf{e}^{-[\sigma-(\kappa-\alpha)a]t} + k_3 \|\mathbf{x}_0\|^{\alpha-1} \right\} \mathsf{e}^{(\alpha a+\sigma)t} \|\mathbf{x}_0\| \\ &\leq \left[k_1 + k_3 \delta^{\alpha-1} \right] \mathsf{e}^{(\alpha a+\sigma)t} \|\mathbf{x}_0\| \\ &= k\, \mathsf{e}^{(\alpha a+\sigma)t} \|\mathbf{x}_0\| . \end{aligned}$$

$\square$

Remark 5.3: If $\kappa > \alpha$ then we can take $\sigma = 0$ in (5.9). This principle, in fact, applies throughout this chapter.

5.1.5 Crucial Obstacle

In Chapters 3 and 4, we were able to "flip the integral" in the general integral equation (5.5) and write

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \mathsf{e}^{t\mathbf{A}} \left[\mathbf{x}_0 + \int_0^\infty \mathsf{e}^{-s\mathbf{A}} \mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \, ds \right] - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}} \mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \, ds.$$

However, we cannot do this in this chapter. Why? The estimates (5.2), (5.7), and (5.8) tell us that there are $\delta, k > 0$ such that

$$\left\| \mathsf{e}^{-s\mathbf{A}} \mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \right\| \leq k\, \mathsf{e}^{(\alpha-\kappa)as} \|\mathbf{x}_0\|^\alpha \quad \text{for all} \quad (s, \mathbf{x}_0) \in \Omega_\delta.$$

The condition (5.4) prevents us from concluding that $\left\| \mathsf{e}^{-s\mathbf{A}} \mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \right\|$ decays exponentially. This in turn means that we cannot, in general, "flip the integral" in (5.5). Hence, we cannot find the initial condition $\mathbf{y}_0$ and define the iterates as easily as with the case of closely-spaced eigenvalues.

5.1.6 David Siegel

The basic idea for the iterates, which we will explore momentarily, is due to David Siegel. In particular, the idea involves iterating in the first component and later iterating in the second component.

5.2 "Flipping the Integral" in the First Component

We know that we cannot "flip" both integrals in (5.6). However, we observe the following.

Claim 5.4: *There are $\delta, k > 0$ such that*

$$\left| e^{-as} b_1 \left(\boldsymbol{\phi}(s, \boldsymbol{x}_0) \right) \right| \leq k \, e^{(\alpha-1)as} \left\| \boldsymbol{x}_0 \right\|^{\alpha} \quad \textit{for all} \quad (s, \boldsymbol{x}_0) \in \Omega_\delta. \tag{5.10}$$

Proof: It follows from (5.2) and (5.8). □

Since $\alpha > 1$, we see from (5.10) that we can "flip the integral" in the first component of (5.6). This gives us the following.

Claim 5.5: *There is a $\delta > 0$ such that*

$$\boldsymbol{\phi}(t, \boldsymbol{x}_0) = \begin{pmatrix} e^{at} y_{01} - \int_t^\infty e^{a(t-s)} b_1 \left(\boldsymbol{\phi}(s, \boldsymbol{x}_0) \right) ds \\ e^{\kappa a t} x_{02} + \int_0^t e^{\kappa a (t-s)} b_2 \left(\boldsymbol{\phi}(s, \boldsymbol{x}_0) \right) ds \end{pmatrix} \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta, \tag{5.11}$$

where

$$y_{01} := \psi_1(\boldsymbol{x}_0) \quad \textit{and} \quad \psi_1(\boldsymbol{x}_0) := x_{01} + \int_0^\infty e^{-as} b_1 \left(\boldsymbol{\phi}(s, \boldsymbol{x}_0) \right) ds. \tag{5.12}$$

Claim 5.6: *There are $\delta, k > 0$ such that*

$$\left| x_{01} - \psi_1(\boldsymbol{x}_0) \right| \leq k \left\| \boldsymbol{x}_0 \right\|^{\alpha} \quad \textit{for all} \quad \boldsymbol{x}_0 \in B_\delta. \tag{5.13}$$

Proof: It follows from (5.10) and (5.12). □

Claim 5.7: *There is a $\delta > 0$ such that*

$$\psi_1 \left(\boldsymbol{\phi}(t, \boldsymbol{x}_0) \right) = e^{at} \psi_1 \left(\boldsymbol{x}_0 \right) \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in B_\delta.$$

Proof: The proof is essentially identical to the proof of Theorem 3.16 on page 51 and makes use of the integral equation (5.11) for $\phi_1(t, \mathbf{x}_0)$, the definition (5.12) of $\psi_1(\mathbf{x}_0)$, a change of variables, and the semi-group property. □

5.3 First Group of Iterates

We will now introduce the *iterates*, which will be denoted by $\left\{ \boldsymbol{\chi}^{(m)} \left(t, \mathbf{y}_0 \right) \right\}_{m=1}^{\infty}$ and, in component form,

$$\boldsymbol{\chi}^{(m)} \left(t, \mathbf{y}_0 \right) = \begin{pmatrix} \chi_1^{(m)} \left(t, \mathbf{y}_0 \right) \\ \chi_2^{(m)} \left(t, \mathbf{y}_0 \right) \end{pmatrix}.$$

However, we cannot specify all the iterates just yet since we must split the iterates into two groups. Let $y_{01} := \psi_1(\mathbf{x}_0)$ and let $\|\mathbf{x}_0\|$ be sufficiently small.

5.3.1 Definition of the Iterates

Define

$$p := \left\lfloor \frac{\kappa - \alpha}{\beta} \right\rfloor + 2.$$

Observe that[1]

$$p \in \{2, 3, \ldots\} \quad \text{and} \quad [\alpha + (p-1)\beta]\, a < \kappa a \leq [\alpha + (p-2)\beta]\, a. \tag{5.14}$$

Take as the first iterate

$$\boldsymbol{\chi}^{(1)}(t, y_{01}) := \begin{pmatrix} \mathsf{e}^{at} y_{01} \\ 0 \end{pmatrix} \tag{5.15a}$$

and (if $p > 2$) define recursively

$$\boldsymbol{\chi}^{(m+1)}(t, y_{01}) := \begin{pmatrix} \mathsf{e}^{at} y_{01} - \int_t^\infty \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds \\ \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds \end{pmatrix}, \quad 1 \leq m \leq p-2. \tag{5.15b}$$

Remarks 5.8:

(i) The purpose of the first group of iterates is to get $\boldsymbol{\chi}^{(p-1)}(t, y_{01})$ close enough to $\boldsymbol{\phi}(t, \mathbf{x}_0)$ so that we can perform another "trick" in the second component of the integral equation (5.11).

(ii) Since the first group of iterates does not depend on y_{02}, we use the notation $\boldsymbol{\chi}^{(m)}(t, y_{01})$ instead of $\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)$. This is a necessary distinction since $y_{02} := \psi_2(\mathbf{x}_0)$ will be defined in terms of $\boldsymbol{\chi}^{(p-1)}(t, y_{01})$.

(iii) The definition of the iterates $\left\{\boldsymbol{\chi}^{(m)}(t, y_{01})\right\}_{m=1}^{p-1}$ follows naturally from the integral equation (5.11) except for the absence of the term $\mathsf{e}^{\kappa at} x_{02}$. There are three reasons why we omit this term. First, we do not yet have an appropriate interpretation of y_{02} and so we should not include the term $\mathsf{e}^{\kappa at} y_{02}$. Second, we cannot use the term $\mathsf{e}^{\kappa at} x_{02}$ since we want the iterates to be functions of $\mathbf{y}_0$ and not of $\mathbf{x}_0$. Finally, it turns out that the term $\mathsf{e}^{\kappa at} x_{02}$ is dominated by the integral $\int_0^t \mathsf{e}^{\kappa a(t-s)} b_2(\boldsymbol{\phi}(s, \mathbf{x}_0))\, ds$ and the presence of the term $\mathsf{e}^{\kappa at} y_{02}$ (or $\mathsf{e}^{\kappa at} x_{02}$) would not factor into decay rates until the second group of iterates.

[1]For $r \in \mathbb{R}$, we know $\lfloor r \rfloor \leq r < \lfloor r \rfloor + 1$. With $r = \frac{\kappa - \alpha}{\beta}$ and $\lfloor r \rfloor = p - 2$, we see $p - 2 \leq \frac{\kappa-\alpha}{\beta} < p - 1$. Hence, $\alpha + (p-2)\beta \leq \kappa < \alpha + (p-1)\beta$.

5.3.2 Existence and Decay Rate of the Iterates

We will now establish the decay rate of the first group of iterates. This basic exponential decay rate is the same as for $\boldsymbol{\phi}(t, \mathbf{x}_0)$ uniformly in m.

Proposition 5.9: *Consider the first group of iterates defined by* (5.15)*. Then, there is a* $\delta > 0$ *(independent of* m*) such that if* $\|\boldsymbol{x}_0\| < \delta$ *then* $\boldsymbol{\chi}^{(m)}(t, y_{01})$ *exists for each* $m \in \{1, \dots, p-1\}$*. Moreover, there is a* $k > 0$ *(independent of* m*) such that*

$$\left\|\boldsymbol{\chi}^{(m)}(t, y_{01})\right\| \leq k\, \mathsf{e}^{at} \|\boldsymbol{x}_0\| \quad \text{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \{1, \dots, p-1\}. \tag{5.16}$$

Proof: Since we are dealing with a finite number of iterates, we do not need to be careful in finding $\delta > 0$ and $k > 0$. The proof will be by induction on m.

Consider first the base case $m = 1$. It follows easily from (5.13) and (5.15a) that $\boldsymbol{\chi}^{(m)}(t, y_{01})$ exists and

$$\left\|\boldsymbol{\chi}^{(m)}(t, y_{01})\right\| = \mathcal{O}\big(\mathsf{e}^{at} \|\mathbf{x}_0\|\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

Thus, the result is true for $m = 1$.

If $p = 2$ then we are finished. Suppose that $p > 2$ and that the result is true for $m \in \{1, \dots, p-2\}$. It follows from (5.2), (5.13), and the induction hypothesis that

$$\int_t^\infty \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds = \mathcal{O}\big(\mathsf{e}^{\alpha a t} \|\mathbf{x}_0\|^\alpha\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0$$

and, for any $\sigma > 0$,

$$\int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds = \mathcal{O}\Big(\mathsf{e}^{(\alpha a + \sigma)t} \|\mathbf{x}_0\|^\alpha\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

Since $\sigma > 0$ is arbitrary and $\alpha > 1$, it follows from (5.15b) that $\boldsymbol{\chi}^{(m+1)}(t, y_{01})$ exists and

$$\left\|\boldsymbol{\chi}^{(m+1)}(t, y_{01})\right\| = \mathcal{O}\big(\mathsf{e}^{at} \|\mathbf{x}_0\|\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

Thus, the result is true for $m + 1$ and, by induction, the result is true for all $m \in \{1, \dots, p-1\}$. □

It is worth emphasizing the decay rate for $\chi_2^{(m)}(t, y_{01})$ as a separate result. This decay rate was established in the proof of Proposition 5.9.

Claim 5.10: *Consider the first group of iterates defined by* (5.15) *and let* $\sigma > 0$ *be sufficiently small. There are* $\delta, k > 0$ *such that*

$$\left|\chi_2^{(m)}(t, y_{01})\right| \leq k\, \mathsf{e}^{(\alpha a + \sigma)t} \|\boldsymbol{x}_0\|^\alpha \quad \text{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \in \{1, \dots, p-1\}.$$

5.3.3 Closeness of the Iterates to the Actual Solution

Here, we establish how good the iterate $\boldsymbol{\chi}^{(m)}(t, y_{01})$, for $m \in \{1, \ldots, p-1\}$, is as an asymptotic approximation to $\boldsymbol{\phi}(t, \mathbf{x}_0)$. As this theorem shows, each iteration improves the accuracy by a factor which is $\mathcal{O}\big(\mathsf{e}^{\beta a t}\big)$ as $t \to \infty$.

Theorem 5.11: *Consider the first group of iterates defined by* (5.15) *and let $\sigma > 0$ be sufficiently small. There are constants $\delta > 0$ and $\{k_m\}_{m=1}^{p-1} \subset \mathbb{R}_+$ such that*

$$\left\|\boldsymbol{\phi}(t, \boldsymbol{x}_0) - \boldsymbol{\chi}^{(m)}(t, y_{01})\right\| \leq k_m \mathsf{e}^{[\alpha+(m-1)\beta][a+\sigma]t} \|\boldsymbol{x}_0\| \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta, \; m \in \{1, \ldots, p-1\}\,. \tag{5.17}$$

Proof: Since we are dealing with a finite number of iterates, we do not need to be careful in finding $\delta > 0$ and $\{k_m\}_{m=1}^{p-1} \subset \mathbb{R}_+$. The proof will be by induction on m.

Consider first the base case $m = 1$. Using (5.9), (5.10), (5.11) and (5.15a), we know that

$$\phi_1(t, \mathbf{x}_0) - \chi_1^{(1)}(t, y_{01}) = \mathcal{O}\big(\mathsf{e}^{\alpha a t} \|\mathbf{x}_0\|^\alpha\big) \quad \text{and} \quad \phi_2(t, \mathbf{x}_0) - \chi_2^{(1)}(t, y_{01}) = \mathcal{O}\Big(\mathsf{e}^{\alpha(a+\sigma)t} \|\mathbf{x}_0\|\Big)$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$. Thus,

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(1)}(t, y_{01})\right\| = \mathcal{O}\Big(\mathsf{e}^{\alpha(a+\sigma)t} \|\mathbf{x}_0\|\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0$$

and the result is true for $m = 1$.

If $p = 2$ then we are done. Assume that $p > 2$ and that the result is true for a fixed index $m \in \{1, \ldots, p-2\}$. Using (5.3), (5.8), (5.11), (5.15b), (5.16), the Mean Value Theorem, and the induction hypothesis, we know that

$$\phi_1(t, \mathbf{x}_0) - \chi_1^{(m+1)}(t, y_{01}) = \mathcal{O}\Big(\mathsf{e}^{[\alpha+m\beta][a+\sigma]t} \|\mathbf{x}_0\|^{\beta+1}\Big)$$

and

$$\phi_2(t, \mathbf{x}_0) - \chi_2^{(m+1)}(t, y_{01}) = \mathsf{e}^{\kappa a t} x_{02} + \mathcal{O}\Big(\mathsf{e}^{[\alpha+m\beta][a+\sigma]t} \|\mathbf{x}_0\|^{\beta+1}\Big)$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$. Note that (5.14) and the fact that $m \in \{1, \ldots, p-2\}$ imply

$$\kappa a \leq [\alpha + (p-2)\,\beta]\, a \leq [\alpha + m\beta]\, a.$$

It follows that

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(m)}(t, y_{01})\right\| = \mathcal{O}\Big(\mathsf{e}^{[\alpha+m\beta][a+\sigma]t} \|\mathbf{x}_0\|\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

Hence, the result is true for $m+1$ and, by mathematical induction, the result is true for all $m \in \{1, \ldots, p-2\}$. $\square$

5.4 "Flipping the Integral" in the Second Component

5.4.1 Performing the "Flip"

Let $y_{01} := \psi_1(\mathbf{x}_0)$, where we assume $\|\mathbf{x}_0\|$ is sufficiently small. Consider the integral equation (5.11) for which the first integral has been "flipped" but the second integral has not. We will manipulate the expression for the second component of the flow, $\phi_2(t, \mathbf{x}_0)$, so that we can "flip the integral" in some way. Write

$$\begin{aligned}\phi_2(t, \mathbf{x}_0) = \mathsf{e}^{\kappa a t} x_{02} + \mathsf{e}^{\kappa a t} \int_0^t \mathsf{e}^{-\kappa a s} b_2 \left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) \, ds \\ + \mathsf{e}^{\kappa a t} \left[\int_0^t \mathsf{e}^{-\kappa a s} b_2 \left(\boldsymbol{\chi}^{(p-1)} \left(s, y_{01}\right) \right) \, ds - \int_0^t \mathsf{e}^{-\kappa a s} b_2 \left(\boldsymbol{\chi}^{(p-1)} \left(s, y_{01}\right) \right) \, ds \right].\end{aligned}$$

Re-arranging,

$$\begin{aligned}\phi_2(t, \mathbf{x}_0) = \mathsf{e}^{\kappa a t} x_{02} + \mathsf{e}^{\kappa a t} \int_0^t \mathsf{e}^{-\kappa a s} \left[b_2 \left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - b_2 \left(\boldsymbol{\chi}^{(p-1)} \left(s, y_{01}\right) \right) \right] \, ds \\ + \mathsf{e}^{\kappa a t} \int_0^t \mathsf{e}^{-\kappa a s} b_2 \left(\boldsymbol{\chi}^{(p-1)} \left(s, y_{01}\right) \right) \, ds. \qquad (5.18)\end{aligned}$$

We want to "flip the first integral" in (5.18). To do this, we need to check the exponential decay rate of the integrand.

Claim 5.12: *Let $\sigma > 0$ be sufficiently small. There are $\delta, k > 0$ such that*

$$\left| \mathsf{e}^{-\kappa a s} \left[b_2 \left(\boldsymbol{\phi}(s, \boldsymbol{x}_0)\right) - b_2 \left(\boldsymbol{\chi}^{(p-1)} \left(s, y_{01}\right) \right) \right] \right| \leq k \, \mathsf{e}^{[\alpha + (p-1)\beta - \kappa][a+\sigma] s} \left\| \boldsymbol{x}_0 \right\|^{\beta+1} \qquad (5.19)$$

for all $(s, \boldsymbol{x}_0) \in \Omega_\delta$.

Proof: It follows from (5.3), (5.8), (5.16), and (5.17) in conjunction with the Mean Value Theorem. $\square$

We know that by virtue of (5.14), we have exponential decay for the integrand of the first integral in (5.18). Furthermore, we see that (in general) we would not have exponential decay if we replaced $\boldsymbol{\chi}^{(p-1)}(s, y_{01})$ by $\boldsymbol{\chi}^{(p-2)}(s, y_{01})$. That is, we iterated just enough times so that we could perform this "integral flip." Hence, define

$$y_{02} := \psi_2(\mathbf{x}_0) \quad \text{and} \quad \psi_2(\mathbf{x}_0) := x_{02} + \int_0^\infty \mathsf{e}^{-\kappa a s}\left[b_2\left(\boldsymbol{\phi}(s,\mathbf{x}_0)\right) - b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds. \tag{5.20}$$

Claim 5.13: *There are $\delta, k > 0$ such that*

$$\|x_{02} - \psi_2(\boldsymbol{x}_0)\| \leq k\,\|\boldsymbol{x}_0\|^{\beta+1} \quad \textit{for all} \quad \boldsymbol{x}_0 \in B_\delta. \tag{5.21}$$

Proof: It follows from (5.19) and (5.20). □

Using y_{02}, we can thus write (5.18) as

$$\begin{aligned}\phi_2(t,\mathbf{x}_0) = &\left[\mathsf{e}^{\kappa a t} y_{02} + \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) ds\right] \\ &- \int_t^\infty \mathsf{e}^{\kappa a(t-s)}\left[b_2\left(\boldsymbol{\phi}(s,\mathbf{x}_0)\right) - b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds.\end{aligned} \tag{5.22}$$

Note that, using (5.11), the first component of the flow satisfies

$$\begin{aligned}\phi_1(t,\mathbf{x}_0) = &\left[\mathsf{e}^{a t} y_{01} - \int_t^\infty \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) ds\right] \\ &- \int_t^\infty \mathsf{e}^{a(t-s)}\left[b_1\left(\boldsymbol{\phi}(s,\mathbf{x}_0)\right) - b_1\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds.\end{aligned} \tag{5.23}$$

5.4.2 The Function $\boldsymbol{\psi}$

Since we now have $\psi_1(\mathbf{x}_0)$ and $\psi_2(\mathbf{x}_0)$, we can define $\boldsymbol{\psi}(\mathbf{x}_0)$:

$$\boldsymbol{\psi}(\mathbf{x}_0) := \begin{pmatrix}\psi_1(\mathbf{x}_0)\\ \psi_2(\mathbf{x}_0)\end{pmatrix} = \begin{pmatrix} x_{01} + \int_0^\infty \mathsf{e}^{-as} b_1\left(\boldsymbol{\phi}(s,\mathbf{x}_0)\right) ds \\ x_{02} + \int_0^\infty \mathsf{e}^{-\kappa a s}\left[b_2\left(\boldsymbol{\phi}(s,\mathbf{x}_0)\right) - b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, \psi_1(\mathbf{x}_0)\right)\right)\right] ds\end{pmatrix}. \tag{5.24}$$

Note that the definition of $\psi_2(\mathbf{x}_0)$ depends on $\psi_1(\mathbf{x}_0)$.

Claim 5.14: *There are $\delta, k > 0$ such that*

$$\|\boldsymbol{x}_0 - \boldsymbol{\psi}(\boldsymbol{x}_0)\| \leq k\,\|\boldsymbol{x}_0\|^{\mathsf{min}\{\alpha,\beta+1\}} \quad \textit{for all} \quad \boldsymbol{x}_0 \in B_\delta.$$

Furthermore, $\boldsymbol{\psi}$ is a near-identity transformation.

Proof: The estimate follows from (5.13) and (5.21). Since $\alpha > 1$ and $\beta > 0$ it follows from the estimate that $\boldsymbol{\psi}$ is near-identity. □

5.5 Second Group of Iterates

We are now in a position to define the remainder of the iterates, $\left\{\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\}_{m=p}^{\infty}$. Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, where $\boldsymbol{\psi}$ is defined in (5.24) and $\|\mathbf{x}_0\|$ is sufficiently small.

5.5.1 Definition of the Iterates

With inspiration from (5.22) and (5.23), we will define the p^{th} iterate by

$$\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0) := \begin{pmatrix} \mathsf{e}^{at} y_{01} - \int_t^\infty \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right) ds \\ \mathsf{e}^{\kappa a t} y_{02} + \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right) ds \end{pmatrix} \tag{5.25a}$$

and define the subsequent iterates recursively by

$$\boldsymbol{\chi}^{(m+1)}(t, \mathbf{y}_0) := \boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0) - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}} \left[\mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right)\right] ds, \quad m \geq p. \tag{5.25b}$$

Observe that we can combine (5.22), (5.23), and (5.25a) to write an integral equation for $\boldsymbol{\phi}(t, \mathbf{x}_0)$ in terms of $\boldsymbol{\chi}^{(p-1)}(t, y_{01})$ and $\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0)$.

Claim 5.15: *There is a $\delta > 0$ such that*

$$\boldsymbol{\phi}(t, \boldsymbol{x}_0) = \boldsymbol{\chi}^{(p)}(t, \boldsymbol{y}_0) - \int_t^\infty \mathsf{e}^{(t-s)\boldsymbol{A}} \left[\boldsymbol{b}(\boldsymbol{\phi}(s, \boldsymbol{x}_0)) - \boldsymbol{b}\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right)\right] ds \tag{5.26}$$

for all $(t, \boldsymbol{x}_0) \in \Omega_\delta$.

Remark 5.16: We have been using the notation $\left\{\boldsymbol{\chi}^{(m)}(t, y_{01})\right\}_{m=1}^{p-1}$ for the first group of iterates. However, if we need to refer to all the iterates at once we will use, for simplicity, the notation $\left\{\boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\}_{m=1}^{\infty}$. The reader should remain mindful of the fact that y_{02} is defined in terms of y_{01} and $\boldsymbol{\chi}^{(p-1)}(t, y_{01})$.

5.5.2 Existence and Decay Rate of the Iterates

Proposition 5.17: *Consider the second group of iterates defined by* (5.25). *Then, there is a $\delta > 0$ (independent of m) such that if $\|\boldsymbol{x}_0\| < \delta$ then $\boldsymbol{\chi}^{(m)}(t, \boldsymbol{y}_0)$ exists for each $m \geq p$. Moreover, there is a $k > 0$ (independent of m) such that*

$$\left\|\boldsymbol{\chi}^{(m)}(t, \boldsymbol{y}_0)\right\| \leq k\, \mathsf{e}^{at} \|\boldsymbol{x}_0\| \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \geq p.$$

Proof: For brevity, we will omit the careful construction of the constants $\delta > 0$ and $k > 0$. See the proof of Proposition 4.8 for how one could be more careful. The proof will be by strong induction on m.

Consider the base case $m = p$. Instead of using the definition (5.25a) of $\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0)$, we will calculate the decay rate of $\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0)$ using (5.26). Now, it follows from (5.3), (5.7), (5.8), (5.16), and (5.17) along with the Mean Value Theorem that, for any $\sigma > 0$,

$$\left\| \int_t^{\infty} \mathsf{e}^{(t-s)\mathbf{A}} \left[\mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right) \right] ds \right\| = \mathcal{O}\left(\mathsf{e}^{[\alpha+(p-1)\beta][a+\sigma]t} \left\|\mathbf{x}_0\right\|^{\beta+1}\right) \tag{5.27}$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$. Since $\sigma > 0$ is arbitrary, $p > 1$, $\alpha > 1$, and $\beta > 0$, using (5.8) and (5.26) we see $\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0)$ exists with

$$\left\|\boldsymbol{\chi}^{(p)}(t, \mathbf{y}_0)\right\| = \mathcal{O}\left(\mathsf{e}^{at} \left\|\mathbf{x}_0\right\|\right) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0$$

as required.

Suppose that the result is true for each $\ell \in \{p, \ldots, m\}$ where $m > p$ is fixed. Now, taking the difference of (5.25b) and (5.26), we see that

$$\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(\ell)}(t, \mathbf{y}_0) = -\int_t^{\infty} \mathsf{e}^{(t-s)\mathbf{A}} \left[\mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(\ell-1)}(s, \mathbf{y}_0)\right) \right] ds$$

for any $\ell \in \{p+1, \ldots, m\}$. It follows from (5.3), (5.7), (5.8), the Mean Value Theorem, and the induction hypothesis that

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(\ell)}(t, \mathbf{y}_0)\right\| = \mathcal{O}\left(\mathsf{e}^{\kappa a t} \left[\int_t^{\infty} \mathsf{e}^{(\beta-\kappa)as} \left\|\boldsymbol{\phi}(s, \mathbf{x}_0) - \boldsymbol{\chi}^{(\ell-1)}(s, \mathbf{y}_0)\right\| ds \right] \left\|\mathbf{x}_0\right\|^{\beta}\right)$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$. It follows from a simple inductive argument, using (5.26) and (5.27) along the way, that

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(m)}(t, \mathbf{y}_0)\right\| = \mathcal{O}\left(\mathsf{e}^{[\alpha+(m-1)\beta][a+\sigma]t} \left\|\mathbf{x}_0\right\|^{(m+1-p)\beta+1}\right)$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$.

By the Triangle Inequality,

$$\begin{aligned}
&\left\|\mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right)\right\| \\
&\leq \left\|\mathbf{b}\left(\boldsymbol{\chi}^{(m)}(s, \mathbf{y}_0)\right) - \mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right)\right\| + \left\|\mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}(s, y_{01})\right)\right\|.
\end{aligned}$$

Appealing to (5.3), (5.8), (5.16), the Mean Value Theorem, and the Induction Hypothesis,

$$\left\| \mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(s, \mathbf{y}_0\right)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) \right\| = \mathcal{O}\left(\mathrm{e}^{[\alpha+(p-1)\beta][a+\sigma]s} \left\|\mathbf{x}_0\right\|^{\beta+1}\right)$$

as $s \to \infty$ and $\|\mathbf{x}_0\| \to 0$. Using this fact in the definition (5.25b) tells us $\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right)$ exists with

$$\left\| \boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right) - \boldsymbol{\chi}^{(p)}\left(t, \mathbf{y}_0\right) \right\| = \mathcal{O}\left(\mathrm{e}^{[\alpha+(p-1)\beta][a+\sigma]t} \left\|\mathbf{x}_0\right\|^{\beta+1}\right)$$

and hence

$$\left\| \boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right) \right\| = \mathcal{O}\left(\mathrm{e}^{at} \left\|\mathbf{x}_0\right\|\right)$$

as $t \to \infty$ and $\|\mathbf{x}_0\| \to 0$. Therefore, the proposition is true for $m+1$. By induction, the proposition is true for all $m \geq p$. □

5.5.3 Closeness of the Iterates to the Actual Solution

Theorem 5.18: *Consider the iterates defined by* (5.15) *and let* $\sigma > 0$ *be sufficiently small. There are constants* $\delta > 0$ *and* $\{k_m\}_{m=p}^{\infty} \subset \mathbb{R}_+$ *such that*

$$\left\| \boldsymbol{\phi}(t, \boldsymbol{x}_0) - \boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{y}_0\right) \right\| \leq k_m \mathrm{e}^{[\alpha+(m-1)\beta][a+\sigma]t} \left\|\boldsymbol{x}_0\right\|^{(m+1-p)\beta+1} \quad \textit{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta,\ m \geq p.$$

Proof: Out of necessity, the theorem and Proposition 5.17 were proved concurrently. □

5.5.4 A Simple Example

Consider the system

$$\dot{\mathbf{x}} = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 0 \\ x_1^2 + x_1^3 \end{pmatrix}.$$

Take

$$a = -1, \quad \kappa = 2, \quad \alpha = 2, \quad \beta = 1, \quad \text{and} \quad p = 2.$$

Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$. We will calculate the first two iterates. The reader may wish to compare with the example in §4.7.2 which begins on page 94.

Since $p = 2$, we only have to find one iterate from the first group. Using (5.15a), the first iterate is given by

$$\boldsymbol{\chi}^{(1)}\left(t, y_{01}\right) = \begin{pmatrix} \mathrm{e}^{-t} y_{01} \\ 0 \end{pmatrix}.$$

Using (5.25a), the second iterate (which is the first iterate of the second group) is given by

$$\boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0) = \begin{pmatrix} \mathsf{e}^{-t} y_{01} \\ \mathsf{e}^{-2t}\left[y_{01}^3 + y_{02} + y_{01}^2 t\right] - \mathsf{e}^{-3t} y_{01}^3 \end{pmatrix}.$$

5.5.5 Another Simple Example

Consider the system

$$\dot{\mathbf{x}} = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 0 \\ x_1^2 \end{pmatrix}.$$

Take

$$a = -1, \quad \kappa = 3, \quad \alpha = 2, \quad \beta = 1, \quad \text{and} \quad p = 3.$$

Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$. We will calculate the first three iterates.

Using (5.15), the first two iterates are given by

$$\boldsymbol{\chi}^{(1)}(t, y_{01}) = \begin{pmatrix} \mathsf{e}^{-t} y_{01} \\ 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}(t, y_{01}) = \begin{pmatrix} \mathsf{e}^{-t} y_{01} \\ \mathsf{e}^{-2t} y_{01}^2 - \mathsf{e}^{-3t} y_{01}^2 \end{pmatrix}.$$

Using (5.25a), the third iterate is

$$\boldsymbol{\chi}^{(3)}(t, \mathbf{y}_0) = \begin{pmatrix} \mathsf{e}^{-t} y_{01} \\ \mathsf{e}^{-2t} y_{01}^2 + \mathsf{e}^{-3t}\left[y_{02} - y_{01}^2\right] \end{pmatrix}.$$

5.6 Important Special Case

The special case which we explore in this section is applicable to the Michaelis-Menten mechanism which we will explore in Part II of this thesis. Assume that $\kappa \in \{2, 3, \ldots\}$. Define

$$\mathbf{b}(\mathbf{x}) := \begin{pmatrix} b_{111} x_1^2 + b_{112} x_1 x_2 + b_{122} x_2^2 \\ b_{211} x_1^2 + b_{212} x_1 x_2 + b_{222} x_2^2 \end{pmatrix},$$

where $\{b_{ijk}\}_{i,j,k=1}^{2} \subset \mathbb{R}$ are constants with at least one b_{ijk} being non-zero. Take

$$\alpha = 2, \quad \beta = 1, \quad \text{and} \quad p = \kappa.$$

Observe that there is resonance in the eigenvalues. Hence, consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0. \tag{5.28}$$

Let $\mathbf{y}_0 := \boldsymbol{\psi}(\mathbf{x}_0)$, where $\|\mathbf{x}_0\|$ is assumed to be sufficiently small with $y_{01} > 0$.[2] Furthermore, let $\mathbf{x}(t)$ be the solution to (5.28). Our goal is to obtain an asymptotic expression for x_2 in terms of x_1 as $x_1 \to 0^+$ up to an order for which the initial condition distinguishes solutions.

5.6.1 Case 1: $\kappa = 2$

We will only need to calculate the first two iterates $\boldsymbol{\chi}^{(1)}(t, y_{01})$ and $\boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0)$. Using (5.15a) and (5.25a), the first two iterates are given by

$$\boldsymbol{\chi}^{(1)}(t, y_{01}) = \begin{pmatrix} y_{01}\mathsf{e}^{at} \\ 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}(t, \mathbf{y}_0) = \begin{pmatrix} y_{01}\mathsf{e}^{at} + \left[\dfrac{b_{111}y_{01}^2}{a}\right]\mathsf{e}^{2at} \\ y_{02}\mathsf{e}^{2at} + \left[b_{211}y_{01}^2\right] t\,\mathsf{e}^{2at} \end{pmatrix}.$$

Claim 5.19: *The components $x_1(t)$ and $x_2(t)$ of the solution to (5.28) satisfy*

$$x_1(t) = (y_{01})\,\mathsf{e}^{at} + \left(\frac{b_{111}y_{01}^2}{a}\right)\mathsf{e}^{2at} + \mathsf{o}\big(\mathsf{e}^{2at}\big) \quad \text{as} \quad t \to \infty \tag{5.29a}$$

and

$$x_2(t) = \big(b_{211}y_{01}^2\big)\,t\,\mathsf{e}^{2at} + (y_{02})\,\mathsf{e}^{2at} + \mathsf{o}\big(\mathsf{e}^{2at}\big) \quad \text{as} \quad t \to \infty. \tag{5.29b}$$

Proof: It follows from Theorem 5.18 and our expression for the second iterate. □

Claim 5.20: *We can write e^{at} in terms of x_1 as*

$$\mathsf{e}^{at} = \left(\frac{1}{y_{01}}\right)x_1 - \left(\frac{b_{111}}{a y_{01}}\right)x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+ \tag{5.30a}$$

and e^{2at} in terms of x_1 as

$$\mathsf{e}^{2at} = \left(\frac{1}{y_{01}^2}\right)x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+. \tag{5.30b}$$

Proof: Equation (5.30b) follows from squaring both sides of (5.30a). To obtain (5.30a), first use (5.29a) to write

$$x_1 = (y_{01})\,\mathsf{e}^{at}\left[1 + \left(\frac{b_{111}y_{01}}{a}\right)\mathsf{e}^{at} + \mathsf{o}\big(\mathsf{e}^{at}\big)\right] \quad \text{as} \quad t \to \infty$$

from which it follows

$$\mathsf{e}^{at} = \left(\frac{x_1}{y_{01}}\right)\left[1 + \left(\frac{b_{111}y_{01}}{a}\right)\mathsf{e}^{at} + \mathsf{o}\big(\mathsf{e}^{at}\big)\right]^{-1} = \left(\frac{x_1}{y_{01}}\right)\left[1 - \left(\frac{b_{111}y_{01}}{a}\right)\mathsf{e}^{at} + \mathsf{o}\big(\mathsf{e}^{at}\big)\right] \quad \text{as} \quad t \to \infty.$$

[2] We make the assumption $y_{01} > 0$ since it corresponds to solutions with $x_1 > 0$ approaching the equilibrium point in the slow direction. This is desirable since it corresponds to, for example, solutions that arise in chemical kinetics.

Observe that

$$x_1 = \mathcal{O}\big(\mathsf{e}^{at}\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \mathsf{e}^{at} = \mathcal{O}(x_1) \quad \text{as} \quad x_1 \to 0^+.$$

Back substituting e^{at},

$$\begin{aligned}
\mathsf{e}^{at} &= \left(\frac{1}{y_{01}}\right) x_1 \left\{1 - \left[\frac{b_{111} y_{01}}{a}\right] \left[\left(\frac{1}{y_{01}}\right) x_1 + \mathsf{o}\big(\mathsf{e}^{at}\big)\right] + \mathsf{o}\big(\mathsf{e}^{at}\big)\right\} \quad \text{as} \quad t \to \infty \\
&= \left(\frac{1}{y_{01}}\right) x_1 \left[1 - \left(\frac{b_{111}}{a}\right) x_1 + \mathsf{o}\big(\mathsf{e}^{at}\big)\right] \quad \text{as} \quad t \to \infty \\
&= \left(\frac{1}{y_{01}}\right) x_1 - \left(\frac{b_{111}}{a y_{01}}\right) x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+.
\end{aligned}$$

This is what we needed to show. □

Claim 5.21: *We can write t in terms of x_1 as*

$$t = \left(\frac{1}{a}\right) \mathit{ln}(x_1) - \frac{\mathit{ln}(y_{01})}{a} + \mathit{o}(1) \quad \textit{as} \quad x_1 \to 0^+. \tag{5.31}$$

Proof: Write (5.30a) as

$$\mathsf{e}^{at} = \left[\frac{1}{y_{01}}\right] [x_1] \left[1 + \mathsf{o}(1)\right] \quad \text{as} \quad x_1 \to 0^+.$$

Taking the natural logarithm of both sides,

$$at = -\mathsf{ln}(y_{01}) + \mathsf{ln}(x_1) + \mathsf{ln}(1 + \mathsf{o}(1)) \quad \text{as} \quad x_1 \to 0^+.$$

If we make the observation $\mathsf{ln}(1+u) = \mathsf{o}(1)$ as $u \to 0$, we are left with what we were trying to show. □

Proposition 5.22: *Consider the initial value problem (5.28), where $\kappa = 2$, $\|\boldsymbol{x}_0\|$ is sufficiently small, $\boldsymbol{y}_0 = \boldsymbol{\psi}(\boldsymbol{x}_0)$, and $\psi_1(\boldsymbol{x}_0) > 0$. If $\boldsymbol{x}(t)$ is the solution, then we can write x_2 in terms of x_1 as*

$$x_2 = \left[\frac{b_{211}}{a}\right] x_1^2\, \mathit{ln}(x_1) + \left[\frac{y_{02}}{y_{01}^2} - \frac{b_{211}\, \mathit{ln}(y_{01})}{a}\right] x_1^2 + \mathit{o}\big(x_1^2\big) \quad \textit{as} \quad x_1 \to 0^+.$$

Proof: Substitute (5.30b) and (5.31) into (5.29b) and simplify. □

5.6.2 Case 2: $\kappa > 2$

First, we will find the first two iterates. Using (5.15),

$$\boldsymbol{\chi}^{(1)}(t, y_{01}) = \begin{pmatrix} y_{01}\mathrm{e}^{at} \\ 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(2)}(t, y_{01}) = \begin{pmatrix} y_{01}\mathrm{e}^{at} + \left[\dfrac{b_{111}y_{01}^2}{a}\right]\mathrm{e}^{2at} \\ \left[\dfrac{b_{211}y_{01}^2}{(2-\kappa)\,a}\right]\mathrm{e}^{2at} - \left[\dfrac{b_{211}y_{01}^2}{(2-\kappa)\,a}\right]\mathrm{e}^{\kappa at} \end{pmatrix}.$$

By Theorem 5.11,

$$x_1(t) = y_{01}\mathrm{e}^{at} + \left(\frac{b_{111}y_{01}^2}{a}\right)\mathrm{e}^{2at} + \mathcal{O}\big(\mathrm{e}^{3at}\big) \quad \text{and} \quad x_2(t) = \left[\frac{b_{211}y_{01}^2}{(2-\kappa)\,a}\right]\mathrm{e}^{2at} + \mathcal{O}\big(\mathrm{e}^{3at}\big)$$

as $t \to \infty$. By inspection,

$$x_2 = \left[\frac{b_{211}}{(2-\kappa)\,a}\right]x_1^2 + \mathcal{O}\big(x_1^3\big) \quad \text{as} \quad x_1 \to 0^+.$$

We will take this further. First, we need the following result.

Claim 5.23: *There exist constants $\{\xi_i\}_{i=1}^{\kappa}$ and $\{\rho_i\}_{i=1}^{\kappa-1}$ which do not depend on the initial condition and a constant ϱ which may depend on the initial condition such that*

$$x_1(t) = \sum_{i=1}^{\kappa} \xi_i \left(\mathrm{e}^{at}y_{01}\right)^i + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty \tag{5.32}$$

and

$$x_2(t) = \sum_{i=1}^{\kappa-1} \rho_i \left(\mathrm{e}^{at}y_{01}\right)^i + \varrho\left(\mathrm{e}^{\kappa at}\right) + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty. \tag{5.33}$$

Moreover,

$$\xi_1 = 1, \quad \rho_1 = 0, \quad \text{and} \quad \rho_2 = \frac{b_{211}}{(2-\kappa)\,a}.$$

Proof: It follows from Theorems 5.11 and 5.18, the definition (5.15) of the first $\kappa - 1$ iterates, and the definition (5.25a) of the κ^{th} iterate. □

Proposition 5.24: *Consider the initial value problem (5.28), where $\kappa \in \{3, 4, \ldots\}$, $\|\boldsymbol{x}_0\|$ is sufficiently small, $\boldsymbol{y}_0 = \boldsymbol{\psi}(\boldsymbol{x}_0)$, and $\psi_1(\boldsymbol{x}_0) > 0$. If $\boldsymbol{x}(t)$ is the solution, then we can write x_2 in terms of x_1 as*

$$x_2 = c_2 x_1^2 + \cdots + c_{\kappa-1}x_1^{\kappa-1} + C\,x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+$$

for some constants $\{c_i\}_{i=2}^{\kappa-1}$ (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_2 = \frac{b_{211}}{(2-\kappa)\,a}.$$

Proof: Note that

$$x_1 = \mathcal{O}\big(\mathsf{e}^{at}\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \mathsf{e}^{at} = \mathcal{O}(x_1) \quad \text{as} \quad x_1 \to 0^+,$$

which follows from (5.32). Now, by inverting (5.32) in a process we have done many times before, it follows that there are constants $\{\nu_i\}_{i=1}^{\kappa}$ which do not depend on the initial condition such that

$$\mathsf{e}^{at} y_{01} = \sum_{i=1}^{\kappa} \nu_i x_1^i + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+. \tag{5.34}$$

Substituting (5.34) in (5.33), there must be constants $\{c_i\}_{i=1}^{\kappa-1}$ (which do not depend on the initial condition) and C (which may depend on the initial condition) such that

$$x_2 = \sum_{i=1}^{\kappa-1} c_i x_1^i + C\, x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+.$$

Note that

$$\nu_1 = 1, \quad c_1 = 0, \quad \text{and} \quad c_2 = \frac{b_{211}}{(2-\kappa)\,a}.$$

□

5.6.3 A Simple Example

Consider the initial value problem

$$\dot{\mathbf{x}} = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 0 \\ x_1^2 \end{pmatrix}, \quad \mathbf{x}(0) = \mathbf{x}_0.$$

This can be solved exactly and the solution is given by

$$\mathbf{x}(t) = \begin{pmatrix} x_{01}\mathsf{e}^{-t} \\ \big[x_{02} + x_{01}^2 t\big]\,\mathsf{e}^{-2t} \end{pmatrix}.$$

Since $\mathsf{e}^{-t} = \dfrac{x_1}{x_{01}}$ and $t = \ln(x_{01}) - \ln(x_1)$, we see that

$$x_2 = -x_1^2 \ln(x_1) + \left[\frac{x_{02}}{x_{01}^2} + \ln(x_{01})\right] x_1^2.$$

This is consistent with Proposition 5.22. Note that, here, $\boldsymbol{\psi}(\mathbf{x}_0) = \mathbf{x}_0$.

5.6.4 Another Simple Example

Consider now the initial value problem

$$\dot{\mathbf{x}} = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix} \mathbf{x} + \begin{pmatrix} 0 \\ x_1^2 \end{pmatrix}, \quad \mathbf{x}(0) = \mathbf{x}_0.$$

This can also be solved exactly:

$$\mathbf{x}(t) = \begin{pmatrix} x_{01}\mathsf{e}^{-t} \\ x_{01}^2\mathsf{e}^{-2t} + \left[x_{02} - x_{01}^2\right]\mathsf{e}^{-3t} \end{pmatrix}.$$

Since $\mathsf{e}^{-t} = \dfrac{x_1}{x_{01}}$, we see that

$$x_2 = x_1^2 + \left(\frac{x_{02} - x_{01}^2}{x_{01}^3}\right) x_1^3.$$

This is consistent with Proposition 5.24.

5.7 What if A is Diagonalizable but not Diagonal?

5.7.1 Introduction

Consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{5.35}$$

where the matrix $\mathbf{A}$ and vector field $\mathbf{b}$ are as before except that $\mathbf{A}$ is only assumed to be diagonalizable with eigenvalues a and κa. Since $\mathbf{A}$ is diagonalizable, there exists an invertible matrix $\mathbf{P}$ such that

$$\overline{\mathbf{A}} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P},$$

where $\overline{\mathbf{A}} := \mathsf{diag}\,(a, \kappa a)$. Define

$$\overline{\mathbf{b}}(\mathbf{y}) := \mathbf{P}^{-1}\mathbf{b}\left(\mathbf{P}\mathbf{y}\right) \quad \text{and} \quad \mathbf{y}_0 := \mathbf{P}^{-1}\mathbf{x}_0.$$

Claim 5.25: *If $\boldsymbol{x}(t)$ is a solution of (5.35) then $\boldsymbol{y}(t) := \boldsymbol{P}^{-1}\boldsymbol{x}(t)$ is a solution of*

$$\dot{\boldsymbol{y}} = \overline{\boldsymbol{A}}\boldsymbol{y} + \overline{\boldsymbol{b}}\left(\boldsymbol{y}\right), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0. \tag{5.36}$$

Proof: Clearly, $\mathbf{y}(0) = \mathbf{y}_0$. To establish the differential equation, calculate

$$\dot{\mathbf{y}} = \mathbf{P}^{-1}\dot{\mathbf{x}} = \mathbf{P}^{-1}\left[\mathbf{A}\mathbf{x} + \mathbf{b}\left(\mathbf{x}\right)\right] = \mathbf{P}^{-1}\left[\mathbf{A}\mathbf{P}\mathbf{y} + \mathbf{b}\left(\mathbf{P}\mathbf{y}\right)\right] = \overline{\mathbf{A}}\mathbf{y} + \mathbf{P}^{-1}\mathbf{b}\left(\mathbf{P}\mathbf{y}\right).$$

□

Claim 5.26: *Consider the vector field $\overline{\boldsymbol{b}}$.*

(a) There are $\delta, k > 0$ such that $\left\|\overline{\boldsymbol{b}}\left(\boldsymbol{y}\right)\right\| \leq k\left\|\boldsymbol{y}\right\|^{\alpha}$ for all $\boldsymbol{y} \in B_{\delta}$.

(b) There are $\delta, k > 0$ such that $\left\|\boldsymbol{D}\overline{\boldsymbol{b}}\left(\boldsymbol{y}\right)\right\| \leq k\left\|\boldsymbol{y}\right\|^{\beta}$ for all $\boldsymbol{y} \in B_{\delta}$.

Proof:

(a) We know from (5.2) that there are $\delta_1, k_1 > 0$ such that if $\|\mathbf{x}\| < \delta_1$ then $\|\mathbf{b}\left(\mathbf{x}\right)\| \leq k_1\|\mathbf{x}\|^{\alpha}$. Take $\delta := \frac{\delta_1}{\|\mathbf{P}\|}$ and $k := k_1\left\|\mathbf{P}^{-1}\right\|\|\mathbf{P}\|^{\alpha}$. If $\|\mathbf{y}\| < \delta$ then $\|\mathbf{P}\mathbf{y}\| \leq \|\mathbf{P}\|\|\mathbf{y}\| < \delta_1$. Hence,

$$\|\mathbf{y}\| < \delta \implies \left\|\overline{\mathbf{b}}\left(\mathbf{y}\right)\right\| \leq \left\|\mathbf{P}^{-1}\right\|\|\mathbf{b}\left(\mathbf{P}\mathbf{y}\right)\| \leq k_1\left\|\mathbf{P}^{-1}\right\|\|\mathbf{P}\mathbf{y}\|^{\alpha} \leq k_1\left\|\mathbf{P}^{-1}\right\|\|\mathbf{P}\|^{\alpha}\|\mathbf{y}\|^{\alpha} = k\|\mathbf{y}\|^{\alpha}.$$

(b) First, note that $\mathbf{D}\overline{\mathbf{b}}\left(\mathbf{y}\right) = \mathbf{P}^{-1}\left[\mathbf{D}\mathbf{b}\left(\mathbf{P}\mathbf{y}\right)\right]\mathbf{P}$. We know from (5.3) that there are $\delta_1, k_1 > 0$ such that if $\|\mathbf{x}\| < \delta_1$ then $\|\mathbf{D}\mathbf{b}\left(\mathbf{x}\right)\| \leq k_1\|\mathbf{x}\|^{\beta}$. Taking $\delta := \frac{\delta_1}{\|\mathbf{P}\|}$ and $k := k_1\left\|\mathbf{P}^{-1}\right\|\|\mathbf{P}\|^{\beta+1}$, we see that if $\|\mathbf{y}\| < \delta$ then $\left\|\mathbf{D}\overline{\mathbf{b}}\left(\mathbf{y}\right)\right\| \leq k\|\mathbf{y}\|^{\beta}$.

□

5.7.2 Associated Iterates

The iterates $\left\{\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\mathbf{y}_0\right)\right)\right\}_{m=1}^{\infty}$ defined with respect to $\overline{\mathbf{A}}$ and $\overline{\mathbf{b}}$ allow us to construct associated iterates for the original system. In particular, the associated iterates are $\left\{\mathbf{P}\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\mathbf{P}^{-1}\mathbf{x}_0\right)\right)\right\}_{m=1}^{\infty}$.

Theorem 5.27: *Let $\boldsymbol{x}(t)$ be the solution of the initial value problem* (5.35). *Consider the iterates $\left\{\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\boldsymbol{y}_0\right)\right)\right\}_{m=1}^{\infty}$ defined with respect to $\overline{\boldsymbol{A}}$ and $\overline{\boldsymbol{b}}$. For any sufficiently small $\sigma > 0$ there are constants $\delta > 0$ and $\{k_m\}_{m=1}^{\infty} \subset \mathbb{R}_+$ such that*

$$\left\|\boldsymbol{x}(t) - \boldsymbol{P}\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\boldsymbol{P}^{-1}\boldsymbol{x}_0\right)\right)\right\| \leq k_m \mathrm{e}^{[\alpha+(m-1)\beta][a+\sigma]t}\left\|\boldsymbol{x}_0\right\|$$

$$\text{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_{\delta},\ m \in \{1, \ldots, p-1\}$$

and

$$\left\| \boldsymbol{x}(t) - \boldsymbol{P}\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\boldsymbol{P}^{-1}\boldsymbol{x}_0\right)\right) \right\| \leq k_m \mathsf{e}^{[\alpha+(m-1)\beta][a+\sigma]t} \left\|\boldsymbol{x}_0\right\|^{(m+1-p)\beta+1}$$
$$\text{for all} \quad (t, \boldsymbol{x}_0) \in \Omega_\delta, \; m \geq p.$$

Proof: Let $\delta > 0$ be sufficiently small so that if $\|\mathbf{x}_0\| < \delta$ then the appropriate estimates apply. Hence, assume $\mathbf{x}_0 \in B_\delta$. Let $\mathbf{y}(t) := \mathbf{P}^{-1}\mathbf{x}(t)$, which is the solution to (5.36). Observe that

$$\|\mathbf{y}_0\| \leq \left\|\mathbf{P}^{-1}\right\| \|\mathbf{x}_0\| \quad \text{and} \quad \left\|\mathbf{x}(t) - \mathbf{P}\boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\mathbf{y}_0\right)\right)\right\| \leq \|\mathbf{P}\| \left\|\mathbf{y}(t) - \boldsymbol{\chi}^{(m)}\left(t, \boldsymbol{\psi}\left(\mathbf{y}_0\right)\right)\right\|.$$

Applying Theorems 5.11 and 5.18 give the conclusion. $\square$

5.7.3 A Simple Example

Take

$$\mathbf{A} := \begin{pmatrix} 1 & -2 \\ 4 & -5 \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}) := \begin{pmatrix} 4x_1^2 - 4x_1x_2 + x_2^2 \\ 8x_1^2 - 8x_1x_2 + 2x_2^2 \end{pmatrix}, \quad \text{and} \quad \mathbf{P} := \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}.$$

Then,

$$\mathbf{P}^{-1} = \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}, \quad \overline{\mathbf{A}} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix}, \quad \text{and} \quad \overline{\mathbf{b}}(\mathbf{y}) = \mathbf{P}^{-1}\mathbf{b}(\mathbf{P}\mathbf{y}) = \begin{pmatrix} 0 \\ y_1^2 \end{pmatrix}.$$

Hence, we will consider the associated system

$$\dot{\mathbf{y}} = \begin{pmatrix} -1 & 0 \\ 0 & -3 \end{pmatrix} \mathbf{y} + \begin{pmatrix} 0 \\ y_1^2 \end{pmatrix},$$

which just happens to be the system[3] we explored in §5.5.5 on page 114.

The third iterate for the system in §5.5.5 was

$$\boldsymbol{\chi}^{(3)}(t, \mathbf{z}_0) = \begin{pmatrix} \mathsf{e}^{-t} z_{01} \\ \mathsf{e}^{-2t} z_{01}^2 + \mathsf{e}^{-3t}\left[z_{02} - z_{01}^2\right] \end{pmatrix},$$

where $\mathbf{z}_0 := \boldsymbol{\psi}(\mathbf{y}_0)$. So, the associated third iterate for the original system is

$$\mathbf{P}\boldsymbol{\chi}^{(3)}(t, \mathbf{z}_0) = \begin{pmatrix} \mathsf{e}^{-t} z_{01} + \mathsf{e}^{-2t} z_{01}^2 + \mathsf{e}^{-3t}\left[z_{02} - z_{01}^2\right] \\ \mathsf{e}^{-t} z_{01} + 2\,\mathsf{e}^{-2t} z_{01}^2 + 2\,\mathsf{e}^{-3t}\left[z_{02} - z_{01}^2\right] \end{pmatrix}.$$

[3]Since $\overline{\mathbf{b}}(\mathbf{y}) = \mathbf{P}^{-1}\mathbf{b}(\mathbf{P}\mathbf{y})$ and $\mathbf{y} = \mathbf{P}^{-1}\mathbf{x}$, we have $\mathbf{b}(\mathbf{x}) = \mathbf{P}\overline{\mathbf{b}}\left(\mathbf{P}^{-1}\mathbf{x}\right)$. This enables us to choose $\mathbf{b}(\mathbf{x})$ so that it gives us a desired $\overline{\mathbf{b}}(\mathbf{y})$.

By Theorem 5.27,

$$\left\|\mathbf{x}(t) - \mathbf{P}\boldsymbol{\chi}^{(3)}\left(t, \mathbf{z}_0\right)\right\| = \mathcal{O}\Big(\mathrm{e}^{-4t}\left\|\mathbf{x}_0\right\|^2\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

5.7.4 Writing x_2 as a Function of x_1

Consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}\left(\mathbf{x}\right), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{5.37}$$

where the matrix $\mathbf{A}$ is diagonalizable (but otherwise the same as before) and

$$\mathbf{b}(\mathbf{x}) := \begin{pmatrix} b_{111}x_1^2 + b_{112}x_1x_2 + b_{122}x_2^2 \\ b_{211}x_1^2 + b_{212}x_1x_2 + b_{222}x_2^2 \end{pmatrix},$$

where $\{b_{ijk}\}_{i,j,k=1}^2 \subset \mathbb{R}$ are constants with at least one b_{ijk} being non-zero. We want to be able to write x_2 as a function of x_1 when $\mathbf{x}(t)$ approaches the origin in the slow direction and there is resonance in the eigenvalues, that is, when $\kappa \in \{2, 3, \ldots\}$. Note that the case when there is no resonance in the eigenvalues was covered in Theorem 2.16 on page 28.

Since $\mathbf{x}(t)$ approaches the origin in the slow direction from the right, we can take the slow eigenvector of $\mathbf{A}$ to have positive first component. Since we can take the first column of $\mathbf{P}$ to be the slow eigenvector, it follows we can choose the invertible matrix $\mathbf{P}$ so that it satisfies $p_{11} > 0$. Note that the slope of the slow eigenvector is $\frac{p_{21}}{p_{11}}$ and so we expect $x_2 = \frac{p_{21}}{p_{11}}x_1 + \mathsf{o}(x_1)$ as $x_1 \to 0^+$.

Recall that $\overline{\mathbf{A}} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$, where $\overline{\mathbf{A}} = \mathsf{diag}\left(a, \kappa a\right)$, $\overline{\mathbf{b}}(\mathbf{y}) = \mathbf{P}^{-1}\mathbf{b}(\mathbf{P}\mathbf{y})$, and $\mathbf{y}_0 = \mathbf{P}^{-1}\mathbf{x}_0$. Observe

$$\overline{\mathbf{b}}(\mathbf{y}) = \begin{pmatrix} \overline{b}_{111}y_1^2 + \overline{b}_{112}y_1y_2 + \overline{b}_{122}y_2^2 \\ \overline{b}_{211}y_1^2 + \overline{b}_{212}y_1y_2 + \overline{b}_{222}y_2^2 \end{pmatrix}$$

for some constants $\left\{\overline{b}_{ijk}\right\}_{i,j,k=1}^2$. As we saw before, $\mathbf{y}(t) := \mathbf{P}^{-1}\mathbf{x}(t)$ is the solution of

$$\dot{\mathbf{y}} = \overline{\mathbf{A}}\mathbf{y} + \overline{\mathbf{b}}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0. \tag{5.38}$$

Since the solution $\mathbf{x}(t)$ approaches the origin in the slow direction and is strictly positive for sufficiently large t, we know that $z_{01} > 0$, where $\mathbf{z}_0 := \boldsymbol{\psi}(\mathbf{y}_0)$ with $\boldsymbol{\psi}$ being defined with respect to the diagonalized system (5.38). Observe that we are now in the scenario we considered in §5.6.

Theorem 5.28: *Consider the initial value problem* (5.37)*. Suppose* $\|\boldsymbol{x}_0\|$ *is sufficiently small and* $\kappa \in \{2, 3, \ldots\}$*. Let* $\boldsymbol{x}(t)$ *be a solution which approaches the origin in the slow direction and (for simplicity) is strictly positive for sufficiently large* t*.*

(a) If $\kappa = 2$, then we can write x_2 in terms of x_1 as

$$x_2 = c_1 x_1 + c_2\, x_1^2 \,\mathsf{ln}(x_1) + C\, x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \textit{as} \quad x_1 \to 0^+$$

for some constants c_1, c_2 (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_1 = \frac{p_{21}}{p_{11}} \quad \textit{and} \quad c_2 = \frac{\overline{b}_{211}\,(p_{11}p_{22} - p_{12}p_{21})}{p_{11}^3 a}.$$

(b) If $\kappa \in \{3, 4, \ldots\}$, then we can write x_2 in terms of x_1 as

$$x_2 = c_1 x_1 + \cdots + c_{\kappa-1} x_1^{\kappa-1} + C\, x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \textit{as} \quad x_1 \to 0^+$$

for some constants $\{c_i\}_{i=1}^{\kappa-1}$ (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_1 = \frac{p_{21}}{p_{11}}.$$

Proof:

(a) Applying Proposition 5.22, we can write y_2 in terms of y_1 as

$$y_2 = \left[\frac{\overline{b}_{211}}{a}\right] y_1^2 \,\mathsf{ln}(y_1) + \left[\frac{z_{02}}{z_{01}^2} - \frac{\overline{b}_{211}\mathsf{ln}(z_{01})}{a}\right] y_1^2 + \mathsf{o}\big(y_1^2\big) \quad \text{as} \quad y_1 \to 0^+. \tag{5.39}$$

Now, since $\mathbf{x} = \mathbf{P}\mathbf{y}$ we have

$$x_1 = p_{11}y_1 + p_{12}y_2 \quad \text{and} \quad x_2 = p_{21}y_1 + p_{22}y_2. \tag{5.40}$$

If we substitute (5.39) into the first equation of (5.40) and "solve" for y_1 (in a manner we used before), we obtain (after some tedious simplification)

$$\begin{aligned} y_1 = {} & \left[\frac{1}{p_{11}}\right] x_1 - \left[\frac{p_{12}\overline{b}_{211}}{p_{11}^3 a}\right] x_1^2 \,\mathsf{ln}(x_1) \\ & - \left[\frac{p_{12}}{p_{11}^3}\right]\left[\frac{z_{02}}{z_{01}^2} - \frac{\overline{b}_{211}\mathsf{ln}(p_{11}z_{01})}{a}\right] x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+. \end{aligned} \tag{5.41}$$

Substituting (5.41) into (5.39) yields (after more tedious simplification)

$$y_2 = \left[\frac{\overline{b}_{211}}{p_{11}^2 a}\right] x_1^2 \,\mathsf{ln}(x_1) + \left[\frac{1}{p_{11}^2}\right]\left[\frac{z_{02}}{z_{01}^2} - \frac{\overline{b}_{211}\mathsf{ln}(p_{11}z_{01})}{a}\right] x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+. \tag{5.42}$$

Substituting (5.41) and (5.42) into the second equation of (5.40), we get

$$x_2 = \left[\frac{p_{21}}{p_{11}}\right] x_1 + \left[\frac{\overline{b}_{211}\left(p_{11}p_{22} - p_{12}p_{21}\right)}{p_{11}^3 a}\right] x_1^2 \ln(x_1)$$
$$+ \left[\frac{p_{11}p_{22} - p_{12}p_{21}}{p_{11}^3}\right]\left[\frac{z_{02}}{z_{01}^2} - \frac{\overline{b}_{211}\ln(p_{11}z_{01})}{a}\right] x_1^2 + \mathrm{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+.$$

Note that $\det(\mathbf{P}) \equiv p_{11}p_{22} - p_{12}p_{21} \neq 0$.

(b) Just like in Claim 5.23, there are constants $\left\{\overline{\xi}_i\right\}_{i=1}^{\kappa}$ and $\{\overline{\rho}_i\}_{i=1}^{\kappa-1}$ which do not depend on the initial condition and a constant $\overline{\varrho}$ which may depend on the initial condition such that

$$y_1(t) = \sum_{i=1}^{\kappa} \overline{\xi}_i \left(\mathrm{e}^{at} z_{01}\right)^i + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty$$

and

$$y_2(t) = \sum_{i=1}^{\kappa-1} \overline{\rho}_i \left(\mathrm{e}^{at} z_{01}\right)^i + \overline{\varrho}\left(\mathrm{e}^{\kappa at}\right) + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty.$$

Note that $\overline{\xi}_1 = 1$ and $\overline{\rho}_1 = 0$. Since $\mathbf{x}(t) = \mathbf{P}\mathbf{y}(t)$, clearly there are constants $\{\xi_i\}_{i=1}^{\kappa}$ and $\{\rho_i\}_{i=1}^{\kappa-1}$ which do not depend on the initial condition and a constant ϱ which may depend on the initial condition such that

$$x_1(t) = \sum_{i=1}^{\kappa} \xi_i \left(\mathrm{e}^{at} z_{01}\right)^i + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty$$

and

$$x_2(t) = \sum_{i=1}^{\kappa-1} \rho_i \left(\mathrm{e}^{at} z_{01}\right)^i + \varrho\left(\mathrm{e}^{\kappa at}\right) + \mathcal{O}\Big(\mathrm{e}^{(\kappa+1)at}\Big) \quad \text{as} \quad t \to \infty.$$

Note that $\xi_1 = p_{11}$ and $\rho_1 = p_{21}$. Proceeding exactly as we did in the proof of Proposition 5.24, we see that there are constants $\{c_i\}_{i=1}^{\kappa-1}$ (which do not depend on the initial condition) and C (which may depend on the initial condition) such that

$$x_2 = \sum_{i=1}^{\kappa-1} c_i x_1^i + C\, x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+.$$

Note that $c_1 = \frac{p_{21}}{p_{11}}$.

□

Remarks 5.29:

(i) If $\mathbf{b}(\mathbf{x})$ is polynomial instead of purely quadratic, the expression for x_2 in terms of x_1 as $x_1 \to 0^+$ will generally have terms of the form $x_1^i \ln(x_1)$.

(ii) The second part of Theorem 5.28 can be extended to show that x_2 can be written as a Taylor series in x_1 as $x_1 \to 0^+$.

5.8 Higher Dimensions

In this section, we will briefly mention how the techniques of this chapter can potentially be generalized to the case where the eigenvalues of $\mathbf{A}$ are widely-spaced relative to $\mathbf{b}(\mathbf{x})$ when we are considering the general initial value problem (2.5). Suppose that $\mathbf{J} \in \mathbb{R}^n$ is the Jordan canonical form of $\mathbf{A}$. Then, there is an invertible matrix $\mathbf{P}$ such that $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{J}$. Now, let $\mathbf{A}$ have $\ell \in \{2, \ldots, n\}$ distinct eigenvalues[4] $\{\lambda_i\}_{i=1}^{\ell} \subset \mathbb{C}$ with respective multiplicities $\{m_i\}_{i=1}^{\ell} \subset \mathbb{N}$ where $\sum_{i=1}^{\ell} m_i = n$. Then, we can write $\mathbf{J} = \bigoplus_{i=1}^{\ell} \mathbf{J}_i$ where $\{\mathbf{J}_i\}_{i=1}^{\ell}$ are the Jordan blocks. (See §A.15 of Appendix A which mentions the Jordan canonical form.)

Consider the initial value problem

$$\dot{\mathbf{y}} = \mathbf{J}\mathbf{y} + \mathbf{c}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0,$$

where $\mathbf{y} := \mathbf{P}^{-1}\mathbf{x}$, $\mathbf{y}_0 := \mathbf{P}^{-1}\mathbf{x}_0$, and $\mathbf{c}(\mathbf{y}) := \mathbf{P}^{-1}\mathbf{b}(\mathbf{P}\mathbf{y})$. If we have iterates to approximate $\mathbf{y}(t)$ then we can form associated iterates to approximate $\mathbf{x}(t)$ just like in §5.7. Now, write

$$\mathbf{y} = (\mathbf{y}_1, \ldots, \mathbf{y}_\ell)^T, \quad \mathbf{y}_0 = (\mathbf{y}_{01}, \ldots, \mathbf{y}_{0\ell})^T, \quad \text{and} \quad \mathbf{c}(\mathbf{y}) = (\mathbf{c}_1(\mathbf{y}), \ldots, \mathbf{c}_\ell(\mathbf{y}))^T,$$

where $\mathbf{y}_i \in \mathbb{R}^{m_i}$ and $\mathbf{c}_i : \mathbb{R}^n \to \mathbb{R}^{m_i}$. Then, $\mathbf{y}_i(t)$ satisfies the integral equation

$$\mathbf{y}_i(t) = \mathrm{e}^{t\mathbf{J}_i}\mathbf{y}_{0i} + \int_0^t \mathrm{e}^{(t-s)\mathbf{J}_i}\mathbf{c}_i(\mathbf{y}(s))\, ds \quad (i = 1, \ldots, \ell)\,. \tag{5.43}$$

In general, we could form ℓ groups of iterates to approximate the solution $\mathbf{y}(t)$. However, the construction of the ℓ groups of iterates would be tedious. Define the ratios

$$\kappa_i := \frac{\mu_{i+1}}{\mu_1} \quad (i = 1, \ldots, \ell - 1)$$

which satisfy $1 < \kappa_1 < \cdots < \kappa_{\ell-1}$ and $\kappa_{\ell-1} \geq \alpha$. The i^{th} group of iterates would involve "flipping the integral" in the i^{th} component of (5.43). Moreover, the number of iterates in each group (except for the last group which has infinitely many iterates) would be in terms of α, β, and the ratios $\{\kappa_i\}_{i=1}^{\ell-1}$. The last iterate in each group, except for the final group, would (by design) be close enough to the actual solution so that we can "flip the integral" in the next component.[5]

[4] It must be that $\ell > 1$ since otherwise the eigenvalues would be closely-spaced relative to the nonlinear part.

[5] It is possible that a particular group of iterates will have zero iterates.

5.9 Summary

In this chapter, we explored a special case of widely-spaced eigenvalues. Consider the initial value problem

$$\dot{\mathbf{x}} = \underbrace{\begin{pmatrix} a & 0 \\ 0 & \kappa a \end{pmatrix}}_{\mathbf{A}} \mathbf{x} + \underbrace{\begin{pmatrix} b_1(\mathbf{x}) \\ b_2(\mathbf{x}) \end{pmatrix}}_{\mathbf{b}(\mathbf{x})}. \quad \mathbf{x}(0) = \mathbf{x}_0.$$

In particular, $a < 0$ and $\kappa > 1$. Moreover, $\mathbf{b}$ is C^1 in a neighbourhood of the origin and there are constants $\alpha > 1$ and $\beta > 0$ such that

$$\|\mathbf{b}(\mathbf{x})\| = \mathcal{O}(\|\mathbf{x}\|^{\alpha}) \quad \text{and} \quad \|\mathbf{D}\mathbf{b}(\mathbf{x})\| = \mathcal{O}\Big(\|\mathbf{x}\|^{\beta}\Big) \quad \text{as} \quad \|\mathbf{x}\| \to 0.$$

Importantly, $\kappa \geq \alpha$ which is the defining characteristic of widely-spaced eigenvalues.

We encountered a problem when attempting to "flip the integral" the way we did in Chapter 4. To remedy this, we looked at each component of the solution $\boldsymbol{\phi}(t, \mathbf{x}_0)$ separately. By defining $y_{01} = \psi_1(\mathbf{x})$, where

$$\psi_1(\mathbf{x}_0) = x_{01} + \int_0^{\infty} \mathsf{e}^{-as} b_1\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds,$$

we wrote

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \begin{pmatrix} \mathsf{e}^{at} y_{01} - \int_t^{\infty} \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds \\ \mathsf{e}^{\kappa a t} x_{02} + \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) ds \end{pmatrix}.$$

Using this form of the integral equation, we defined the first group of iterates $\left\{\boldsymbol{\chi}^{(m)}(t, y_{01})\right\}_{m=1}^{p-1}$ by

$$\boldsymbol{\chi}^{(1)}(t, y_{01}) = \begin{pmatrix} \mathsf{e}^{at} y_{01} \\ 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^{(m+1)}(t, y_{01}) = \begin{pmatrix} \mathsf{e}^{at} y_{01} - \int_t^{\infty} \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds \\ \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(m)}(s, y_{01})\right) ds \end{pmatrix},$$

where

$$p := \left\lfloor \frac{\kappa - \alpha}{\beta} \right\rfloor + 2.$$

These iterates satisfy

$$\left\|\boldsymbol{\chi}^{(m)}(t, y_{01})\right\| = \mathcal{O}\big(\mathsf{e}^{at}\|\mathbf{x}_0\|\big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0$$

and, for any $\sigma > 0$,

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(m)}(t, y_{01})\right\| = \mathcal{O}\Big(\mathsf{e}^{[\alpha + (m-1)\beta][a+\sigma]t}\|\mathbf{x}_0\|\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

If $\kappa > \alpha$ then we can take $\sigma = 0$.

By defining $y_{02} = \psi_2(\mathbf{x}_0)$, where

$$\psi_2(\mathbf{x}_0) = x_{02} + \int_0^\infty \mathsf{e}^{-\kappa a s} \left[b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds,$$

we wrote the second component of the flow as

$$\begin{aligned}\phi_2(t, \mathbf{x}_0) = &\left[\mathsf{e}^{\kappa a t} y_{02} + \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) ds\right] \\ &- \int_t^\infty \mathsf{e}^{\kappa a(t-s)} \left[b_2\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds.\end{aligned}$$

Using this form of the integral equation, we defined the second group of iterates $\left\{\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right\}_{m=p}^\infty$ by

$$\boldsymbol{\chi}^{(p)}\left(t, \mathbf{y}_0\right) = \begin{pmatrix} \mathsf{e}^{at} y_{01} - \int_t^\infty \mathsf{e}^{a(t-s)} b_1\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) ds \\ \mathsf{e}^{\kappa a t} y_{02} + \int_0^t \mathsf{e}^{\kappa a(t-s)} b_2\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right) ds \end{pmatrix}$$

and

$$\boldsymbol{\chi}^{(m+1)}\left(t, \mathbf{y}_0\right) = \boldsymbol{\chi}^{(p)}\left(t, \mathbf{y}_0\right) - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}} \left[\mathbf{b}\left(\boldsymbol{\chi}^{(m)}\left(s, \mathbf{y}_0\right)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds.$$

Interestingly, we can write the integral equation for the flow as

$$\boldsymbol{\phi}(t, \mathbf{x}_0) = \boldsymbol{\chi}^{(p)}\left(t, \mathbf{y}_0\right) - \int_t^\infty \mathsf{e}^{(t-s)\mathbf{A}} \left[\mathbf{b}\left(\boldsymbol{\phi}(s, \mathbf{x}_0)\right) - \mathbf{b}\left(\boldsymbol{\chi}^{(p-1)}\left(s, y_{01}\right)\right)\right] ds.$$

These iterates satisfy

$$\left\|\boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right\| = \mathcal{O}\left(\mathsf{e}^{at} \|\mathbf{x}_0\|\right) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0$$

and, for any $\sigma > 0$,

$$\left\|\boldsymbol{\phi}(t, \mathbf{x}_0) - \boldsymbol{\chi}^{(m)}\left(t, \mathbf{y}_0\right)\right\| = \mathcal{O}\left(\mathsf{e}^{[\alpha+(m-1)\beta][a+\sigma]t} \|\mathbf{x}_0\|^{(m+1-p)\beta+1}\right) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0.$$

As before, if $\kappa > \alpha$ then we can take $\sigma = 0$.

Consider now the special case where $\kappa \in \{2, 3, \ldots\}$ and

$$\mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_{111} x_1^2 + b_{112} x_1 x_2 + b_{122} x_2^2 \\ b_{211} x_1^2 + b_{212} x_1 x_2 + b_{222} x_2^2 \end{pmatrix}.$$

Suppose that $\|\mathbf{x}_0\|$ is sufficiently small, $\mathbf{y}_0 = \boldsymbol{\psi}(\mathbf{x}_0)$, and $\psi_1(\mathbf{x}_0) > 0$. If $\kappa = 2$, we were able to write the second component of the flow in terms of the first component as

$$x_2 = \left[\frac{b_{211}}{a}\right] x_1^2 \ln(x_1) + \left[\frac{y_{02}}{y_{01}^2} - \frac{b_{211} \ln(y_{01})}{a}\right] x_1^2 + \mathsf{o}\left(x_1^2\right) \quad \text{as} \quad x_1 \to 0^+.$$

On the other hand, if $\kappa \in \{3, 4, \ldots\}$ we can write

$$x_2 = c_2 x_1^2 + \cdots + c_{\kappa-1} x_1^{\kappa-1} + C\, x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+$$

for some constants $\{c_i\}_{i=2}^{\kappa-1}$ (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_2 = \frac{b_{211}}{(2-\kappa)\, a}.$$

Suppose that $\mathbf{A}$ is merely diagonalizable and $\mathbf{P}$ is an invertible matrix such that $\overline{\mathbf{A}} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$, where $\overline{\mathbf{A}} = \mathsf{diag}\,(a, \kappa a)$ and $\mathbf{b}(\mathbf{x})$ is the general vector field from before. If we define $\mathbf{y}_0 = \mathbf{P}^{-1}\mathbf{x}_0$ and $\overline{\mathbf{b}}(\mathbf{y}) = \mathbf{P}^{-1}\mathbf{b}\,(\mathbf{P}\mathbf{y})$, then $\mathbf{y}(t) = \mathbf{P}^{-1}\mathbf{x}(t)$ is the solution of the initial value problem

$$\dot{\mathbf{y}} = \overline{\mathbf{A}}\mathbf{y} + \overline{\mathbf{b}}\,(\mathbf{y})\,, \quad \mathbf{y}(0) = \mathbf{y}_0.$$

Moreover,

$$\big\|\overline{\mathbf{b}}(\mathbf{y})\big\| = \mathcal{O}(\|\mathbf{y}\|^{\alpha}) \quad \text{and} \quad \big\|\mathbf{D}\overline{\mathbf{b}}(\mathbf{y})\big\| = \mathcal{O}\Big(\|\mathbf{y}\|^{\beta}\Big) \quad \text{as} \quad \|\mathbf{y}\| \to 0.$$

We can define the associated iterates $\big\{\mathbf{P}\boldsymbol{\chi}^{(m)}\,(t, \mathbf{z}_0)\big\}_{m=1}^{\infty}$, where $\mathbf{z}_0 = \boldsymbol{\psi}(\mathbf{y}_0)$ with $\boldsymbol{\psi}$ defined with respect to the diagonalized system. These associated iterates satisfy

$$\Big\|\mathbf{x}(t) - \mathbf{P}\boldsymbol{\chi}^{(m)}\,(t, \mathbf{z}_0)\Big\| = \mathcal{O}\Big(\mathrm{e}^{[\alpha+(m-1)\beta][a+\sigma]t}\,\|\mathbf{x}_0\|\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0,$$

for $m < p$, and

$$\Big\|\mathbf{x}(t) - \mathbf{P}\boldsymbol{\chi}^{(m)}\,(t, \mathbf{z}_0)\Big\| = \mathcal{O}\Big(\mathrm{e}^{[\alpha+(m-1)\beta][a+\sigma]t}\,\|\mathbf{x}_0\|^{(m+1-p)\beta+1}\Big) \quad \text{as} \quad t \to \infty \quad \text{and} \quad \|\mathbf{x}_0\| \to 0,$$

for $m \geq p$.

Consider now the special case where $\mathbf{A}$ is merely diagonalizable with $\kappa \in \{2, 3, \ldots\}$ and

$$\mathbf{b}(\mathbf{x}) = \begin{pmatrix} b_{111}x_1^2 + b_{112}x_1x_2 + b_{122}x_2^2 \\ b_{211}x_1^2 + b_{212}x_1x_2 + b_{222}x_2^2 \end{pmatrix}.$$

Let $\mathbf{P} = \{p_{ij}\}_{i,j=1}^{2}$ be as before and

$$\overline{\mathbf{b}}(\mathbf{y}) = \mathbf{P}^{-1}\mathbf{b}\,(\mathbf{P}\mathbf{y}) = \begin{pmatrix} \overline{b}_{111}y_1^2 + \overline{b}_{112}y_1y_2 + \overline{b}_{122}y_2^2 \\ \overline{b}_{211}y_1^2 + \overline{b}_{212}y_1y_2 + \overline{b}_{222}y_2^2 \end{pmatrix}.$$

Suppose that $\|\mathbf{x}_0\|$ is sufficiently small, $\mathbf{y}_0 = \boldsymbol{\psi}(\mathbf{x}_0)$, and $\psi_1(\mathbf{x}_0) > 0$. Assume that the solution $\mathbf{x}(t)$ approaches the origin in the slow direction and is strictly positive for sufficiently large t.

Consequently, we can assume $p_{11} > 0$. If $\kappa = 2$, then we can write the second component of the solution in terms of the first component as

$$x_2 = c_1 x_1 + c_2\, x_1^2 \,\mathsf{ln}(x_1) + C\, x_1^2 + \mathsf{o}\big(x_1^2\big) \quad \text{as} \quad x_1 \to 0^+$$

for some constants c_1, c_2 (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_1 = \frac{p_{21}}{p_{11}} \quad \text{and} \quad c_2 = \frac{\overline{b}_{211}\,(p_{11}p_{22} - p_{12}p_{21})}{p_{11}^3 a}.$$

On the other hand, if $\kappa \in \{3, 4, \dots\}$ then

$$x_2 = c_1 x_1 + \cdots + c_{\kappa-1} x_1^{\kappa-1} + C\, x_1^{\kappa} + \mathcal{O}\big(x_1^{\kappa+1}\big) \quad \text{as} \quad x_1 \to 0^+$$

for some constants $\{c_i\}_{i=1}^{\kappa-1}$ (which depend only on the differential equation) and C (which depends on the differential equation and the initial condition). Moreover,

$$c_1 = \frac{p_{21}}{p_{11}}.$$

Part II

The Michaelis-Menten Mechanism

Chapter 6

Introduction

The Michaelis-Menten mechanism, which is named after two researchers who worked on the model, is the simplest chemical network modeling the formation of a product from a substrate with the aide of an enzyme. There are different and more complicated networks which involve, for example, multiple enzymes, inhibition, and cooperativity. However, even though the Michaelis-Menten mechanism is relatively simple, there are plenty of results on the mechanism and the standard techniques of analyzing the reaction are easily adapted to the more complicated networks. In this part of the thesis, we will develop many new results regarding the Michaelis-Menten mechanism. These results, as will be apparent, can also be adapted to more complicated networks.

6.1 The Michaelis-Menten Mechanism

6.1.1 History

An enzyme is an organic molecule (usually a protein) which catalyzes a chemical reaction and is not consumed by the reaction. The reactants of such a reaction are called substrates. Enzymes often act upon only one or very few specific substrates. The key effect of the binding of the substrate to the active site of the enzyme is the lowering of the activation energy. It is not uncommon for this binding to speed up the rate of reaction by a factor in the millions.

Emil Fischer (1852–1919) was a German chemist who, in 1894, proposed the "lock and key" model for an enzyme. In this model, the enzyme and substrate have complementary "shapes," with a given enzyme fitting exactly into a specific substrate. See, for example, Fischer's paper [41].

Fischer won the Nobel Prize for Chemistry in 1902 "in recognition of the extraordinary services he has rendered by his work on sugar and purine syntheses." The "induced-fit" model, which was proposed by the American biochemist Daniel Koshland (1920–2007) in 1958 and is the currently accepted model for binding, is a modification of the "lock and key" model. See, for example, Koshland's paper [72].

It was known in the late eighteenth and early nineteenth centuries that there were reactions, such as digestion, which were aided by another substance which was not consumed by the reaction. Anselme Payen (1795–1871) and Jean-Francois Persoz (1805–1868) were French chemists who, in 1833, discovered the first enzyme, amylase, which they called diastase. See, for example, their paper [99]. Diastase is now the generic term for an enzyme which catalyzes the breakdown of starch into maltose.

Louis Pasteur (1822–1895) was a French chemist who studied, among other things, the fermentation of sucrose into alcohol (alcoholic fermentation) by yeast. For much of the nineteenth century, there was debate over whether or not the catalyst in alcoholic fermentation was living or not living. Pasteur believed that the fermentation was catalyzed by a vital force in the yeast, saying "no fermentation without life." See, for example, [86].

Adrian Brown (1852–1920) was a British biochemist who worked at a brewing company until 1899 and later became a professor of malting and brewing at the University of Birmingham. He investigated the fermentation of sucrose by yeast and found in 1892 that the rate of fermentation of sucrose in the presence of yeast appeared to be independent of the amount of sucrose that was present. Furthermore, he suggested that a substance in the yeast (later identified and referred to as the enzyme[1] invertase) was responsible for speeding up the reaction. See, for example, [75] and Brown's paper [17].

Eduard Buchner (1860–1917) was a German chemist. In 1897, Buchner showed that a non-living extract of yeast (namely the invertase) catalyzed alcoholic fermentation. This demonstration is regarded as the birth of biochemistry and death of vitalism[2]. For this discovery, Buchner was awarded the 1907 Nobel Prize for Chemistry. See, for example, Buchner's paper [21]. Brown, in

[1]The word "enzyme," which is Greek for "in leaven," was first used by Wilhelm Kühne. A "leaven" is any substance, yeast being the most common, which causes batter or dough to rise.

[2]Vitalism is a belief system that asserts that processes in living organisms cannot be fully explained as physical or chemical phenomena.

light of Buchner's results, in 1902 suggested that the invertase combines with the substrate to form an enzyme-substrate complex. See, for example, Brown's paper [18].

Victor Henri (1872–1940) was a French physical chemist. Throughout his career he published more than five hundred papers. Interestingly, he co-wrote with Alfred Binet a book on intellectual fatigue. Henri was critical of Brown's model of an enzyme reaction, which asserted that the enzyme-substrate had a fixed lifetime and was abruptly created and destroyed. In 1902, Henri originated the accepted model of an enzyme reaction. See, for example, Henri's paper [58]. Henri, unfortunately, is not usually credited with formulating this model.

Leonor Michaelis (1875–1949) was a German biochemist and Maude Menten (1879–1960) was a Canadian medical researcher and biochemist who was one of the first Canadian female medical doctors. Michaelis and Menten, in 1913, popularized Henri's work and advanced the experimental techniques used in enzymology such as pH-control. See, for example, their paper [88]. Even though Henri originated the enzyme model, the mechanism is generally referred to as the Michaelis-Menten mechanism. Moreover, the equilibrium approximation is frequently attributed to Michaelis and Menten rather than Henri. However, it should be noted that Michaelis and Menten clearly indicated Henri's contribution. Moreover, Michaelis and Menten made very important contributions to enzyme kinetics and are regarded as the founders of enzymology.

There are many good general references on the Michaelis-Menten mechanism. For example, [29, 32, 69, 71, 76]. The goal of this chapter is to introduce the model and make preparations for studying the model mathematically. In Chapter 7, we will explore the properties of the planar reduction, which we will soon introduce, in phase space. In Chapter 8, we will explore time-dependent properties of the planar reduction. In Chapter 9, we briefly explore some alternatives to the Michaelis-Menten mechanism.

6.1.2 The Model

In the scheme of Michaelis and Menten (and Henri), an enzyme reacts with the substrate and reversibly forms an intermediate complex, which decays into the product and original enzyme. Symbolically,

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E, \tag{6.1}$$

where S stands for substrate, E for enzyme, C for complex, and P for product. The constants k_{-1}, k_1, and k_2 are the reaction-rate constants.

Technically, the reaction from C to $P + E$ is reversible, but the rate constant k_{-2} is usually negligible and the reverse reaction is omitted. Henri's original model allowed for the reverse reaction. Moreover, in a cell or laboratory the product is continually removed to be used for other purposes which prevents the reverse reaction from occurring.

6.2 Associated Ordinary Differential Equations

6.2.1 Ordinary Differential Equations

Consider the mechanism (6.1). Let lower-case letters (as is the convention) stand for concentrations, t for time, and $\dot{} = \frac{d}{dt}$. The Law of Mass Action (see §A.1 of Appendix A) gives the set of four ordinary differential equations

$$\dot{s} = k_{-1}c - k_1 se, \tag{6.2a}$$

$$\dot{e} = (k_{-1} + k_2)\, c - k_1 se, \tag{6.2b}$$

$$\dot{c} = k_1 se - (k_{-1} + k_2)\, c, \tag{6.2c}$$

$$\dot{p} = k_2 c. \tag{6.2d}$$

The traditional initial conditions are $s(0) = s_0$, $e(0) = e_0$, $c(0) = 0$, and $p(0) = 0$. However, we will allow the initial conditions to be arbitrary.

These equations can be confirmed to be a successful model of a given enzyme reaction by experiment. For example, observations can be made over time of the changes in certain light absorption properties of the chemical species involved which would enable the experimenter to estimate the respective concentrations over time.

6.2.2 Conservation Laws

There are a couple of important conservation laws that can be deduced from our system of four differential equations. First, adding (6.2b) and (6.2c) and then integrating with respect to t, we see that

$$c(t) + e(t) \equiv e_0. \tag{6.3}$$

Second, adding (6.2a), (6.2b) and (6.2d), and integrating with respect to t, we get

$$s(t) + c(t) + p(t) \equiv s_0. \tag{6.4}$$

We choose s_0 and e_0 to denote the constants since, traditionally, the complex and product are regarded as not being initially present. These conservation laws tell us that solutions of (6.2) are restricted to a two-dimensional surface within the four-dimensional solution space.

6.2.3 Planar Reduction

The system (6.2) consists of four differential equations. However, we can reduce that number. The equation for $p(t)$, (6.2d), can be ignored for our purposes because none of the other three concentrations depend on the value of $p(t)$. Furthermore, we can ignore the equation for $e(t)$, (6.2b), due to the conservation law (6.3) which implies that the time evolution of $e(t)$ can be determined precisely from that of $c(t)$.[3] We can hence consider only the system of two ordinary differential equations

$$\dot{s} = k_{-1}c - k_1 s\,(e_0 - c)\,, \tag{6.5a}$$

$$\dot{c} = k_1 s\,(e_0 - c) - (k_{-1} + k_2)\,c. \tag{6.5b}$$

This is frequently referred to as the planar reduction of the Michaelis-Menten reaction. The traditional initial conditions are $s(0) = s_0$ and $c(0) = 0$. However, we will again allow the initial conditions to be arbitrary.

6.2.4 Scalar Reduction

One further reduction is occasionally made to the system (6.2). The system (6.5) includes the time dependence of the concentrations. However, we will find it useful to reduce the planar reduction to a scalar differential equation. Note that it is of practical importance to chemists to study how the concentration of the complex C varies as a function of the concentration of the substrate S.

The set of points $(s(t), c(t))$ defines a curve in the sc-plane, say $c = c(s)$. Since (6.5) is autonomous, we see that

$$c' = \frac{k_1 s\,(e_0 - c) - (k_{-1} + k_2)\,c}{k_{-1}c - k_1 s\,(e_0 - c)}, \tag{6.6}$$

[3] It is traditional to work with $s(t)$ and $c(t)$ instead of, say, $s(t)$ and $e(t)$.

where $' = \frac{d}{ds}$. We restrict attention to the non-negative quadrant, which corresponds to the physically-real space.[4] The flow of the larger system (6.2), when projected on the sc-plane, is equivalent to the flow of (6.6).

6.3 The Equilibrium and Quasi-Steady-State Approximations

The planar system (6.5) is certainly simpler than the original four-dimensional system (6.2). However, it is still impossible to obtain an explicit solution of the planar system. There are two notable approximations employed by biochemists which are inspired by the fact that chemical reactions have a tendency to approach an equilibrium (where one or more chemical species is produced and consumed at the same rate).

6.3.1 The Equilibrium Approximation (EA)

To obtain an approximate solution to (6.5), Henri applied what is called the (rapid) Equilibrium Approximation (EA). Although Michaelis and Menten did use the EA, it was Henri who originated the approximation. Frequently in the literature, Michaelis and Menten are given credit for inventing the EA which Henri deserves.

In particular, Henri assumed that the substrate is in equilibrium with the complex. That is, the substrate is produced and consumed at roughly the same rate. Mathematically, we can interpret the equilibrium approximation as the condition $\dot{s}(t) \approx 0$ for sufficiently large time t. From (6.5a),

$$k_1 s(t)\,[e_0 - c(t)] \approx k_{-1} c(t).$$

Solving for $c(t)$, we get

$$c(t) \approx \frac{e_0 s(t)}{K_s + s(t)}, \quad \text{where} \quad K_s := \frac{k_{-1}}{k_1}.$$

In terms of the scalar reduction, this gives us the equilibrium approximation

$$c_{\mathrm{EA}}(s) := \frac{e_0 s}{K_s + s}. \tag{6.7}$$

[4]It is also common to restrict attention to $s \geq 0$ and $0 \leq c \leq e_0$ since, using the conservation law (6.3), we know that $c(t)$ cannot exceed e_0.

6.3.2 The Quasi-Steady-State Approximation (QSSA)

John Haldane (1892–1964) was a British evolutionary biologist and geneticist. Haldane made major contributions in many areas of science with, arguably, his most important contribution being his development (along with Ronald Fisher and Sewall Wright) of the mathematical theory of natural selection. Interestingly, Haldane described his service in the infantry during the First World War as a "very enjoyable experience" and admitted that he "enjoyed the opportunity of killing people." Moreover, he is known to have used himself (and those around him) in experiments (involving, for example, oxygen poisoning and decompression sickness). He also wrote a well-known humourous poem shortly before his death about the cancer which killed him. See, for example, [1] and pages 300–303 of [20].

Haldane, along with the British botanist George Briggs (1893–1985), introduced in 1925 a second, more common approximation for the Michaelis-Menten reaction. They suggested that after sufficiently much time has passed, the complex is produced and consumed at roughly the same rate. Since the complex is an intermediate of the reaction, this approximation is known as the Quasi-Steady-State Approximation (QSSA). See, for example, their paper [15].

The reasoning for this approximation is as follows. At the beginning of the reaction, the concentration of the complex increases rapidly as the enzyme combines with the substrate. During the initial period of the reaction there is plenty of substrate and the speed of the reaction is limited only by how fast the enzyme can work. However, as the complex builds up, more complex is consumed producing substrate and product until a quasi-steady-state is reached.

The mathematical interpretation of the quasi-steady-state approximation is that, after sufficiently large time, we have $\dot{c}(t) \approx 0$. From (6.5b),

$$k_1 s(t)\,[e_0 - c(t)] \approx (k_2 + k_{-1})\,c(t).$$

Solving for $c(t)$, we get

$$c(t) \approx \frac{e_0 s(t)}{K_m + s(t)}, \quad \text{where} \quad K_m := \frac{k_{-1} + k_2}{k_1}.$$

In terms of the scalar reduction, the quasi-steady-state approximation is

$$c_{\mathrm{QSSA}}(s) := \frac{e_0 s}{K_m + s}. \tag{6.8}$$

The constant K_m is called the Michaelis-Menten constant (or the Michaelis constant).

6.3.3 Lineweaver-Burk Plots

The velocity V of the reaction (6.1) is defined as the rate of formation of product, that is, $V := \frac{dp}{dt}$. Using (6.2d) and the QSSA (6.8),

$$V \approx \frac{k_2 e_0 s}{K_m + s},$$

which is known as the Michaelis-Menten approximation. This can be re-written as

$$\frac{1}{V} \approx \frac{1}{V_{\max}} + \left(\frac{K_m}{V_{\max}}\right)\frac{1}{s},$$

where $V_{\max} := k_2 e_0$ is the maximum velocity. Observe that $V \approx \frac{1}{2}V_{\max}$ (known as half saturation) when $s = K_m$.

The values of s and V can be experimentally measured. If $\frac{1}{V}$ is plotted versus $\frac{1}{s}$, the resulting curve is approximately a straight line. The slope and intercept can be found yielding a value for $V_{\max}$ and K_m. Such a graph is called a Lineweaver-Burk plot, after Hans Lineweaver and Dean Burk who, in 1934, suggested this technique for measuring $V_{\max}$ and K_m. See, for example, their paper [83]. There are other techniques for measuring some of the constants associated with the Michaelis-Menten reaction, but this method is the most well-known.

6.4 Dimensionless Ordinary Differential Equations

It is very helpful for future analysis to re-scale the differential equations (6.5) and (6.6) into dimensionless form. First, we note that the dimensions of the involved quantities are

$$[s, c, e_0] = \frac{Q}{L^3}, \quad [\dot{s}, \dot{c}] = \frac{Q}{L^3 T}, \quad [k_{-1}, k_2] = \frac{1}{T}, \quad \text{and} \quad [k_1] = \frac{L^3}{QT},$$

where Q stands for quantity of substance (usually measured in moles), L stands for length, and T stands for time. To improve the presentation, we use for example $[s, c, e_0]$ in place of $[s], [c], [e_0]$ since all three of the quantities have the same dimension.

6.4.1 Dimensionless Variables and Parameters

The system (6.5) can be written in dimensionless form in several ways. See, for example, [35, 84, 91, 98, 112]. Usually, a parameter ε with $0 < \varepsilon \ll 1$ is introduced. The more traditional choice is $\varepsilon = \frac{e_0}{s_0}$. We, however, will use a different scaling which was used, for example, in [109].

Define[5]

$$\tau := k_1 e_0 t, \quad x := \left(\frac{k_1}{k_{-1}+k_2}\right) s, \quad y := \frac{c}{e_0}, \quad \varepsilon := \frac{k_1 e_0}{k_{-1}+k_2}, \quad \text{and} \quad \eta := \frac{k_2}{k_{-1}+k_2},$$

which are all dimensionless, and note that

$$\varepsilon > 0 \quad \text{and} \quad 0 < \eta < 1.$$

Thus, τ, x, and y are, respectively, a scaled time, substrate concentration, and complex concentration.

The parameter ε measures the ratio of the time scales and a small value of ε is indicative of high efficiency of the enzyme. Moreover, the parameter η can be regarded as the probability that the complex C decays to product P. It is apparent from the mechanism (6.1) that the EA reduces to the QSSA when $\eta \to 0^+$. Also, when $\eta \to 1^-$ we see that the conversion of substrate S to product proceeds with little or no resistance, which suggests that the complex cannot be near a quasi-steady state.

Throughout this part of the thesis, it will be our philosophy that both $\varepsilon > 0$ and $\eta \in (0, 1)$ are arbitrary parameters of any permissible size. In particular, we do not need to make the usual assumption that ε is small.

6.4.2 Planar System

It is easy to verify that the differential equation (6.5) takes on the dimensionless form

$$\dot{x} = -x + (1 - \eta + x)\, y, \quad \dot{y} = \varepsilon^{-1} \left[x - (1 + x)\, y\right], \tag{6.9}$$

where $\dot{} = \frac{d}{dt}$ and (for simplicity) we are using t when we really are using the scaled time τ. We will occasionally need to refer to the vector field of the planar system (6.9). Hence, define

$$\mathbf{g}(\mathbf{x}) := \begin{pmatrix} -x + (1 - \eta + x)\, y \\ \varepsilon^{-1} \left[x - (1 + x)\, y\right] \end{pmatrix}, \tag{6.10}$$

where $\mathbf{x} := (x, y)^T$. In Chapter 7 and Chapter 8, we will explore properties of solutions of (6.9).

[5]Instead of using $\varepsilon = \frac{e_0}{s_0}$, which is the ratio of initial enzyme concentration to initial substrate concentration, we are using $\varepsilon = \frac{e_0}{K_m}$, which is the ratio of initial enzyme concentration to half-saturation substrate concentration.

6.4.3 Scalar Differential Equation

We can also write the scalar differential equation (6.6) in the form

$$y' = \frac{x - (1+x)\,y}{\varepsilon\,[-x + (1-\eta+x)\,y]}, \tag{6.11}$$

where $' = \frac{d}{dx}$. Furthermore, define the function

$$f(x,y) := \frac{x - (1+x)\,y}{\varepsilon\,[-x + (1-\eta+x)\,y]}. \tag{6.12}$$

In Chapter 7, we will explore the properties of solutions of (6.11).

Remark 6.1: The function $f(x,y)$ can be written

$$f(x,y) = \frac{g_2(x,y)}{g_1(x,y)},$$

where $g_1(x,y)$ and $g_2(x,y)$ are the components of the function $\mathbf{g}(\mathbf{x})$ given in (6.10). Note the use of the row vector (x,y) in the arguments of g_1 and g_2 as opposed to the column vector $\mathbf{x}$. To alleviate notational headaches that arise from competing conventions involving row and column vectors, when there will be no confusion we will use the notation appropriate for the given situation.

6.4.4 The EA and QSSA

With this new scaling, it is easy to show that Equations (6.7) and (6.8), for EA and QSSA, take the respective forms

$$y_{\mathrm{EA}}(x) := \frac{x}{1-\eta+x} \quad \text{and} \quad y_{\mathrm{QSSA}}(x) := \frac{x}{1+x}. \tag{6.13}$$

These can, of course, be obtained by setting $\dot{x} = 0$ and $\dot{y} = 0$ in (6.9). Alternatively, we see that $y_{\mathrm{EA}}(x)$ is the vertical isocline of the system (6.11) and $y_{\mathrm{QSSA}}(x)$ is the horizontal isocline. One may refer to $y = y_{\mathrm{EA}}(x)$ as the rapid equilibrium manifold and $y = y_{\mathrm{QSSA}}(x)$ as the quasi-steady-state manifold.

6.5 Phase Portrait

The goal of this section is to develop a reasonable phase portrait for the planar system (6.9). We will restrict our attention to the non-negative quadrant S since, physically, we are only concerned with non-negative concentrations.[6] In Chapter 7, we will develop more precise results on the properties of the phase portrait.

To develop the phase portrait, we will find the isoclines, establish the positive invariance of the non-negative quadrant S, look at the linearization at the origin (which is the only equilibrium point), and specify the slopes of solutions of (6.11) in different regions.

6.5.1 Isoclines

To find the horizontal and vertical isoclines, set, respectively, $\dot{y} = 0$ and $\dot{x} = 0$ in Equation (6.9) to obtain

$$H(x) := \frac{x}{1+x} \quad \text{and} \quad V(x) := \frac{x}{1-\eta+x}. \tag{6.14}$$

Comparing this with Equation (6.13), we see that the EA corresponds to the vertical isocline and the QSSA corresponds to the horizontal isocline. Interestingly, neither the horizontal isocline nor the vertical isocline depends on ε.

It is obvious from (6.14) that

$$H(0) = 0 = V(0), \quad 0 < H(x) < V(x) \quad \text{for all} \quad x > 0, \quad \text{and} \quad \lim_{x\to\infty} H(x) = 1 = \lim_{x\to\infty} V(x).$$

The region between the isoclines,

$$\Gamma_0 := \{\ (x,y)\ :\ x > 0,\ H(x) \le y \le V(x)\ \},$$

will be of importance. To illustrate Remark 6.1, suppose that x and y are such that $x > 0$ and $H(x) \le y \le V(x)$. Then, we may write $(x,y) \in \Gamma_0$ as well as $\mathbf{x} \in \Gamma_0$, where $\mathbf{x} = (x,y)^T$.

6.5.2 Positive Invariance of the Non-Negative Quadrant S

The origin is the only equilibrium point of the system (6.9). To see why, set $\dot{x} = 0$ and $\dot{y} = 0$ which gives $y = H(x)$ and $y = V(x)$. Since the isoclines only intersect at $x = 0$, we obtain $(x,y) = (0,0)$.

If $x = 0$ and $y > 0$ then $\dot{x} = (1-\eta)\,y > 0$. Thus, on the positive y-axis, the vector field $\mathbf{g}$ points into the positive quadrant. Similarly, if $x > 0$ and $y = 0$ then $\dot{y} = \varepsilon^{-1}x > 0$. Thus, on the positive x-axis, the vector field $\mathbf{g}$ points into the positive quadrant. It follows that the non-negative quadrant S is positively invariant.

[6] It is also common to limit the analysis to $x \ge 0$ and $0 \le y \le 1$. This additional restriction on y results from the conservation law (6.3) and the fact that $y = \frac{c}{e_0}$.

6.5.3 Linearization at the Origin

The Jacobian matrix for the system (6.9) at $(0, 0)$ is

$$\mathbf{A} := \begin{pmatrix} -1 & 1-\eta \\ \varepsilon^{-1} & -\varepsilon^{-1} \end{pmatrix}. \tag{6.15}$$

We will find the eigenvalues and associated eigenvectors of this matrix. With the aid of Hartman's Theorem, these will tell us how the phase portrait of the system (6.9) looks near the origin.

The Eigenvalues $\lambda_\pm$ of the Matrix A

The characteristic equation of the matrix **A** is given by

$$\lambda^2 + \left(\frac{1}{\varepsilon} + 1\right)\lambda + \frac{\eta}{\varepsilon} = 0. \tag{6.16}$$

Observe that -1 and 0 cannot be roots of the characteristic equation since $\varepsilon > 0$ and $0 < \eta < 1$. The eigenvalues of **A** are hence given by

$$\lambda_\pm := \frac{-(\varepsilon+1) \pm \sqrt{(\varepsilon+1)^2 - 4\varepsilon\eta}}{2\varepsilon}. \tag{6.17}$$

Claim 6.2: *The eigenvalues λ_+ and λ_- are real-valued and distinct.*

Proof: Observe that the radicand of (6.17) satisfies

$$(\varepsilon+1)^2 - 4\varepsilon\eta > (\varepsilon+1)^2 - 4\varepsilon = (\varepsilon-1)^2 \geq 0,$$

where we used the facts that $\varepsilon > 0$ and $0 < \eta < 1$. The claim follows. □

Claim 6.3: *The eigenvalues λ_+ and λ_- satisfy the limits*

$$\lim_{\varepsilon\to 0^+} \lambda_+ = -\eta, \quad \lim_{\varepsilon\to\infty} \lambda_+ = 0, \quad \lim_{\varepsilon\to 0^+} \lambda_- = -\infty, \quad \textit{and} \quad \lim_{\varepsilon\to\infty} \lambda_- = -1. \tag{6.18}$$

Proof: The proof is a simple exercise in limits. □

Claim 6.4: *In terms of η and either eigenvalue λ, ε can be written*

$$\varepsilon = -\frac{\lambda+\eta}{\lambda(1+\lambda)}. \tag{6.19}$$

Proof: Solve the characteristic equation (6.16) for ε. □

Claim 6.5: *Either eigenvalue* λ *satisfies*

$$\frac{\partial\lambda}{\partial\varepsilon} = \frac{\lambda^2 (\lambda+1)^2}{(\lambda+\eta)^2 + \eta(1-\eta)}. \tag{6.20}$$

Proof: Differentiate (6.16) with respect to ε, solve for $\frac{\partial\lambda}{\partial\varepsilon}$, and substitute (6.19) to get

$$\frac{\partial\lambda}{\partial\varepsilon} = -\frac{\lambda(\lambda+1)}{2\varepsilon\lambda+\varepsilon+1} = \frac{\lambda^2(\lambda+1)^2}{(\lambda+\eta)^2+\eta(1-\eta)}.$$

□

Claim 6.6: *The eigenvalues* λ_+ *and* λ_- *satisfy the inequalities*

$$\lambda_- < -1 < -\eta < \lambda_+ < 0. \tag{6.21}$$

Proof: It follows from (6.20) (and the fact that neither eigenvalue is -1 or 0) that

$$\frac{\partial\lambda_+}{\partial\varepsilon} > 0 \quad \text{and} \quad \frac{\partial\lambda_-}{\partial\varepsilon} > 0.$$

This in conjunction with the limits (6.18) give the conclusion. □

Since $\lambda_- < \lambda_+ < 0$, the eigenvalue λ_+ is referred to as the slow eigenvalue since it corresponds to the slow exponential decay rate $\mathcal{O}\left(\mathrm{e}^{\lambda_+ t}\right)$. Similarly, λ_- is the fast eigenvalue since it corresponds to the fast exponential decay rate $\mathcal{O}\left(\mathrm{e}^{\lambda_- t}\right)$.

Claim 6.7: *There is resonance in the eigenvalues* λ_+ *and* λ_- *of* $\boldsymbol{A}$ *if and only if* $\kappa \in \{2, 3, \ldots\}$, *where* $\kappa := \frac{\lambda_-}{\lambda_+}$.

Proof: It follows from Proposition 2.15 and the fact that $\kappa > 1$. □

The Ratio κ of the Eigenvalues

Part I of this thesis made it clear that the ratio of the eigenvalues,

$$\kappa := \frac{\lambda_-}{\lambda_+}, \tag{6.22}$$

will be of importance. Using the definition (6.17) of the eigenvalues $\lambda_\pm$ and the definition (6.22) of κ, we see that κ can be written in terms of ε and η as

$$\kappa = \frac{\varepsilon+1+\sqrt{(\varepsilon+1)^2-4\varepsilon\eta}}{\varepsilon+1-\sqrt{(\varepsilon+1)^2-4\varepsilon\eta}}. \tag{6.23}$$

Claim 6.8: *The ratio κ satisfies*

$$\kappa > \mathsf{max}\left\{\varepsilon, \varepsilon^{-1}\right\}. \tag{6.24}$$

Proof: For any $\varepsilon > 0$ and $\eta \in (0,1)$, we have

$$(\varepsilon+1)^2 - 4\varepsilon\eta > (\varepsilon+1)^2 - 4\varepsilon = (\varepsilon-1)^2.$$

It follows from (6.23) that

$$\kappa > \frac{(\varepsilon+1)+|\varepsilon-1|}{(\varepsilon+1)-|\varepsilon-1|} = \begin{cases} \varepsilon, & \text{if} \quad \varepsilon \geq 1 \\ \varepsilon^{-1}, & \text{if} \quad 0 < \varepsilon < 1 \end{cases} = \mathsf{max}\left\{\varepsilon, \varepsilon^{-1}\right\}.$$

□

Remark 6.9: It follows from (6.24) that κ satisfies

$$\kappa > 1, \quad \lim_{\varepsilon \to 0^+} \kappa = \infty, \quad \text{and} \quad \lim_{\varepsilon \to \infty} \kappa = \infty.$$

Moreover, if ε is very small, which is the case traditionally considered, then κ is very large. Many results that follow in this part of the thesis will involve κ and so it is a good idea to keep this in mind.

Claim 6.10: *In terms of ε and κ, η can be written*

$$\eta = \frac{\kappa\left(\varepsilon+1\right)^2}{\varepsilon(\kappa+1)^2}. \tag{6.25}$$

Proof: Solve (6.23) for η. □

Figure 6.1 sketches κ as a function of ε for a fixed η and Figure 6.2 sketches η as a function of κ for a fixed value of ε. The details of these sketches are easily verified.

Remark 6.11: Equation (6.25) can tell us when the parameter κ takes any desired value. For example, we may want to design a numerical simulation with $\kappa = 3$ and $\varepsilon = 1$. Then, we need to take $\eta = \frac{3(1+1)^2}{1(3+1)^2} = \frac{3}{4}$. However, for a given $\varepsilon > 0$ and $\kappa > 1$, there may not be a corresponding physically valid $\eta \in (0,1)$.

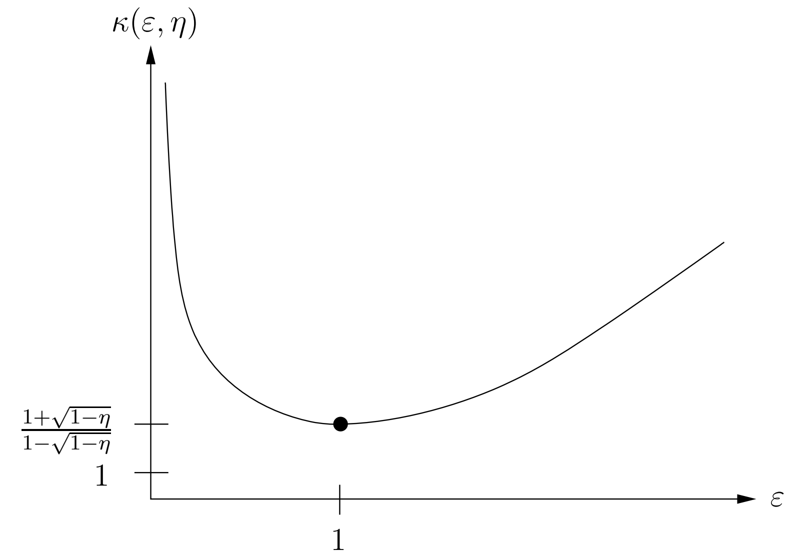

Figure 6.1: The graph of $\kappa(\varepsilon, \eta)$ versus $\varepsilon > 0$ for an arbitrary, fixed $\eta \in (0, 1)$. It is easy to show that $\frac{\partial \kappa}{\partial \eta} < 0$ for all $\varepsilon > 0$ and $\eta \in (0, 1)$.

The Eigenvectors $\mathbf{v}_\pm$ of the Matrix A

Eigenvectors associated with the eigenvalues $\lambda_\pm$ are easily calculated. We will take as the eigenvectors

$$\mathbf{v}_\pm := \begin{pmatrix} 1 - \eta \\ \lambda_\pm + 1 \end{pmatrix}. \tag{6.26}$$

Since $\lambda_- < \lambda_+ < 0$, the eigenvector $\mathbf{v}_+$ is referred to as the slow eigenvector since solutions approaching the origin in the direction of $\mathbf{v}_+$ do so at the slow exponential decay rate $\mathcal{O}\big(\mathrm{e}^{\lambda_+ t}\big)$. Similarly, $\mathbf{v}_-$ is the fast eigenvector since solutions approaching the origin in the direction of $\mathbf{v}_-$ do so at the slow exponential decay rate $\mathcal{O}\big(\mathrm{e}^{\lambda_- t}\big)$.

Applying the bounds of (6.21) to the expression (6.26) for the eigenvectors, we see that $\mathbf{v}_+$ points into the positive quadrant while $\mathbf{v}_-$ does not.

The Slope σ of the Slow Eigenvector $\mathbf{v}_+$

The slope of the slow eigenvector $\mathbf{v}_+$ at the origin is very important, and will be denoted by

$$\sigma := \frac{\lambda_+ + 1}{1 - \eta}. \tag{6.27}$$

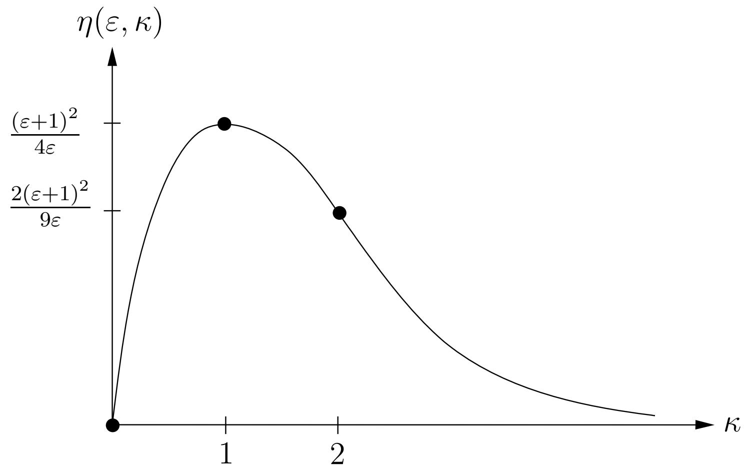

Figure 6.2: The graph of $\eta(\varepsilon,\kappa)$ for an arbitrary, fixed $\varepsilon > 0$. The physically relevant values of κ are $\kappa > 1$. It can be shown that the maximum value satisfies $\frac{(\varepsilon+1)^2}{4\varepsilon} \geq 1$ for all $\varepsilon > 0$ with equality only for $\varepsilon = 1$. Moreover, it is easy to show that for any κ, $\frac{\partial\eta}{\partial\varepsilon} > 0$ for $\varepsilon > 1$ and $\frac{\partial\eta}{\partial\varepsilon} < 0$ for $0 < \varepsilon < 1$.

Claim 6.12: *The slope σ of the slow eigenvector $\boldsymbol{v}_+$ satisfies*

$$1 < \sigma < \frac{1}{1-\eta}. \tag{6.28}$$

Proof: It follows from the definition (6.27) of σ and the inequalities in (6.21). □

Claim 6.13: *The slope σ satisfies the limits*

$$\lim_{\varepsilon\to 0^+} \sigma = 1 \quad \textit{and} \quad \lim_{\varepsilon\to\infty} \sigma = \frac{1}{1-\eta}.$$

Proof: It follows from (6.18) and (6.27). □

Phase Portrait for the Linear System

Figure 6.3 gives a sketch of the phase portrait for the linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$. We will make a few observations.

- If $y < \frac{x}{1-\eta}$ then $\dot{x} < 0$. Similarly, if $y > \frac{x}{1-\eta}$ then $\dot{x} > 0$.
- If $y < x$ then $\dot{y} > 0$. Similarly, if $y > x$ then $\dot{y} < 0$.

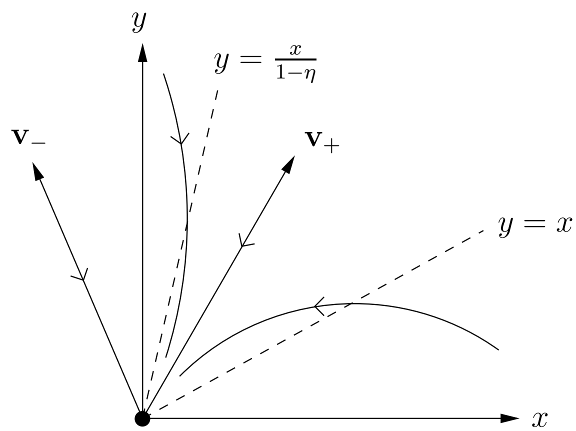

Figure 6.3: A phase portrait of the linearized system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$ near the origin.

- Since $\lambda_- < \lambda_+ < 0$, we know that the origin is asymptotically stable with all solutions approaching the origin in the slow direction (except those on the fast eigenvector).
- Equation (6.28) implies that the slow eigenvector $\mathbf{v}_+$ is between the horizontal isocline $y = x$ and the vertical isocline $y = \frac{x}{1-\eta}$.

Since the origin is a hyperbolic equilibrium point and the vector field $\mathbf{g}$, where $\mathbf{g}$ is defined in (6.10), is C^2 in a neighbourhood of the origin, Hartman's Theorem tells us that the phase portrait of the nonlinear system (6.9) looks like the phase portrait of the linear system in a neighbourhood of the origin. In particular, the origin is a stable node. See §A.8 of Appendix A for an overview of some different types of equilibrium points.

6.5.4 The Slopes of Solutions of the Scalar Differential Equation

Table 6.1 summarizes the slopes of solutions of the scalar differential equation (6.11). These results can be obtained easily by manipulating the differential equation.

6.5.5 Phase Portrait

The Portraits

Five computer-generated phase portraits for (6.9) are depicted in Figures 6.4 through 6.8 for various values of the parameters ε and η. The chosen values of the parameters are not entirely random. It

Region	Values of the Slopes of Solutions
$x = 0,\ y = 0$	undefined
$x = 0,\ y > 0$	$f = -\varepsilon^{-1}(1-\eta)^{-1}$
$x > 0,\ y = 0$	$f = -\varepsilon^{-1}$
$x > 0,\ 0 < y < H(x)$	$-\varepsilon^{-1} < f < 0$
$x > 0,\ y = H(x)$	$f = 0$
$x > 0,\ H(x) < y < V(x)$	$0 < f < \infty$
$x > 0,\ y = V(x)$	undefined
$x > 0,\ V(x) < y < 1$	$-\infty < f < -\varepsilon^{-1}(1-\eta)^{-1}$
$x > 0,\ y = 1$	$f = -\varepsilon^{-1}(1-\eta)^{-1}$
$x > 0,\ y > 1$	$-\varepsilon^{-1}(1-\eta)^{-1} < f < -\varepsilon^{-1}$

Table 6.1: This table lists the slopes of solutions of (6.11) in different regions of the non-negative quadrant. The function f is defined in (6.12).

is important to recognize the differences and the similarities in the phase portraits for ε less than one and greater than one and for η near one and near zero.

The EA and QSSA

We can see from the phase portraits why the EA and QSSA have proven so useful. Both isoclines sketch out similar curves and define a so-called "trapping region" which we have already denoted Γ_0. After solutions enter this trapping region, they follow both the isoclines. It appears that solutions follow the horizontal isocline more closely for small ε which is consistent with the fact that QSSA is the favoured approximation.

The phrase "pre-steady-state period" is often used to describe the period of time before the reaction (6.1) exhibits steady-state behaviour. Similarly, the "steady-state period" is the period when the reaction does exhibit steady-state behaviour. Consider the system (6.9) with initial condition $x(0) = x_0 > 0$ and $y(0) = 0$. We will refer to the period before the solution $\mathbf{x}(t)$ enters the trapping region Γ_0 as the pre-steady-state period. The time afterwards, when the solution forever remains in Γ_0, will be referred to as the steady-state period.

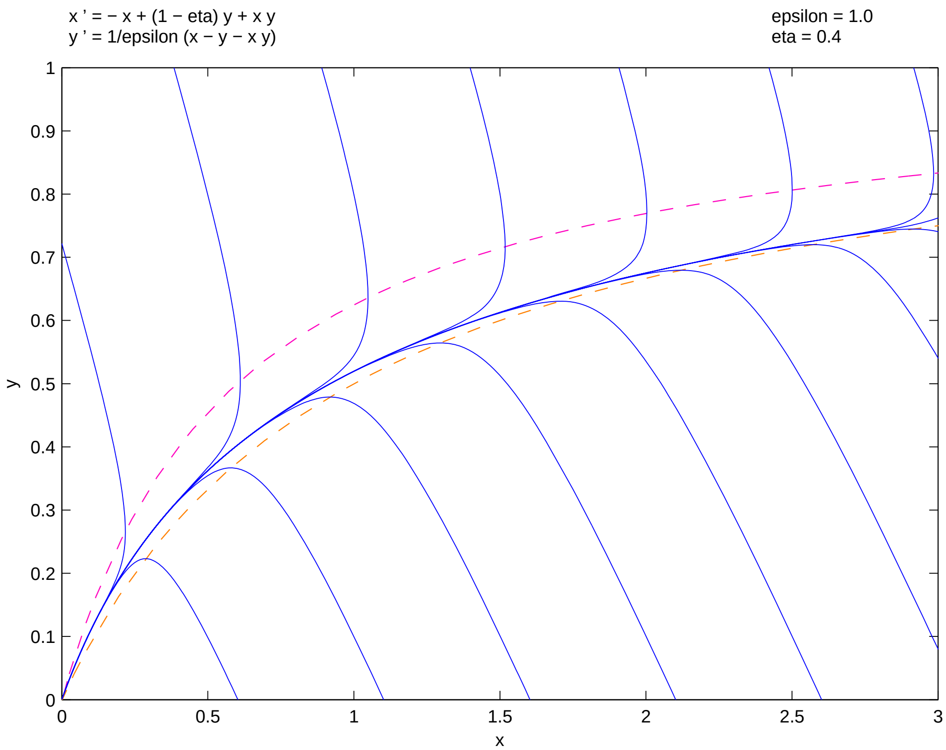

Figure 6.4: A phase portrait for (6.9) for $\varepsilon = 1.0$ and $\eta = 0.4$ in which $\sigma \approx 1.3$ and $\kappa \approx 7.9$, generated by MATLAB using the programs dfield7 and pplane7. The dashed lines are the horizontal and vertical isoclines.

The Slow Manifold

We can see from the phase portraits that there appears to be an exceptional solution that stays inside the trapping region and attracts all other solutions. This exceptional solution to the scalar differential equation (6.11) will be referred to as the *slow manifold* and denoted by $y = \mathcal{M}(x)$ which is defined for all $x > 0$. In Chapter 7, we will rigorously define the slow manifold and show that it exists and is unique.

Davis and Skodje, in [33] for example, take the slow manifold to be the trajectory joining a saddle at infinity and a stable node which approaches in a slow direction. Fraser and Roussel, for example in [43, 104, 106, 109], take (as we do here) the slow manifold as the exceptional solution between

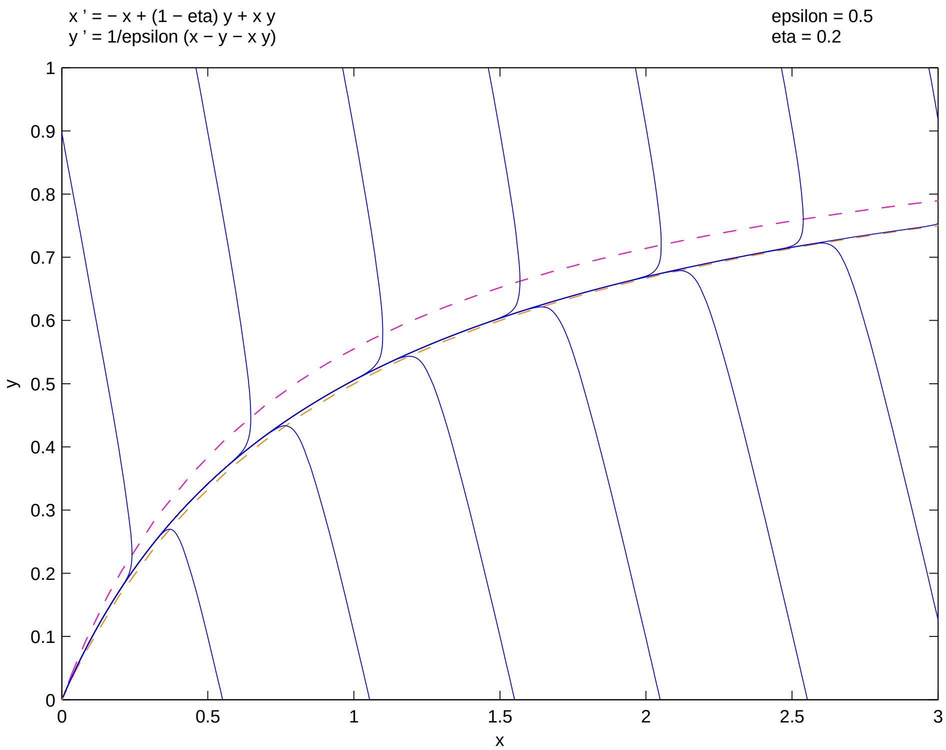

Figure 6.5: A phase portrait for (6.9) for $\varepsilon = 0.5$ and $\eta = 0.2$ in which $\sigma \approx 1.1$ and $\kappa \approx 20.5$.

the isoclines. For general references on invariant manifolds, see for example [25, 49, 126, 127].

The slow manifold is an invariant manifold and is important from a dynamical systems point of view in the same sense that a centre manifold or stable manifold is important. Solutions approach the slow manifold exponentially fast and then follow it as time proceeds. Hence, it is of value to study the dynamics on the slow manifold which is of lesser dimension than the original system.

The slow manifold represents a much better long-term approximation than EA and QSSA. Moreover, knowing the position of the slow manifold accurately allows, for example, all rate constants to be determined independently from steady-state data. See, for example, [108].

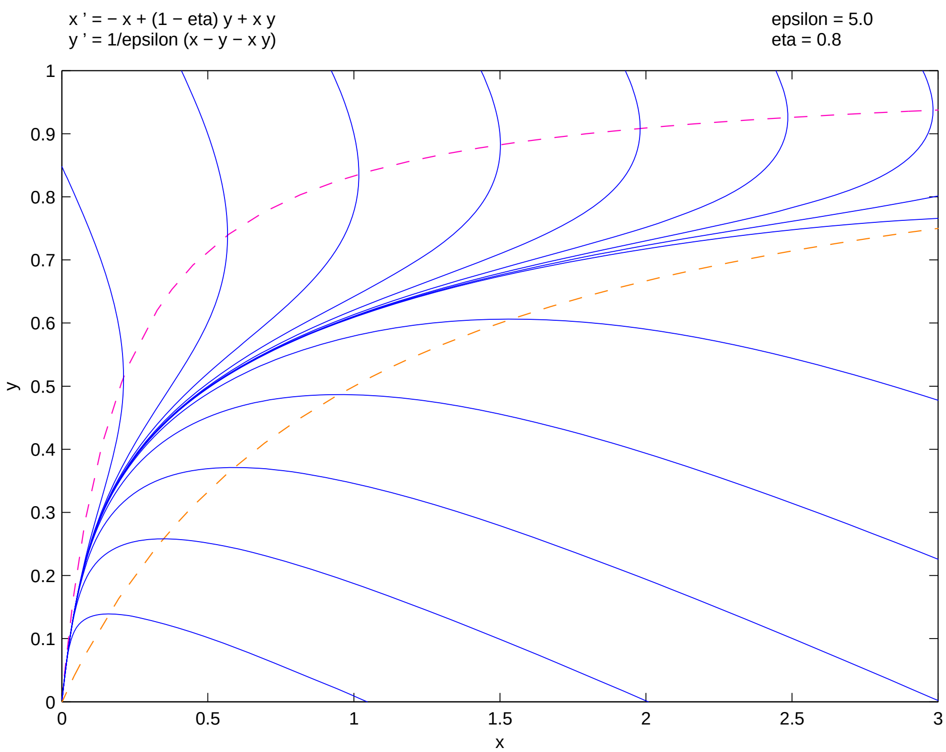

Figure 6.6: A phase portrait for (6.9) for $\varepsilon = 5.0$ and $\eta = 0.8$ in which $\sigma \approx 4.2$ and $\kappa \approx 6.9$.

6.5.6 Domain of Existence for Solutions of the Differential Equations

Any solution $\mathbf{x}(t)$ of the planar system (6.9) is defined for all $t \geq 0$. We will only ever consider $\mathbf{x}_0 \in S$, where $\mathbf{x}(0) = \mathbf{x}_0$ is the initial condition. Recall that S is positively invariant. However, we need to be a little more careful in specifying the domain for solutions $y(x)$ to the scalar differential equation (6.11). There are five possibilities.

- If $(x, y) = (0, 0)$ or if $x > 0$ and $y = V(x)$, the function f is not defined, where f is given in (6.12). We will not consider there to be a scalar solution y through the origin or along the vertical isocline.

- If y is the slow manifold, that is $y = \mathcal{M}$, then y is defined for $x > 0$.

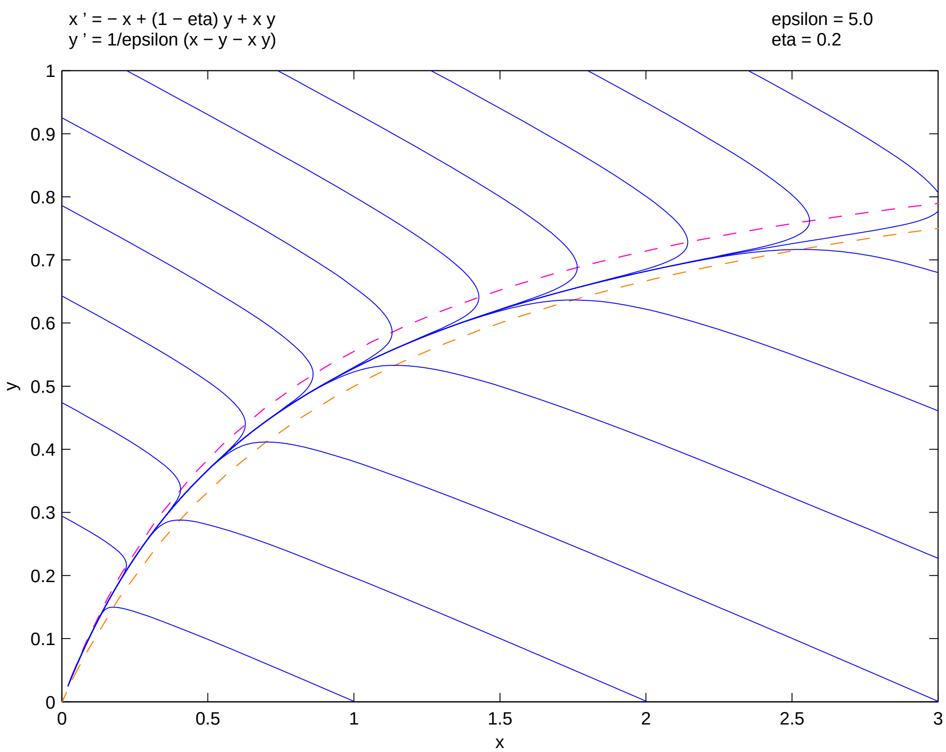

Figure 6.7: A phase portrait for (6.9) for $\varepsilon = 5.0$ and $\eta = 0.2$ in which $\sigma \approx 1.2$ and $\kappa \approx 34.0$.

- If y lies below the slow manifold, y will intersect the x-axis for some $a > 0$. Thus, y is defined for $(0, a]$ with $y(a) = 0$.
- If y lies below the vertical isocline, y will intersect V for some $a > 0$. Thus, y is defined for $(0, a)$ with $\lim_{x \to a^-} y(x) = V(a)$.
- If y lies above the vertical isocline, y will intersect V for some $a > 0$. Thus, y is defined for $[0, a)$ with $\lim_{x \to a^-} y(x) = V(a)$.

Since $\mathbf{g}$ in Equation (6.10) is analytic, solutions $\mathbf{x}(t)$ are also analytic. Furthermore, since f in Equation (6.12) is analytic except at $(0, 0)$ and along the vertical isocline V, scalar solutions $y(x)$ are analytic except at $(0, 0)$ and along the vertical isocline.

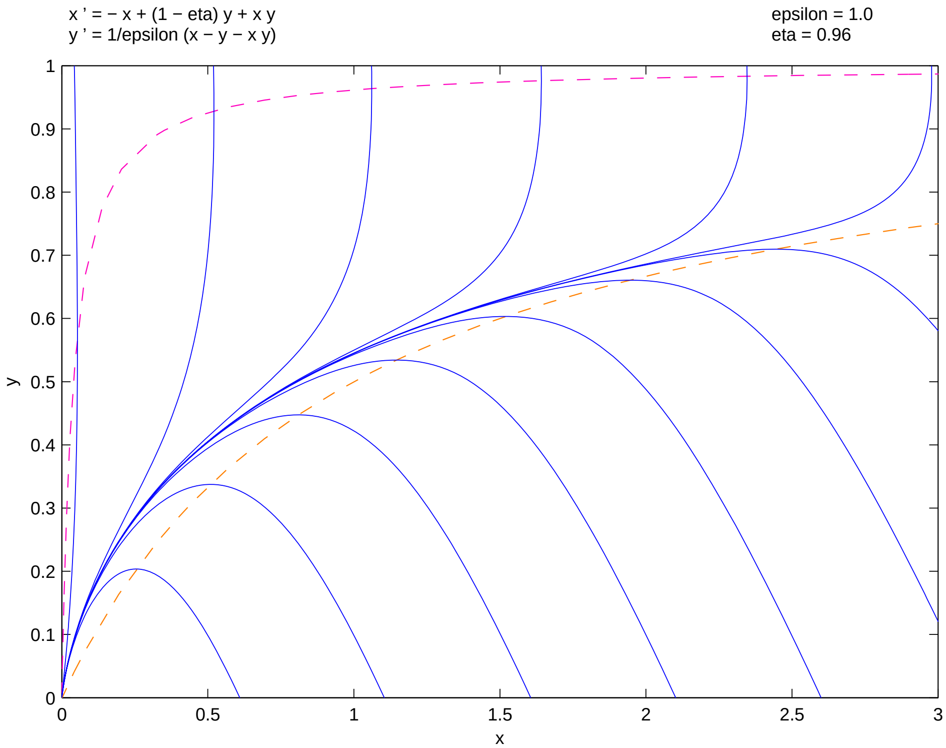

Figure 6.8: A phase portrait for (6.9) for $\varepsilon = 1.0$ and $\eta = 0.96$ in which $\sigma = 5$ and $\kappa = 1.5$.

6.6 The Matrix Exponential

The goal of this section is to find an explicit expression for the matrix exponential $\mathsf{e}^{t\mathbf{A}}$, where $\mathbf{A}$ is given in (6.15). Recall the fast $\mathbf{v}_+$ and slow $\mathbf{v}_-$ eigenvectors of $\mathbf{A}$, which were specified in (6.26). Observe that the eigenvectors have respective slopes[7]

$$\sigma_\pm := \frac{\lambda_\pm + 1}{1 - \eta}.$$

Define the matrix

$$\mathbf{P} := \begin{pmatrix} 1 & 1 \\ \sigma_+ & \sigma_- \end{pmatrix}$$

[7]We have already defined σ as the slope of $\mathbf{v}_+$, but in this section we want to refer to the slopes of both eigenvectors.

which has inverse

$$\mathbf{P}^{-1} = \frac{1}{\sigma_+ - \sigma_-}\begin{pmatrix} -\sigma_- & 1 \\ \sigma_+ & -1 \end{pmatrix}.$$

It follows that

$$\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{\Lambda},$$

where $\mathbf{\Lambda} := \mathsf{diag}\,(\lambda_+, \lambda_-)$. Moreover,

$$\mathbf{A} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^{-1}, \quad \mathsf{e}^{t\mathbf{\Lambda}} = \mathsf{diag}\left(\mathsf{e}^{\lambda_+ t}, \mathsf{e}^{\lambda_- t}\right), \quad \text{and} \quad \mathsf{e}^{t\mathbf{A}} = \mathbf{P}\mathsf{e}^{t\mathbf{\Lambda}}\mathbf{P}^{-1}.$$

Thus, we can write

$$\mathsf{e}^{t\mathbf{A}} = \mathsf{e}^{\lambda_+ t}\mathbf{B}_+ + \mathsf{e}^{\lambda_- t}\mathbf{B}_-,$$

where

$$\mathbf{B}_+ := \frac{1}{\sigma_+ - \sigma_-}\begin{pmatrix} -\sigma_- & -\sigma_- \\ \sigma_+ & \sigma_+ \end{pmatrix} \quad \text{and} \quad \mathbf{B}_- := \frac{1}{\sigma_+ - \sigma_-}\begin{pmatrix} \sigma_+ & \sigma_- \\ -\sigma_+ & -\sigma_- \end{pmatrix}.$$

Consider the initial value problem

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x}_0. \tag{6.29}$$

It is interesting to see how the exact solution of (6.29), which is given by $\mathsf{e}^{t\mathbf{A}}\mathbf{x}_0$, depends on the eigenvectors $\mathbf{v}_\pm$ in addition to the initial condition $\mathbf{x}_0$. Define the vectors and constants

$$\mathbf{w}_\pm := \begin{pmatrix} \varepsilon^{-1} \\ \lambda_\pm + 1 \end{pmatrix} \quad \text{and} \quad c_\pm := \frac{\mathbf{w}_\pm^T \mathbf{x}_0}{\mathbf{w}_\pm^T \mathbf{v}_\pm}.$$

Note that $\mathbf{w}_+$ and $\mathbf{w}_-$ are left eigenvectors of $\mathbf{A}$ which satisfy the orthogonality condition $\mathbf{w}_\pm^T \mathbf{v}_\mp = 0$. (See §A.14 of Appendix A for a review of left and right eigenvectors.) It can be shown that the unique solution of (6.29)

$$\mathbf{x}(t) = c_+\mathsf{e}^{\lambda_+ t}\mathbf{v}_+ + c_-\mathsf{e}^{\lambda_- t}\mathbf{v}_-.$$

Remarks 6.14:

(i) Observe that $c_\pm = 0$ if and only if $\mathbf{x}_0 \parallel \mathbf{v}_\mp$.

(ii) Note that $\mathbf{v}_+$ and $\mathbf{w}_+$ both point into the first quadrant and $\mathbf{v}_-$ and $\mathbf{w}_-$ both point into the second quadrant. This means that $\mathbf{w}_\pm^T \mathbf{v}_\pm > 0$. Furthermore, if we assume $\mathbf{x}_0 \neq \mathbf{0}$ then $\mathbf{x}_0$ points into the non-negative quadrant, thus $\mathbf{w}_+^T \mathbf{x}_0 > 0$ and $c_+ > 0$. Moreover, $c_- > 0$ if $\mathbf{x}_0$ is to the left of $\mathbf{v}_+$ and $c_- < 0$ if $\mathbf{x}_0$ is to the right of $\mathbf{v}_+$.

6.7 Literature Review

Throughout this introductory chapter, we included historical notes on the development of the Michaelis-Menten reaction. In this section, we will single out some other contributions to the literature, particularly those which apply to the mathematical study of the mechanism. Where mathematical expressions occur, we have converted them (if necessary) into the notation of this thesis.

Traditionally, the parameter ε is considered to be small. Hence, the system (6.9) with initial conditions $x(0) = x_0 > 0$ and $y(0) = 0$ can be treated as a singular perturbation problem. See, for example, [14, 45, 57, 67, 84]. A matched-asymptotic analysis yields the zeroth-order term of the outer solution

$$x^{(0)}_{\text{outer}}(t) = W\left(x_0 \mathsf{e}^{x_0 - \eta t}\right) \quad \text{and} \quad y^{(0)}_{\text{outer}} = H\left(x^{(0)}_{\text{outer}}(t)\right),$$

where W is the Lambert W function (see §A.16 of Appendix A). Observe that the QSSA is the zeroth-order term in the outer solution. Note that originally $x^{(0)}_{\text{outer}}(t)$ was given implicitly. Later, $x^{(0)}_{\text{outer}}(t)$ was given explicitly in terms of W as an example in [31] (which was where the Lambert W function was first given its name). The uniform approximation for $t \geq 0$ turns out to be

$$x_{\text{uniform}}(t) = W\left(x_0\, \mathsf{e}^{x_0 - \eta t}\right) \quad \text{and} \quad y_{\text{uniform}}(t) = H\left(x_{\text{uniform}}(t)\right) - H\left(x_0\right) \mathsf{e}^{-\varepsilon^{-1}(1+x_0)t}.$$

The correctness of the above analysis is proved using Tikhonov-Levinson Theory. In particular, the solution to initial value problem converges uniformly over a time interval $[0, T]$ as $\varepsilon \to 0^+$ to the uniform approximation. See, for example, [80, 98, 120, 125]. Moreover, explicit bounds on the approximations have been obtained for small ε. See, for example, [112]. Frank Hoppensteadt showed that we can take the interval $[0, T]$ for uniform convergence to be $[0, \infty)$. See, for example, [62, 63]. In Chapter 8, we will find estimates for the concentrations and time lengths, which are valid for all ε and η, for both the pre-steady-state period and the steady-state period.

Lee A. Segel and Marshall Slemrod, in [112], have argued that there is an optimal scaling for the singular perturbation approach. In particular, they choose $\varepsilon = \frac{e_0}{s_0 + K_m}$, where e_0 is the initial enzyme concentration, s_0 is the initial substrate concentration, and K_m is the Michaelis-Menten constant. Recall that the traditional scaling has $\varepsilon = \frac{e_0}{s_0}$ and that the scaling we are using in this thesis is $\varepsilon = \frac{e_0}{K_m}$. In a sense, the scaling we are using is an intermediate of the traditional and Segel-Slemrod choices for ε. Segel and Slemrod also extended and simplified the estimates of the two time scales in the singular perturbation problem.

The matrix **A** given in (6.15) has two strictly negative eigenvalues and so the Centre Manifold Theorem cannot be applied directly at the origin. However, Jack Carr in [23] on pages 8-10 used the system (6.9) as an example of approximating a parameter-based centre manifold. Re-scale the time by letting $\tau := \varepsilon^{-1}t$ and denote $' = \frac{d}{d\tau}$. Then, the system (6.9) can be written in the equivalent form

$$x' = \varepsilon r(x,z), \quad z' = -z + x^2 - xz + \varepsilon r(x,z), \quad \varepsilon' = 0,$$

where

$$r(x,z) := -x + (1-\eta+x)(x-z) \quad \text{and} \quad z := x - y.$$

The Centre Manifold Theorem applies to this system and hence there is a centre manifold $z = z(x,\varepsilon)$ which is C^∞ in a neighbourhood of the origin $(x,z,\varepsilon) = (0,0,0)$. To leading order,

$$z(x,\varepsilon) = -\varepsilon\eta x + y^2 + \mathcal{O}\big(x^3+\varepsilon^3\big) \quad \text{as} \quad x,\varepsilon \to 0^+$$

and thus[8]

$$y(x,\varepsilon) = (1+\varepsilon\eta)\,x - x^2 + \mathcal{O}\big(x^3+\varepsilon^3\big) \quad \text{as} \quad x,\varepsilon \to 0^+.$$

In Chapter 7, we will show that the slow manifold can be constructed as a centre manifold for a fixed point at infinity.

The phase portrait of the system (6.9) has been investigated by Simon J. Fraser, An Hoang Nguyen, Marc R. Roussel (formerly Fraser's Ph.D. student), and others. See, for example, [44, 92, 104]. The work for this part of the thesis is inspired by this dynamical systems approach. Two main themes of this work has been the recognition of the EA and QSSA as the isoclines and the approximation of the slow manifold.

Fraser and Roussel have argued informally that a unique slow manifold must indeed exist between the horizontal and vertical isoclines and be unique. See, for example, [43, 104, 106]. These arguments make use of the idea of antifunnels. See, for example, [64]. In Chapter 7, we will rigorously prove that the slow manifold exists and is unique.

[8] The slope σ of the slow eigenvector $\mathbf{v}_+$, which we defined earlier, satisfies

$$\sigma = 1 + \varepsilon\eta + \mathcal{O}\big(\varepsilon^2\big) \quad \text{as} \quad \varepsilon \to 0^+.$$

It was argued in [92] and [104], for example, that the slow manifold can be written as a Taylor series at the origin, $\mathcal{M}(x) = \sum_{n=0}^{\infty} \sigma_n x^n$. Obviously,

$$\sigma_0 = 0 \quad \text{and} \quad \sigma_1 = \sigma$$

and, for $n > 1$, it was found

$$\sigma_n = -\frac{\sum_{k=2}^{n-1} \left[(n-k)\sigma_{n-k} + (1-\eta)(n-k+1)\sigma_{n-k+1}\right]\sigma_k + \left[(n-1)\sigma_1 + \varepsilon^{-1}\right]\sigma_{n-1}}{\varepsilon^{-1} + (1-\eta)(n+1)\sigma_1 - n}.$$

In Chapter 7, we will show that this is not quite correct.

It was argued by Roussel, for example in [104], that the slow manifold, for large x, can be written $\mathcal{M}(x) \sim \sum_{n=0}^{\infty} \rho_n x^{-n}$ as $x \to \infty$. The coefficients are found to be

$$\rho_0 = 1, \quad \rho_1 = -1, \quad \rho_2 = 1, \quad \text{and} \quad \rho_n = -\rho_{n-1} + \varepsilon \sum_{i=1}^{n-2} i\rho_i \left[\rho_{n-i-1} + (1-\eta)\rho_{n-i-2}\right] \quad \text{for} \quad n > 2.$$

In Chapter 7, we will show that this asymptotic series is fully correct.

Fraser and Roussel have introduced and investigated an iteration procedure to approximate the slow manifold for all $x > 0$. See, for example, [43, 92, 104, 106, 107, 109]. These iterates are defined by $y_{n+1}(x) := F(x, y_n'(x))$, where $F(x,c)$ is found by solving $f(x,y) = c$ for $y = F(x,c)$ and f is the function defined in (6.12). A definitive proof of convergence of this scheme for all values of ε and η has not yet been given.

Roussel and Fraser, for example in [107], have used a linearized stability analysis to argue convergence for all $x \geq 0$ if ε is small. Furthermore, Roussel noted, for example in [104, 106], that if the initial function y_0 is analytic at the origin with $y_0'(0) \geq 0$, then the sequence of iterates $\{y_n\}_{n=1}^{\infty}$ converges to $\mathcal{M}$ at $x = 0$. We will extend this result in Appendix B. Finally, Roussel, in [104] on page 57 and 58, showed inductively that if

$$y_n(x) = \sum_{i=0}^{m} \rho_i x^{-i} + \mathcal{O}\Big(x^{-(m+1)}\Big) \quad \text{as} \quad x \to \infty$$

then

$$y_{n+1}(x) = \sum_{i=0}^{m+2} \rho_i x^{-i} + \mathcal{O}\Big(x^{-(m+3)}\Big) \quad \text{as} \quad x \to \infty,$$

where $\{\rho_i\}_{i=0}^{\infty}$ are as in the asymptotic series $\mathcal{M}(x) \sim \sum_{n=0}^{\infty} \rho_n x^{-n}$. Hence, two coefficients of the asymptotic expansion of $\mathcal{M}$ are gained for each iteration.

The Fraser scheme $y_{n+1}(x) := F(x, y_n'(x))$ is fairly reliable but does not converge in some cases. See, for example, [104]. Roussel suggested an alteration to the Fraser scheme in an attempt to force convergence. First, he wrote $y = F(x, y')$ equivalently as

$$y(x) + \xi(x)y(x) = F(x, y'(x)) + \xi(x)y(x),$$

where $\xi(x)$ is a yet-to-be-determined weighting function, which has the same fixed points as the original equation. New iterates are formed by writing

$$y_{n+1}(x) := \frac{F(x, y_n'(x)) + \xi(x)y_n(x)}{1 + \xi(x)}.$$

Choosing

$$\xi(x) := \frac{\varepsilon\eta x}{(1+x)^2}$$

preserves the good behaviour near $x = 0$ and $x = \infty$ that the Fraser scheme possesses but also suppresses any erratic behaviour in the intermediate values of x (based on a linearized stability analysis).

A Geometric singular perturbation approximation has been obtained for the slow manifold, for example, by Hans and Tasso Kaper, who are father and son mathematicians. See, for example, [68]. Here, they compared the Fraser iterates with initial function $y_0 := H$ and the perturbation series. They found that

$$y_n(x) = \sum_{m=0}^{n} \mathcal{M}_m(x)\varepsilon^m + \mathcal{O}\big(\varepsilon^{n+1}\big) \quad \text{as} \quad \varepsilon \to 0^+$$

for each n where $\{y_n\}_{n=0}^{\infty}$ are the Fraser iterates and

$$\mathcal{M}(x) = \sum_{m=0}^{\infty} \mathcal{M}_m(x)\varepsilon^m \quad \text{as} \quad \varepsilon \to 0^+$$

is the perturbation series.

The use of Intrinsic Low-Dimensional Manifolds (ILDMs) in chemical kinetics has been explored, for example, by Hans and Tasso Kaper in [68], U. Maas and S.B. Pope in [85], and Roussel on pages 50–56 of [104]. For the system (6.9), an example of an ILDM is the slow tangent manifold. The slow tangent manifold is not a solution of the differential equation but it does approximate the slow manifold. Let $\mathbf{v}_+(\mathbf{x})$ be a slow eigenvector for the Jacobian matrix $\mathbf{Dg}(\mathbf{x})$. The slow-tangent manifold $\mathcal{T}$ is the set of points $\mathbf{x}$ such that $\mathbf{v}_+(\mathbf{x})$ is parallel to $\mathbf{g}(\mathbf{x})$. By equating the slope of the slow eigenvector $\mathbf{v}_+(\mathbf{x})$ to the slope of the vector field $\mathbf{g}(\mathbf{x})$, one finds that the slow-tangent manifold $x = \mathcal{T}(y)$ is given by

$$\mathcal{T}(y) = \frac{y\left\{\left[1-\varepsilon\left(1-y\right)^2\right] + \sqrt{\left[1-\varepsilon\left(1-y\right)^2\right]^2 + 4\varepsilon\left(1-\eta\right)\left(1-y\right)^2}\right\}}{2\left(1-y\right)}.$$

In Chapter 7, we discuss another interpretation for the slow-tangent manifold.

6.8 Summary

We have seen the Michaelis-Menten mechanism for an enzyme reaction,

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E,$$

where S is the substrate, E is the enzyme, C is the complex, P is the product, and k_{-1}, k_1, and k_2 are the reaction-rate constants. The traditional equilibrium approximation (EA) and quasi-steady-state approximation (QSSA) yield, respectively,

$$c \approx \frac{e_0 s}{K_s + s} \quad \text{and} \quad c \approx \frac{e_0 s}{K_m + s},$$

where s is the concentration of the substrate, c is the concentration of the complex, e_0 is the initial concentration of the enzyme, and $K_s = \frac{k_{-1}+k_2}{k_1}$ and $K_m = \frac{k_{-1}}{k_1}$.

The Law of Mass Action, conservation laws, and a re-scaling give the dimensionless planar system

$$\dot{x} = -x + \left(1-\eta+x\right)y, \quad \varepsilon\dot{y} = x - \left(1+x\right)y,$$

where x is a scaled substrate concentration, y is a scaled complex concentration, $\dot{} = \frac{d}{dt}$, $\varepsilon > 0$ is a measure of the ratio of the different time scales involved, and $\eta \in (0,1)$ is another parameter. Furthermore, we form the equivalent scalar system

$$y' = \frac{x - \left(1+x\right)y}{\varepsilon\left[-x + \left(1-\eta+x\right)y\right]},$$

where $' = \frac{d}{dx}$. In this introductory chapter, we initiated our study of the solutions for the scalar and planar systems in the (physically relevant) non-negative quadrant S.

The horizontal and vertical isoclines for the planar system are, respectively,

$$H(x) = \frac{x}{1+x} \quad \text{and} \quad V(x) = \frac{x}{1-\eta+x}.$$

It turns out that the horizontal isocline is equivalent to the QSSA and the vertical isocline is equivalent to the EA. The region between the isoclines will be of importance and is denoted by

$$\Gamma_0 = \{ \ (x, y) \ : \ x > 0, \ H(x) \leq y \leq V(x) \ \} \, .$$

The linearization matrix at the origin, which is the sole equilibrium point of the planar system, is given by

$$\mathbf{A} = \begin{pmatrix} -1 & 1-\eta \\ \varepsilon^{-1} & -\varepsilon^{-1} \end{pmatrix}.$$

The fast and slow eigenvalues of $\mathbf{A}$ are

$$\lambda_{\pm} = \frac{-\left(\varepsilon+1\right) \pm \sqrt{\left(\varepsilon+1\right)^2 - 4\varepsilon\eta}}{2\varepsilon},$$

which are both real-valued and satisfy

$$\lambda_- < -1 < -\eta < \lambda_+ < 0.$$

There is resonance in the eigenvalues if and only if $\kappa \in \{2, 3, \ldots\}$, where

$$\kappa = \frac{\lambda_-}{\lambda_+}$$

is the ratio of the eigenvalues which satisfies $\kappa > 1$. Moreover, the slope of the slow eigenvector $\mathbf{v}_+$ of the matrix $\mathbf{A}$ is

$$\sigma = \frac{\lambda_+ + 1}{1-\eta},$$

which satisfies

$$1 < \sigma < \frac{1}{1-\eta}.$$

As we will show in Chapter 7, all solutions to the planar system enter the region Γ_0 and approach the origin in the slow direction with slope σ.

Figures 6.4 through 6.8 give computer-generated phase portraits for the planar system. In these phase portraits, there appears to be an exceptional solution between the horizontal and vertical isoclines. In Chapter 7, we will prove that this exceptional solution, which is called the slow manifold and is denoted by $y = \mathcal{M}(x)$, exists and is unique.

Chapter 7

Properties of Solutions in Phase Space

7.1 Introduction

The Michaelis-Menten mechanism, recall, is

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E,$$

where S, E, C, and P are, respectively, the substrate, enzyme, complex, and product. The Law of Mass Action, reduction via conservation laws, and a re-scaling give us the planar differential equation

$$\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x}) \tag{7.1}$$

and the corresponding scalar differential equation

$$y' = f(x, y), \tag{7.2}$$

where

$$\mathbf{g}(\mathbf{x}) = \begin{pmatrix} -x + (1 - \eta + x)\, y \\ \varepsilon^{-1}\, [x - (1 + x)\, y] \end{pmatrix} \quad \text{and} \quad f(x, y) = \frac{x - (1 + x)\, y}{\varepsilon\, [-x + (1 - \eta + x)\, y]}. \tag{7.3}$$

Note that t is a scaled time, x is a scaled substrate concentration, y is a scaled complex concentration, $\varepsilon > 0$ is a parameter, $\eta \in (0, 1)$ is another parameter, $\dot{} = \frac{d}{dt}$, and $' = \frac{d}{dx}$. The physically relevant portion of the xy-plane is the non-negative quadrant, which is denoted by S. Note also that the Jacobian of the vector field $\mathbf{g}$ at the origin is

$$\mathbf{A} = \begin{pmatrix} -1 & 1 - \eta \\ \varepsilon^{-1} & -\varepsilon^{-1} \end{pmatrix},$$

which has eigenvalues

$$\lambda_{\pm} = \frac{-(\varepsilon+1) \pm \sqrt{(\varepsilon+1)^2 - 4\varepsilon\eta}}{2\varepsilon}. \tag{7.4}$$

In this chapter, we will explore properties of solutions of the planar differential equation (7.1) in phase space for non-negative x and y. Equivalently, we will be studying solutions of the scalar differential equation (7.2).

7.2 Isoclines

The horizontal and vertical isoclines are usually the only two isoclines that are considered. However, we will make tremendous use of all of the isoclines for the planar system (7.1). Recall that the horizontal and vertical isoclines are, respectively,

$$H(x) = \frac{x}{1+x} \quad \text{and} \quad V(x) = \frac{x}{1-\eta+x}, \tag{7.5}$$

with the region between the isoclines denoted by

$$\Gamma_0 = \{\ (x,y)\ :\ x>0,\ H(x) \le y \le V(x)\ \}.$$

The most important isocline will turn out to be the isocline for slope σ, where σ is the slope of the slow eigenvector. From Chapter 6,

$$\sigma = \frac{\lambda_+ + 1}{1-\eta}, \tag{7.6}$$

where the slow eigenvalue λ_+ was given in (7.4).

7.2.1 Finding the Isoclines

The curve $y = w(x)$ is an isocline for slope $c \in \mathbb{R}$ if $f(x, w(x)) = c$ for all $x > 0$, where f is given in (7.3). Solving $f(x,y) = c$ for y gives

$$y = \frac{x}{K(c)+x},$$

where

$$K(c) := \frac{1+\varepsilon(1-\eta)c}{1+\varepsilon c}, \quad c \neq -\varepsilon^{-1}. \tag{7.7}$$

Hence, define the function

$$F(x,c) := \frac{x}{K(c)+x}, \quad c \neq -\varepsilon^{-1}, \quad x \neq -K(c). \tag{7.8}$$

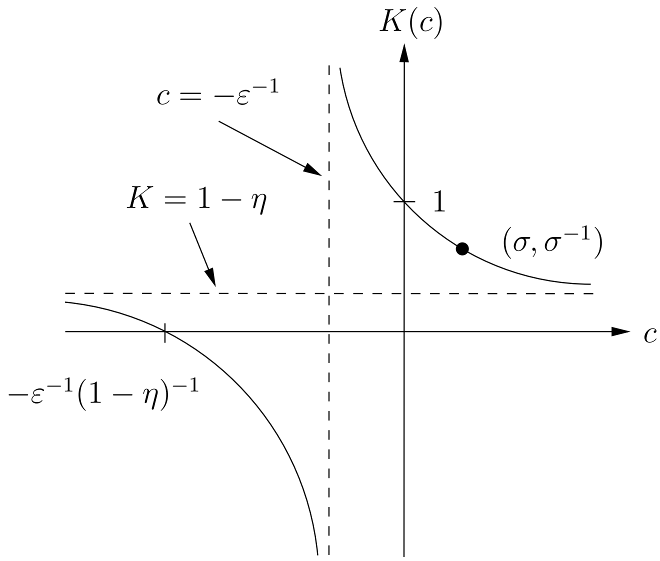

Figure 7.1: Graph of the function $K(c)$ for arbitrary $\varepsilon > 0$ and $\eta \in (0, 1)$.

It follows that $y = F(x, c)$ is the isocline for slope c. Observe that each isocline is a hyperbola (except when $K(c) = 0$) with vertical asymptote at $x = -K(c)$. Observe also that

$$y'(x) = f(x, y(x)) \quad \text{if and only if} \quad y(x) = F(x, y'(x)).$$

Claim 7.1: *Any of the isoclines w satisfy the differential equation*

$$w(w-1) + xw' = 0. \tag{7.9}$$

Proof: It is easy to show that $w(x) := \frac{x}{r+x}$ satisfies the given differential equation for any r. □

7.2.2 The Function K

In this subsection, we will establish some properties of the function K. Note that K is a transformed hyperbola since

$$K(c) = 1 - \eta \left[\frac{c}{\varepsilon^{-1} + c}\right].$$

A sketch of the graph of $r = K(c)$ is given in Figure 7.1.

Claim 7.2: *The function K satisfies*

$$K(\sigma) = \sigma^{-1}. \tag{7.10}$$

Proof: It can be shown by substituting (7.4) and (7.6) into (7.7) and simplifying. □

Claim 7.3: *We can invert $K(c) = r$ for $r \neq 1-\eta$ and differentiate $K(c)$ for $c \neq -\varepsilon^{-1}$ with*

$$K^{-1}(r) = \frac{r-1}{\varepsilon(1-\eta-r)}, \quad r \neq 1-\eta \quad \textit{and} \quad K'(c) = -\frac{\varepsilon\eta}{(1+\varepsilon c)^2}, \quad c \neq -\varepsilon^{-1}. \tag{7.11}$$

Proof: The proof is easy. □

Claim 7.4: *The functions K and F satisfy, for all $c \neq -\varepsilon^{-1}$,*

$$F(K(c), c) = \tfrac{1}{2} \quad \textit{and} \quad f\left(K(c), \tfrac{1}{2}\right) = c.$$

Proof: These can be shown directly by using the definitions (7.7) and (7.8) of K and F. □

Claim 7.5: *Let $u(c) := cK(c)$. Then,*

$$u(0) = 0, \quad u(\sigma) = 1 \quad \textit{and} \quad u'(c) \geq 1-\eta \quad \textit{for all} \quad c \geq 0. \tag{7.12}$$

Proof: See Figure 7.2, which gives a sketch of $u = cK(c)$. The fact that $u(0) = 0$ is obvious since $K(0) = 1$. Furthermore, the fact that $u(\sigma) = 1$ follows from (7.10). Finally, we show that $u'(c) \geq 1$. Since $u'(c) = K(c) + cK'(c)$, substituting (7.7) and (7.11) yields

$$u'(c) = \left(\frac{1}{1+\varepsilon c}\right)\left[1 + \varepsilon(1-\eta)c - \frac{\varepsilon\eta c}{1+\varepsilon c}\right] \geq \left(\frac{1}{1+\varepsilon c}\right)\left[1+\varepsilon(1-\eta)c - \eta\right] = 1-\eta.$$

□

Remarks 7.6:

(i) The interior of Γ_0 corresponds to $0 < c < \infty$ and $1-\eta < K(c) < 1$. Furthermore, $K(0) = 1$ corresponds to the horizontal isocline H and $\lim_{c\to\infty} K(c) = 1-\eta$ corresponds to the vertical isocline V.

(ii) There are two exceptional isoclines, namely $w(x) = 0$ and $w(x) = 1$. These correspond, respectively, to slope $c = -\varepsilon^{-1}$ and $c = -\varepsilon^{-1}(1-\eta)^{-1}$. For completeness, we will agree that $F\left(x, -\varepsilon^{-1}\right) = 0$.

(iii) The vertical isocline, V, also is somewhat of an exceptional case. Approaching it from below, one encounters increasing c up to $+\infty$. After passing through V, the slopes increase from $-\infty$ to $-\varepsilon^{-1}$. The reader is encouraged to compare Figure 7.3 and Table 6.1 for consistency.

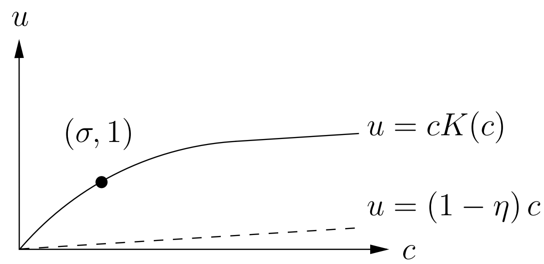

Figure 7.2: Graph of the function $u(c) := cK(c)$ for arbitrary $\varepsilon > 0$ and $\eta \in (0,1)$. The function is strictly increasing for $c > 0$ for every admissible ε and η. Furthermore, $u'(0) = 1$ and $\lim\limits_{c\to\infty} u'(c) = 1 - \eta$.

7.2.3 The Isocline Structure

Figure 7.3 sketches the isocline structure for the planar system (7.1). Occasionally, we will appeal to the isocline structure. For example, since the slow manifold is between the horizontal and vertical isoclines, the isocline structure shows that the slope of the slow manifold is always strictly positive.

7.3 Global Asymptotic Stability

The following result, which is formulated in terms of solutions of (7.1) which are functions of time, is necessary for understanding solutions in the phase plane.

Theorem 7.7: *Consider the planar system* (7.1)*.*

(a) The region Γ_0 is positively invariant.

(b) Let $\boldsymbol{x}(t)$ be the solution to (7.1) *with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in S \setminus \{\boldsymbol{0}\}$. Then, there is a $t^* \geq 0$ such that $\boldsymbol{x}(t) \in \Gamma_0$ for all $t \geq t^*$.*

(c) Let $\boldsymbol{x}(t)$ be the solution to (7.1) *with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in S$. Then,*

$$\lim_{t\to\infty} \boldsymbol{x}(t) = \boldsymbol{0}.$$

Proof:

(a) It follows from the definition (7.3) of the vector field $\mathbf{g}$ and Figure 7.4 that $\mathbf{g} \bullet \boldsymbol{\nu} < 0$ along V and H, where $\boldsymbol{\nu}$ is the outward unit normal vector. Thus, solutions cannot exit Γ_0 through

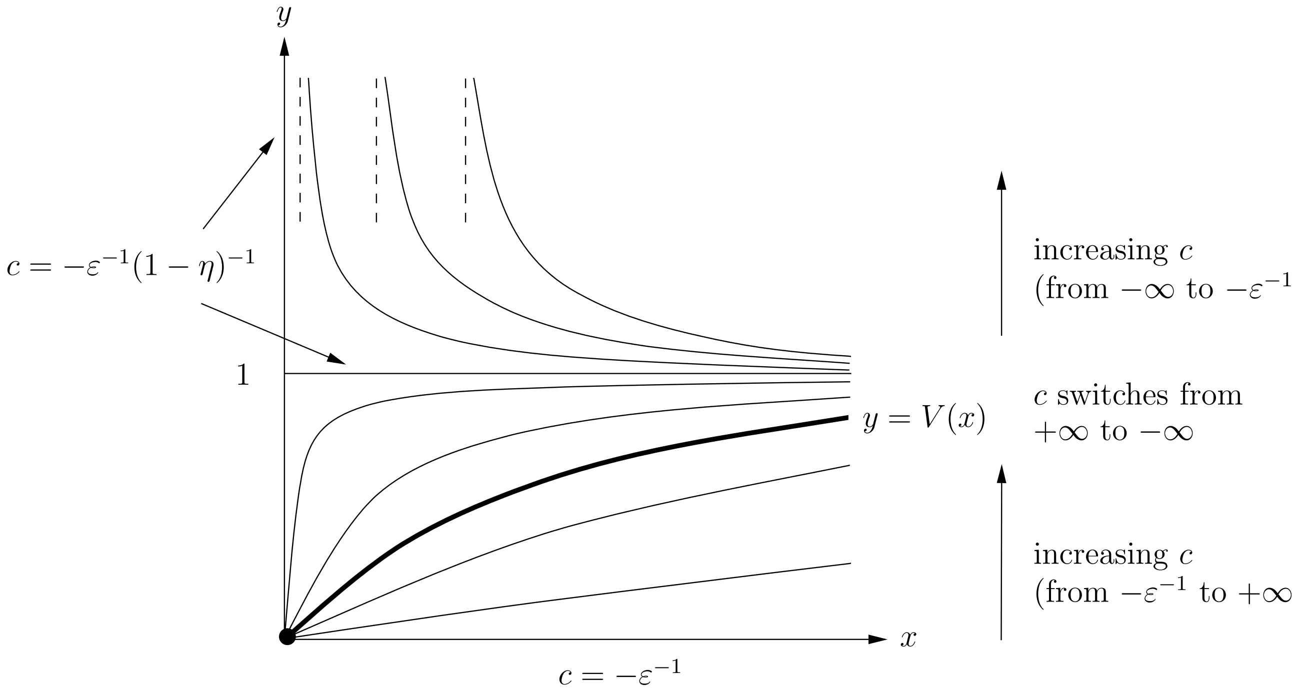

Figure 7.3: Sketch of the isocline structure of (7.1).

the horizontal or vertical isoclines. Furthermore, solutions cannot escape from Γ_0 through the origin since solutions do not intersect. Hence, Γ_0 is positively invariant.

(b) We will break the proof into cases.

Case 1: $(x_0, y_0) \in \Gamma_0$**.** Since Γ_0 is positively invariant, $\mathbf{x}(t) \in \Gamma_0$ for all $t \geq 0$.

Case 2: $x_0 > 0$ **and** $y_0 > V(x_0)$**.** Suppose, on the contrary, that $\mathbf{x}(t)$ does not enter Γ_0. It follows that $y(t) > V(x(t))$ for all $t \geq 0$. Using the differential equation (7.1), we know $\dot{x}(t) > 0$ and $\dot{y}(t) < 0$ for all $t \geq 0$. Now, we see from the definition (7.3) of the function f and Table 6.1 that

$$\frac{\dot{y}(t)}{\dot{x}(t)} = f(x(t), y(t)) < -\varepsilon^{-1} \quad \text{for all} \quad t \geq 0.$$

Thus,

$$\dot{y}(s) < -\varepsilon^{-1}\dot{x}(s) \quad \text{for all} \quad s \geq 0.$$

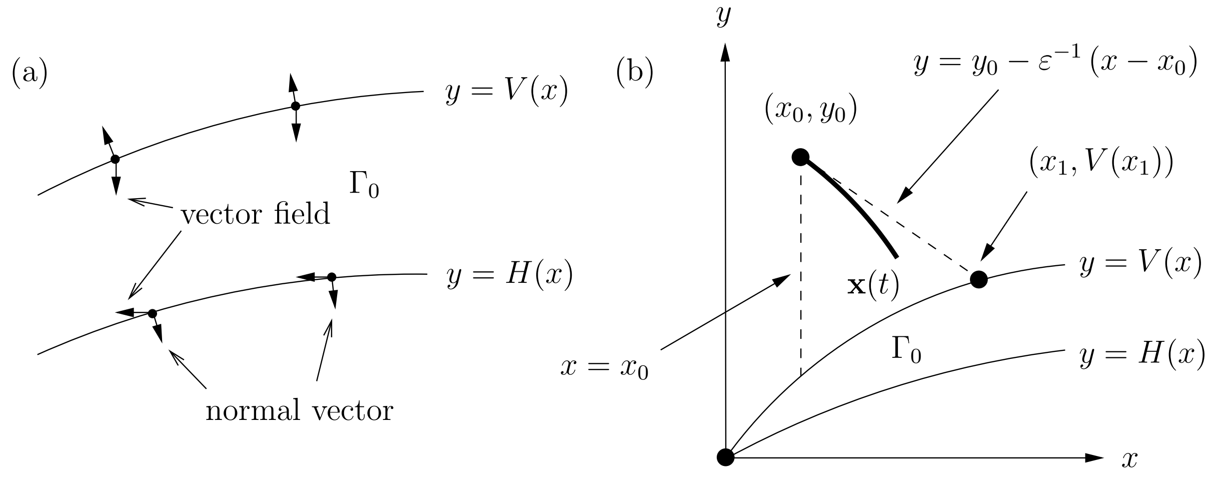

Figure 7.4: (a) The positive invariance of Γ_0. (b) Suppose that $x_0 > 0$ and $y_0 > V(x_0)$. If the solution $\mathbf{x}(t)$ never enters Γ_0, then $\mathbf{x}(t)$ is bounded by the line $x = x_0$, the vertical isocline $y = V(x)$, and the line $y = y_0 - \varepsilon^{-1}(x - x_0)$.

Integrating with respect to s from 0 to t and re-arranging, we obtain

$$y(t) \le y_0 - \varepsilon^{-1}[x(t) - x_0] \quad \text{for all} \quad t \ge 0.$$

Let $(x_1, V(x_1))$ be the point of intersection of the vertical isocline $y = V(x)$ and the straight line $y = y_0 - \varepsilon^{-1}(x - x_0)$. See Figure 7.4. Obviously, $x_1 > x_0$. Since $x(t)$ is monotone increasing and bounded above by x_1, we see that there is an $\overline{x} \in [x_0, x_1]$ such that $\lim_{t\to\infty} x(t) = \overline{x}$. Similarly, since $y(t)$ is monotone decreasing and bounded below by $V(x_0)$, we see that there is a $\overline{y} \in [y_0, V(x_0)]$ such that $\lim_{t\to\infty} y(t) = \overline{y}$. Thus, the ω-limit set is $\omega(x_0, y_0) = \{(\overline{x}, \overline{y})\}$. Since $\omega(x_0, y_0)$ is invariant and $(0,0)$ is the only equilibrium point of the system, $\overline{x} = 0$ and $\overline{y} = 0$. This is a contradiction.

Case 3: $x_0 > 0$ **and** $y_0 < H(x_0)$**.** This case is proved in a manner similar to Case 2.

Case 4: $x_0 = 0$ **and** $y_0 > 0$**.** It follows from the differential equation that $\dot{x}(0) = (1 - \eta)\, y_0 > 0$. So, $x(t) > 0$ and $y(t) > V(x(t))$ for sufficiently small $t > 0$. Thus, we can apply Case 2.

Case 5: $x_0 > 0$ **and** $y_0 = 0$**.** It follows from the differential equation that $\dot{y}(0) = \varepsilon^{-1} x_0 > 0$. So, $x(t) > 0$ and $0 < y(t) < H(x(t))$ for sufficiently small $t > 0$. Thus, we can apply Case 3.

(c) We can assume that $(x_0, y_0) \in \Gamma_0$ (since the trivial solution obviously satisfies the given limit and all other solutions eventually enter Γ_0). It follows from the differential equation (7.1) and the fact that Γ_0 is positively invariant that $\dot{x}(t) \leq 0$ and $\dot{y}(t) \leq 0$ for all $t \geq 0$. Since both $x(t)$ and $y(t)$ are strictly decreasing and bounded below by zero, by the Monotone Convergence Theorem we know that there are $\overline{x}$ and $\overline{y}$ such that $\lim_{t\to\infty} x(t) = \overline{x}$ and $\lim_{t\to\infty} y(t) = \overline{y}$. Thus, the ω-limit set is $\omega(x_0, y_0) = \{(\overline{x}, \overline{y})\}$. Since $\omega(x_0, y_0)$ is invariant and $(0, 0)$ is the only equilibrium point of the system, $\overline{x} = 0$ and $\overline{y} = 0$.

□

Remark 7.8: In the preceding proof, we twice had a situation in which $\lim_{t\to\infty} \mathbf{x}(t) = \overline{\mathbf{x}}$, where $\mathbf{x}(t)$ is a solution of (7.1). We can show that $\overline{\mathbf{x}} = \mathbf{0}$ without using the ω-limit set. Since $\mathbf{x}(t)$ is bounded, it follows from the differential equation that $\ddot{\mathbf{x}}(t)$ is bounded and hence $\dot{\mathbf{x}}(t)$ is uniformly continuous. Therefore, by Barbălat's Lemma (see §A.7 of Appendix A) $\mathbf{g}(\overline{\mathbf{x}}) = \mathbf{0}$ and hence $\overline{\mathbf{x}} = \mathbf{0}$.

7.4 Existence and Uniqueness of the Slow Manifold

In this section, we will prove the existence and uniqueness of a solution to the scalar differential equation (7.2) which lies entirely in the region Γ_0. To accomplish this, we will use the so-called Antifunnel Theorem. The reader may wish to consult §A.3 of Appendix A. A very good reference for funnels and antifunnels is [64].

7.4.1 Introduction

It is tempting to refer to Γ_0, the region between the horizontal and vertical isoclines, as an antifunnel. However, this would be incorrect. The reason is that the function f is infinite along the vertical isocline.

There are three possible courses of action to remedy this situation. First, we could extend the results to include the case where slopes are vertical along a fence. Second, we could develop analogous results for solutions that are curves as functions of time. The third possibility is the simplest and perhaps most rewarding. It turns out that there is a smaller, valid, traditional antifunnel within Γ_0. Hence, we would have better bounds on a unique solution lying within this new antifunnel.[1]

[1] In some ways, it would be simpler to consider only Γ_0. For example, we would only need to work with the intuitive region Γ_0.

The key to the proof is considering the isocline α for slope σ, where σ is the slope of the slow eigenvector. Equations (7.7), (7.8), and (7.10) tell us that α is given by the simple expression

$$\alpha(x) = \frac{x}{\sigma^{-1} + x}. \tag{7.13}$$

Claim 7.9: *The isocline α satisfies*

$$\alpha'(0) = \sigma, \quad \sigma = f(x, \alpha(x)) \quad \textit{for all} \quad x > 0, \quad \textit{and} \quad \alpha''(x) < 0 \quad \textit{for all} \quad x > 0.$$

Proof: The first property follows from differentiating (7.13) with respect to x and setting $x = 0$. The second property follows from the fact that α is the isocline for slope σ. Finally, the third property can be shown easily by differentiating (7.13) twice. □

Claim 7.10: *The curve $y = \alpha(x)$ is a strong lower fence and the curve $y = H(x)$ is a strong upper fence for the differential equation* (7.2) *for $x > 0$.*

Proof: The derivative of solutions to (7.2) along the concave-down curve $y = \alpha(x)$ is identically equal to σ. Thus,

$$\alpha'(x) < \alpha'(0) = \sigma = f(x, \alpha(x)) \quad \text{for all} \quad x > 0.$$

Hence, by definition, $y = \alpha(x)$ is a strong lower fence for $x > 0$. To show that $y = H(x)$ is a strong upper fence for $x > 0$, consider that

$$f(x, H(x)) = 0 < H'(x) \qquad \text{for all} \quad x > 0.$$

□

Remark 7.11: If $c \geq \sigma$ then the isocline $w(x) := F(x, c)$ is a strong lower fence. To see why, first let $r := K(c)$. Since w is concave down for all $x > 0$, we know $w'(x) < w'(0) = r^{-1}$ for all $x > 0$. Now, by virtue of (7.12), $r^{-1} \leq c$. Thus,

$$w'(x) < r^{-1} \leq c = f(x, w(x)) \quad \text{for all} \quad x > 0.$$

Claim 7.12: *The region*

$$\Gamma_1 := \{\ (x, y)\ :\ x > 0,\ H(x) \leq y \leq \alpha(x)\ \}$$

is a narrowing antifunnel for the differential equation (7.2)*.*

Proof: We know already that $y = \alpha(x)$ and $y = H(x)$ are strong fences for (7.2). Furthermore, the fences satisfy $\alpha(x) > H(x)$ for $x > 0$ and

$$\lim_{x\to\infty} |\alpha(x) - H(x)| = 0.$$

By definition, Γ_1 is a narrowing antifunnel. □

7.4.2 The Existence-Uniqueness Theorem

Theorem 7.13:

(a) There exists a unique slow manifold $y = \mathcal{M}(x)$ in Γ_1 for the scalar differential equation (7.2).

(b) The slow manifold $y = \mathcal{M}(x)$ is also the only solution that lies entirely in Γ_0.

Proof:

(a) We know from the isocline structure that $\frac{\partial f}{\partial y} \geq 0$ in Γ_1. So, all the conditions for the Antifunnel Theorem (Theorem A.4 on page 309) have been established. Therefore, there exists a unique solution $y = \mathcal{M}(x)$ to (7.2) that lies entirely in Γ_1.

(b) Let y be a solution in Γ_0 lying below $\mathcal{M}$. Since $\mathcal{M}$ is the only solution contained in Γ_1, y must leave Γ_1 through the horizontal isocline.

Now, let y be a solution in Γ_0 lying above $\mathcal{M}$. Suppose on the contrary that y never leaves Γ_0 and thus $\mathcal{M}(x) < y(x) < V(x)$ for all $x > 0$. Since $\mathcal{M}$ is the only solution contained in Γ_1, y must leave Γ_1 through the α isocline, say at $x = a$ for some $a > 0$. Since $\alpha'(x) < \sigma$ for all $x > 0$ and $y'(x) \geq \sigma$ if $y(x) \geq \alpha(x)$, we can conclude via a simple comparison argument that $\alpha(x) < y(x) < V(x)$ for all $x > a$. Hence, $y(x) > y(a) + \sigma\,(x - a)$ for all $x > a$. This implies that $y(x) > 1 > V(x)$ for sufficiently large x, which is a contradiction.

□

Remarks 7.14:

(i) Slow manifolds, like centre manifolds, are generally not unique and are defined locally. In our case, all solutions that have slope σ at the origin are slow manifolds. However, we look at the global phase portrait and refer to the unique solution within Γ_1 as *the* slow manifold.

(ii) It is easy to show

$$|\alpha(x) - H(x)| \leq \frac{\sigma - 1}{(\sqrt{\sigma} + 1)^2} \quad \text{and} \quad \frac{\sigma - 1}{(\sqrt{\sigma} + 1)^2} = \left(\tfrac{1}{4}\,\eta\right)\varepsilon + \mathcal{O}\big(\varepsilon^2\big) \quad \text{as} \quad \varepsilon \to 0^+.$$

Theorem 7.13 shows that $H(x) < \mathcal{M}(x) < \alpha(x)$. It follows that, uniformly in x, we have

$$\mathcal{M}(x) - H(x) = \mathcal{O}(\varepsilon) \quad \text{as} \quad \varepsilon \to 0^+.$$

(iii) If $w_1(x) < \mathcal{M}(x) < w_2(x)$ for all $x > 0$, where w_1 and w_2 are isoclines, then $w_1(x) \leq H(x)$ and $w_2(x) \geq \alpha(x)$ for all $x > 0$. This follows from the isocline structure and the fact (which we will show later) that $\lim_{x \to 0^+} \mathcal{M}'(x) = \sigma$ and $\lim_{x \to \infty} \mathcal{M}'(x) = 0$.

(iv) The isocline α gives the improved hyperbolic rate law

$$V \approx \frac{k_2 e_0 s}{(K_m \sigma^{-1}) + s}$$

for the velocity of the Michaelis-Menten reaction.

7.4.3 Nested Antifunnels

We can find a family of nested antifunnels using the isoclines as boundaries. These antifunnels will not be valid for all $x > 0$. Note that the antifunnel Γ_1, which we used to prove the existence and uniqueness of the slow manifold, can be regarded as a limiting case.

For an isocline $w(x) := F(x, c)$ to be a strong lower fence on an interval, we need $w'(x) < f(x, w(x))$. Now, solving the equation $w'(x) = f(x, w(x))$, as we shall see, yields $x = \sqrt{c^{-1}K(c)} - K(c)$. Hence, we define the function

$$\xi(c) := \sqrt{c^{-1}K(c)} - K(c), \quad c \in (0, \sigma). \tag{7.14}$$

We will now establish a few properties of the function $\xi(c)$. See Figure 7.5 for a sketch of $\xi(c)$.

Claim 7.15: *The function $\xi(c)$ satisfies*

$$\lim_{c \to 0^+} \xi(c) = +\infty, \quad \lim_{c \to \sigma^-} \xi(c) = 0, \quad \text{and} \quad \xi'(c) < 0 \quad \text{for all} \quad c \in (0, \sigma). \tag{7.15}$$

Proof: The first limit follows from the fact that $K(0) = 1$ and the second limit follows from the fact that $K(\sigma) = \sigma^{-1}$. To show that $\xi(c)$ is strictly decreasing on $(0, \sigma)$, we begin by writing

$$\xi(c) = \left[\sqrt{c^{-1}K(c)}\right]\left[1 - \sqrt{cK(c)}\right].$$

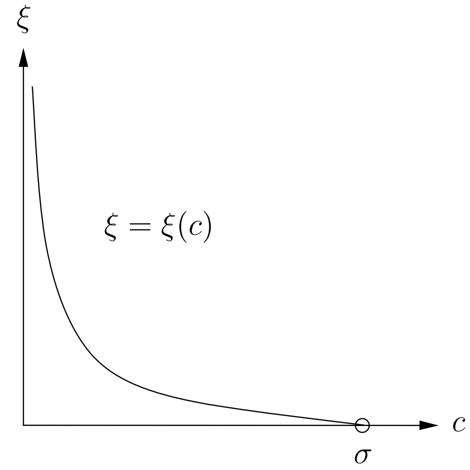

Figure 7.5: Graph of the function $\xi(c)$ for arbitrary $\varepsilon > 0$ and $\eta \in (0, 1)$.

Now, it follows from (7.7), (7.11), and (7.12) that, for any $c \in (0, \sigma)$,

$$\sqrt{c^{-1}K(c)} > 0, \quad 1 - \sqrt{cK(c)} > 0, \quad K(c) - cK'(c) > 0, \quad \text{and} \quad \frac{d}{dc}\left(cK(c)\right) > 0.$$

If we differentiate $\xi(c)$, for any $c \in (0, \sigma)$ we have

$$\xi'(c) = \left[\frac{cK'(c) - K(c)}{2c^2\sqrt{c^{-1}K(c)}}\right]\left[1 - \sqrt{cK(c)}\right] + \left[\sqrt{c^{-1}K(c)}\right]\left[-\left(\frac{1}{2\sqrt{cK(c)}}\right)\frac{d}{dc}\left(cK(c)\right)\right] < 0.$$

□

Claim 7.16: *The function $\xi(c)$ is analytic for all $c \in (0, \sigma)$. Furthermore, $\xi(c)$ has analytic inverse $\xi^{-1}(x)$ defined for all $x > 0$.*

Proof: It is clear from the definition (7.14) that $\xi(c)$ is analytic for all $c \in (0, \sigma)$. Using (7.15) in conjunction with the Real Analytic Inverse Function Theorem, we know that $\xi(c)$ is invertible for all $c \in (0, \sigma)$ and that $\xi^{-1}(x)$ is analytic for all $x > 0$. □

We are now in a position to establish on what interval a given isocline is a strong lower fence (or a strong upper fence). Observe that no isocline between the horizontal isocline and the α isocline is strong fence for all $x > 0$. That is, there are no isoclines between H and α that would give us a thinner antifunnel valid for all $x > 0$ with which to prove the existence and uniqueness of the slow manifold.

Proposition 7.17: *Let $c \in (0, \sigma)$ be fixed and let $w(x) := F(x, c)$ be the isocline for slope c.*

(a) The isocline w satisfies

$$w'(x) \begin{cases} > f(x, w(x)), & \text{if} \quad 0 < x < \xi(c) \\ = f(x, w(x)), & \text{if} \quad x = \xi(c) \\ < f(x, w(x)), & \text{if} \quad x > \xi(c) \end{cases} .$$

(b) The slow manifold satisfies

$$H(x) < \mathcal{M}(x) < w(x) \quad \text{for all} \quad x > \xi(c).$$

Proof:

(a) We know that

$$f(x, w(x)) = c \quad \text{and} \quad w'(x) = \frac{K(c)}{[K(c) + x]^2} \quad \text{for all} \quad x > 0.$$

We will show only the third case (the one that results in an antifunnel) since the first two cases are similar. Thus,

$$x > \sqrt{c^{-1}K(c)} - K(c) \implies \frac{K(c)}{[K(c) + x]^2} < c \implies w'(x) < f(x, w(x)).$$

(b) It follows from the Antifunnel Theorem.

∎

7.5 Behaviour Near $x = 0$: Introduction

We already know that all solutions $\mathbf{x}(t)$ to (7.1), except the trivial solution, eventually enter Γ_0. We also know that the slow manifold $\mathcal{M}$ separates the solutions; solutions either lie above $\mathcal{M}$ and enter Γ_0 through the vertical isocline or lie below $\mathcal{M}$ and enter Γ_0 through the horizontal isocline.

Proposition 7.18: *Let y be a solution to (7.2) lying inside Γ_0 for $x \in (0, a)$, where $a > 0$. Then, we can extend $y(x)$ and $y'(x)$ to say $y(0) = 0$ and $y'(0) = \sigma$.*

Proof: We should begin by emphasizing that solutions $\mathbf{x}(t)$ to (7.1) enter and forever remain in the interior of Γ_0. By hypothesis, $H(x) < y(x) < V(x)$ for all $x \in (0, a)$. The Squeeze Theorem establishes $y(0) = 0$ since $H(0) = V(0) = 0$.

To establish $y'(0) = \sigma$, observe that the function $\mathbf{g}$, as in (7.3), is C^2 with $\mathbf{g}(\mathbf{0}) = \mathbf{0}$ and the matrix $\mathbf{A} = \mathbf{Dg}(\mathbf{0})$ has strictly negative eigenvalues. It follows from Hartman's Theorem (see, for example, page 127 of [100]), which is a stronger version of the Hartman-Grobman Theorem and applies even in cases of resonance, that the phase portrait of (7.1) behaves like the phase portrait of the linear system $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$ diffeomorphically in a neighbourhood of the origin. Therefore, solutions to the nonlinear system have slope σ as they approach the origin too. □

7.6 Concavity

The goal of this section is to establish the concavity of solutions $y(x)$ to the scalar system (7.2) in all regions of the non-negative quadrant except for along the slow manifold. The concavity of the slow manifold will be established separately in §7.10. To achieve these results, we find and analyze an auxiliary function h which has the same sign as y''.

7.6.1 Introduction

Let y be a solution to (7.2), which we will assume is not the slow manifold because we will deal with that case later. Then, $y'(x) = f(x, y(x))$ where f is given in (7.3). By the Chain Rule,

$$y''(x) = \frac{\partial f}{\partial x}(x, y(x)) + \frac{\partial f}{\partial y}(x, y(x))f(x, y(x)).$$

A quick calculation shows that we can write

$$y''(x) = p(x, y(x))h(x, y(x)), \tag{7.16}$$

where

$$p(x, y) := \frac{\eta}{\varepsilon\left[-x + (1 - \eta + x)\, y\right]^2} \quad \text{and} \quad h(x, y) := y\,(y - 1) + xf(x, y). \tag{7.17}$$

The function $p(x, y)$ is positive everywhere except along the vertical isocline, where it is undefined. For a given solution y, we will overload the definitions of h and p and write

$$h(x) := h(x, y(x)) \quad \text{and} \quad p(x) := p(x, y(x)).$$

Claim 7.19: *For a given $x \geq 0$ with $y(x) \neq V(x)$, the sign of $h(x)$ is the same as the sign of $y''(x)$. Furthermore, the function h has derivative*

$$h'(x) = 2y(x)y'(x) + xp(x)h(x). \tag{7.18}$$

Proof: The first part follows from (7.16) and the fact that $p(x) > 0$. To show the second part, write

$$h(x) = y(x)^2 - y(x) + xy'(x).$$

Differentiating,

$$h'(x) = 2y(x)y'(x) - y'(x) + y'(x) + xy''(x) = 2y(x)y'(x) + xp(x)h(x),$$

where we applied (7.16). □

Remark 7.20: The function h cannot tell us anything about the concavity of solutions at $x = 0$, not even by taking a limit.

Claim 7.21: *Let $y(x)$ be a solution to (7.2) and let $x_0 \geq 0$ be such that $y(x_0) \neq V(x_0)$. Define $w(x) := F(x, y'(x_0))$, which is the isocline through the point $(x_0, y(x_0))$. Then,*

$$h(x_0) = x_0 \left[y'(x_0) - w'(x_0)\right]. \tag{7.19}$$

Furthermore, $y''(x_0) > 0$ if and only if $y'(x_0) > w'(x_0)$ and $y''(x_0) < 0$ if and only if $y'(x_0) < w'(x_0)$.

Proof: The first part follows from (7.9) and (7.17). The second part follows from the first. □

The concavity of all solutions in all regions of the non-negative quadrant can be deduced using the auxiliary function h. Table 7.1 summarizes what we will develop in this section. They are all suggested by the phase portraits in Figures 6.4 through 6.8 from Chapter 6.

7.6.2 Establishing the Results

A Lemma

Many of the following proofs will involve the following elementary lemma, so we single it out here.

Lemma 7.22: *Let I be one of the intervals $[a, b]$, (a, b), $[a, b)$, and $(a, b]$. Suppose that $\phi \in C(I)$ is a function having at least one zero in I.*

Region	Concavity of Solutions
$0 \le y < \mathcal{M}$	concave down
$\mathcal{M} < y < \alpha$	concave down, then inflection point, then concave up
$\alpha \le y < V$	concave up
$V < y < 1$	concave down
$y \ge 1$	concave up, then inflection point, then concave down

Table 7.1: This table gives a summary of the concavity of solutions of (7.2) in the non-negative quadrant.

(a) If $I = (a, b]$ or $I = [a, b]$, then the function ϕ has a right-most zero in I. Likewise, if $I = [a, b)$ or $I = [a, b]$, then the function ϕ has a left-most zero in I.

(b) If $\phi \in C^1(I)$ and $\phi'(x) > 0$ for every zero of ϕ in I, then ϕ has exactly one zero in I.

Proof: Let $R := \{x \in I \ : \ \phi(x) = 0\}$.

(a) We will prove that ϕ has a right-most zero in the case that $I = (a, b]$ or $I = [a, b]$. Let $c := \sup\limits_{x \in R} \{x\} \in [a, b]$, which exists by the Least Upper Bound Principle. Consider the sequence $\{u_n\}_{n=1}^{\infty} \subset R$ satisfying $c - \frac{1}{n} < u_n \le c$, which exists because R is non-empty and c is a least upper bound. Letting $n \to \infty$, we have that $u_n \to c$ and, by continuity, $\phi(u_n) \to \phi(c)$. However, $\phi(u_n) = 0$ for all n which implies that $\phi(c) = 0$ and hence $c \in R$. Therefore, c is the right-most zero of ϕ.

(b) For a contradiction, assume that there are two or more zeros. Let $[a', b'] \subset I$ be such that at least two of these zeros are in $[a', b']$. Let $x_2 \in R$ be the right-most zero of ϕ in $[a', b']$. Since $\phi'(x_2) > 0$, there is a $\delta > 0$ such that $\phi(x) < 0$ over $(x_2 - \delta, x_2)$. Let $d \in (x_2 - \delta, x_2)$ with $d > a'$. Now, ϕ has one or more zeros in $[a', d]$ and hence has a right-most zero in $[a', d]$, say $x_1 < d$. By construction, ϕ has no zeros in (x_1, x_2). However, since $\phi'(x_1) > 0$, there is a $c \in (x_1, d)$ such that $\phi(c) > 0$. Because $\phi(d) < 0$, ϕ has a zero in $(c, d) \subset (x_1, x_2)$, by the Intermediate Value Theorem. This is a contradiction.

$\square$

Remark 7.23: The condition that the endpoint be included for there to be a left-most or right-most zero is essential. For example, consider the function $x\ \mathsf{sin}\big(x^{-1}\big)$ which is extended continuously to be 0 at $x = 0$. This function does not have a left-most zero over $(0, 1)$ but does have a left-most zero over $[0, 1)$.

Concavity Below $\mathcal{M}$

Proposition 7.24: *Let $y(x)$ be any solution to* (7.2) *lying below the slow manifold, say with domain* $(0, a]$ *where $a > 0$ and $y(a) = 0$. Then, y is concave down for all $x \in (0, a]$.*

Proof: Let h be defined as in (7.17) with respect to the solution y. There are two regions to consider, namely where $y(x) > H(x)$ and where $y(x) \leq H(x)$.

First, we show that $y''(x) < 0$ when $y(x) \leq H(x)$. It is clear from (7.16) and (7.17) that $y''(x) < 0$ for $y(x) \leq H(x)$, noting that $0 \leq y(x) < 1$ and $y'(x) < 0$.

Second, we show that $y''(x) < 0$ when $H(x) < y(x) < \mathcal{M}(x)$. The solution $y(x)$ crosses the horizontal isocline, say at $x = x_2 \in (0, a)$. We see from (7.17) that $h(x_2) < 0$. By continuity, we need only show that h has no zeros in $(0, x_2]$. Suppose on the contrary that h has one or more zeros in $(0, x_2]$. Applying Lemma 7.22, let $x_1 \in (0, x_2)$ be the right-most zero of h. Using (7.18), $h'(x_1) = 2y(x_1)y'(x_1) > 0$. Then, h is positive in a neighbourhood to the right of x_1. Since $h(x_2) < 0$, by the Intermediate Value Theorem, h has a zero in (x_1, x_2) which contradicts the fact that x_1 is the right-most zero. □

Concavity Between $\mathcal{M}$ and α

Proposition 7.25: *Let y be any solution to* (7.2) *lying between $\mathcal{M}$ and α, say with domain* $(0, a]$ *where $a > 0$ and $y(a) = \alpha(a)$. Then, there is a unique $x_1 \in (0, a)$ such that $y''(x_1) = 0$. Moreover, y is concave down on $(0, x_1)$ and concave up on $(x_1, a]$.*

Proof: We know $y'(0) = \sigma$ and $y'(a) = \sigma$. Hence, by Rolle's Theorem, y has an inflection point $x_1 \in (0, a)$. To prove uniqueness of the inflection point, let h be as in (7.17) with respect to the solution y. Now, if x is a zero of h, then $h'(x) = 2y(x)y'(x) > 0$. By Lemma 7.22, h has no other inflection point in $(0, a)$. Moreover, since $h'(x_1) > 0$, y is concave down on $(0, x_1)$ and concave up on $(x_1, a]$. □

Concavity Between α and V

Proposition 7.26: *Let y be any solution to (7.2) lying between α and V, say with domain (a,b) where $0 < a < b$, $\lim_{x\to a^+} y(x) = \alpha(a)$, and $\lim_{x\to b^-} y(x) = V(b)$. Then, y is concave up on (a,b).*

Proof: Fix $x_0 \in (a,b)$. Let $c := y'(x_0)$ and $r := K(c)$. Since $c > \sigma$, (7.12) tells us that $rc > 1$ which in turn implies $r < \sqrt{rc^{-1}}$. Let $w(x) := F(x,c)$ be the isocline through $(x_0, y(x_0))$. With h defined as in (7.17) with respect to y, we have

$$h(x_0) = x_0 \left[c - \frac{r}{(r+x_0)^2}\right] = x_0 \left[\frac{c\,(r+x_0)^2 - r}{(r+x_0)^2}\right],$$

where we used the expression for h in Equation (7.19). Suppose, on the contrary, that $y''(x_0) \le 0$. Then, $c\,(r+x_0)^2 - r \le 0$ which implies $x_0 \le \sqrt{rc^{-1}} - r < 0$. This is a contradiction. □

Concavity Between V and $y = 1$

Proposition 7.27: *Let y be a solution to (7.2) which lies above V and below 1, with domain $[a,b)$ where $0 \le a < b$, $y(a) < 1$, and $\lim_{x\to b^-} y(x) = V(b)$. Then, y is concave down for all $x \in [a,b)$.*

Proof: It is clear from the expression for h, Equation (7.17), where h is defined with respect to the solution y, and the fact that $y' < 0$ in that region. □

Concavity Above $y = 1$

Proposition 7.28: *Let y be a solution to (7.2) which lies above 1, with domain $[0,a]$ where $a > 0$ and $y(a) = 1$. Then, there is a unique $x_1 \in (0,a)$ such that $y''(x_1) = 0$. Moreover, y is concave up over $[0,x_1)$ and concave down over $(x_1,a]$.*

Proof: Let h be defined as in Equation (7.17) with respect to the solution y. We know that $y'(0) = -\varepsilon^{-1}(1-\eta)^{-1}$ and $y'(a) = -\varepsilon^{-1}(1-\eta)^{-1}$. By Rolle's Theorem, there exists $x_1 \in (0,a)$ such that $y''(x_1) = 0$. The uniqueness of the inflection point follows from the fact that any zero x of h in $(0,a)$ satisfies $h'(x) < 0$ and an application of Lemma 7.22. Moreover, since $h'(x_1) < 0$, y is concave up on $[0,x_1)$ and concave down on $(x_1,a]$. □

Remark 7.29: The above result does not cover the point $(0,1)$. If y is the solution to (7.2) through the point $(0,1)$, then (7.17) shows us that $(0,1)$ is an inflection point.

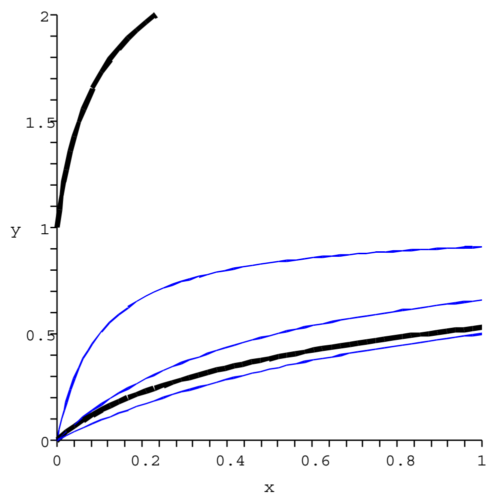

Figure 7.6: The two thick curves are curves along which solutions of (7.2) have inflection points, for parameter values $\varepsilon = 0.6$ and $\eta = 0.9$. The thin curves are the horizontal, α, and vertical isoclines.

7.6.3 Curves of Inflection Points

We now know that solutions can only have inflection points between $\mathcal{M}$ and α and above $y = 1$. There are, in fact, curves along which solutions have zero second derivative. Using the definition (7.3) of f and the definition (7.17) of h,

$$h(x,y) = \frac{\varepsilon\,(1-\eta+x)\,y^3 - \varepsilon\,(1-\eta+2x)\,y^2 + \left[(\varepsilon-1)\,x - x^2\right]y + x^2}{\varepsilon\left[-x + (1-\eta+x)\,y\right]}.$$

Thus, there are three curves along which solutions have zero second derivative, given implicitly by

$$\varepsilon\,(1-\eta+x)\,y^3 - \varepsilon\,(1-\eta+2x)\,y^2 + \left[(\varepsilon-1)\,x - x^2\right]y + x^2 = 0.$$

One curve lies below the x-axis and is discarded. The other two curves are in the positive quadrant, one lying between $\mathcal{M}$ and α, the other starting at the point $(0, 1)$ and increasing with x. See Figure 7.6.

We know that, for a given slope $c \in (0, \sigma)$, the isocline $w(x) := F(x, c)$ switches from being a strong upper fence to being a strong lower fence at $x = \xi(c)$, where $F(x, c)$ was defined in (7.8) and $\xi(c)$ was defined in (7.14). Thus, we expect the point $(\xi(c), F(\xi(c), c))$ to be an inflection point for the scalar solution through this point. To put this another way, for a given $x > 0$ we expect the point $\left(x, F(x, \xi^{-1}(x)\right)$ to be an inflection point for the scalar solution through this point. Hence, we define the function

$$\mathcal{Y}(x) := F\left(x, \xi^{-1}(x)\right), \quad x > 0. \tag{7.20}$$

We claim that $y = \mathcal{Y}(x)$ is a curve between $y = \mathcal{M}(x)$ and $y = \alpha(x)$ along which solutions to the scalar differential equation (7.2) have inflection points. Note that, by virtue of the isocline structure, $H(x) < F(x, c) < \alpha(x)$ for all $x > 0$ and $c \in (0, \sigma)$. Note also that $0 < \xi^{-1}(x) < \sigma$ for all $x > 0$. It follows from the definition of $\mathcal{Y}(x)$ that $H(x) < \mathcal{Y}(x) < \alpha(x)$ for all $x > 0$.

Claim 7.30: *Suppose that $x_0 > 0$ and $H(x_0) < y_0 < \alpha(x_0)$. Define the slope $c := f(x_0, y_0)$ and isocline $w(x) := F(x, c)$. Then, the isocline w satisfies*

$$w'(x_0) \begin{cases} > f(x_0, y_0), & \textit{if} \quad H(x_0) < y_0 < \mathcal{Y}(x_0) \\ = f(x_0, y_0), & \textit{if} \quad y_0 = \mathcal{Y}(x_0) \\ < f(x_0, y_0), & \textit{if} \quad \mathcal{Y}(x_0) < y_0 < \alpha(x_0) \end{cases}.$$

Proof: Note that $0 < c < \sigma$ and $y_0 = w(x_0)$. We will only show the third case since the other two cases are similar. Assume that $\mathcal{Y}(x_0) < y_0 < \alpha(x_0)$. Appealing to the isocline structure, we know $\frac{\partial f}{\partial y}(x, y) > 0$ if $x > 0$ and $H(x) < y < \alpha(x)$. Thus, $f(x_0, y_0) > f(x_0, \mathcal{Y}(x_0))$. Since $c = f(x_0, y_0)$ and $\xi^{-1}(x_0) = f(x_0, \mathcal{Y}(x_0))$, we have $c > \xi^{-1}(x_0)$. Since ξ is strictly decreasing, $x_0 > \xi(c)$. By virtue of Proposition 7.17, we can conclude $w'(x_0) < f(x_0, y_0)$. $\square$

Claim 7.31: *The curve $y = \mathcal{Y}(x)$ is analytic for all $x > 0$.*

Proof: We know that $\xi^{-1}(x)$ is analytic and $0 < \xi^{-1}(x) < \sigma$ for all $x > 0$. Since $F(x, c)$ is analytic if $x > 0$ and $0 < c < \sigma$, we see from the definition (7.20) that $\mathcal{Y}(x)$ is analytic for all $x > 0$. $\square$

Proposition 7.32: *The function h, defined in* (7.17), *satisfies*

$$h(x, y) \begin{cases} < 0, & \textit{if} \quad x > 0, \ H(x) < y < \mathcal{Y}(x) \\ = 0, & \textit{if} \quad x > 0, \ y = \mathcal{Y}(x) \\ > 0, & \textit{if} \quad x > 0, \ \mathcal{Y}(x) < y < \alpha(x) \end{cases}.$$

Proof: Let $x_0 > 0$ and $H(x_0) < y_0 < \alpha(x_0)$ be fixed. Consider the slope $c := f(x_0, y_0)$ and isocline $w(x) := F(x, c)$. We know from Claim 7.21 that

$$h(x_0, y_0) = x_0 \left[f(x_0, y_0) - w'(x_0) \right].$$

The result follows from Claim 7.30. □

Proposition 7.33: *The curve $y = \mathcal{Y}(x)$ satisfies*

$$\mathcal{M}(x) < \mathcal{Y}(x) < \alpha(x) \quad \textit{for all} \quad x > 0.$$

Proof: We know already that $H(x) < \mathcal{Y}(x) < \alpha(x)$ for all $x > 0$. From our results on concavity, we know $h(x, y) < 0$ if $x > 0$ and $H(x) < y < \mathcal{M}(x)$, where h is the function defined in (7.17). By continuity, we can conclude $h(x, \mathcal{M}(x)) \leq 0$ for all $x > 0$. It follows from Proposition 7.32 that $\mathcal{M}(x) \leq \mathcal{Y}(x)$ for all $x > 0$.

To establish a strict inequality, let h be defined along the solution $y = \mathcal{M}(x)$. Assume, on the contrary, that there is an $x_0 > 0$ such that $h(x_0) = 0$. Using (7.18), $h'(x_0) > 0$. This contradicts the fact that $h(x) \leq 0$ for all $x > 0$. □

Claim 7.34: *The slope of the curve of inflection points $y = \mathcal{Y}(x)$ satisfies*

$$\lim_{x \to 0^+} \mathcal{Y}'(x) = \sigma.$$

Proof: We know that $\mathcal{M}(x) < \mathcal{Y}(x) < \alpha(x)$ for all $x > 0$. We also know that

$$\lim_{x \to 0^+} \mathcal{M}(x) = 0, \quad \lim_{x \to 0^+} \mathcal{M}'(x) = \sigma, \quad \lim_{x \to 0^+} \alpha(x) = 0, \quad \text{and} \quad \lim_{x \to 0^+} \alpha'(x) = \sigma.$$

Letting $x \to 0^+$ and applying the Squeeze Theorem, we see

$$\lim_{x \to 0^+} \mathcal{Y}(x) = 0.$$

Now,

$$\frac{\mathcal{M}(x) - 0}{x} < \frac{\mathcal{Y}(x) - 0}{x} < \frac{\alpha(x) - 0}{x} \quad \text{for all} \quad x > 0.$$

Letting $x \to 0^+$ and applying the Squeeze Theorem again gives the conclusion. □

7.6.4 The Slow Tangent Manifold

The slow tangent manifold $\mathcal{T}$ is an approximation used by, for example, Marc Roussel to approximate the slow manifold. Recall that the slow tangent manifold consists of the points for which the tangent vector for a flow points in the slow direction. Explicitly, $x = \mathcal{T}(y)$ is given by

$$\mathcal{T}(y) = \frac{y\left\{\left[1 - \varepsilon(1-y)^2\right] + \sqrt{\left[1 - \varepsilon(1-y)^2\right]^2 + 4\varepsilon(1-\eta)(1-y)^2}\right\}}{2(1-y)}.$$

We will show that, in general, a curve of points where the second derivative of a scalar solution is zero is actually equivalent to a tangent manifold. This result will be specialized to the planar system (7.1) and the scalar system (7.2). Similar results have been obtained by Masami Okuda in [94, 95, 96].

The General Systems

Consider the general planar system

$$\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x}), \tag{7.21}$$

where $\dot{} = \frac{d}{dt}$ and $\mathbf{g} \in C^1(\mathbb{R}^2, \mathbb{R}^2)$. To make the expressions less cumbersome, we will use the notation $g_{ij} := \frac{\partial g_i}{\partial x_j}$ and suppress the dependence on $\mathbf{x}$ where there will be no confusion. Consider also the scalar system

$$y' = \frac{g_2(x,y)}{g_1(x,y)}, \tag{7.22}$$

where $' = \frac{d}{dx}$.

The Jacobian of the vector field $\mathbf{g}$ is the matrix

$$\mathbf{A} := \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}.$$

The characteristic equation of $\mathbf{A}$ is

$$(\lambda - g_{11})(\lambda - g_{22}) - g_{12}g_{21} = 0. \tag{7.23}$$

Alternatively, the characteristic equation can be written

$$\lambda^2 - \tau\lambda + \Delta = 0, \tag{7.24}$$

where

$$\tau := g_{11} + g_{22} \quad \text{and} \quad \Delta := g_{11}g_{22} - g_{12}g_{21}.$$

The slow tangent manifold will be constructed in terms of the eigenvalues and eigenvectors of the Jacobian matrix.

Claim 7.35: *Suppose $4\Delta < \tau^2$ and $g_{12} \neq 0$. Then, $\boldsymbol{A}$ has real and distinct eigenvalues*

$$\lambda_\pm := \frac{\tau \pm \sqrt{\tau^2 - 4\Delta}}{2}. \tag{7.25}$$

Furthermore, the matrix $\boldsymbol{A}$ has distinct eigenvectors

$$\boldsymbol{v}_{\pm} := \begin{pmatrix} 1 \\ \sigma_{\pm} \end{pmatrix}, \quad \textit{where} \quad \sigma_{\pm} := \frac{\lambda_{\pm} - g_{11}}{g_{12}}. \tag{7.26}$$

Proof: First, solving the characteristic equation (7.24) yields the eigenvalues $\lambda_{\pm}$. The restriction on τ and Δ ensures that the eigenvalues are distinct and real with $\lambda_{-} < \lambda_{+}$. Second, it is clear that $\mathbf{v}_{\pm} \neq \mathbf{0}$ and $\mathbf{v}_{+} \neq \mathbf{v}_{-}$. Finally, it is easy to confirm using the definitions of $\mathbf{A}$, $\mathbf{v}_{\pm}$, and $\sigma_{\pm}$ in conjunction with the characteristic equation (7.23) that $(\lambda_{\pm}\mathbf{I} - \mathbf{A})\,\mathbf{v}_{\pm} = \mathbf{0}$. Thus, $\mathbf{v}_{\pm}$ is an eigenvector of $\mathbf{A}$ with associated eigenvalue $\lambda_{\pm}$. ☐

Proposition 7.36: *Consider the planar system* (7.21) *and the scalar system* (7.22)*. Suppose that $g_1 \neq 0$, $g_{12} \neq 0$, and $4\Delta < \tau^2$ at some fixed point (a, b). Let $y(x)$ be a scalar solution through (a, b). Then, $y''(a) = 0$ if and only if $\boldsymbol{g} \parallel \boldsymbol{v}_{+}$ or $\boldsymbol{g} \parallel \boldsymbol{v}_{-}$ at (a, b).*

Proof: By the Chain Rule, if we differentiate (7.22) with respect to x we get

$$y'' = \frac{g_1\left[g_{21} + g_{22}\left(\frac{g_2}{g_1}\right)\right] - \left[g_{11} + g_{12}\left(\frac{g_2}{g_1}\right)\right] g_2}{g_1^2}.$$

It is routine (but tedious) to show, using (7.25) and (7.26), that

$$y'' = \frac{-g_{12}\left[\left(\frac{g_2}{g_1}\right) - \sigma_{+}\right]\left[\left(\frac{g_2}{g_1}\right) - \sigma_{-}\right]}{g_1}.$$

Recall that $\sigma_{\pm}$ is the slope of the eigenvector $\mathbf{v}_{\pm}$. Thus, $\mathbf{g} \parallel \mathbf{v}_{\pm}$ is equivalent to $\sigma_{\pm} = \frac{g_2}{g_1}$. The conclusion follows. ☐

The Michaelis-Menten Mechanism

We now return to the specific planar system (7.1) and scalar system (7.2) for the Michaelis-Menten mechanism. Here,

$$\mathbf{A} = \begin{pmatrix} y - 1 & 1 - \eta + x \\ \frac{1-y}{\varepsilon} & -\frac{1+x}{\varepsilon} \end{pmatrix}, \quad \tau = y - 1 - \frac{1+x}{\varepsilon}, \quad \text{and} \quad \Delta = \frac{\eta\,(1-y)}{\varepsilon}.$$

To apply Proposition 7.36, we need to check the conditions. Observe that $g_1 \neq 0$ except along the vertical isocline. Furthermore, $g_{12} > 0$ if $x \geq 0$. Finally, to show that $\tau^2 > 4\Delta$ for $x \geq 0$, observe that

$$\tau^2 - 4\Delta = \left[y - \frac{\varepsilon + 1 - 2\eta + x}{\varepsilon}\right]^2 + \frac{4\eta\,(1 - \eta + x)}{\varepsilon^2} \geq \frac{4\eta\,(1 - \eta + x)}{\varepsilon^2} > 0.$$

It follows from Proposition 7.36 that the curve of inflection points $y = \mathcal{Y}(x)$ is a tangent manifold. Furthermore, the curve of inflection points above the line $y = 1$ (see Figure 7.6) is also a tangent manifold.

7.7 Behaviour Near $x = 0$: Conclusion

We have already shown that scalar solutions $y(x)$ inside the trapping region Γ_0 satisfy $y(0) = 0$ and $y'(0) = \sigma$. The goal of this section is obtain an improved asymptotic expression for $y(x)$ as $x \to 0^+$. It is at this point in the chapter that we need to start worrying about the ratio of the eigenvalues

$$\kappa = \frac{\lambda_-}{\lambda_+}.$$

Recall that $\kappa > 1$. Moreover, $\kappa \in \{2, 3, \ldots\}$ if and only if there is resonance in the eigenvalues.

7.7.1 The Power Series Method

Recall that it was argued by Fraser and Roussel that the slow manifold can be written as a Taylor series $\mathcal{M}(x) = \sum_{n=0}^{\infty} \sigma_n x^n$ at the origin. Clearly,

$$\sigma_0 = 0 \quad \text{and} \quad \sigma_1 = \sigma. \tag{7.27a}$$

To obtain the remaining coefficients $\{\sigma_n\}_{n=2}^{\infty}$, the series can be substituted into the differential equation yielding the recursive expression

$$\sigma_n = -\frac{\sum_{k=2}^{n-1} \left[(n-k)\,\sigma_{n-k} + (1-\eta)\,(n-k+1)\,\sigma_{n-k+1}\right]\sigma_k + \left[(n-1)\,\sigma_1 + \varepsilon^{-1}\right]\sigma_{n-1}}{\varepsilon^{-1} + (1-\eta)\,(n+1)\,\sigma_1 - n}, \quad n \geq 2. \tag{7.27b}$$

We need to make two observations about the Taylor series. First, suppose that $\varepsilon = 1$ and $\eta = \frac{24}{25}$. Then, $\kappa = \frac{3}{2}$, $\sigma_1 = 5$, and $\sigma_2 = 75$. However, Propositions 7.32 and 7.33 imply that $\mathcal{M}''(x) < 0$ for all $x > 0$. Therefore, for these parameter values we cannot write the slow manifold as the Taylor series $\mathcal{M}(x) = \sum_{n=0}^{\infty} \sigma_n x^n$ at the origin. Second, since the slow manifold is defined according to its global behaviour, we expect that the conclusions we draw regarding coefficients $\{\sigma_n\}_{n=0}^{\infty}$ can be applied to all scalar solutions lying inside Γ_0.

Let $y(x)$ be a scalar solution to (7.2) lying inside the trapping region Γ_0. We will show that

$$y(x) \sim \sum_{n=0}^{\ell} \sigma_n x^n \quad \text{as} \quad x \to 0^+$$

for some $\ell \in \mathbb{N}_0$ which is determined by the ratio κ of the eigenvalues. In the very least, we expect $\ell \geq 1$ for all values of the parameters ε and η. Traditionally, ε is taken to satisfy $0 < \varepsilon \ll 1$ and consequently ℓ will be very large. First, we need to establish the source of the problem mentioned earlier regarding the coefficient σ_2 and the concavity of solutions at the origin.

Consider the coefficient σ_2. Using (6.25), (7.4), (7.6), and (7.27b), we can write σ_2 in terms of κ and ε as

$$\sigma_2 = -\frac{\kappa\,(\kappa+1)^2}{(\kappa-2)\,(\kappa-\varepsilon)^2}.$$

Moreover, we know from (6.24) that $\kappa > \max\left\{\varepsilon, \varepsilon^{-1}\right\}$. This gives us the following.

Claim 7.37: *The coefficient σ_2 satisfies*

$$\sigma_2 \begin{cases} < 0, \quad \textit{if} \quad \kappa > 2 \\ > 0, \quad \textit{if} \quad 1 < \kappa < 2 \\ \textit{is undefined}, \quad \textit{if} \quad \kappa = 2 \end{cases}. \tag{7.28}$$

We see that if $\kappa = 2$ then σ_2 is not defined. This can be generalized to say that σ_κ is undefined for $\kappa \in \{2, 3, \ldots\}$. Note also that (7.28) suggests that there must be a term between $\sigma_1 x$ and $\sigma_2 x^2$ in the asymptotic expansion of $\mathcal{M}(x)$ in order to account for the concavity.

Proposition 7.38: *Consider the ratio $\kappa > 1$ and the coefficients $\{\sigma_n\}_{n=0}^{\infty}$.*

(a) If $\kappa \notin \{2, 3, \ldots\}$, then all of $\{\sigma_n\}_{n=0}^{\infty}$ are defined.

(b) If $\kappa \in \{2, 3, \ldots\}$, then $\{\sigma_n\}_{n=0}^{\kappa-1}$ are all defined but σ_κ is not defined (and hence all subsequent σ_n are not defined).

Proof: We know that the coefficients σ_0 and σ_1 are always defined. Consider the expression (7.27b), which gives the recursive expressions for the remaining coefficients. Solving

$$\varepsilon^{-1} + (1-\eta)\,(n+1)\,\sigma - n = 0, \quad n \in \{2, 3, \ldots\}$$

for η gives

$$\eta = \frac{n\,(\varepsilon+1)^2}{\varepsilon(n+1)^2}. \tag{7.29}$$

Note that this requires we use the definition (7.6) for σ and the definition (7.4) for λ_+. Appealing to (6.25), we know that (7.29) is true if and only if $\kappa = n$. Hence, if $\kappa \in \{2, 3, \ldots\}$ then $\{\sigma_n\}_{n=0}^{\kappa-1}$ are all defined but σ_κ is not defined. If $\kappa \notin \{2, 3, \ldots\}$, then all the coefficients are defined. $\square$

7.7.2 Asymptotic Expressions

We want to find the detailed asymptotic behaviour of scalar solutions $y(x)$ to the system (7.2) as $x \to 0^+$. However, as we have seen, the power series method, as we have seen, will not work in general in this case. To remedy this problem, we will employ results from Part I of this thesis.

The planar system (7.1) along with the initial condition $\mathbf{x}(0) = \mathbf{x}_0$ can be written in the form

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{7.30}$$

where the matrix $\mathbf{A}$ and vector field $\mathbf{b}$ are given by

$$\mathbf{A} = \begin{pmatrix} -1 & 1-\eta \\ \varepsilon^{-1} & -\varepsilon^{-1} \end{pmatrix} \quad \text{and} \quad \mathbf{b}(\mathbf{x}) := xy \begin{pmatrix} 1 \\ -\varepsilon^{-1} \end{pmatrix}.$$

Observe that

$$0 \le (x-y)^2 = x^2 + y^2 - 2xy = \|\mathbf{x}\|^2 - \left(\frac{2}{\sqrt{1+\varepsilon^{-2}}}\right) \|\mathbf{b}(\mathbf{x})\|$$

and

$$\|\mathbf{D}\mathbf{b}(\mathbf{x})\| = \max_{\|\mathbf{u}\|=1} \{\|\mathbf{D}\mathbf{b}(\mathbf{x})\mathbf{u}\|\} = \left(\sqrt{1+\varepsilon^{-2}}\right) \max_{\|\mathbf{u}\|=1} \{|yu_1 + xu_2|\}.$$

It follows that

$$\|\mathbf{b}(\mathbf{x})\| \le \left(\tfrac{1}{2}\sqrt{1+\varepsilon^{-2}}\right) \|\mathbf{x}\|^2 \quad \text{and} \quad \|\mathbf{D}\mathbf{b}(\mathbf{x})\| \le \left(\sqrt{1+\varepsilon^{-2}}\right) \|\mathbf{x}\|.$$

Note that, for the bound on $\|\mathbf{D}\mathbf{b}(\mathbf{x})\|$, we used the Cauchy-Schwarz Inequality and the fact that $\|\mathbf{x}\| = \left\|(y,x)^T\right\|$.

We will also need to consider the initial value problem which results from diagonalizing the matrix $\mathbf{A}$. In §6.6, we defined the matrices

$$\mathbf{P} = \begin{pmatrix} 1 & 1 \\ \sigma_+ & \sigma_- \end{pmatrix}, \quad \mathbf{P}^{-1} = \frac{1}{\sigma_+ - \sigma_-} \begin{pmatrix} -\sigma_- & 1 \\ \sigma_+ & -1 \end{pmatrix}, \quad \text{and} \quad \mathbf{\Lambda} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix},$$

where

$$\sigma_\pm = \frac{\lambda_\pm + 1}{1-\eta}$$

are the slopes of the eigenvectors. Then, $\mathbf{\Lambda} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$. If we define

$$\mathbf{y} := \mathbf{P}^{-1}\mathbf{x}, \quad \mathbf{y}_0 := \mathbf{P}^{-1}\mathbf{x}_0, \quad \text{and} \quad \overline{\mathbf{b}}(\mathbf{y}) := \mathbf{P}^{-1}\mathbf{b}\left(\mathbf{P}\mathbf{y}\right),$$

then the initial value problem (7.30) is transformed into the initial value problem

$$\dot{\mathbf{y}} = \mathbf{\Lambda y} + \overline{\mathbf{b}}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0.$$

Note that

$$\overline{\mathbf{b}}(\mathbf{y}) = \frac{\sigma_+ y_1^2 + (\sigma_+ + \sigma_-)\, y_1 y_2 + \sigma_- y_2^2}{\sigma_+ - \sigma_-} \begin{pmatrix} -\sigma_- - \varepsilon^{-1} \\ \sigma_+ + \varepsilon^{-1} \end{pmatrix},$$

for which the coefficient of the y_1^2 term in the second component is

$$\overline{b}_{211} := \frac{\sigma_+ \left(\sigma_+ + \varepsilon^{-1}\right)}{\sigma_+ - \sigma_-} > 0.$$

Theorem 7.39: *Let $y(x)$ be a scalar solution to (7.2) lying inside Γ_0 and consider the coefficients $\{\sigma_n\}_{n=1}^{\infty}$ given in (7.27).*

(a) If $\kappa \notin \{2, 3, \ldots\}$, then

$$y(x) = \sum_{n=1}^{\lfloor \kappa \rfloor} \sigma_n x^n + C\, x^{\kappa} + o(x^{\kappa}) \quad \text{as} \quad x \to 0^+$$

for some constant C (which depends on the differential equation and the initial condition).

(b) If $\kappa = 2$, then

$$y(x) = \sigma\, x + c\, x^2 \ln(x) + C\, x^2 + o\big(x^2\big) \quad \text{as} \quad x \to 0^+$$

where

$$c := \frac{\sigma \left(\sigma + \varepsilon^{-1}\right)}{-\lambda_+} > 0 \tag{7.31}$$

and some constant C (which depends on the differential equation and the initial condition).

(c) If $\kappa \in \{3, 4, \ldots\}$, then

$$y(x) = \sum_{n=1}^{\kappa - 1} \sigma_n x^n + C\, x^{\kappa} + \mathcal{O}\big(x^{\kappa+1}\big) \quad \text{as} \quad x \to 0^+$$

for some constant C (which depends on the differential equation and the initial condition).

Proof:

(a) The result follows immediately from Theorem 2.16 on page 28. Note that the coefficients of the integer powers of x must indeed be $\{\sigma_n\}_{n=1}^{\lfloor \kappa \rfloor}$ since they are generated uniquely by the differential equation.

(b) The result is an immediate consequence of Theorem 5.28 on page 122.

(c) The result is also an immediate consequence of Theorem 5.28 on page 122.

□

Proposition 7.40: *If $\kappa \notin \{2, 3, \ldots\}$ then there exists a scalar solution $y(x)$ to* (7.2) *such that*

$$y(x) \sim \sum_{n=1}^{\infty} \sigma_n x^n \quad \text{as} \quad x \to 0^+,$$

where the coefficients $\{\sigma_n\}_{n=1}^{\infty}$ are given in (7.27).

Proof: It follows immediately from Corollary 2.18 on page 32 that there is at least one solution $y(x)$ for which the coefficients of the non-integral powers of x are zero. Note that the coefficients must indeed be $\{\sigma_n\}_{n=1}^{\infty}$ since they are generated uniquely by the differential equation. □

7.8 All or Most Solutions Must Enter Γ_1

Theorem 7.7 established that the trapping region Γ_0 is positively invariant and that all solutions to the planar system eventually enter this region. Now, we investigate whether or not the antifunnel Γ_1 is positively invariant and all solutions enter this region.

Theorem 7.41: *Consider the planar system* (7.1).

(a) The antifunnel Γ_1 is positively invariant.

(b) Suppose that $\kappa \geq 2$. Let $\boldsymbol{x}(t)$ be the solution to (7.1) *with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in S \setminus \{\boldsymbol{0}\}$. Then, there is a $t^* \geq 0$ such that $\boldsymbol{x}(t) \in \Gamma_1$ for all $t \geq t^*$.*

(c) Suppose that $1 < \kappa < 2$. Then, there exists non-trivial solutions to (7.1) *which do not enter Γ_1. Moreover, solutions that do not enter Γ_1 must enter Γ_0 through the vertical isocline V to the left of the line $y = \sigma x$.*

Proof:

(a) It follows from the fact that $\mathbf{g} \bullet \boldsymbol{\nu} < 0$ along α and H, where $\boldsymbol{\nu}$ is the outward unit normal vector.

(b) We know that eventually $\mathbf{x}(t)$ will enter Γ_0. Let y be the corresponding scalar solution lying in Γ_0. If $\kappa > 2$, applying Theorem 7.39 gives

$$y(x) = \sigma x + \sigma_2 x^2 + \mathsf{o}\big(x^2\big) \quad \text{as} \quad x \to 0^+.$$

A routine (but tedious) calculation shows

$$y'(x) = f(x, y(x)) = \sigma + 2\sigma_2 x + \mathsf{o}(x) \quad \text{as} \quad x \to 0^+.$$

(Note that we have not justified that direct differentiation of the asymptotic expression for $y(x)$ is permissible.) We know from (7.28) that $\sigma_2 < 0$ and thus there is a $\delta > 0$ such that $0 < y'(x) < \sigma$ for all $x \in (0, \delta)$. By virtue of the isocline structure, $\mathbf{x}(t)$ must enter Γ_1. If instead $\kappa = 2$, then we know from Theorem 7.39 that

$$y(x) = \sigma x + c\,x^2 \ln(x) + \mathcal{O}\big(x^2\big) \quad \text{as} \quad x \to 0^+$$

where $c > 0$. Another routine (and also tedious) calculation shows

$$y'(x) = f(x, y(x)) = \sigma + 2c\,x \ln(x) + \mathcal{O}(x) \quad \text{as} \quad x \to 0^+.$$

Since $c > 0$, we see there is a $\delta > 0$ with $0 < y'(x) < \sigma$ for all $x \in (0, \delta)$. Hence, $\mathbf{x}(t)$ enters Γ_1.

(c) Let $y(x)$ be the scalar solution in Proposition 7.40. It can be shown that

$$y'(x) = f(x, y(x)) = \sigma + 2\sigma_2 x + \mathcal{O}\big(x^2\big) \quad \text{as} \quad x \to 0^+.$$

Now, (7.28) assures us that $\sigma_2 > 0$. Thus, there is a $\delta > 0$ such that $y'(x) > \sigma$ for all $x \in (0, \delta)$. Appealing to the isocline structure, $y(x) > \alpha(x)$ for all $x \in (0, \delta)$ and so $\mathbf{x}(t)$ does not enter Γ_1.

Suppose now that $\mathbf{x}(t)$ is a non-trivial solution which does not enter Γ_1. Since $\mathbf{x}(t)$ must enter Γ_0, we can conclude that $\mathbf{x}(t)$ enters Γ_0 through the vertical isocline. Denote by (x^*, y^*) the point of intersection of the line $y = \sigma x$ and the vertical isocline $y = V(x)$. See Figure 7.7. Assume, for a contradiction, that $\mathbf{x}(t)$ enters Γ_0 through the vertical isocline to the right of (x^*, y^*). We claim that $\mathbf{x}(t)$ must also enter Γ_1. Suppose that $y(x)$ intersects the vertical isocline at $x = x_1$, where $y(x)$ is the corresponding scalar solution. Observe that $x_1 \geq x^*$, by assumption, and $y(x_1) \leq \sigma x_1$. By the Mean Value Theorem, there is an $x_0 \in (0, x_1)$ such that

$$y'(x_0) = \frac{y(x_1) - 0}{x_1 - 0} = \frac{y(x_1)}{x_1} \leq \frac{\sigma x_1}{x_1} = \sigma.$$

By virtue of the isocline structure, we conclude that $\mathbf{x}(t)$ enters Γ_1. This is a contradiction.

$\square$

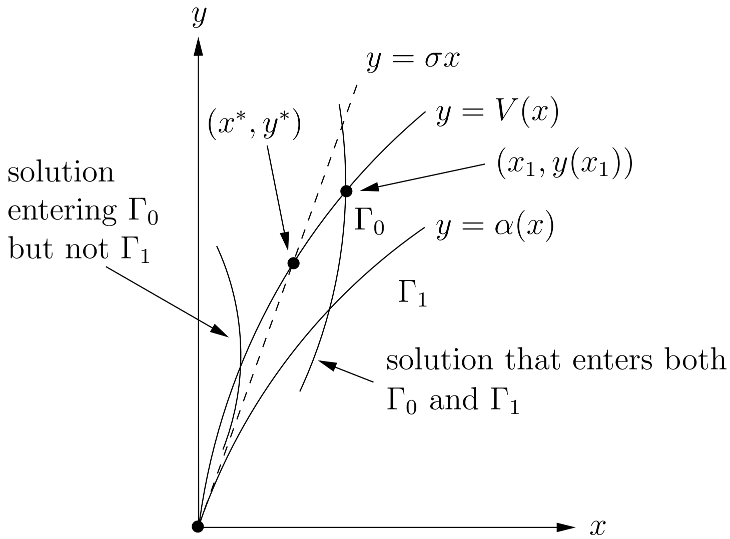

Figure 7.7: Sketch demonstrating Theorem 7.41(c).

7.9 Bounds on $y(x)$

Let $y(x)$ be the solution of the scalar differential equation (7.2) with initial condition $y(x_0) = y_0$, where $x_0 > 0$ and $y_0 \geq 0$. We will consider three cases, namely $y_0 = 0$, $y_0 = H(x_0)$, and $y_0 = \alpha(x)$. Here, $H(x)$ is the horizontal isocline which is given in (7.5), $\alpha(x)$ is the isocline for slope σ which is given in (7.13), and σ is the slope given in (7.6). Our goal is to obtain simple bounds on $y(x)$ over $(0, x_0]$. Moreover, we will use these bounds to state bounds on the slow manifold. To realize these goals, we will use Chaplygin's method (see §A.5 of Appendix A).

If $x > 0$ and $0 \leq y < V(x)$ then

$$\frac{\partial f}{\partial y}(x,y) = \frac{\eta x}{\varepsilon\left[x - (1-\eta+x)\,y\right]^2} > 0 \quad \text{and} \quad \frac{\partial^2 f}{\partial y^2}(x,y) = \frac{2\eta\,(1-\eta+x)\,x}{\varepsilon\left[x-(1-\eta+x)\,y\right]^3} > 0,$$

where f is the function given in (7.3) and $V(x)$ is the vertical isocline given in (7.5). Note that

$$f(x,0) = -\varepsilon^{-1}, \quad f(x,H(x)) = 0, \quad \text{and} \quad f(x,\alpha(x)) = \sigma \quad \text{for all} \quad x > 0.$$

Furthermore, note that

$$\frac{\partial f}{\partial y}(x,0) = \frac{\eta}{\varepsilon x}, \quad \frac{\partial f}{\partial y}(x,H(x)) = \frac{(1+x)^2}{\varepsilon\eta x}, \quad \text{and} \quad \frac{\partial f}{\partial y}(x,\alpha(x)) = \frac{\eta\,(1+\sigma x)^2}{\varepsilon\lambda_+^2 x} \quad \text{for all} \quad x > 0,$$

where λ_+ is the slow eigenvalue.

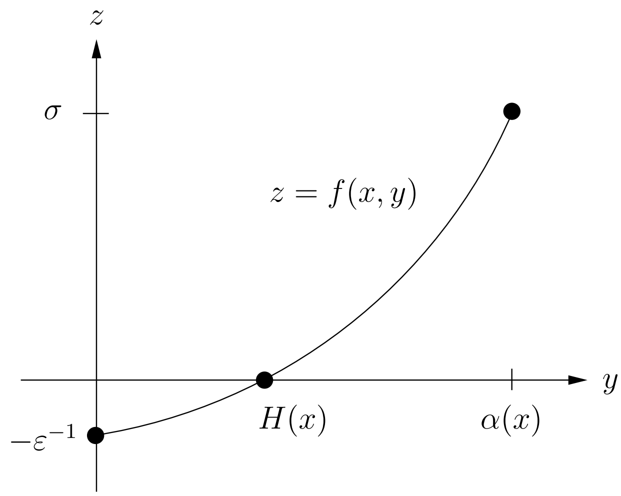

Figure 7.8: For a fixed $x \in (0, x_0]$, the curve $z = f(x, y)$ is concave up on the interval $[0, \alpha(x)]$. This allows us to obtain bounds on $f(x, y)$ over the interval $[0, \alpha(x)]$ using secants and tangents.

Consider $x \in (0, x_0]$ to be fixed. Then, the curve $z = f(x, y)$ as a function of y is concave up on the interval $[0, \alpha(x)]$. See Figure 7.8. This fact enables us to state bounds on $f(x, y)$ using secants and tangents.

- The tangent to $z = f(x, y)$ at $y = 0$ is $z = T_1(x, y)$, where
$$T_1(x, y) := -\frac{1}{\varepsilon} + \frac{\eta}{\varepsilon x}\, y. \tag{7.32a}$$
- The tangent to $z = f(x, y)$ at $y = H(x)$ is $z = T_2(x, y)$, where
$$T_2(x, y) := \frac{(1+x)^2}{\varepsilon \eta x}\left(y - \frac{x}{1+x}\right). \tag{7.32b}$$
- The tangent to $z = f(x, y)$ at $y = \alpha(x)$ is $z = T_3(x, y)$, where
$$T_3(x, y) := \sigma + \frac{\eta\,(1+\sigma x)^2}{\varepsilon \lambda_+^2 x}\left(y - \frac{x}{\sigma^{-1} + x}\right). \tag{7.32c}$$
- The secant line through $\left(0, -\varepsilon^{-1}\right)$ and $(\alpha(x), \sigma)$ is $z = S_1(x, y)$, where
$$S_1(x, y) := -\frac{1}{\varepsilon} + \frac{(1+\varepsilon\sigma)\,(1+\sigma x)}{\varepsilon \sigma x}\, y. \tag{7.32d}$$
- The secant line through $(H(x), 0)$ and $(\alpha(x), \sigma)$ is $z = S_2(x, y)$, where
$$S_2(x, y) := \frac{\sigma\,(1+\sigma x)\,(1+x)}{(\sigma - 1)\,x}\left(y - \frac{x}{1+x}\right). \tag{7.32e}$$

7.9.1 Case 1: $x_0 > 0$ and $y_0 = 0$

Suppose that $y_0 = 0$. Thus, $y(x)$ is a solution which terminates on the x-axis at $x = x_0$. Since $y(x)$ is a solution lying below the slow manifold which in turn lies below the isocline $\alpha(x)$, we know that

$$0 \le y(x) \le \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Now, we can see from Figure 7.8 that

$$T_3(x,y) \le f(x,y) \le S_1(x,y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,,$$

where $T_3(x,y)$ is as in (7.32c) and $S_1(x,y)$ is as in (7.32d). (Note that we could have used $T_1(x,y)$, given in (7.32a), instead of $T_3(x,y)$ but $T_3(x,y)$ usually yields a better bound.)

Define, for $x \in (0, x_0]$, the functions

$$a_1(x) := -\varepsilon^{-1}, \quad b_1(x) := \frac{(1+\varepsilon\sigma)\,(1+\sigma x)}{\varepsilon\sigma x}, \quad \mu_1(x) := \mathsf{exp}\left(\int_x^{x_0} b_1(z)\,dz\right)$$

along with

$$a_2(x) := \sigma\left[1 - \frac{\eta\,(1+\sigma x)}{\varepsilon\lambda_+^2}\right], \quad b_2(x) := \frac{\eta\,(1+\sigma x)^2}{\varepsilon\lambda_+^2 x}, \quad \text{and} \quad \mu_2(x) := \mathsf{exp}\left(\int_x^{x_0} b_2(z)\,dz\right).$$

Note that

$$\mu_i(x_0) = 1, \quad \mu_i(x) > 0, \quad \text{and} \quad \mu_i'(x) = -b_i(x)\mu_i(x) \quad (i = 1, 2)\,.$$

Thus, we can write

$$a_2(x) + b_2(x)y(x) \le y'(x) \le a_1(x) + b_1(x)y(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Re-arranging and replacing x with z,

$$\frac{d}{dz}\left(\mu_2(z)y(z)\right) \ge \mu_2(z)a_2(z) \quad \text{and} \quad \frac{d}{dz}\left(\mu_1(z)y(z)\right) \le \mu_1(z)a_1(z) \quad \text{for all} \quad z \in (0, x_0]\,.$$

If we integrate with respect to z from x to x_0, where $x \in (0, x_0]$, apply the initial condition $y(x_0) = 0$, and re-arrange, we obtain

$$-\frac{1}{\mu_1(x)}\int_x^{x_0} \mu_1(z)a_1(z)\,ds \le y(x) \le -\frac{1}{\mu_2(x)}\int_x^{x_0} \mu_2(z)a_2(z)\,ds \quad \text{for all} \quad x \in (0, x_0]\,. \tag{7.33}$$

Figure 7.9 gives two numerical examples of the bounds given in (7.33).

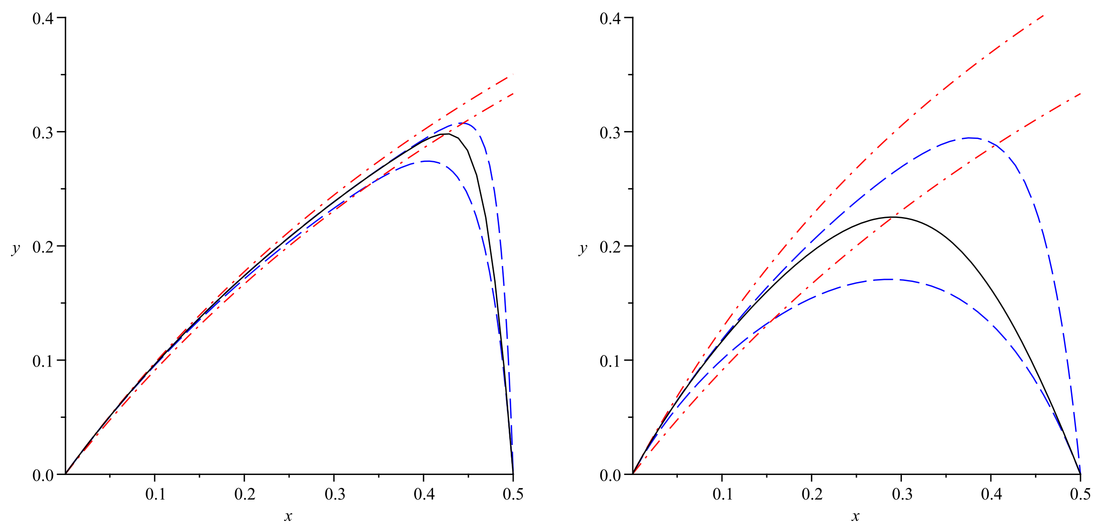

Figure 7.9: For the first picture, suppose $\varepsilon = 0.1$, $\eta = 0.75$, and $x_0 = 0.5$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (7.33). The solid curve represents the actual solution (found numerically) with $y(x_0) = 0$. The dash-dot curves are the horizontal and α isoclines. The second picture is the same as the first except with $\varepsilon = 1.0$, $\eta = 0.75$, and $x_0 = 0.5$.

7.9.2 Case 2: $x_0 > 0$ and $y_0 = H(x_0)$

Suppose now that $y_0 = H(x_0)$. Then, $y(x)$ is a solution which terminates on the horizontal isocline at $x = x_0$. We know that

$$H(x) \le y(x) \le \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Now, we can see from Figure 7.8 that

$$T_3(x,y) \le f(x,y) \le S_2(x,y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,,$$

where $T_3(x,y)$ is as in (7.32c) and $S_2(x,y)$ is as in (7.32e). (Note that we could have used $T_2(x,y)$, given in (7.32b), instead of $T_3(x,y)$ but $T_3(x,y)$ usually yields a better bound.)

Define, for $x \in (0, x_0]$, the functions

$$a_1(x) := -\frac{\sigma\,(1+\sigma x)}{(\sigma-1)}, \quad b_1(x) := \frac{\sigma\,(1+\sigma x)\,(1+x)}{(\sigma-1)\,x}, \quad \mu_1(x) := \mathsf{exp}\left(\int_x^{x_0} b_1(z)\,dz\right) \tag{7.34}$$

along with

$$a_2(x) := \sigma\left[1 - \frac{\eta\,(1+\sigma x)}{\varepsilon\lambda_+^2}\right], \quad b_2(x) := \frac{\eta\,(1+\sigma x)^2}{\varepsilon\lambda_+^2 x}, \quad \text{and} \quad \mu_2(x) := \mathsf{exp}\left(\int_x^{x_0} b_2(z)\,dz\right). \tag{7.35}$$

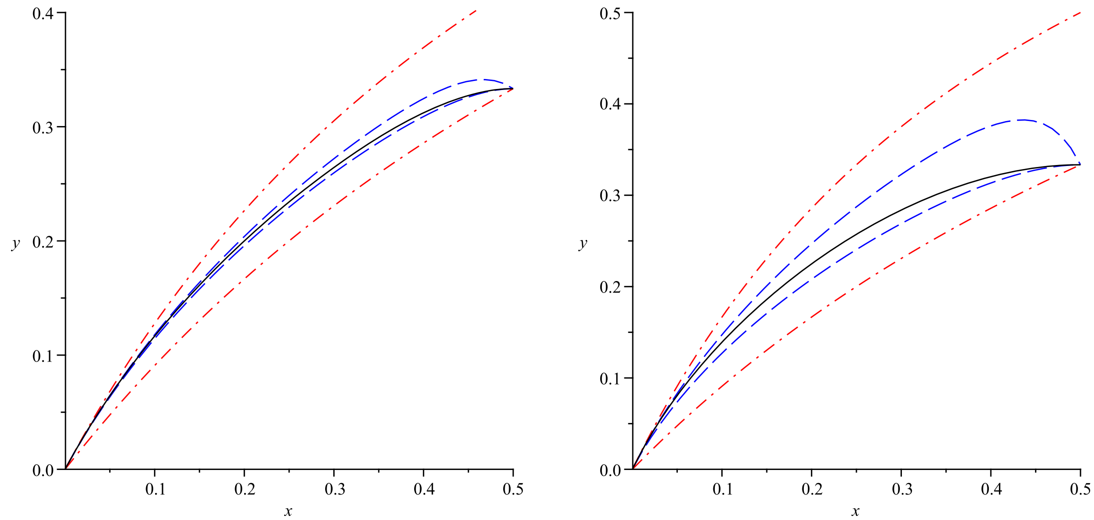

Figure 7.10: For the first picture, suppose $\varepsilon = 0.5$, $\eta = 0.75$, and $x_0 = 0.5$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (7.36). The solid curve represents the actual solution (found numerically) with $y(x_0) = H(x_0)$. The two dash-dot curves are the horizontal and α isoclines. The second picture is the same as the first except with $\varepsilon = 1.0$, $\eta = 0.75$, and $x_0 = 0.5$.

Proceeding as before, we obtain

$$\frac{H(x_0) - \int_x^{x_0} \mu_1(z) a_1(z)\, ds}{\mu_1(x)} \leq y(x) \leq \frac{H(x_0) - \int_x^{x_0} \mu_2(z) a_2(z)\, ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,. \tag{7.36}$$

Figure 7.10 gives two numerical examples of the bounds given in (7.36).

7.9.3 Case 3: $x_0 > 0$ and $y_0 = \alpha(x_0)$

Suppose now that $y_0 = \alpha(x_0)$. Then, $y(x)$ is a solution which terminates on the α isocline at $x = x_0$. We know that

$$H(x) \leq y(x) \leq \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Now, we can see from Figure 7.8 that

$$T_3(x,y) \leq f(x,y) \leq S_2(x,y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,.$$

Proceeding as before, we obtain

$$\frac{\alpha(x_0) - \int_x^{x_0} \mu_1(z) a_1(z)\, ds}{\mu_1(x)} \leq y(x) \leq \frac{\alpha(x_0) - \int_x^{x_0} \mu_2(z) a_2(z)\, ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,, \tag{7.37}$$

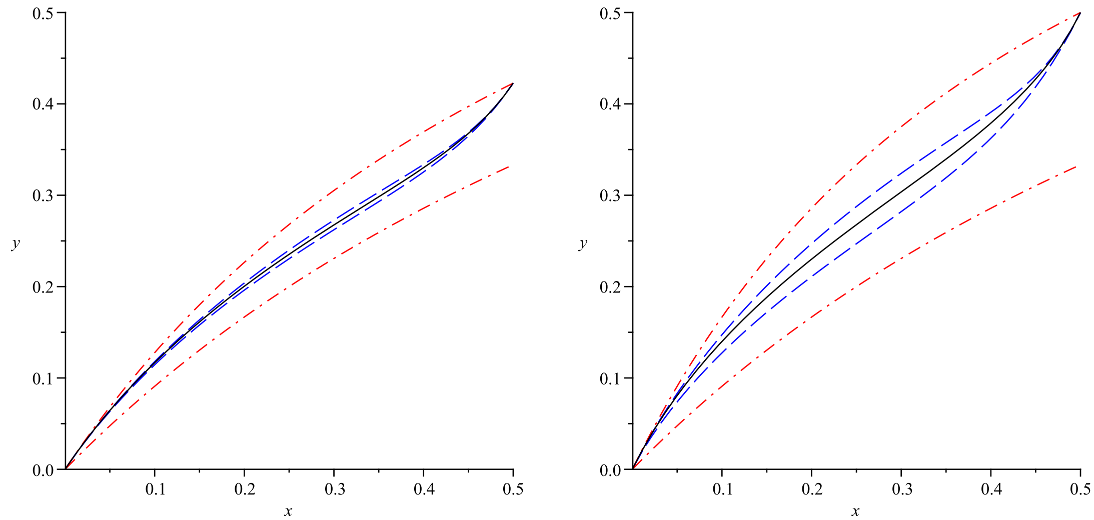

Figure 7.11: For the first picture, suppose $\varepsilon = 0.5$, $\eta = 0.75$, and $x_0 = 0.5$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (7.37). The solid curve represents the actual solution (found numerically) with $y(x_0) = \alpha(x_0)$. The two dash-dot curves are the horizontal and α isoclines. The second picture is the same as the first except with $\varepsilon = 1.0$, $\eta = 0.75$, and $x_0 = 0.5$.

where $a_i(x)$, $b_i(x)$, and $\mu_i(x)$ for $i = 1, 2$ are as in (7.34) and (7.35). Figure 7.11 gives two numerical examples of the bounds given in (7.37).

7.9.4 Bounds on the Slow Manifold

We can use the material from the previous two subsections to state bounds on the slow manifold. Suppose that $y_1(x)$ is the solution of (7.2) with initial condition $y(x_0) = H(x_0)$. Suppose also that $y_2(x)$ is the solution of (7.2) with initial condition $y(x_0) = \alpha(x_0)$. It follows that the slow manifold satisfies $y_1(x) \leq \mathcal{M}(x) \leq y_2(x)$ for all $x \in (0, x_0]$. If we combine (7.36), which gives bounds for $y_1(x)$, and (7.37), which gives bounds for $y_2(x)$, we can conclude that

$$\frac{H(x_0) - \int_x^{x_0} \mu_1(z) a_1(z)\, ds}{\mu_1(x)} \leq \mathcal{M}(x) \leq \frac{\alpha(x_0) - \int_x^{x_0} \mu_2(z) a_2(z)\, ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,,$$

where $a_i(x)$, $b_i(x)$, and $\mu_i(x)$ for $i = 1, 2$ (which all depend on x_0) are as in (7.34) and (7.35). It is worth reiterating the fact that $x_0 > 0$ is arbitrary.

7.10 Properties of the Slow Manifold

The focus of this chapter is the properties of all scalar solutions to the differential equation (7.2). In this section, we single out important properties of the exceptional solution $y = \mathcal{M}(x)$, namely the slow manifold.

7.10.1 Bounds on the Slow Manifold

Proposition 7.42: *The slow manifold $y = \mathcal{M}(x)$ satisfies*

$$0 < H(x) < \mathcal{M}(x) < \mathcal{Y}(x) < \alpha(x) < 1 \quad \textit{for all} \quad x > 0.$$

Furthermore,

$$\lim_{x \to 0^+} \mathcal{M}(x) = 0 \quad \textit{and} \quad \lim_{x \to \infty} \mathcal{M}(x) = 1.$$

Proof: The first result follows from Theorem 7.13, Proposition 7.33, and the definition (7.13) of α. To establish the limits, note that the functions H, α, and $\mathcal{M}$ are all continuous for $x > 0$. Since

$$\lim_{x \to 0^+} H(x) = 0 = \lim_{x \to 0^+} \alpha(x) \quad \text{and} \quad \lim_{x \to \infty} H(x) = 1 = \lim_{x \to \infty} \alpha(x),$$

the limits for the slow manifold follow from the Squeeze Theorem. $\square$

7.10.2 Concavity of the Slow Manifold

Proposition 7.43: *The slow manifold $y = \mathcal{M}(x)$ is concave down for all $x > 0$.*

Proof: It follows from Propositions 7.32 and 7.33 that $h\left(x, \mathcal{M}(x)\right) < 0$ for all $x > 0$, where h is the function defined in (7.17). Since $\mathsf{sgn}(\mathcal{M}''(x)) = \mathsf{sgn}(h(x, \mathcal{M}(x)))$, it must be that the slow manifold is concave down for all $x > 0$. $\square$

7.10.3 The Slope of the Slow Manifold

Proposition 7.44: *The slope of the slow manifold $y = \mathcal{M}(x)$ satisfies*

$$0 < \mathcal{M}'(x) < \sigma \quad \textit{for all} \quad x > 0, \quad \lim_{x \to 0^+} \mathcal{M}'(x) = \sigma, \quad \textit{and} \quad \lim_{x \to \infty} \mathcal{M}'(x) = 0.$$

Proof: Since the slow manifold satisfies $H(x) < \mathcal{M}(x) < \alpha(x)$ for all $x > 0$, by virtue of the isocline structure we can conclude that $0 < \mathcal{M}'(x) < \sigma$ for all $x > 0$. This establishes the first part of the result. The second part of the result is a special case of Proposition 7.18.

To prove the third part of the result, we note that, since $\mathcal{M}$ is strictly increasing and concave down, there is a $c \in [0, \sigma)$ such that

$$\lim_{x \to \infty} \mathcal{M}'(x) = c.$$

Suppose, on the contrary, that $c > 0$. By the Fundamental Theorem of Calculus,

$$\mathcal{M}(x) = \int_0^x \mathcal{M}'(u)\, du > \int_0^x c\, du = cx.$$

However, for sufficiently large x, $cx > \alpha(x)$, which is a contradiction. $\square$

7.10.4 Asymptotic Series for the Slow Manifold at the Origin

Proposition 7.45: *Asymptotically, the slow manifold can be written in the form*

$$\mathcal{M}(x) = \begin{cases} \displaystyle\sum_{n=1}^{\lfloor\kappa\rfloor} \sigma_n x^n + C\,x^\kappa + o(x^\kappa), & \text{if} \quad \kappa \notin \{2, 3, \ldots\} \\ \sigma\,x + c\,x^2 \ln(x) + C\,x^2 + o\big(x^2\big), & \text{if} \quad \kappa = 2 \\ \displaystyle\sum_{n=1}^{\kappa-1} \sigma_n x^n + C\,x^\kappa + \mathcal{O}\big(x^{\kappa+1}\big), & \text{if} \quad \kappa \in \{3, 4, \ldots\} \end{cases} \qquad \text{as} \quad x \to 0^+,$$

where $\{\sigma_n\}_{n=1}^{\infty}$ *are as in* (7.27) *and* c *is as in* (7.31).

Proof: The asymptotic expressions follow immediately from Theorem 7.39. $\square$

Remark 7.46: In the statement of Proposition 7.45, the constant C (in all three cases) distinguishes the slow manifold from other scalar solutions. Suppose that you want to approximate C for a given choice of ε and η. We could use the following "higher-lower algorithm."

1. Choose a small $x_0 > 0$.

2. Define $r_1 := \frac{1}{2}\,[H(x_0) + \alpha(x_0)]$.

3. Assuming r_n is known, find numerically the solution $y_n(x)$ of $y' = f(x, y)$ with initial condition $y(x_0) = r_n$. If $y = y_n(x)$ intersects $y = H(x)$ to the right of x_0 then $r_n < \mathcal{M}(x_0)$ and so take $r_{n+1} := \frac{1}{2}\,[r_n + \alpha(x_0)]$. Otherwise, take $r_{n+1} := \frac{1}{2}\,[H(x_0) + r_n]$.

4. The sequence of approximations $\{r_n\}_{n=1}^{\infty}$ satisfies

$$|\mathcal{M}(x_0) - r_n| \leq \frac{1}{2^n}\left[\alpha(x_0) - H(x_0)\right] \quad \text{and} \quad \lim_{n\to\infty} r_n = \mathcal{M}(x_0).$$

5. The constant C can be approximated by the appropriate expression in Proposition 7.45.

Corollary 7.47: *The slow manifold satisfies*

$$\mathcal{M}(x) = \alpha(x) + o(x) \quad \textit{as} \quad x \to 0^+.$$

Moreover, this statement would not be true if we replace $\alpha(x)$ with any other isocline $F(x,c)$.

Proof: It follows from a comparison of the asymptotic expansions for $\mathcal{M}(x)$, $\alpha(x)$, and $F(x,c)$. □

7.10.5 Asymptotic Series for the Slow Manifold at Infinity

Recall that it was argued by Roussel, for example in [104], that the slow manifold can be written as the asymptotic series $\mathcal{M}(x) \sim \sum_{n=0}^{\infty} \rho_n x^{-n}$ as $x \to \infty$. Substitution of the series into the differential equation (7.2) in conjunction with known properties of the slow manifold yields

$$\begin{aligned} & \rho_0 = 1, \quad \rho_1 = -1, \quad \rho_2 = 1, \\ \text{and} \quad & \rho_n = -\rho_{n-1} + \varepsilon \sum_{i=1}^{n-2} i\rho_i \left[\rho_{n-i-1} + (1-\eta)\,\rho_{n-i-2}\right] \quad \text{for} \quad n > 2. \end{aligned} \tag{7.38}$$

This series, as we will show momentarily, is fully correct. To establish this, we will use the Centre Manifold Theorem. First, we will show that $\mathcal{M}(x) \sim 1 - x^{-1}$ as $x \to \infty$ using the isoclines. This will motivate our choice of a change of variables.

Let $c \in (0, \sigma)$. We know from Proposition 7.17 that

$$H(x) < \mathcal{M}(x) < F(x,c) \quad \text{for all} \quad x > \xi(c),$$

where F and ξ are given, respectively, in (7.8) and (7.14). (Alternatively, we could obtain the inequality for all $x > x^*$ for some $x^* > 0$ by using the fact that $\mathcal{M}$ is concave down and $\lim_{x\to\infty} \mathcal{M}'(x) = 0$.) Manipulating the inequalities,

$$\frac{F(x,c)-1}{-x^{-1}} < \frac{\mathcal{M}(x)-1}{-x^{-1}} < \frac{H(x)-1}{-x^{-1}} \quad \text{for all} \quad x > \xi(c). \tag{7.39}$$

Now,

$$H(x) = \frac{x}{1+x} = 1 - x^{-1} + \mathcal{O}\big(x^{-2}\big) \quad \text{as} \quad x \to \infty.$$

Thus, if we let $x \to \infty$ in (7.39) we see

$$\limsup_{x\to\infty} \frac{\mathcal{M}(x) - 1}{-x^{-1}} \le 1.$$

Furthermore, since

$$F(x,c) = \frac{x}{K(c)+x} = 1 - K(c)\, x^{-1} + \mathcal{O}\big(x^{-2}\big) \quad \text{as} \quad x \to \infty,$$

if we let $x \to \infty$ in (7.39) we see

$$\liminf_{x\to\infty} \frac{\mathcal{M}(x) - 1}{-x^{-1}} \ge K(c).$$

Since $c \in (0, \sigma)$ was arbitrary and $K(c) \to 1^-$ as $c \to 0^+$, we can deduce

$$1 \le \liminf_{x\to\infty} \frac{\mathcal{M}(x) - 1}{-x^{-1}} \le \limsup_{x\to\infty} \frac{\mathcal{M}(x) - 1}{-x^{-1}} \le 1.$$

Therefore,

$$\lim_{x\to\infty} \frac{\mathcal{M}(x) - 1}{-x^{-1}} = 1 \quad \text{and} \quad \mathcal{M}(x) = 1 - x^{-1} + \mathsf{o}\big(x^{-1}\big) \quad \text{as} \quad x \to \infty.$$

Unfortunately, this is as much information that we can extract using the isoclines. To obtain the remaining terms of the asymptotic series, we will use the Centre Manifold Theorem.

Proposition 7.48: *The slow manifold satisfies*

$$\mathcal{M}(x) \sim \sum_{n=0}^{\infty} \rho_n x^{-n} \quad \textit{as} \quad x \to \infty,$$

where $\{\rho_i\}_{i=0}^{\infty}$ *are as in* (7.38).

Proof: Define the new variables

$$X := x^{-1} \quad \text{and} \quad Y := y - \left(1 - x^{-1}\right). \tag{7.40}$$

Differentiating with respect to time and using the differential equation (7.1), we arrive at the system

$$\begin{aligned}
\dot{X} &= -X^2 g_1\left(X^{-1}, 1 - X + Y\right), \\
\dot{Y} &= -X^2 g_1\left(X^{-1}, 1 - X + Y\right) + g_2\left(X^{-1}, 1 - X + Y\right),
\end{aligned} \tag{7.41}$$

where g_1 and g_2 are as in (7.3). The system (7.41) is not polynomial but there is no harm, because the resulting scalar differential equation will be the same, in considering instead the system

$$\begin{aligned}\dot{X} &= -X^3 g_1\left(X^{-1}, 1 - X + Y\right),\\ \dot{Y} &= -X^3 g_1\left(X^{-1}, 1 - X + Y\right) + X g_2\left(X^{-1}, 1 - X + Y\right),\end{aligned} \tag{7.42}$$

which is indeed polynomial. Expanding the key expressions, we get

$$\begin{aligned}X^3 g_1\left(X^{-1}, 1 - X + Y\right) &= -X^2\left[\eta X - Y + (1-\eta) X (X - Y)\right],\\ X g_2\left(X^{-1}, 1 - X + Y\right) &= \varepsilon^{-1}\left(X^2 - XY - Y\right).\end{aligned}$$

The system (7.42), as we see, is a bit more messy than the original system (7.1). The eigenvalues of the matrix for the linear part of the new system (7.42), which is diagonal by construction, are 0 and $-\varepsilon^{-1}$. We know from centre manifold theory that there is a C^∞ centre manifold $Y = \mathcal{C}(X)$ which, we claim, must be the slow manifold.

For the scalar differential equation in the original coordinates, all other solutions except for the slow manifold leave the antifunnel Γ_1 and $\mathcal{M}(x)$ is the only solution which is $1 + \mathsf{o}(1)$ as $x \to \infty$. Thus, to establish that the slow manifold in the original coordinates is the same as the centre manifold in the new coordinates, it is sufficient to show that the centre manifold $Y = \mathcal{C}(X)$ is the only scalar solution in the new coordinates which is $\mathsf{o}(1)$ as $X \to 0^+$.

Observe that the Y-axis is invariant. Moreover, the fixed point $(X, Y) = (0, 0)$ is a saddle node (also known as a degenerate saddle). The physically relevant portion of the phase portrait, namely $X \geq 0$ and $Y \geq -1$, consists of two hyperbolic sectors, one with the positive Y-axis and the centre manifold as boundaries and the other with the negative Y-axis and the centre manifold as boundaries. See Figure 7.12. This can be shown using techniques in §9.21 of [2] (in particular Theorem 65 on page 340) and §2.11 of [100]. Therefore, $\mathcal{C}(X)$ is the only scalar solution in the new coordinates which is $\mathsf{o}(1)$ as $X \to 0^+$. It follows that the centre manifold is indeed the slow manifold.

By the Centre Manifold Theorem, the slow manifold (in the new coordinates) can be written

$$\mathcal{M}(X) \sim \sum_{i=2}^{\infty} \widehat{\rho}_i X^i \quad \text{as} \quad X \to 0^+,$$

for some coefficients $\{\widehat{\rho}_i\}_{i=2}^{\infty}$. Reverting back to the original coordinates,

$$\mathcal{M}(x) \sim 1 - x^{-1} + \sum_{i=2}^{\infty} \widehat{\rho}_i x^{-i} \quad \text{as} \quad x \to \infty.$$

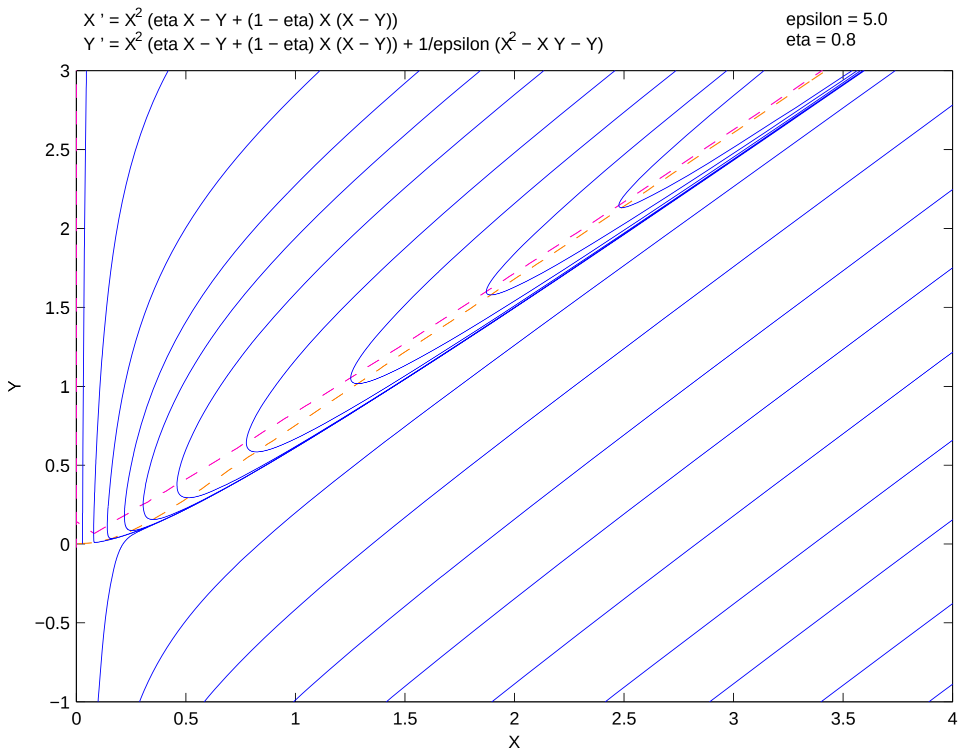

Figure 7.12: A phase portrait for (7.42) for $\varepsilon = 5.0$ and $\eta = 0.8$.

Observing that the coefficients in (7.38) are generated uniquely from the differential equation, the conclusion follows. □

Remark 7.49: We use the ad hoc transformation (7.40) because it is inspired by the series for $\mathcal{M}$ which we wish to obtain and it also results in a system which is in the canonical form of the Centre Manifold Theorem. Others, for example [33, 47], have used Poincaré compactification to study the behaviour of $\mathcal{M}$ at infinity and found that the fixed point is a saddle node.

Corollary 7.50: *The slow manifold satisfies*

$$\mathcal{M}(x) = H(x) + \mathcal{O}\left(\frac{1}{x^2}\right) \quad \textit{as} \quad x \to \infty.$$

Moreover, this statement would not be true if we replace $H(x)$ with any other isocline $F(x,c)$.

Proof: It follows from a comparison of the asymptotic expansions for $\mathcal{M}(x)$, $H(x)$, and $F(x,c)$. $\square$

7.10.6 Curvature of the Slow Manifold at the Origin

Proposition 7.51: *The second derivative of the slow manifold satisfies*

$$\lim_{x\to 0^+} \mathcal{M}''(x) = \begin{cases} 2\sigma_2, & \text{if} \quad \kappa > 2 \\ -\infty, & \text{if} \quad \kappa \leq 2 \end{cases} .$$

Proof: Suppose first that $\kappa > 2$. We know from (7.28) that $\sigma_2 < 0$ and from Proposition 7.45 that

$$\mathcal{M}(x) = \sigma x + \sigma_2 x^2 + \mathsf{o}\big(x^2\big) \quad \text{as} \quad x \to 0^+.$$

It can be shown that

$$\mathcal{M}''(x) = \frac{\partial f}{\partial x}(x, \mathcal{M}(x)) + \frac{\partial f}{\partial y}(x, \mathcal{M}(x)) f(x, \mathcal{M}(x)) = 2\sigma_2 + \mathsf{o}(1) \quad \text{as} \quad x \to 0^+.$$

The limit in the proposition for $\kappa > 2$ follows.

Now, suppose that $\kappa = 2$. We know from Proposition 7.45 that

$$\mathcal{M}(x) = \sigma x + c\,x^2 \ln(x) + \mathcal{O}\big(x^2\big) \quad \text{as} \quad x \to 0^+.$$

for some $c > 0$. It can be shown that

$$\mathcal{M}''(x) = c\,[2\ln(x) + 3] + \mathsf{o}(1) \quad \text{as} \quad x \to 0^+.$$

The limit in the proposition for $\kappa = 2$ follows.

Finally, suppose that $1 < \kappa < 2$. Note that (7.28) implies $\sigma_2 > 0$. If we apply Proposition 7.45 and appeal to Remark 2.17 on page 31, we know that

$$\mathcal{M}(x) = \sigma x + C\,x^\kappa + \sigma_2 x^2 + \mathsf{o}\big(x^2\big) \quad \text{as} \quad x \to 0^+$$

for some constant C. Note that the coefficient of the x^2 term must be σ_2 since it is generated uniquely by the differential equation. It can be shown that

$$\mathcal{M}''(x) = C\kappa\,(\kappa - 1)\,x^{\kappa-2} + 2\sigma_2 + \mathsf{o}(1) \quad \text{as} \quad x \to 0^+.$$

Since the slow manifold is concave down for all $x > 0$ and $\sigma_2 > 0$, it must be that $C < 0$. The limit in the proposition for $1 < \kappa < 2$ follows. $\square$

7.10.7 Final Remarks on the Slow Manifold

The quasi-steady-state approximation has traditionally been used to approximate the long-term behaviour (in time) of solutions to (7.1). Is this justified? Recall that

$$H(x) = \frac{x}{1+x}, \quad V(x) = \frac{x}{1-\eta+x}, \quad \text{and} \quad \alpha(x) = \frac{x}{\sigma^{-1}+x}.$$

It follows that the QSSA is good for large time when $\sigma \approx 1$ and the EA is good for large time when $\sigma \approx (1-\eta)^{-1}$. Recall also that $\sigma = 1 + \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0^+$ and $\sigma = (1-\eta)^{-1} + \mathcal{O}\big(\varepsilon^{-1}\big)$ as $\varepsilon \to \infty$. Hence, the QSSA is a good approximation for large time when ε is small and the EA is a good approximation for large time when ε is large. Furthermore, since $\kappa > \mathsf{max}\left\{\varepsilon, \varepsilon^{-1}\right\}$, a large number of Taylor coefficients are correct in the asymptotic expansion at the origin for the slow manifold if ε is very small or very large.

7.11 Summary

The Michaelis-Menten mechanism

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P + E$$

gives rise to the planar and scalar differential equations

$$\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x}), \quad \dot{} = \frac{d}{dt} \quad \text{and} \quad y' = f(x,y), \quad ' = \frac{d}{dx},$$

where

$$\mathbf{g}(\mathbf{x}) = \begin{pmatrix} -x + (1-\eta+x)\,y \\ \varepsilon^{-1}\left[x - (1+x)\,y\right] \end{pmatrix} \quad \text{and} \quad f(x,y) = \frac{x-(1+x)\,y}{\varepsilon\left[-x+(1-\eta+x)\,y\right]}.$$

The main subject of this chapter was properties of scalar solutions $y(x)$. In the next chapter, we explore properties of solutions $\mathbf{x}(t)$ to the planar system that explicitly involve time t.

The Jacobian matrix $\mathbf{A} = \mathbf{Dg}(\mathbf{0})$ has two real and distinct eigenvalues, λ_- and λ_+. These eigenvalues satisfy $\lambda_- < \lambda_+ < 0$. Consequently, λ_+ and $\mathbf{v}_+$ are referred to, respectively, as the slow eigenvalue and slow eigenvector. Similarly, λ_- and $\mathbf{v}_-$ are the fast eigenvalue and fast eigenvector. Two important quantities associated with the eigenvalues is the slope σ of the slow eigenvector and the ratio κ of the eigenvalues, which are given by

$$\sigma = \frac{\lambda_+ + 1}{1-\eta} \quad \text{and} \quad \kappa = \frac{\lambda_-}{\lambda_+}.$$

The isoclines of the scalar system are all hyperbolas of the form

$$w(x) = \frac{x}{r+x}.$$

There are three special isoclines, namely the horizontal, vertical, and α isoclines. Explicitly,

$$H(x) = \frac{x}{1+x}, \quad V(x) = \frac{x}{1-\eta+x}, \quad \text{and} \quad \alpha(x) = \frac{x}{\sigma^{-1}+x}.$$

Note that the horizontal isocline corresponds to the QSSA, the vertical isocline corresponds to the EA, and the α isocline is the isocline for slope σ (which is the slope of the slow eigenvector at the origin). These three isoclines allowed us to define the positively invariant regions

$$\Gamma_0 = \{\ (x,y)\ :\ x>0,\ H(x) \le y \le V(x)\ \} \quad \text{and} \quad \Gamma_1 = \{\ (x,y)\ :\ x>0,\ H(x) \le y \le \alpha(x)\ \}.$$

All solutions of the planar system, we showed, enter the region Γ_0. Provided $\kappa \ge 2$, all solutions enter the region Γ_1 (which is a subset of Γ_0). However, if $1 < \kappa < 2$, then most (but not all) solutions enter Γ_1. Furthermore, we showed that the origin is globally asymptotically stable.

The Antifunnel Theorem applied to the region Γ_1 enabled us to prove the existence and uniqueness of a solution contained in Γ_1 for all $x > 0$. This solution is referred to as the slow manifold and is denoted by $y = \mathcal{M}(x)$. The slow manifold is so named since it, as is apparent from the phase portrait, attracts all other solutions and approaches the origin in the slow direction.

We determined the concavity of solutions to the scalar differential equation in the non-negative quadrant. This was accomplished by considering the auxiliary function

$$h(x) = y(x)\,[y(x)-1] + xy'(x),$$

where $y(x)$ is a solution of the scalar system, which determines the sign of the second derivative of the solution. Table 7.1 summarizes the concavity in all the regions.

Our investigation of concavity led us to construct the curve $y = \mathcal{Y}(x)$, which is between $y = \mathcal{M}(x)$ and $y = \alpha(x)$, along which scalar solutions $y(x)$ have inflection points. Furthermore, we showed that this curve is equivalent to the slow tangent manifold which has been explored by others.

Assuming the existence of a power series solution to the scalar differential equation, substitution of the series in to the differential equation formally gives a recursive expression for the Taylor coefficients $\{\sigma_n\}_{n=0}^{\infty}$, where $\sigma_0 = 0$ and $\sigma_1 = \sigma$. We showed that if $\kappa \notin \{2,3,\ldots\}$ then $\{\sigma_n\}_{n=0}^{\infty}$ are all defined. However, if $\kappa \in \{2,3,\ldots\}$ then only $\{\sigma_n\}_{n=0}^{\kappa-1}$ are defined. Furthermore, we showed the behaviour of scalar solutions $y(x)$ inside Γ_0 is in general not given by a Taylor series. In particular, $y(x)$ can be written in the form

$$y(x) = \begin{cases} \displaystyle\sum_{n=1}^{\lfloor\kappa\rfloor} \sigma_n x^n + C\,x^\kappa + \mathsf{o}(x^\kappa), & \text{if} \quad \kappa \notin \{2,3,\ldots\} \\ \sigma\,x + c\,x^2 \ln(x) + C\,x^2 + \mathsf{o}\big(x^2\big), & \text{if} \quad \kappa = 2 \\ \displaystyle\sum_{n=1}^{\kappa-1} \sigma_n x^n + C\,x^\kappa + \mathcal{O}\big(x^{\kappa+1}\big), & \text{if} \quad \kappa \in \{3,4,\ldots\} \end{cases} \qquad \text{as} \quad x \to 0^+.$$

For a given $x_0 > 0$, the scalar solution $y(x)$ with initial condition $y(x_0) = y_0$, with $0 \leq y_0 \leq \alpha(x_0)$, satisfies $0 \leq y(x) \leq \alpha(x)$ for all $x \in (0, x_0]$. Using Chaplygin's method, we derived tighter bounds on $y(x)$ valid over the interval $x \in (0, x_0]$ for the three cases $y_0 = 0$, $y_0 = H(x_0)$, and $y_0 = \alpha(x_0)$. Furthermore, we used these bounds to state bounds on the slow manifold over the interval $x \in (0, x_0]$.

We concluded this chapter with a summary of properties of the slow manifold $y = \mathcal{M}(x)$. For example, the slow manifold is concave down, is strictly increasing, and for large x has an asymptotic series of the form $\mathcal{M}(x) \sim \sum_{n=0}^{\infty} \rho_n x^{-n}$ as $x \to \infty$. To establish the asymptotic series, we used the isoclines to obtain leading-order behaviour and we constructed the slow manifold as a centre manifold for a fixed point at infinity.

Chapter 8

Time Estimates

The goal of this chapter is to briefly explore a few properties of solutions to the planar system for the Michaelis-Menten mechanism. These properties will fundamentally involve time as opposed to being expressible in terms of the corresponding scalar solution. In particular, we will obtain a low-order asymptotic expression for $\mathbf{x}(t)$ as $t \to \infty$. Furthermore, we will obtain bounds on $\mathbf{x}(t)$ during the steady-state period and as well as bounds on the length of the pre-steady-state period.

The Michaelis-Menten mechanism, recall, for the single enzyme-substrate reaction results in the planar system of ordinary differential equations

$$\dot{x} = -x + (1-\eta+x)\,y, \quad \dot{y} = \varepsilon^{-1}\left[x - (1+x)\,y\right], \tag{8.1}$$

where $\dot{} = \frac{d}{dt}$, $\varepsilon > 0$, and $\eta \in (0,1)$. The horizontal and vertical isoclines, along with the α isocline (which corresponds to the slope σ of the slow manifold at the origin), are given by

$$H(x) = \frac{x}{1+x}, \quad V(x) = \frac{x}{1-\eta+x}, \quad \text{and} \quad \alpha(x) = \frac{x}{\sigma^{-1}+x}. \tag{8.2}$$

In Chapter 7, we showed that all non-trivial solutions eventually enter the region

$$\Gamma_0 = \{\ (x,y)\ :\ x > 0,\ H(x) \le y \le V(x)\ \}.$$

Furthermore, most solutions enter the region

$$\Gamma_1 = \{\ (x,y)\ :\ x > 0,\ H(x) \le y \le \alpha(x)\ \}.$$

See Theorems 7.7 and 7.41 for more precise statements.

8.1 Behaviour as $t \to \infty$

Let $\mathbf{x}(t)$ be the solution of (8.1) with initial condition $\mathbf{x}(0) = \mathbf{x}_0$, where $\mathbf{x}_0 \in \Gamma_0$. We will use the isocline structure and differential inequalities to obtain a leading-order estimate of the components of the solution. We know already from Theorem 2.12 on page 22 that $x(t) = \mathcal{O}\big(\mathrm{e}^{\lambda_+ t}\big)$ and $x(t) = \mathcal{O}\big(\mathrm{e}^{\lambda_+ t}\big)$ as $t \to \infty$, where λ_+ is the slow eigenvalue. Note that the matrix $\mathbf{A}$ is diagonalizable so the σ in the statement of the theorem (which has a different meaning than in this part of the thesis) can be taken as zero.

The origin is globally asymptotically stable (see Theorem 7.7). Thus, our first estimate is

$$x(t) = \mathsf{o}(1) \quad \text{and} \quad y(t) = \mathsf{o}(1) \quad \text{as} \quad t \to \infty. \tag{8.3}$$

Let $\delta \in (0, \sigma)$ be fixed and arbitrary and define $c_1 := \sigma - \delta$ and $c_2 := \sigma + \delta$. Now, we know from Equation (8.3), Proposition 7.18, and the isocline structure that there is a $T \geq 0$ such that

$$F(x(t), c_1) \leq y(t) \leq F(x(t), c_2) \quad \text{for all} \quad t \geq T, \tag{8.4}$$

where F is the function given in (7.8). Using (7.8), (8.1), and (8.4), we see that $x(t)$ must satisfy the differential inequalities

$$-\frac{a_1 x(t)}{1 + b_1 x(t)} \leq \dot{x}(t) \leq -\frac{a_2 x(t)}{1 + b_2 x(t)} \quad \text{for all} \quad t \geq T, \tag{8.5}$$

where

$$a_1 := \frac{K(c_1) - (1 - \eta)}{K(c_1)}, \quad b_1 := \frac{1}{K(c_1)}, \quad a_2 := \frac{K(c_2) - (1 - \eta)}{K(c_2)}, \quad \text{and} \quad b_2 := \frac{1}{K(c_2)},$$

with the function K being defined in (7.7). Note that, courtesy of Figure 7.1, we can conclude $a_1, a_2, b_1, b_2 > 0$. Note also that

$$-a_1 < \lambda_+ < -a_2, \quad \lim_{\delta \to 0^+} a_i = -\lambda_+, \quad \text{and} \quad \lim_{\delta \to 0^+} b_i = \sigma, \quad \text{and} \quad (\ i = 1, 2\ ), \tag{8.6}$$

which follows from Equations (7.6) and (7.10) as well as Figure 7.1.

We can apply the Initial-Value Comparison Theorem (see Theorem A.6 in Appendix A on page 310) to the differential inequalities (8.5). Now, Claim A.25 (which is in Appendix A on page 323) gives us the solution of the corresponding differential equalities. Hence,

$$\chi_{a_1, b_1}(t) \leq x(t) \leq \chi_{a_2, b_2}(t) \quad \text{for all} \quad t \geq T, \tag{8.7}$$

where

$$\chi_{a,b}(t) := \frac{1}{b}\, W\Big(\Big[bx_0 \mathsf{e}^{bx_0}\Big]\, \mathsf{e}^{-at}\Big) \quad \text{for} \quad a, b > 0. \tag{8.8}$$

Remark 8.1: We can obtain simpler-looking bounds for $x(t)$ than those given in (8.7). First, observe that the lower bound in (8.5) can be taken one step further to give $\dot{x}(t) \geq -a_1 x(t)$ for all $t \geq T$. Second, we use the fact that $W(u) \leq u$ for all $u \geq 0$ in (8.7) and (8.8). Thus,

$$x_0 \mathsf{e}^{-a_1 t} \leq x(t) \leq x_0 \mathsf{e}^{b_2 x_0} \mathsf{e}^{-a_2 t} \quad \text{for all} \quad t \geq T.$$

A standard property of the Lambert W function is

$$W(x) = x + \mathcal{O}\big(x^2\big) \quad \text{as} \quad x \to 0^+.$$

It follows that

$$\chi_{a,b}(t) = \Big[x_0 \mathsf{e}^{bx_0}\Big]\, \mathsf{e}^{-at}\, \big[1 + \mathcal{O}\big(\mathsf{e}^{-at}\big)\big] \quad \text{as} \quad t \to \infty$$

and[1]

$$\ln(\chi_{a,b}(t)) = \ln\Big(x_0 \mathsf{e}^{bx_0}\Big) - at + \mathcal{O}\big(\mathsf{e}^{-at}\big) \quad \text{as} \quad t \to \infty. \tag{8.9}$$

We can conclude from (8.7) and (8.9) that

$$\liminf_{t\to\infty} \frac{\ln(x(t))}{t} \geq -a_1 \quad \text{and} \quad \limsup_{t\to\infty} \frac{\ln(x(t))}{t} \leq -a_2.$$

Since this is true for all $\delta \in (0, \sigma)$, if we let $\delta \to 0^+$ and apply (8.6), we get

$$\lim_{t\to\infty} \frac{\ln(x(t))}{t} = \lambda_+.$$

Furthermore, since

$$y(t) = \sigma x(t)\, [1 + \mathsf{o}(1)] \quad \text{and} \quad \ln(y(t)) = \ln(\sigma) + \ln(x(t)) + \mathsf{o}(1) \quad \text{as} \quad t \to \infty$$

which we know from Theorem 7.39 in conjunction with (8.3), we also have

$$\lim_{t\to\infty} \frac{\ln(y(t))}{t} = \lambda_+.$$

We have thus proven the following.

[1]Since $\ln(1+u) = u + \mathcal{O}\big(u^2\big)$ as $u \to 0$, it must be that $\ln(1 + \mathcal{O}(u)) = \mathcal{O}(u)$ as $u \to 0$.

Proposition 8.2: *Let $\boldsymbol{x}(t)$ be the solution of* (8.1) *with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in \Gamma_0$. Then,*

$$\lim_{t\to\infty} \frac{\ln(x(t))}{t} = \lambda_+ \quad \textit{and} \quad \lim_{t\to\infty} \frac{\ln(y(t))}{t} = \lambda_+.$$

Remark 8.3: If

$$\lim_{t\to\infty} \frac{\ln(z(t))}{t} = \mu$$

for some function $z(t)$ and constant μ, it does not follow that

$$z(t) = \mathcal{O}\left(\mathrm{e}^{\mu t}\right) \quad \text{as} \quad t \to \infty.$$

For a simple counter-example, consider

$$\lim_{t\to\infty} \frac{\ln\left(t\,\mathrm{e}^{-t}\right)}{t} = \lim_{t\to\infty} \left[\frac{\ln(t)}{t} - 1\right] = -1.$$

8.2 Bounds on Solutions while in Γ_1

Let $\mathbf{x}(t)$ be the solution of the planar system (8.1) with initial condition $\mathbf{x}(0) = \mathbf{x}_0$, where $\mathbf{x}_0 \in \Gamma_1$. We will use differential inequalities to obtain simple bounds on the components of the solution. These estimates will be valid for all $t \geq 0$.

Since the region Γ_1 is positively invariant, which we know from Theorem 7.41, we can conclude that

$$H(x(t)) \leq y(t) \leq \alpha(x(t)) \quad \text{for all} \quad t \geq 0. \tag{8.10}$$

The period of time while a solution is inside Γ_1 (or Γ_0) may be referred to as the "steady-state period" since the solution roughly obeys the QSSA. Here, we are assuming that the solution begins in the steady-state period. Using (7.6), (8.1), (8.2), and (8.10), we see that $x(t)$ satisfies the differential inequalities

$$-\frac{\eta x(t)}{1 + x(t)} \leq \dot{x}(t) \leq \frac{\lambda_+ x(t)}{1 + \sigma x(t)} \quad \text{for all} \quad t \geq 0. \tag{8.11}$$

Using the Initial-Value Comparison Theorem (Theorem A.6) and Claim A.25, we get

$$\chi_{\eta,1}(t) \leq x(t) \leq \chi_{-\lambda_+,\sigma}(t) \quad \text{for all} \quad t \geq 0,$$

where $\chi_{a,b}(t)$ was defined in (8.8). Figure 8.1 demonstrates the bounds on $x(t)$. Furthermore, since both H and α are strictly increasing functions and $y(t)$ satisfies (8.10), we have thus proven the following.

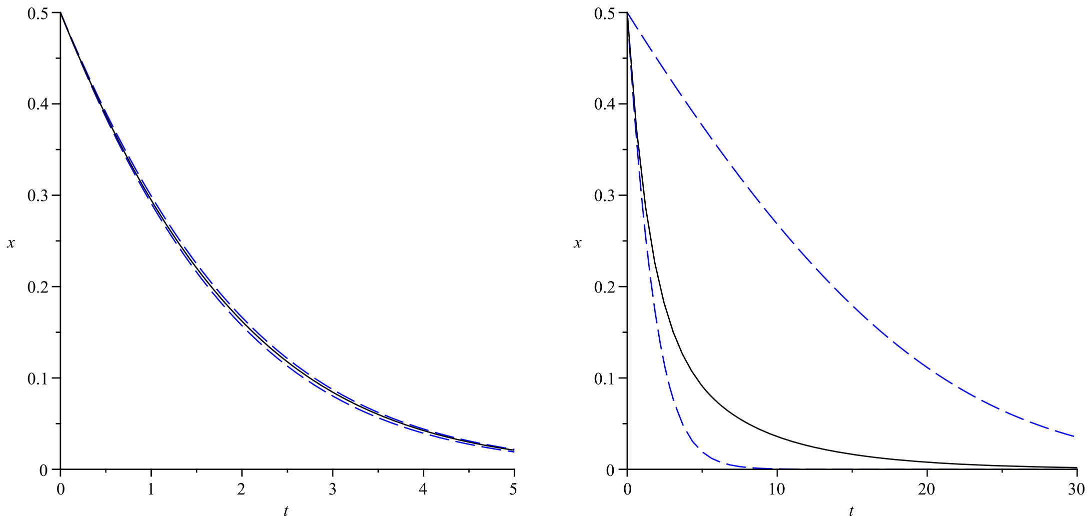

Figure 8.1: For the first picture, suppose $\varepsilon = 0.1$, $\eta = 0.75$, and $x_0 = 0.5$. The two dashed curves represent the lower and upper bounds for $x(t)$, given in Equation (8.12), while inside Γ_1. The solid curve represents the actual solution (found numerically) with $x(0) = x_0$ and $y(0) = H(x_0)$. The second picture is the same as the first except with $\varepsilon = 5.0$, $\eta = 0.75$, and $x_0 = 0.5$.

Proposition 8.4: *Let $\boldsymbol{x}(t)$ be the solution of* (8.1) *with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in \Gamma_1$. Then,*

$$\chi_{\eta,1}(t) \leq x(t) \leq \chi_{-\lambda_+,\sigma}(t) \quad \textit{and} \quad H\left(\chi_{\eta,1}(t)\right) \leq y(t) \leq \alpha\left(\chi_{-\lambda_+,\sigma}(t)\right) \quad \textit{for all} \quad t \geq 0. \tag{8.12}$$

Remark 8.5: We can obtain simpler-looking (but weaker) bounds for $x(t)$ than (8.12). First, we take the lower bound in (8.11) one step further and observe that $\dot{x}(t) \geq -\eta x(t)$ for all $t \geq 0$. Second, we use the fact that $W(u) \leq u$ for all $u \geq 0$ in (8.8) and (8.11). Thus,

$$x_0 \mathsf{e}^{-\eta t} \leq x(t) \leq x_0 \mathsf{e}^{\sigma x_0} \mathsf{e}^{\lambda_+ t} \quad \text{for all} \quad t \geq 0.$$

8.3 Time to Enter Γ_1

Suppose that $x_0 > 0$. Let $\mathbf{x}(t)$ be the solution of (8.1) with $x(0) = x_0$ and $y(0) = 0$. Let $\bar{t} > 0$ be the time it takes for the solution $\mathbf{x}(t)$ to enter Γ_1. Moreover, let $(\overline{x}, \overline{y})$ be the point at which $\mathbf{x}(t)$ enters Γ_1. The goal of this section is to find easily-computable bounds for $\bar{t}$, which equals the length of the "pre-steady-state period." See Figure 8.2. These bounds will be decidedly crude. Estimates

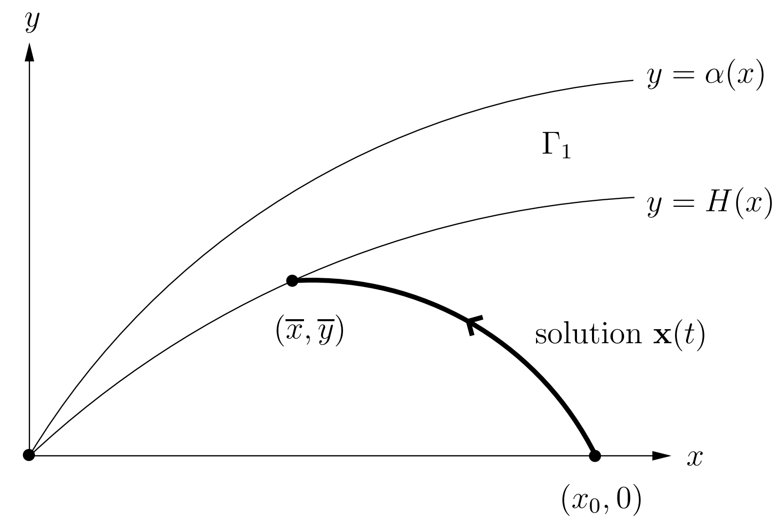

Figure 8.2: Estimating the time it takes for a solution starting at $x(0) = x_0$ and $y(0) = 0$ to enter the antifunnel Γ_1. The solution enters Γ_1 through $(\overline{x}, \overline{y})$ at time $\overline{t}$.

of the length of (one definition or another of) the pre-steady-state period have been considered before. See, for example, [93, 112].

8.3.1 Bounds on $\overline{t}$ in terms of $\overline{x}$

We know that $y(t)$ satisfies

$$0 \le y(t) \le H(x(t)) \quad \text{for all} \quad t \in \left[0, \overline{t}\right].$$

Using this fact in conjunction with (8.1) and (8.2), we see that $x(t)$ satisfies

$$-x(t) \le \dot{x}(t) \le -\frac{\eta x(t)}{1 + x(t)} \quad \text{for all} \quad t \in \left[0, \overline{t}\right].$$

By inspection,

$$x_0 \mathsf{e}^{-t} \le x(t) \le W\left(x_0 \mathsf{e}^{x_0} \mathsf{e}^{-\eta t}\right) \quad \text{for all} \quad t \in \left[0, \overline{t}\right],$$

where we used the expression (8.8) for $\chi_{a,b}(t)$. Setting $t = \overline{t}$ and $x(t) = \overline{x}$ and solving for $\overline{t}$, we get[2]

$$-\ln\left(\frac{\overline{x}}{x_0}\right) \le \overline{t} \le \frac{1}{\eta}\left[(x_0 - \overline{x}) - \ln\left(\frac{\overline{x}}{x_0}\right)\right]. \tag{8.13}$$

[2] If $u \le W(v)$ then $\mathsf{e}^u \le \mathsf{e}^{W(v)}$. Multiplying these two inequalities gives $u\,\mathsf{e}^u \le W(v)\,\mathsf{e}^{W(v)}$. By definition of the Lambert W function, $W(v)\,\mathsf{e}^{W(v)} = v$. Thus, $u\,\mathsf{e}^u \le v$.

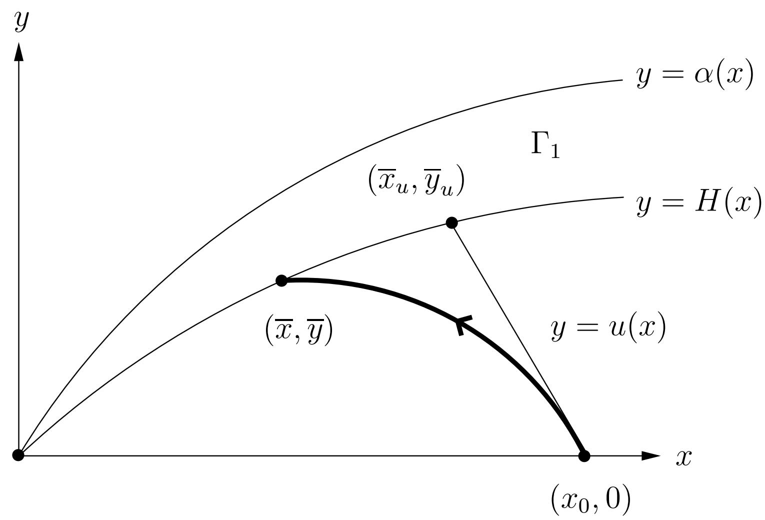

Figure 8.3: The point of intersection $(\overline{x}_u, \overline{y}_u)$ of $y = u(x)$ and $y = H(x)$, where $u(x)$ is the tangent to the scalar solution $y(x)$ at $x = x_0$ and H is the horizontal isocline. Obviously, $\overline{x}_u$ is an upper bound for $\overline{x}$.

These bounds on $\overline{t}$, unfortunately, are currently unusable since we do not have a value for $\overline{x}$. However, if we have upper and lower bounds on $\overline{x}$ which depend only on ε, η, and x_0, then we have usable bounds on $\overline{t}$.

8.3.2 Upper Bound $\overline{x}_u$ for $\overline{x}$

Let $y(x)$ be the corresponding scalar solution. We know that $y(x_0) = 0$ and $y'(x_0) = -\varepsilon^{-1}$, the latter of which follows from Table 6.1 on page 150. Thus, the tangent line to $y(x)$ at $x = x_0$ is given by

$$u(x) := -\varepsilon^{-1}(x - x_0).$$

This line will intersect the horizontal isocline twice (once to the left and once to the right of the y-axis). Let $(\overline{x}_u, \overline{y}_u)$ be the point of intersection to the right of the y-axis. See Figure 8.3. Hence,

$$\frac{\overline{x}_u}{1 + \overline{x}_u} = -\varepsilon^{-1}(\overline{x}_u - x_0) \quad \text{and} \quad (\overline{x}_u)^2 - (x_0 - 1 - \varepsilon)\,\overline{x}_u - x_0 = 0.$$

Solving for the positive root,

$$\overline{x}_u = \tfrac{1}{2}(x_0 - 1 - \varepsilon) + \tfrac{1}{2}\sqrt{(x_0 - 1 - \varepsilon)^2 + 4x_0}. \tag{8.14}$$

Observe that

$$\overline{x}_u = x_0 + \mathcal{O}(\varepsilon) \quad \text{and} \quad \overline{y}_u = \frac{x_0}{1+x_0} + \mathcal{O}(\varepsilon) \quad \text{as} \quad \varepsilon \to 0^+. \tag{8.15}$$

We know from Table 7.1 that $y(x)$ is concave down on $[\overline{x}, x_0]$. Thus, $y(x) \le u(x)$ on $[\overline{x}, x_0]$. Furthermore, the horizontal isocline is strictly increasing. Therefore, we indeed have the bounds $\overline{x} \le \overline{x}_u$ and $\overline{y} \le \overline{y}_u$.

8.3.3 Lower Bound $\overline{x}_\ell$ for $\overline{x}$

Finding a lower bound for $\overline{x}$ will not be quite as easy as for the upper bound. Let $y(x)$ be the corresponding scalar solution, which satisfies $y(x_0) = 0$ and $y'(x_0) = -\varepsilon^{-1}$. A straight-line lower bound for $y(x)$ can be found, at least on some interval with right-endpoint x_0, which can be used to find a lower bound on $\overline{x}$. However, there are some computational issues associated with using this straight line which we want to avoid. Instead, consider the hyperbola

$$\ell_r(x) := \frac{x_0 - x}{r + (x_0 - x)} \quad \text{for} \quad r > \varepsilon.$$

We will use the Comparison Theorem to find an interval with right-endpoint x_0 on which this hyperbola is below the solution. Note that

$$\ell_r(x_0) = 0, \quad \ell_r'(x_0) = -\frac{1}{r}, \quad \text{and} \quad \ell_r'(x), \ell_r''(x) < 0 \quad \text{for all} \quad x \le x_0.$$

Note also that the restriction $r > \varepsilon$ ensures $y'(x_0) < \ell_r'(x_0) < 0$.

The hyperbola and horizontal isocline intersect at $x = \frac{x_0}{1+r}$. Moreover, $f(x, \ell_r(x))$ decreases monotonically on $\left[\frac{x_0}{1+r}, x_0\right]$ from 0 to $-\varepsilon^{-1}$, which follows from the Chain Rule and the fact that $\frac{\partial f}{\partial x}(x, \ell_r(x)) \le 0$, $\frac{\partial f}{\partial y}(x, \ell_r(x)) > 0$, and $\ell_r'(x) < 0$. It follows that there is a unique $a_r \in \left(\frac{x_0}{1+r}, x_0\right)$ such that

$$f(a_r, \ell_r(a_r)) = -\frac{1}{r} \quad \text{and} \quad f(x, \ell_r(x)) \le -\frac{1}{r} \quad \text{for all} \quad x \in [a_r, x_0].$$

Since $\ell_r'(x) \ge -\frac{1}{r}$ for all $x \le x_0$, we see $f(x, \ell_r(x)) \le \ell_r'(x)$ for all $x \in [a_r, x_0]$. By the Final-Value Comparison Theorem (see Theorem A.7 in Appendix A on page 311),

$$y(x) \ge \ell_r(x) \quad \text{for all} \quad x \in [a_r, x_0].$$

The value of a_r is easy to find: solving $f(a_r, \ell_r(a_r)) = -r^{-1}$ yields

$$a_r = \frac{[r - (1-\eta)\,\varepsilon]\, x_0}{r\,(r-\varepsilon) + r - (1-\eta)\,\varepsilon} = x_0 \left\{ 1 + r \left[\frac{(r-\varepsilon)}{r - (1-\eta)\,\varepsilon} \right] \right\}^{-1}.$$

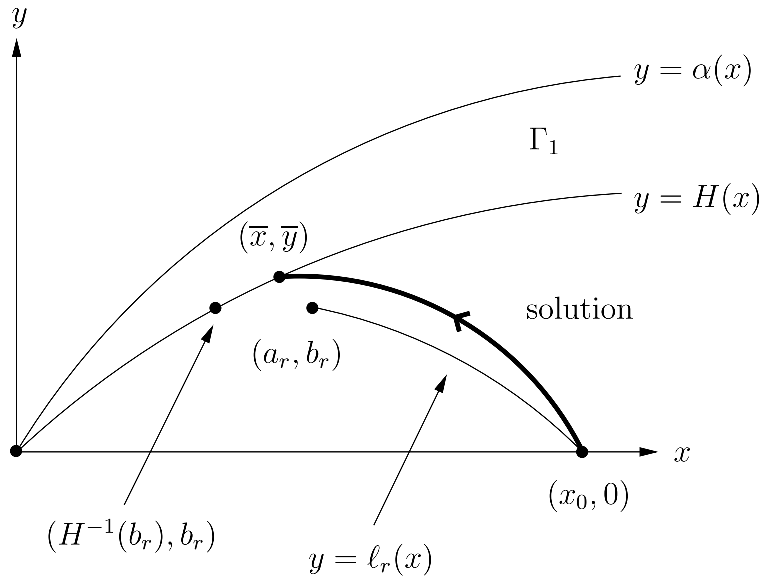

Figure 8.4: This figure depicts a hyperbolic lower bound $y = \ell_r(x)$, for any $r > \varepsilon$, for the solution curve $y = y(x)$. The point (a_r, b_r), where $b_r = \ell_r(a_r)$, is found using the Comparison Theorem and allows us to find lower bounds on $\overline{x}$ and $\overline{y}$. In particular, $\overline{y} \geq b_r$ and $\overline{x} \geq H^{-1}(b_r)$.

Since $\varepsilon > 0$, $\eta \in (0,1)$, and $r > \varepsilon$, it is easy to check that indeed $a_r \in \left(\frac{x_0}{1+r}, x_0\right)$. Let $b_r := \ell(a_r)$. As we can see from Figure 8.4, the point (a_r, b_r) can be to the left or to the right of $(\overline{x}, \overline{y})$. However, it must be the case that (a_r, b_r) is below $(\overline{x}, \overline{y})$. That is, $b_r \leq \overline{y}$. Thus, we want to maximize b_r with respect to $r > \varepsilon$. A simple Calculus argument will verify that the optimal choice of r is $\sqrt{\varepsilon\eta} + \varepsilon$. Hence, we will take

$$r := \sqrt{\varepsilon\eta} + \varepsilon, \quad \ell(x) := \frac{x_0 - x}{\left(\sqrt{\varepsilon\eta} + \varepsilon\right) + (x_0 - x)}, \quad \text{and} \quad a := \frac{\left(\sqrt{\varepsilon\eta} + 1\right) x_0}{2\sqrt{\varepsilon\eta} + \varepsilon + 1}.$$

It is apparent from Figure 8.4 that $\ell(a)$ is a lower bound for $\overline{y}$ and $H^{-1}(\ell(a))$ is a lower bound for $\overline{x}$. Note that

$$H^{-1}(y) = \frac{y}{1-y}.$$

Therefore, we take

$$\overline{x}_\ell := \frac{x_0}{2\sqrt{\varepsilon\eta} + \varepsilon + 1} \quad \text{and} \quad \overline{y}_\ell := \frac{x_0}{2\sqrt{\varepsilon\eta} + \varepsilon + (1 + x_0)}, \tag{8.16}$$

which satisfy $\overline{x} \geq \overline{x}_\ell$ and $\overline{y} \geq \overline{y}_\ell$. Figure 8.5 gives two examples of locating the points $(\overline{x}_\ell, \overline{y}_\ell)$ and $(\overline{x}_u, \overline{y}_u)$ and demonstrates how the actual point of entry $(\overline{x}, \overline{y})$ is between the two points along the horizontal isocline.

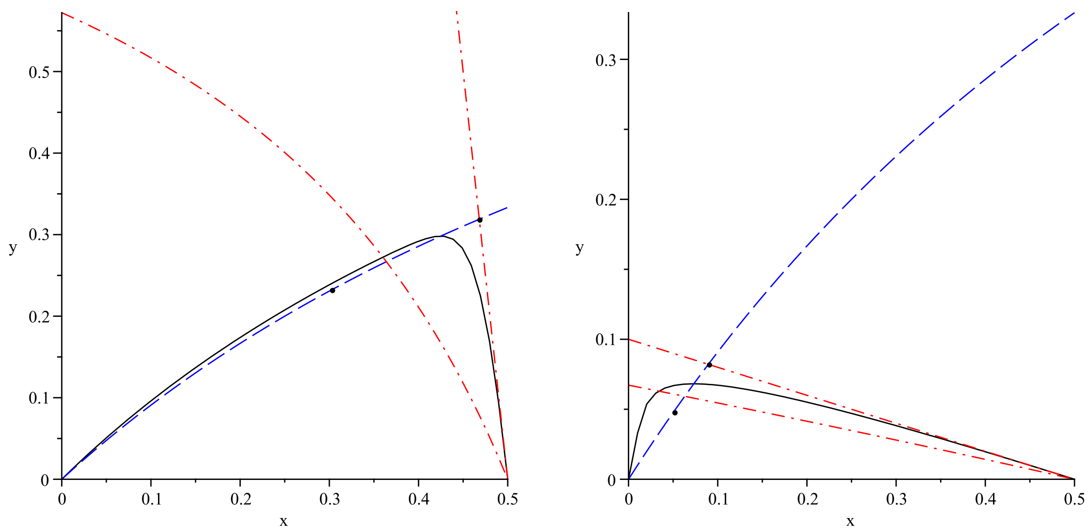

Figure 8.5: For the first picture, suppose $\varepsilon = 0.1$, $\eta = 0.75$, and $x_0 = 0.5$. The actual solution (solid line) and horizontal isocline (dashed line, the quasi-steady-state approximation) are shown. Also shown are the hyperbola $y = \ell(x)$ (left dash-dot line) and tangent line $y = -\varepsilon^{-1}(x - x_0)$ (right dash-dot line). The points $(\overline{x}_\ell, \overline{y}_\ell)$ and $(\overline{x}_u, \overline{y}_u)$ are indicated by the solid circles. The second picture is the same as the first except with $\varepsilon = 5.0$, $\eta = 0.75$, and $x_0 = 0.5$.

Observe that

$$\overline{x}_\ell = x_0 + \mathcal{O}\big(\sqrt{\varepsilon}\big) \quad \text{and} \quad \overline{y}_\ell = \frac{x_0}{1 + x_0} + \mathcal{O}\big(\sqrt{\varepsilon}\big) \quad \text{as} \quad \varepsilon \to 0^+. \tag{8.17}$$

Equations (8.15) and (8.17) give us the following.

Proposition 8.6: *Suppose that $x_0 > 0$. Let $\boldsymbol{x}(t)$ be the solution of (8.1) with $x(0) = x_0$ and $y(0) = 0$. If $(\overline{x}, \overline{y})$ is the point where $\boldsymbol{x}(t)$ enters Γ_1, then*

$$\lim_{\varepsilon \to 0^+} \overline{x} = x_0 \quad \textit{and} \quad \lim_{\varepsilon \to 0^+} \overline{y} = \frac{x_0}{1 + x_0}. \tag{8.18}$$

8.3.4 Bounds on $\overline{t}$ in terms of $\overline{x}_\ell$ and $\overline{x}_u$

We are now in a position to state non-trivial bounds on the time $\overline{t}$ it takes for the solution $\mathbf{x}(t)$ to enter the region Γ_1 (that is, the length of the pre-steady-state period). Recall Equation (8.13), which gives bounds on $\overline{t}$ in terms of the x-value $\overline{x}$ of the point of entry into Γ_1. The expressions on the left and right are both strictly decreasing functions of $\overline{x}$. With the aid of (8.18), we therefore have proven the following.

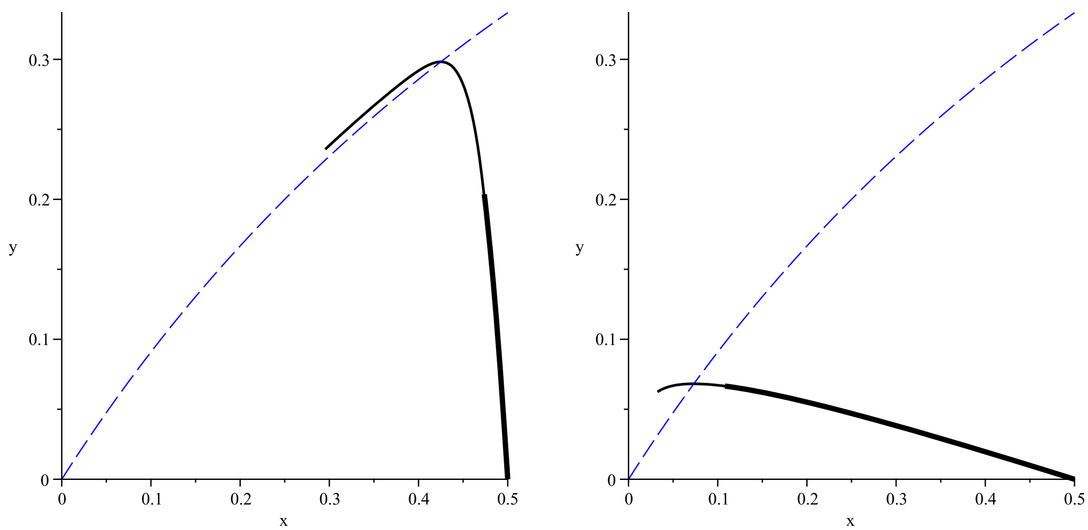

Figure 8.6: For the first picture, suppose $\varepsilon = 0.1$, $\eta = 0.75$, and $x_0 = 0.5$. With these values, we can calculate the bounds on $\overline{t}$ (the time it takes for the solution to cross the horizontal isocline) to be $\overline{t}_\ell \approx 0.0659$ and $\overline{t}_u \approx 0.928$ using (8.14), (8.16), and (8.20). The actual solution (solid line) and horizontal isocline (dashed line) are shown. The thick portion of the solution corresponds to $t \in \left[0, \overline{t}_\ell\right]$ and the thin portion of the solution corresponds to $t \in \left[\overline{t}_\ell, \overline{t}_u\right]$. Indeed, $\overline{t} \in \left[\overline{t}_\ell, \overline{t}_u\right]$. The second picture is the same as the first except with $\varepsilon = 5.0$, $\eta = 0.75$, and $x_0 = 0.5$. The lower and upper bounds for $\overline{t}$ respectively are $\overline{t}_\ell \approx 1.72$ and $\overline{t}_u \approx 3.65$.

Proposition 8.7: *Suppose that $x_0 > 0$. Let $\boldsymbol{x}(t)$ be the solution of* (8.1) *with $x(0) = x_0$ and $y(0) = 0$. If $\overline{t}$ is the time it takes for $\boldsymbol{x}(t)$ to enter Γ_1, then*

$$-\mathit{ln}\left(\frac{\overline{x}_u}{x_0}\right) \le \overline{t} \le \frac{1}{\eta}\left[(x_0 - \overline{x}_\ell) - \mathit{ln}\left(\frac{\overline{x}_\ell}{x_0}\right)\right], \tag{8.19}$$

where $\overline{x}_\ell$ is given in (8.16) *and $\overline{x}_u$ is given in* (8.14). *Furthermore,*

$$\lim_{\varepsilon \to 0^+} \overline{t} = 0.$$

Figure 8.6 gives two examples of using (8.19) to find bounds on $\overline{t}$. Define

$$\overline{t}_\ell := -\ln\left(\frac{\overline{x}_u}{x_0}\right) \quad \text{and} \quad \overline{t}_u := \frac{1}{\eta}\left[(x_0 - \overline{x}_\ell) - \ln\left(\frac{\overline{x}_\ell}{x_0}\right)\right] \tag{8.20}$$

which are the lower and upper bounds for $\overline{t}$. It can be shown that

$$\overline{t}_\ell = \left(\frac{1}{1 + x_0}\right)\varepsilon + \mathcal{O}(\varepsilon^2) \quad \text{and} \quad \overline{t}_u = \left[\frac{2\,(1 + x_0)}{\sqrt{\eta}}\right]\sqrt{\varepsilon} + \mathcal{O}(\varepsilon) \quad \text{as} \quad \varepsilon \to 0^+.$$

Remark 8.8: There is an interesting consequence of these bounds on $\bar{t}$. Since $0 < \overline{x} \leq \overline{x}_u$, it follows from (8.14) that

$$\lim_{\varepsilon\to\infty} \overline{x} = 0.$$

Appealing to (8.13), we can conclude

$$\lim_{\varepsilon\to\infty} \bar{t} = \infty.$$

That is, when ε is large the pre-steady-state period is long. (When ε is small, the pre-steady-state period is brief.)

8.4 Summary

The purpose of this chapter was to develop some basic time estimates for solutions $\mathbf{x}(t)$, with initial condition $\mathbf{x}_0$, to the planar system

$$\dot{x} = -x + (1 - \eta + x)\, y, \quad \varepsilon\dot{y} = x - (1 + x)\, y,$$

which arises from the Michaelis-Menten mechanism.

First, we used differential inequalities and properties we have developed in this thesis to establish the long-term asymptotic behaviour of $\mathbf{x}(t)$ when $\mathbf{x}_0 \in \Gamma_0$, where

$$\Gamma_0 = \{\ (x, y)\ :\ x > 0,\ H(x) \leq y \leq V(x)\ \}$$

with H being the horizontal isocline and V being the vertical isocline. In particular, we showed

$$\lim_{t\to\infty} \frac{\ln(x(t))}{t} = \lambda_+ \quad \text{and} \quad \lim_{t\to\infty} \frac{\ln(y(t))}{t} = \lambda_+,$$

where λ_+ is the slow eigenvalue.

Second, we obtained bounds on the solution if $\mathbf{x}_0 \in \Gamma_1$, where

$$\Gamma_1 = \{\ (x, y)\ :\ x > 0,\ H(x) \leq y \leq \alpha(x)\ \}$$

with α being the isocline for slope σ (the slope of the slow manifold at the origin). Specifically,

$$\chi_{\eta,1}(t) \leq x(t) \leq \chi_{-\lambda_+,\sigma}(t) \quad \text{and} \quad H\left(\chi_{\eta,1}(t)\right) \leq y(t) \leq \alpha\left(\chi_{-\lambda_+,\sigma}(t)\right) \quad \text{for all} \quad t \geq 0,$$

where

$$\chi_{a,b}(t) = \frac{1}{b}\, W\left(\left[bx_0 \mathsf{e}^{bx_0}\right] \mathsf{e}^{-at}\right) \quad \text{for} \quad a, b > 0.$$

Note that $W(x)$ is the Lambert W function. Alternatively, we showed that

$$x_0 \mathsf{e}^{-\eta t} \leq x(t) \leq x_0 \mathsf{e}^{\sigma x_0} \mathsf{e}^{\lambda_+ t} \quad \text{for all} \quad t \geq 0.$$

Finally, we found lower and upper bounds on the time $\overline{t}$ for the solution to enter Γ_1 (which it does through the point $(\overline{x}, \overline{y})$) when the initial condition is on the positive x-axis. In particular, using the Comparison Theorem and other tricks we showed that

$$-\ln\left(\frac{\overline{x}_u}{x_0}\right) \leq \overline{t} \leq \frac{1}{\eta}\left[(x_0 - \overline{x}_\ell) - \ln\left(\frac{\overline{x}_\ell}{x_0}\right)\right],$$

where

$$\overline{x}_\ell = \frac{x_0}{2\sqrt{\varepsilon\eta} + \varepsilon + 1} \quad \text{and} \quad \overline{x}_u = \tfrac{1}{2}\left(x_0 - 1 - \varepsilon\right) + \tfrac{1}{2}\sqrt{\left(x_0 - 1 - \varepsilon\right)^2 + 4x_0}$$

are lower and upper bounds on $\overline{x}$. Moreover, we showed that

$$\lim_{\varepsilon \to 0^+} \overline{x} = x_0, \quad \lim_{\varepsilon \to 0^+} \overline{y} = \frac{x_0}{1 + x_0}, \quad \text{and} \quad \lim_{\varepsilon \to 0^+} \overline{t} = 0.$$

At the other extreme, we showed

$$\lim_{\varepsilon \to \infty} \overline{x} = 0, \quad \lim_{\varepsilon \to \infty} \overline{y} = 0, \quad \text{and} \quad \lim_{\varepsilon \to \infty} \overline{t} = \infty.$$

Chapter 9

Modifications to the Michaelis-Menten Mechanism

The Michaelis-Menten mechanism is the simplest chemical network which models the formation of a product from a substrate with the help of a catalytic enzyme. Symbolically, this mechanism is

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\to} P + E,$$

where S is the substrate, E is the enzyme, C is the complex, P is the product, and k_{-1}, k_1, and k_2 are the reaction-rate constants. There are, of course, many more complicated enzyme reactions and chemical networks which are studied in biochemistry and chemical kinetics. The goal of this chapter is to make it apparent that the techniques and results we developed in Chapters 7 and 8 can be extended to other chemical networks.

9.1 Henri Mechanism

A mechanism in chemical kinetics is the complete set of elementary reactions which encompass a reaction. However, a given reaction may have many different possible mechanisms which are consistent with the known information. Since knowing which mechanism is correct is of fundamental theoretical importance, much attention in chemical kinetics is devoted to the distinguishing of mechanisms.

Victor Henri, who originated the traditional Michaelis-Menten mechanism (which involves a productive enzyme-substrate complex), also proposed another mechanism for a simple enzyme reaction (which involves a nonproductive enzyme-substrate complex). This second mechanism is often called the Henri mechanism or the Nuisance-Complex mechanism. See, for example, [108, 111, 121].

Henri preferred what is now referred to as the Michaelis-Menten mechanism, but recognized that both mechanisms explain the observed kinetics yet are kinetically indistinguishable using the equilibrium approximation. Presently, the Michaelis-Menten mechanism is considered the probable mechanism. However, more complicated mechanisms with nonproductive enzyme-substrate complexes are important in many other reactions. Thus, techniques of kinetically distinguishing the Michaelis-Menten and Henri mechanisms are of theoretical value.

9.1.1 The Model and Differential Equations

Symbolically, the Henri mechanism is

$$C \underset{k_1}{\overset{k_{-1}}{\rightleftharpoons}} S + E \overset{k_2}{\rightarrow} P + E,$$

where S is the substrate, E is the enzyme, C is the complex, and P is the product. The constants k_{-1}, k_1, and k_2 are the reaction-rate constants. Using the Law of Mass Action, we have the system of ordinary differential equations

$$\begin{aligned}
\dot{s} &= k_{-1}c - (k_1 + k_2)\, se, \\
\dot{e} &= k_{-1}c - k_1 se, \\
\dot{c} &= k_1 se - k_{-1}c, \\
\dot{p} &= k_2 se,
\end{aligned}$$

where $\dot{} = \frac{d}{dt}$. The traditional initial conditions are $s(0) = s_0$, $e(0) = e_0$, $c(0) = 0$, and $p(0) = 0$. However, we will allow the initial conditions to be arbitrary.

Observe that

$$e(t) + c(t) \equiv e_0 \quad \text{and} \quad s(t) + c(t) + p(t) \equiv s_0,$$

which are the same two conservation laws, (6.3) and (6.4), which we had for the standard Michaelis-Menten mechanism. We denoted the constants by s_0 and e_0 since, traditionally, the complex and product are not considered to be initially present.

9.1.2 Reduction and Re-scaling

Using the first conservation law and ignoring the differential equation for p (which is decoupled from the other three differential equations), we have the planar reduction

$$\dot{s} = k_{-1}c - (k_1 + k_2)\, s\,(e_0 - c)\,, \quad \dot{c} = k_1 s\,(e_0 - c) - k_{-1}c. \tag{9.1}$$

The dimensions of the involved quantities in (9.1) are

$$[s, c, e_0] = \frac{Q}{L^3}, \quad [\dot{s}, \dot{c}] = \frac{Q}{L^3 T}, \quad [k_{-1}] = \frac{1}{T}, \quad \text{and} \quad [k_1, k_2] = \frac{L^3}{QT}.$$

Now, define the dimensionless quantities

$$\tau := (k_1 + k_2)\, e_0 t, \quad x := \left(\frac{k_1}{k_{-1}}\right) s, \quad y := \frac{c}{e_0}, \quad \varepsilon := \frac{e_0\,(k_1 + k_2)}{k_{-1}}, \quad \text{and} \quad \eta := \frac{k_2}{k_1 + k_2}.$$

Observe $\varepsilon > 0$ and $0 < \eta < 1$. With these scaled variables, (9.1) becomes

$$x' = -x + (1 - \eta + x)\, y, \quad y' = \varepsilon^{-1}\left[x - (1 + x)\, y\right], \tag{9.2}$$

where $' = \frac{d}{d\tau}$.

The planar system (9.2) is exactly the same planar system as for the standard Michaelis-Menten mechanism. This was noted by Roussel in [104]. When two different reactions give the same system of differential equations (in this case the planar reduction), the mechanisms are said to be homeomorphic or kinetically equivalent. Thus, everything we established in Chapters 7 and 8 for the system for the Michaelis-Menten mechanism carries forward to (9.2). Physically, the two mechanisms can be distinguished on the basis of product formation: The velocity of the standard mechanism is $V = \dot{p} = k_2 c$ and the velocity of the Henri mechanism is $V = \dot{p} = k_2 s e$. See, for example, [108, 111].

9.2 Reversible Michaelis-Menten Mechanism

Traditionally, it is assumed for the Michaelis-Menten mechanism that the reaction from the complex to the product is irreversible. The rational for this assumption is that the rate of the reverse reaction is negligible compared to the rate of the forward reaction. Moreover, in practice the product is frequently removed as it is produced[1] and hence the reverse reaction cannot occur.

[1] For example, the product may be consumed as the reactant of another reaction in the metabolic pathway.

9.2.1 The Model and Differential Equations

Symbolically, the Reversible Michaelis-Menten mechanism is

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} P + E,$$

where S is the substrate, E is the enzyme, C is the complex, and P is the product. The constants k_{-1}, k_1, k_{-2}, and k_2 are the reaction-rate constants. By the Law of Mass Action, we have the system of four ordinary differential equations

$$\begin{aligned}
\dot{s} &= k_{-1}c - k_1 se, \\
\dot{e} &= (k_{-1} + k_2)\, c - k_1 se - k_{-2}ep, \\
\dot{c} &= k_1 se + k_{-2}ep - (k_{-1} + k_2)\, c, \\
\dot{p} &= k_2 c - k_{-2}ep.
\end{aligned}$$

Traditionally, the initial conditions are $s(0) = s_0$, $e(0) = e_0$, $c(0) = 0$, and $p(0) = 0$. However, we will allow the initial conditions to be arbitrary.

Two conservations laws which follow from these differential equations are

$$e(t) + c(t) = e_0 \quad \text{and} \quad s(t) + c(t) + p(t) = s_0.$$

We denote the two constants by s_0 and e_0 since, traditionally, the complex and product are not considered to be initially present.

9.2.2 Reduction and Re-scaling

Using the two conservation laws, we have the planar reduction

$$\dot{s} = k_{-1}c - k_1 s\,(e_0 - c)\,, \quad \dot{c} = k_1 s\,(e_0 - c) + k_{-2}\,(e_0 - c)\,(s_0 - s - c) - (k_{-1} + k_2)\, c. \tag{9.3}$$

The dimensions of the involved quantities in (9.3) are

$$[s, s_0, c, e_0] = \frac{Q}{L^3}, \quad [\dot{s}, \dot{c}] = \frac{Q}{L^3 T}, \quad [k_{-1}, k_2] = \frac{1}{T}, \quad \text{and} \quad [k_1, k_{-2}] = \frac{L^3}{QT}.$$

Define now the new variables

$$\tau := k_1 e_0 t, \quad x := \left(\frac{k_1}{k_{-1} + k_2}\right) s, \quad \text{and} \quad y := \frac{c}{e_0}$$

and new parameters

$$\varepsilon := \frac{k_1 e_0}{k_{-1}+k_2}, \quad \eta := \frac{k_2}{k_{-1}+k_2}, \quad \mu := \frac{s_0}{e_0}, \quad \text{and} \quad \theta := \frac{k_{-2}}{k_1}.$$

Hence, we are left with the system

$$x' = -x + (1-\eta+x)\,y, \quad y' = \varepsilon^{-1}\left[x-(1+x)\,y\right] + \theta\left[\mu - \varepsilon^{-1}x - y\right]\left[1-y\right], \tag{9.4}$$

where $' = \frac{d}{d\tau}$. Observe that if $k_{-2}=0$ then $\theta=0$ and the system reduces to the system for the (irreversible) Michaelis-Menten mechanism. Observe also that the origin is not an equilibrium point. In fact, there is a positive equilibrium point. See Figures 9.1 and 9.2, which strongly suggest the existence of a trapping region and a slow manifold. Proving the existence of a unique slow manifold may be as simple as constructing an antifunnel bounded by the horizontal isocline and the isocline for the slope of the slow eigenvector (associated with the Jacobian at the positive equilibrium).

9.3 Competitive Inhibition

Another simple variation of the basic Michaelis-Menten mechanism is the presence of a competitive inhibitor. Such an inhibitor is occasionally referred to as an "imposter substrate" since the inhibitor is similar to the substrate and binds with the enzyme at the active site. This competition between substrate and inhibitor effectively inhibits the conversion of the true substrate into product. See, for example, Chapter 1 of [69] and Chapter 5 of [71]. We will show that all concentrations approach equilibrium.

9.3.1 The Model and Differential Equations

Symbolically, the Michaelis-Menten mechanism with a single competitive inhibitor H is

$$S+E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \overset{k_2}{\rightarrow} P+E, \quad H+E \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} B,$$

where B is the inactive enzyme-inhibitor complex. Using the Law of Mass Action, we arrive at the system of ordinary differential equations

$$\begin{aligned} \dot{s} &= k_{-1}c - k_1 se, & \dot{e} &= (k_{-1}+k_2)\,c + k_{-3}b - k_1 se - k_3 eh, \\ \dot{c} &= k_1 se - (k_{-1}+k_2)\,c, & \dot{p} &= k_2 c, \\ \dot{h} &= k_{-3}b - k_3 eh, & \dot{b} &= k_3 eh - k_{-3}b. \end{aligned} \tag{9.5}$$

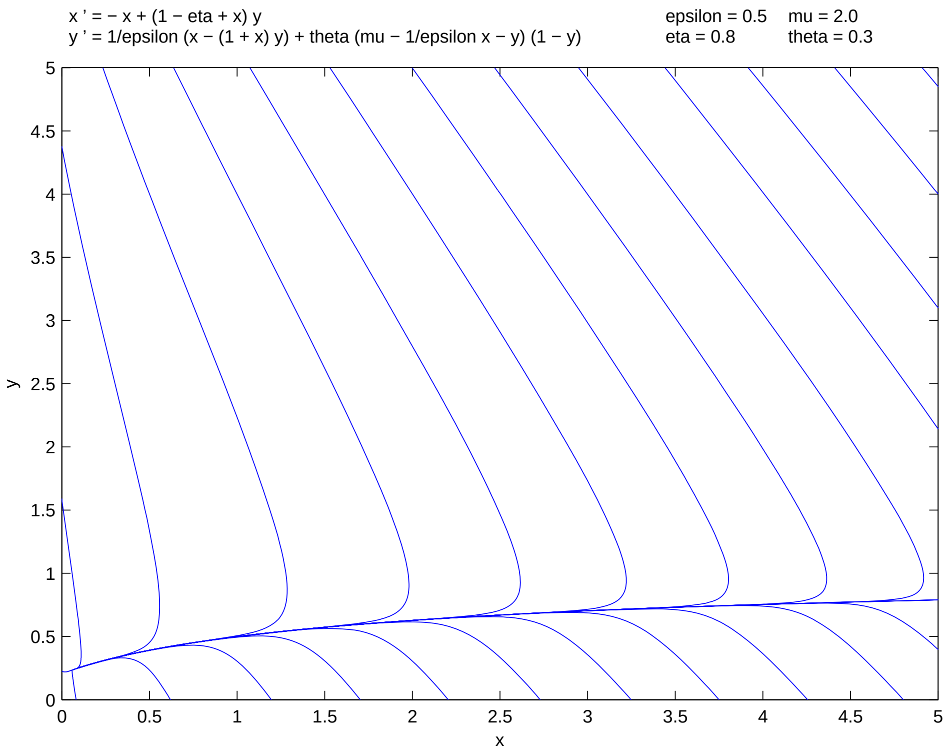

Figure 9.1: Phase portrait for the system (9.4) for $\varepsilon = 0.5$, $\eta = 0.8$, $\mu = 2.0$, and $\theta = 0.3$.

An immediate consequence of these equations are the three conservation laws

$$s(t) + c(t) + p(t) \equiv s_0, \quad c(t) + b(t) + e(t) \equiv e_0, \quad \text{and} \quad h(t) + b(t) \equiv h_0. \tag{9.6}$$

We use s_0, e_0, and h_0 to denote the constants since, traditionally, the two complexes and the product are not considered to be initially present. We will assume that $e_0 > 0$ which is physically reasonable; if $e_0 = 0$ then all concentrations are constant.

9.3.2 Global Asymptotic Stability

We will now show that all six concentrations tend to a constant as time tends to infinity. Consequently, this proves global asymptotic stability of a unique equilibrium point. Marc Roussel, in his thesis [104], performed a linearized analysis about this equilibrium point using the Jacobian.

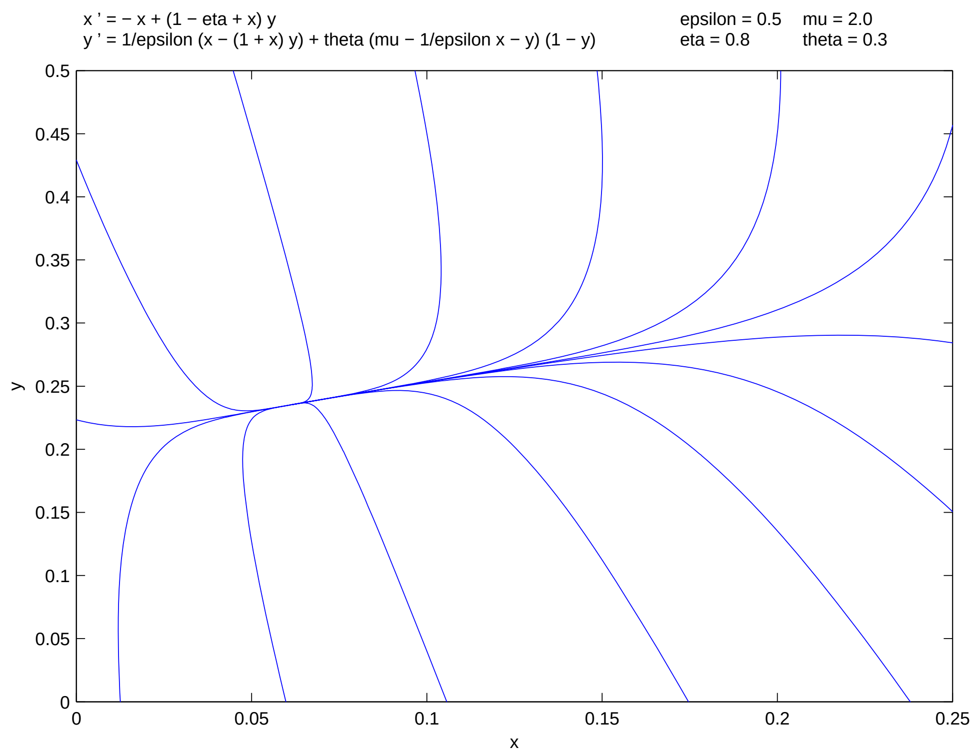

Figure 9.2: The positive equilibrium point for the system (9.4) for $\varepsilon = 0.5$, $\eta = 0.8$, $\mu = 2.0$, and $\theta = 0.3$.

Proposition 9.1:

(a) The concentrations $s(t)$, $e(t)$, $c(t)$, $p(t)$, $h(t)$, and $b(t)$ are all non-negative.

(b) The concentrations $s(t)$, $e(t)$, $c(t)$, $p(t)$, $h(t)$, and $b(t)$ are all bounded.

(c) The substrate, complex, and product concentrations satisfy

$$\lim_{t\to\infty} s(t) = 0, \quad \lim_{t\to\infty} c(t) = 0, \quad \textit{and} \quad \lim_{t\to\infty} p(t) = s_0.$$

(d) Let

$$r := \frac{-\left[k_{-3} + k_3\left(e_0 - h_0\right)\right] + \sqrt{\left[k_{-3} + k_3\left(e_0 - h_0\right)\right]^2 + 4k_{-3}k_3h_0}}{2k_3}.$$

Then, the enzyme, inhibitor, and enzyme-inhibitor complex concentrations satisfy[2]

$$\lim_{t\to\infty} e(t) = e_0 + r - h_0, \quad \lim_{t\to\infty} h(t) = r, \quad \textit{and} \quad \lim_{t\to\infty} b(t) = h_0 - r.$$

Proof:

(a) Trivial.

(b) It follows from the previous part and the conservation laws (9.6).

(c) First, we show the limit for $c(t)$. If we add the differential equations for $s(t)$ and $c(t)$ in (9.5), we obtain

$$\dot{s}(t) + \dot{c}(t) = -k_2 c(t) \quad \text{for all} \quad t \geq 0$$

and thus $u(t) := s(t) + c(t)$ is non-increasing. Since $u(t) \geq 0$ for all $t \geq 0$, there is some $\overline{u} \geq 0$ such that $\lim_{t\to\infty} u(t) = \overline{u}$. Note that $\ddot{u}(t)$ is bounded, which follows from the differential equations (9.5) and the boundedness of the concentrations, and thus $\dot{u}(t)$ is uniformly continuous for all $t \geq 0$. By Barbălat's Lemma (see §A.7 of Appendix A), $\lim_{t\to\infty} \dot{u}(t) = 0$. Since $\dot{u}(t) = -k_2 c(t)$, we conclude $\lim_{t\to\infty} c(t) = 0$.

Since $u(t) = s(t) + c(t)$, $\lim_{t\to\infty} u(t) = \overline{u}$, and $\lim_{t\to\infty} c(t) = 0$, it follows $\lim_{t\to\infty} s(t) = \overline{u}$. Using the first conservation law in (9.6), $\lim_{t\to\infty} p(t) = s_0 - \overline{u}$. Thus, we need only show that $\overline{u} = 0$.

Suppose, on the contrary, that $\overline{u} > 0$. If we let $t \to \infty$ in the differential equation for $s(t)$ and apply limits we know along with Barbălat's Lemma, we see that $\lim_{t\to\infty} e(t) = 0$. It follows from the second and third conservation laws in (9.6) that $\lim_{t\to\infty} b(t) = e_0 > 0$ and $\lim_{t\to\infty} h(t) = h_0 - e_0$. By Barbălat's Lemma, $\lim_{t\to\infty} \dot{h}(t) = 0$. Appealing to the differential equation for $h(t)$, we see $\lim_{t\to\infty} b(t) = 0$ which is a contradiction. Therefore, $\overline{u} = 0$, $\lim_{t\to\infty} s(t) = 0$, and $\lim_{t\to\infty} p(t) = s_0$.

(d) Consider the initial value problem

$$\dot{x} = a_2 x^2 + a_1 x + a_0, \quad x(t_0) = x_0,$$

where $a_0 > 0$ and $a_2 < 0$. Define $f(x) := a_2 x^2 + a_1 x + a_0$. Since f is a parabola opening downwards with $f(0) > 0$, f clearly has two distinct real roots, say r_1, r_2 where $r_1 < 0 < r_2$.

[2]Observe that $\lim_{e_0\to 0^+} r = h_0$.

Thus $f(x) > 0$ for $x \in (r_1, r_2)$ and $f(x) < 0$ for $x > r_2$. It is easy to verify that if $x_0 > r_1$ then the solution $x(t)$ satisfies $\lim_{t\to\infty} x(t) = r_2$.

We will use the above fact and the Comparison Theorem to show that $\lim_{t\to\infty} h(t) = r$. By virtue of the conservation laws (9.6), this will complete the proof of this part of the proposition.

Using the differential equation for $h(t)$ in (9.5) in conjunction with the conservation laws (9.6), we see that

$$\dot{h}(t) = -k_3 h(t)^2 - \left[k_{-3} + k_3\left(e_0 - h_0 - c(t)\right)\right] h(t) + k_{-3} h_0.$$

Let $\delta > 0$ be arbitrary. Since $\lim_{t\to\infty} c(t) = 0$, there is a $T \geq 0$ such that $0 \leq c(t) \leq \delta$ for any $t \geq T$. It follows that

$$f_0(h(t)) \leq \dot{h}(t) \leq f_\delta(h(t)) \quad \text{for all} \quad t \geq T,$$

where

$$f_\gamma(x) := -k_3 x^2 - \left[k_{-3} + k_3\left(e_0 - h_0 - \gamma\right)\right] x + k_{-3} h_0.$$

Observe that r, which is in the statement of this part of the proposition, is the positive root of $f_0(x) = 0$. Now, let r_δ be the positive root of $f_\delta(x) = 0$. It follows from the Comparison Theorem and the discussion at the beginning of the proof that

$$\liminf_{t\to\infty} h(t) \geq r \quad \text{and} \quad \limsup_{t\to\infty} h(t) \leq r_\delta.$$

Since $\delta > 0$ is arbitrary and $\lim_{\delta\to 0^+} r_\delta = r$, we can conclude $\lim_{t\to\infty} h(t) = r$.

□

9.3.3 Reduction and Re-scaling

Consider the system (9.5) and conservation laws (9.6). Clearly, there are only three independent concentrations. Following convention, (9.5) is reduced to

$$\begin{aligned}
\dot{s} &= k_{-1} c - k_1 s\left(e_0 - c - b\right), \\
\dot{c} &= k_1 s\left(e_0 - c - b\right) - \left(k_{-1} + k_2\right) c, \\
\dot{b} &= k_3\left(e_0 - c - b\right)\left(h_0 - b\right) - k_{-3} b.
\end{aligned} \tag{9.7}$$

Observe that the differential equation for b does not depend on s.

The dimensions of the quantities in (9.7) are

$$[s, c, b, h_0, e_0] = \frac{Q}{L^3}, \quad \left[\dot{s}, \dot{c}, \dot{b}\right] = \frac{Q}{L^3 T}, \quad [k_{-1}, k_2, k_{-3}] = \frac{1}{T}, \quad \text{and} \quad [k_1, k_3] = \frac{L^3}{QT}.$$

Now, define the new variables

$$\tau := k_1 e_0 t, \quad x := \left(\frac{k_1}{k_{-1} + k_2}\right) s, \quad y := \frac{c}{e_0}, \quad \text{and} \quad z := \frac{b}{h_0}$$

and the new parameters

$$\varepsilon := \frac{k_1 e_0}{k_{-1} + k_2}, \quad \eta := \frac{k_2}{k_{-1} + k_2}, \quad \mu := \frac{h_0}{e_0}, \quad \theta := \frac{k_{-3}}{k_1 e_0}, \quad \text{and} \quad \omega := \frac{k_3}{k_1}.$$

Hence, (9.7) becomes

$$\begin{aligned} x' &= -x + (1 - \eta + x)\, y + \mu x z, \\ y' &= \varepsilon^{-1} \left[x - (1 + x)\, y - \mu x z\right], \\ z' &= -\theta z + \omega \,(1 - y - \mu z)\,(1 - z)\,, \end{aligned}$$

where $' = \frac{d}{d\tau}$. Observe that the origin is not an equilibrium point. Note also that the x, y, and z isoclines, respectively, are given by $y = \mathcal{N}_x(x, z)$, $y = \mathcal{N}_z(x, z)$, and $y = \mathcal{N}_z(x, z)$, where

$$\mathcal{N}_x(x, z) := \frac{(1 - \mu z)\, x}{1 - \eta + x}, \quad \mathcal{N}_y(x, z) := \frac{(1 - \mu z)\, x}{1 + x}, \quad \text{and} \quad \mathcal{N}_z(x, z) := 1 - \mu z - \frac{\theta z}{\omega\,(1 - z)}.$$

The equilibrium approximation (EA) assumes that the substrate is in equilibrium and thus corresponds to the isocline $y = \mathcal{N}_x(x, z)$ (which is a surface). The quasi-steady-state approximation (QSSA), on the other hand, assumes that both of the complexes are in equilibrium and thus corresponds to the intersection of the isoclines $y = \mathcal{N}_y(x, z)$ and $y = \mathcal{N}_z(x, z)$ (which is a curve).

We conjecture that we can form a three-dimensional trapping region containing a unique solution by using the isoclines as boundaries. To prove this, we would need to formulate a higher-dimensional version of the Antifunnel Theorem. Note that this would likely involve the characterization of the antifunnel being narrowing in one direction (most likely the x-direction here).

Part III

The Lindemann Mechanism

Chapter 10

Introduction

We turn our attention to a different reaction, namely the Lindemann mechanism for unimolecular decay, which we will study from a dynamical systems point of view. A unimolecular reaction, as the name suggests, occurs when a single molecule undergoes a chemical change. In the scheme of Lindemann, for a given molecule to decay (or isomerize) it must be activated by another molecule and this activated molecule decays into the product molecule. This idea of a multi-step mechanism for unimolecular reactions, which originated with Lindemann, is now ubiquitous.

The Lindemann mechanism will lead to a planar differential equation and corresponding scalar differential equation which we will explore. As with the Michaelis-Menten mechanism, there will be a trapping region in phase space containing a unique slow manifold. In this part of the thesis, we will adapt the techniques of Part II to this mechanism.

10.1 The Lindemann Mechanism

Radioactive decay involves the emission of energy from an unstable atomic nucleus. For unimolecular decay, however, a certain amount of energy must be supplied externally, namely the activation energy. For some time, it was unknown just how the molecules became activated. Jean-Baptiste Perrin (1870–1942), the French physicist who won the Nobel Prize for Physics in 1926, suggested in 1919 that the activation was due to the absorption of infrared radiation. However, this idea was quickly shown to be false.

The British physicist Frederick Lindemann (1886–1957) suggested in 1922 that unimolecular decay involves two steps, namely the activation/deactivation by collision step and the reaction step. See, for example, [82] which is a "discussion on the radiation theory of chemical action" that includes Perrin and Lindemann as its participants. The British chemist Cyril Norman Hinshelwood (1897–1967) made further contributions to the Lindemann model in 1926 and, consequently, the Lindemann mechanism is occasionally referred to as the Lindemann-Hinshelwood mechanism. See, for example, Hinshelwood's paper [61]. For general references on unimolecular reactions and the Lindemann mechanism, see, for example, [11, 42, 48, 90].

Suppose that the reactant A is to decay into the product P. Then, according to the Lindemann mechanism, A is activated by a collision with another molecule M, typically from a gas bath, producing the activated complex B. This activation can also be reversed. The complex then decays into the product. Symbolically,

$$A + M \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B + M, \quad B \overset{k_2}{\rightarrow} P,$$

where k_1, k_{-1}, and k_2 are the reaction rate constants. There are alternatives to this model which include the presence of multiple products.

Observe that the concentration of M is constant and the resulting system of differential equations is linear. However, when the reactant A is activated by colliding with itself, the resulting system of differential equations is nonlinear. Symbolically, this model, which is the standard Lindemann mechanism, is

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \overset{k_2}{\rightarrow} P. \tag{10.1}$$

This is the model which we will be using.

10.2 Associated Ordinary Differential Equations

10.2.1 Ordinary Differential Equations

Consider the Lindemann mechanism (10.1). The Law of Mass Action gives the system of ordinary differential equations

$$\dot{a} = k_{-1}ab - k_1a^2, \tag{10.2a}$$

$$\dot{b} = k_1a^2 - k_{-1}ab - k_2b, \tag{10.2b}$$

$$\dot{p} = k_2b, \tag{10.2c}$$

where $\dot{} = \frac{d}{dt}$. The traditional initial conditions are $a(0) = a_0$, $b(0) = 0$, and $p(0) = 0$. However, we will allow the initial conditions to be arbitrary.

10.2.2 Conservation Law

By adding Equations (10.2a), (10.2b), and (10.2c), we arrive at the conservation law

$$a(t) + b(t) + p(t) \equiv a_0. \tag{10.3}$$

We choose a_0 to denote the constant since, traditionally, the complex and product are not initially present.

10.2.3 Planar Reduction

The system (10.2) consists of three ordinary differential equations. Since the differential equations for a and b are decoupled from the differential equation for p, we need only study the planar reduction

$$\dot{a} = k_{-1}ab - k_1a^2, \tag{10.4a}$$

$$\dot{b} = k_1a^2 - k_{-1}ab - k_2b. \tag{10.4b}$$

The traditional initial conditions are $a(0) = a_0$ and $b(0) = 0$. However, we will again allow the initial conditions to be arbitrary.

10.2.4 Scalar Reduction

The scalar reduction is formed by eliminating t from the (autonomous) planar reduction (10.4) and considering b as a function of a. Observe that $\frac{db}{da} = \frac{\dot{b}}{\dot{a}}$. Hence, consider the system

$$b' = \frac{k_1a^2 - k_{-1}ab - k_2b}{-k_1a^2 + k_{-1}ab}, \tag{10.5}$$

where $' = \frac{d}{da}$. We will, of course, restrict attention to the non-negative quadrant which consists of non-negative concentrations.

10.3 The Equilibrium and Quasi-Steady-State Approximations

The Equilibrium Approximation (EA) and the Quasi-Steady-State Approximation (QSSA), which have proved successful for the Michaelis-Menten mechanism, have also been applied to the Lindemann mechanism. See, for example, §2.2 of [48] and pages 122–126 and 313–317 of [90].

10.3.1 The Equilibrium Approximation (EA)

Assume that the reversible reaction in (10.1) is in equilibrium. That is, the activation and deactivation reactions are occurring at roughly the same rate. Mathematically, $\dot{a}(t) \approx 0$ for sufficiently large time t. Using (10.4a),

$$k_{-1}a(t)b(t) \approx k_1 a(t)^2.$$

It is reasonable to assume that $a(t) > 0$. Thus, we have the equilibrium approximation

$$b(t) \approx \frac{k_1}{k_{-1}} a(t).$$

In terms of the scalar reduction (10.5), the EA is

$$b_{\mathrm{EA}}(a) := \frac{k_1}{k_{-1}}\, a. \tag{10.6}$$

10.3.2 The Quasi-Steady-State Approximation (QSSA)

Assume that the activated complex B of the mechanism (10.1) is in a quasi-steady state. Mathematically, $\dot{b}(t) \approx 0$ for sufficiently large time t. The differential equation (10.4b) gives

$$k_1 a(t)^2 \approx k_{-1}a(t)b(t) + k_2 b(t).$$

Solving for $b(t)$,

$$b(t) \approx \frac{k_1 a(t)^2}{k_2 + k_{-1}a(t)}.$$

In terms of the scalar reduction (10.5), the QSSA is

$$b_{\mathrm{QSSA}}(a) := \frac{k_1 a^2}{k_2 + k_{-1}a}. \tag{10.7}$$

10.4 Dimensionless Ordinary Differential Equations

We will now re-scale the variables to produce dimensionless planar and scalar systems. Note that the dimensions of the involved quantities are

$$[a, b] = \frac{Q}{L^3}, \quad \left[\dot{a}, \dot{b}\right] = \frac{Q}{L^3 T}, \quad [k_2] = \frac{1}{T}, \quad \text{and} \quad [k_{-1}, k_1] = \frac{L^3}{QT}.$$

10.4.1 Dimensionless Variables and Parameter

Define[1]

$$\tau := k_2 t, \quad x := \left(\frac{k_1}{k_2}\right) a, \quad y := \left(\frac{k_1}{k_2}\right) b, \quad \text{and} \quad \varepsilon := \frac{k_{-1}}{k_1},$$

which are all dimensionless. Thus, τ, x, and y are, respectively, a scaled time, reactant concentration, and complex concentration. Moreover, the parameter $\varepsilon > 0$ measures how slow the deactivation of the reactant is compared to the activation. Traditionally, one may want to consider ε to be small. In our analysis, the size of ε does not matter.

10.4.2 Planar System

It is easy to verify that, with the re-scaling, the planar system (10.4) becomes

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = x^2 - (1 + \varepsilon x)\, y, \tag{10.8}$$

where $\dot{} = \frac{d}{dt}$ and (for simplicity) we are using t when we really are using the scaled time τ. Observe that the system (10.8) is a regular perturbation problem, whereas the planar system for the Michaelis-Menten mechanism is a singular perturbation problem. Occasionally, we will need to refer to the vector field of this planar system. Hence, define

$$\mathbf{g}(\mathbf{x}) := \begin{pmatrix} -x^2 + \varepsilon xy \\ x^2 - (1 + \varepsilon x)\, y \end{pmatrix}, \tag{10.9}$$

where $\mathbf{x} := (x, y)^T$. In Chapter 11 and Chapter 12, we will explore properties of solutions of (10.8).

[1] This is the re-scaling used, for example, by Marc Roussel in lecture notes available on his website http://people.uleth.ca/∼roussel at the University of Lethbridge.

10.4.3 Scalar Differential Equation

With the re-scaling, the scalar system (10.5) assumes the dimensionless form

$$y' = \frac{x^2 - (1 + \varepsilon x)\, y}{-x^2 + \varepsilon xy}, \tag{10.10}$$

where $' = \frac{d}{dx}$. Furthermore, we will define the function

$$f(x, y) := \frac{x^2 - y - \varepsilon xy}{-x^2 + \varepsilon xy}. \tag{10.11}$$

In Chapter 11, we will explore properties of solutions of (10.10).

10.4.4 The EA and QSSA

In terms of this scaling, Equations (10.6) and (10.7), for the EA and QSSA, take the respective forms

$$y_{\text{EA}}(x) := \frac{x}{\varepsilon} \quad \text{and} \quad y_{\text{QSSA}}(x) := \frac{x^2}{1 + \varepsilon x}. \tag{10.12}$$

Alternatively, these can be found by setting, respectively, $\dot{x} = 0$ and $\dot{y} = 0$ in (10.8). The EA can be interpreted as the vertical isocline, just like with the Michaelis-Menten mechanism, and the QSSA can be interpreted as the horizontal isocline.

10.5 Phase-Plane Analysis

Later in this section, we will present two computer-generated phase portraits. Our goal here is to provide rudimentary justification for these phase portraits. In Chapter 11, we will develop more precise results. The phase portraits, for physical reasons, will be restricted to the non-negative quadrant S.

We will use, like in Part II, a casual notation with regard to column and row vectors. For example, by $\mathbf{x} \in S$ we mean the (column) vector $\mathbf{x} = (x, y)^T$ satisfies $x, y \geq 0$. Similarly, by $(x, y) \in S$ we mean the point (x, y) satisfies $x, y \geq 0$.

To motivate the phase portrait, we will find the isoclines, establish the positive invariance of the non-negative quadrant S, classify the origin (which is the only equilibrium point), and specify the slopes of solutions of (10.10) in different regions of S.

10.5.1 Isoclines

To find the horizontal and vertical isoclines for the planar system (10.8), respectively set $\dot{y} = 0$ and $\dot{x} = 0$ to get

$$H(x) := \frac{x^2}{1 + \varepsilon x} \quad \text{and} \quad V(x) := \frac{x}{\varepsilon}.$$

We pointed out earlier that the EA corresponds to the vertical isocline and the QSSA corresponds to the horizontal isocline. See Equation (10.12). Note that the line $x = 0$ may also be regarded as a vertical isocline. Note also that both of the isoclines depend on ε, whereas neither did in the Michaelis-Menten mechanism.

Observe that the isoclines satisfy

$$H(0) = 0 = V(0), \quad 0 < H(x) < V(x) \quad \text{for all} \quad x > 0, \quad \text{and} \quad \lim_{x\to\infty} H(x) = \infty = \lim_{x\to\infty} V(x).$$

The region between the isoclines will be important and is denoted by

$$\Gamma_0 := \{\ (x, y)\ :\ x > 0,\ H(x) \leq y \leq V(x)\ \}.$$

Note that, unlike for the Michaelis-Menten mechanism, this region is not narrowing as $x \to \infty$ since

$$\lim_{x\to\infty} [V(x) - H(x)] = \varepsilon^{-2}.$$

10.5.2 Positive Invariance of the Non-Negative Quadrant S

It is easy to confirm that the origin $(0, 0)$ is the only equilibrium point of the system (10.8). Observe that two simple solutions of (10.8) are $\mathbf{x}(t) \equiv \mathbf{0}$ and $\mathbf{x}(t) \equiv \left(0, \mathsf{e}^{-t} y_0\right)^T$ (for any $y_0 > 0$). Hence, the non-negative y-axis is positively invariant. Now, if $x > 0$ and $y = 0$, then $\dot{y} = x^2 > 0$. Thus, on the positive x-axis, the vector field $\mathbf{g}$ points into S. It follows that the non-negative quadrant is positively invariant.

10.5.3 Classifying the Origin

The Jacobian matrix at the origin for the planar system (10.8) is

$$\mathbf{A} := \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}.$$

Region	Values of the Slopes of Solutions
$x = 0,\ y \geq 0$	undefined
$x > 0,\ y = 0$	$f = -1$
$x > 0,\ 0 < y < H(x)$	$-1 < f < 0$
$x > 0,\ y = H(x)$	$f = 0$
$x > 0,\ H(x) < y < V(x)$	$0 < f < \infty$
$x > 0,\ y = V(x)$	undefined
$x > 0,\ y > V(x)$	$-\infty < f < -1$

Table 10.1: This table lists the slopes of solutions of (10.10) in different regions of the non-negative quadrant. The function f is defined in (10.11).

By inspection, $\mathbf{A}$ has eigenvalues and associated eigenvectors

$$\lambda_+ := 0, \quad \lambda_- := -1, \quad \mathbf{v}_+ := \mathbf{e}_1, \quad \text{and} \quad \mathbf{v}_- := \mathbf{e}_2.$$

We are thus confronted with the first significant difference with the Michaelis-Menten mechanism: the origin is a non-hyperbolic fixed point. The Hartman-Grobman Theorem, unfortunately, cannot be applied here.

Using Theorem 65 in §9.21 of [2], the origin is a saddle node (see Figure A.3 in §A.8) which consists of two hyperbolic sectors and one parabolic sector. As we will effectively show later, S is contained in the parabolic sector.

10.5.4 The Slopes of Solutions of the Scalar Differential Equation

Table 10.1 summarizes the slopes of solutions of the scalar differential equation (10.10) in all regions of the non-negative quadrant. These results can easily be confirmed using the differential equation.

10.5.5 Phase Portrait

The Portraits

We now present, in Figures 10.1 and 10.2, two computer-generated phase portraits for the system (10.8). In one figure ε is small and in the other figure ε is larger.

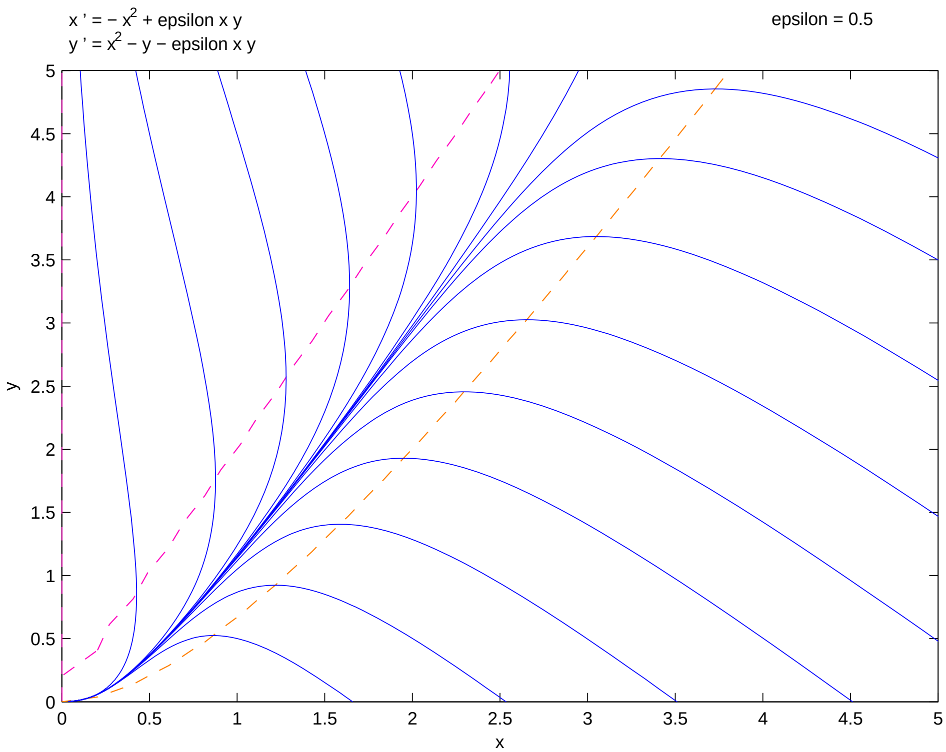

Figure 10.1: A phase portrait for (10.8) for parameter value $\varepsilon = 0.5$ along with the isoclines. Curiously, MATLAB could not find the vertical isocline, which is a straight line, sufficiently accurately.

The EA and QSSA

The phase portraits have many similarities with the phase portraits for the Michaelis-Menten mechanism. The isoclines again define a so-called trapping region which we have already called Γ_0. Moreover, the horizontal isocline (QSSA) appears to capture the long-term behaviour of solutions of the planar system (10.8). The vertical isocline (EA) also appears to capture the long-term behaviour, but decidedly less so than the horizontal isocline.

The Slow Manifold

The phase portraits suggest that there is a unique exceptional solution to (10.10) contained in the region Γ_0 between the isoclines. As with the Michaelis-Menten mechanism, we will refer to this

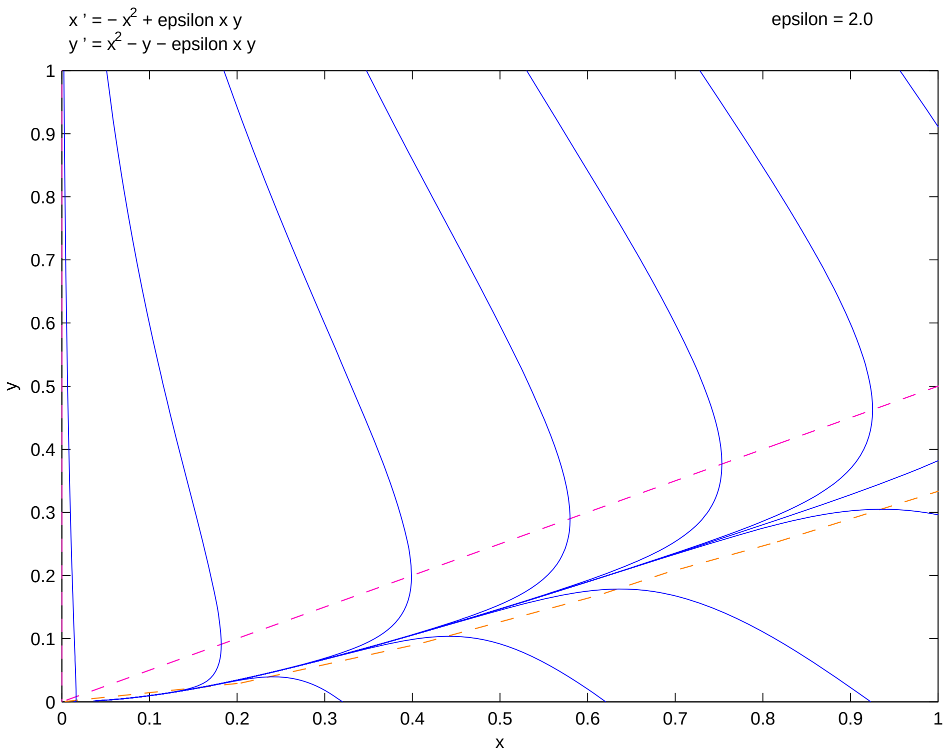

Figure 10.2: A phase portrait for (10.8) for parameter value $\varepsilon = 2.0$ along with the isoclines.

exceptional solution as the slow manifold and it will be denoted by $y = \mathcal{M}(x)$. In Chapter 11, we will show that this solution indeed exists and is unique.

10.5.6 Domain of Existence for Solutions of the Differential Equations

For any initial condition $\mathbf{x}_0 \in S$, the solution $\mathbf{x}(t)$ to the planar system (10.8) is defined for all $t \geq 0$. However, we need to be more careful with the domain for scalar solutions $y(x)$ to (10.10). There are five possibilities.

- If $x = 0$ and $y \geq 0$ or if $x > 0$ and $y = V(x)$, the function f is not defined, where f is given in (10.11). We will not consider there to be a scalar solution along the y-axis or the vertical isocline.

- If y is the slow manifold, that is $y = \mathcal{M}$, then y is defined for $x > 0$.
- If y lies below the slow manifold, y will intersect the x-axis for some $a > 0$. Thus, y is defined for $(0, a]$ with $y(a) = 0$.
- If y lies below the vertical isocline, y will intersect V for some $a > 0$. Thus, y is defined for $(0, a)$ with $\lim_{x \to a^-} y(x) = V(a)$.
- If y lies above the vertical isocline, y will intersect V for some $a > 0$. Thus, y is defined for $(0, a)$ with $\lim_{x \to a^-} y(x) = V(a)$.

Since $\mathbf{g}$ in Equation (10.9) is analytic, solutions $\mathbf{x}(t)$ are also analytic. Furthermore, since f in Equation (10.11) is analytic except along the non-negative y-axis and along the vertical isocline V, scalar solutions $y(x)$ are analytic there as well.

10.6 Literature Review

The Lindemann mechanism is a less prominent model than the Michaelis-Menten mechanism. Consequently, the relevant literature for the Lindemann mechanism is much more limited than for the Michaelis-Menten mechanism. However, when the Michaelis-Menten mechanism is studied mathematically, the Lindemann mechanism is occasionally used as an alternate example (just like in this thesis). The literature mentioned in Part II and particularly §6.7 can, broadly, be extended to this part of the thesis.

The planar system (10.8) has been studied as a perturbation problem. See, for example, [102, 113]. Furthermore, Simon Fraser has used the Lindemann mechanism as an alternate example in his work on the dynamical systems approach to chemical kinetics. See, for example, [43, 46]. Finally, two of the three authors of [35] also looked at some mathematical properties of the Lindemann mechanism in [34].

10.7 Summary

The nonlinear Lindemann mechanism for unimolecular decay is

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \xrightarrow{k_2} P,$$

where A is the molecule that decays, B is the activated complex, and P is the product of the decay. The Law of Mass Action and a re-scaling gives the dimensionless planar system

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = x^2 - y - \varepsilon xy,$$

where x is a scaled concentration of A, y is a scaled concentration of B, $\varepsilon > 0$ is a parameter, and $\dot{} = \frac{d}{dt}$. Traditionally, one may assume $0 < \varepsilon \ll 1$ but we will consider $\varepsilon > 0$ to be general. Furthermore, one can form a corresponding scalar system

$$y' = \frac{x^2 - y - \varepsilon xy}{-x^2 + \varepsilon xy},$$

where $' = \frac{d}{dx}$. We will be studying the planar and scalar systems in the non-negative quadrant S.

The horizontal and vertical isoclines for the planar system are, respectively,

$$H(x) = \frac{x^2}{1 + \varepsilon x} \quad \text{and} \quad V(x) = \frac{x}{\varepsilon}.$$

Physically, the horizontal isocline corresponds to the QSSA and the vertical isocline corresponds to the EA. The important region between the isoclines will be denoted by

$$\Gamma_0 = \{ \ (x, y) \ : \ x > 0, \ H(x) \leq y \leq V(x) \ \}.$$

The origin for the planar system is a saddle node and a non-hyperbolic equilibrium point. This is one major difference between the Lindemann and the Michaelis-Menten mechanism. Two computer-generated phase portraits were given in Figures 10.1 and 10.2. In Chapter 11, we will prove that there is a unique solution (namely the slow manifold) that lies entirely in the region Γ_0.

Chapter 11

Properties of Solutions in Phase Space

11.1 Introduction

The nonlinear Lindemann mechanism for unimolecular decay is

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \overset{k_2}{\rightarrow} P,$$

where A is reactant, B is the activated complex, and P is the product of the decay. The Law of Mass Action and a re-scaling gave us the planar system

$$\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x}) \tag{11.1}$$

and the scalar system

$$y' = f(x, y), \tag{11.2}$$

where

$$\mathbf{g}(\mathbf{x}) = \begin{pmatrix} -x^2 + \varepsilon xy \\ x^2 - (1 + \varepsilon x)\, y \end{pmatrix} \quad \text{and} \quad f(x, y) = \frac{x^2 - y - \varepsilon xy}{-x^2 + \varepsilon xy}. \tag{11.3}$$

Note that t is a scaled time, x is a scaled reactant concentration, y is a scaled complex concentration, $\varepsilon > 0$ is a parameter, $\dot{} = \frac{d}{dt}$, and $' = \frac{d}{dx}$.

In this chapter, we make precise statements about the phase portrait of the planar system (11.1). Equivalently, we will study the scalar solutions of the differential equation (11.2). The physically relevant portion of the xy-plane is S, the non-negative quadrant, and so we will only work in that region.

11.2 Isoclines

The isocline structure for the phase portrait of the Michaelis-Menten mechanism proved to be a valuable tool and the same will be true for the Lindemann mechanism. From Chapter 10, the horizontal and vertical isoclines are given by

$$H(x) = \frac{x^2}{1+\varepsilon x} \quad \text{and} \quad V(x) = \frac{x}{\varepsilon}. \tag{11.4}$$

We will show that the region between the isoclines,

$$\Gamma_0 = \{ \ (x,y) \ : \ x > 0, \ H(x) \le y \le V(x) \ \},$$

is a "trapping region."

11.2.1 Finding the Isoclines

The curve $y = w(x)$ is an isocline for slope $c \in \mathbb{R}$ if $f(x, w(x)) = c$ for all $x > 0$, where f is the slope function given in (11.3). Solving $f(x,y) = c$ for y gives

$$y = \frac{x^2}{K(c) + \varepsilon x},$$

where

$$K(c) := \frac{1}{1+c}, \quad c \neq -1. \tag{11.5}$$

Hence, define the function

$$F(x,c) := \frac{x^2}{K(c)+\varepsilon x}, \quad c \neq -1, \quad x \neq -\varepsilon^{-1}K(c). \tag{11.6}$$

Figure 11.1 gives a sketch of K. It follows that $y = F(x,c)$ is the isocline for slope c. Note that each isocline, except the vertical isocline which corresponds to $\lim\limits_{c\to\infty} K(c) = 0$ and which is a straight line, has a vertical asymptote at $x = -\varepsilon^{-1}K(c)$. Observe also that

$$y'(x) = f(x, y(x)) \quad \text{if and only if} \quad y(x) = F(x, y'(x)).$$

Claim 11.1: *Let $c \in \mathbb{R}\setminus\{-1\}$ and let $w(x) := F(x,c)$ be the isocline for slope c. Then, the derivative of w satisfies*

$$\lim_{x\to\infty} w'(x) = \varepsilon^{-1}. \tag{11.7}$$

Furthermore, w is concave up for all $x > 0$ and satisfies the differential equation

$$x^2 w' + w(\varepsilon w - 2x) = 0. \tag{11.8}$$

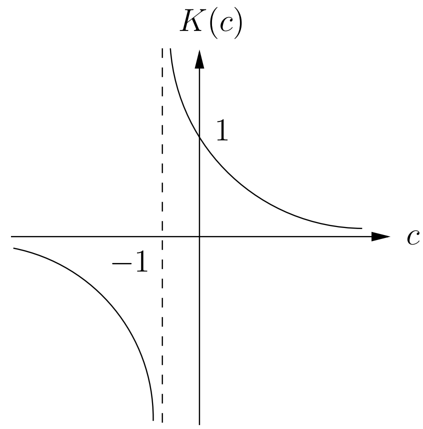

Figure 11.1: Graph of the function $K(c)$.

Proof: We can write

$$w(x) := \frac{x^2}{r + \varepsilon x},$$

where $r := K(c)$. Calculate

$$w'(x) = \frac{x\,(2r + \varepsilon x)}{(r + \varepsilon x)^2} \quad \text{and} \quad w''(x) = \frac{2r^2}{(r + \varepsilon x)^3}.$$

Clearly, $\lim_{x \to \infty} w'(x) = \varepsilon^{-1}$ and $w''(x) > 0$ for all $x > 0$. The differential equation is easy to verify. □

Claim 11.2: *We can invert $K(c) = r$ for $r \neq 0$ and differentiate $K(c)$ for $c \neq -1$ with*

$$K^{-1}(r) = \frac{1 - r}{r}, \quad r \neq 0 \quad \textit{and} \quad K'(c) = -\frac{1}{(1 + c)^2}, \quad c \neq -1.$$

Proof: The proof is trivial. □

Remarks 11.3:

(i) The interior of the region Γ_0 corresponds to $0 < c < \infty$ and $0 < K(c) < 1$. Furthermore, $K(0) = 1$ corresponds to the horizontal isocline H and $\lim_{c \to \infty} K(c) = 0$ corresponds to the vertical isocline V.

(ii) The vertical isocline, which is a straight line, is an exceptional isocline. Another exceptional isocline is $w(x) = 0$, which corresponds to slope -1. For completeness, we will write $F(x, -1) = 0$.

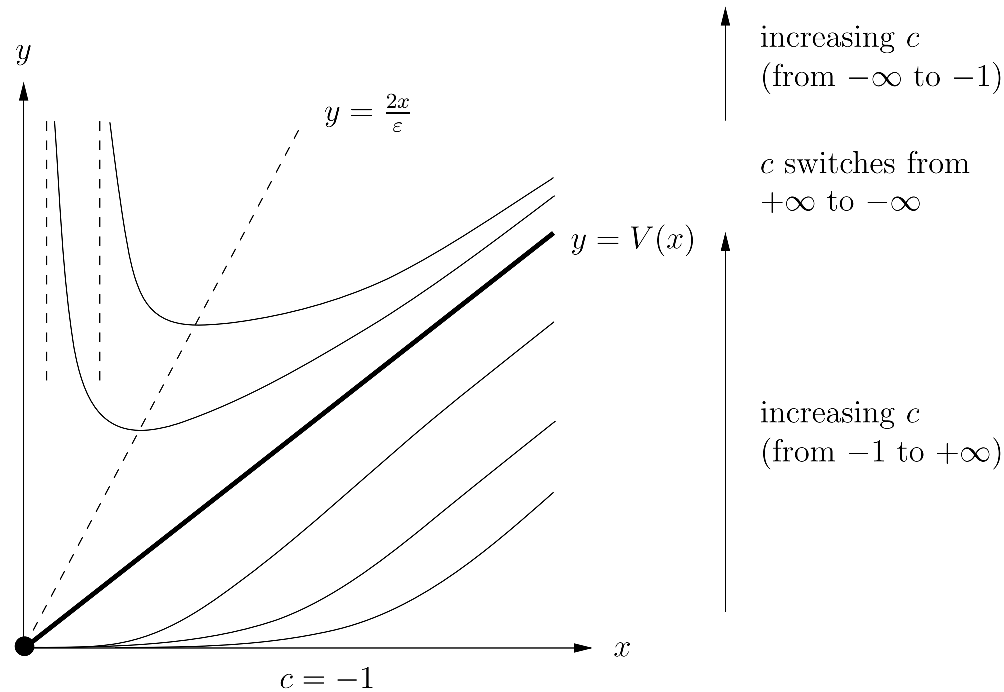

Figure 11.2: Sketch of the isocline structure of (11.2). The isoclines above the vertical isocline have zero slope along the line $y = \frac{2x}{\varepsilon}$.

(iii) The vertical isocline satisfies the limit (11.7) and the differential equation (11.8). The isocline $w(x) = 0$ (the isocline for slope -1) also satisfies the differential equation but does not satisfy the limit.

11.2.2 The Isocline Structure

The isocline structure is sketched in Figure 11.2. As with the Michaelis-Menten mechanism, we will often appeal to the isocline structure. For example, if a scalar solution is above the line $y = 0$ and below the horizontal isocline $y = H(x)$, we know that $-1 < y'(x) < 0$.

11.3 Global Asymptotic Stability

We have referred to the region Γ_0 as a "trapping region." As we will now show, all solutions $\mathbf{x}(t)$ to the planar system (11.1) eventually enter Γ_0. Moreover, all solutions to the planar system approach the origin in time. That is, the origin is globally (at least, in terms of the non-negative quadrant) asymptotically stable.

Theorem 11.4: *Consider the planar system* (11.1).

(a) The region Γ_0 *is positively invariant.*

(b) Let $\boldsymbol{x}(t)$ *be the solution to* (11.1) *with initial condition* $\boldsymbol{x}(0) = \boldsymbol{x}_0$*, where* $\boldsymbol{x}_0 \in S \setminus \{\boldsymbol{0}\}$*. Then, there is a* $t^* \geq 0$ *such that* $\boldsymbol{x}(t) \in \Gamma_0$ *for all* $t \geq t^*$*.*

(c) Let $\boldsymbol{x}(t)$ *be the solution to* (11.1) *with initial condition* $\boldsymbol{x}(0) = \boldsymbol{x}_0$*, where* $\boldsymbol{x}_0 \in S$*. Then,*

$$\lim_{t\to\infty} \boldsymbol{x}(t) = \boldsymbol{0}.$$

Proof: The proof is essentially identical to the corresponding proof in Theorem 7.7 of Chapter 8 on page 167. Note that for (b), in the case where $x_0 > 0$ and $y_0 > V(x_0)$, if $\mathbf{x}(t)$ is assumed to not enter Γ_0 then

$$f(x(t), y(t)) < -1 \quad \text{and} \quad y(t) \leq y_0 - [x(t) - x_0] \quad \text{for all} \quad t \geq 0.$$

$\square$

11.4 Existence and Uniqueness of the Slow Manifold

In this section, we will prove that there is a unique solution $y = \mathcal{M}(x)$ to the scalar differential equation (11.2) that lies entirely inside the trapping region Γ_0. The proof will be similar to the corresponding proof in §7.4. However, there are two notable differences. First, the isocline α which we will use for the strong lower fence is actually the isocline for the slope of the slow manifold at $x = \infty$ and not $x = 0$. Second, the antifunnel formed by the horizontal and α isoclines will not be narrowing. Recall that, in order to use the Antifunnel Theorem, we needed the antifunnel to be narrowing.

11.4.1 Introduction

Suppose that we want the isocline

$$w(x) := \frac{x^2}{r + \varepsilon x}, \quad 0 < r < 1$$

to be a strong lower fence for the differential equation (11.2) for all $x > 0$. Note that the condition on r restricts the isocline to being between the horizontal and vertical isoclines. Note also that

$$f(x, w(x)) = K^{-1}(r) \quad \text{for all} \quad x > 0.$$

Since w is concave up and satisfies the limit $\lim_{x\to\infty} w'(x) = \varepsilon^{-1}$, we know that $w'(x) < \varepsilon^{-1}$ for all $x > 0$. Hence,

$$\varepsilon^{-1} \leq K^{-1}(r) \implies w'(x) < f(x, w(x)) \quad \text{for all} \quad x > 0.$$

Since we want the isocline that will give us the thinnest antifunnel, we choose

$$\alpha(x) := \frac{x^2}{K(\varepsilon^{-1}) + \varepsilon x}. \tag{11.9}$$

Note that

$$K\left(\varepsilon^{-1}\right) = \frac{\varepsilon}{1+\varepsilon}.$$

Claim 11.5: *The isocline α is a strong lower fence and the horizontal isocline H is a strong upper fence for the differential equation* (11.2) *for all $x > 0$.*

Proof: We have already shown that α is a strong lower fence. To show that H is a strong upper fence, observe

$$f(x, H(x)) = 0 < H'(x) \quad \text{for all} \quad x > 0.$$

□

Claim 11.6: *The region*

$$\Gamma_1 := \{\ (x, y)\ :\ x > 0,\ H(x) \leq y \leq \alpha(x)\ \}$$

is an antifunnel for the differential equation (11.2).

Proof: We know $y = \alpha(x)$ and $y = H(x)$ are strong fences for (11.2). Moreover, $\alpha(x) > H(x)$ for all $x > 0$. By definition, Γ_1 is an antifunnel. □

11.4.2 The Existence-Uniqueness Theorem

Now, we will prove the existence and uniqueness of the slow manifold. To this end, we will use an alternate form of the Antifunnel Theorem which does not require the antifunnel to be narrowing.

Theorem 11.7:

(a) There exists a unique slow manifold $y = \mathcal{M}(x)$ in Γ_1 for the scalar differential equation (11.2).

(b) The slow manifold $y = \mathcal{M}(x)$ is also the only solution that lies entirely in Γ_0.

Proof:

(a) Suppose that $x > 0$ and $H(x) < y < V(x)$. Using (11.4),

$$\frac{\varepsilon x^2}{1+\varepsilon x} < \varepsilon y < x \quad \text{and} \quad 0 < x - \varepsilon y < x - \frac{\varepsilon x^2}{1+\varepsilon x}.$$

Re-arranging, we have

$$0 < \frac{1+\varepsilon x}{x} < \frac{1}{x-\varepsilon y} \quad \text{and} \quad 0 < \left(\frac{1}{x} + \varepsilon\right)^2 < \frac{1}{(x-\varepsilon y)^2}.$$

Thus, using the definition (11.3) of f we have

$$\frac{\partial f}{\partial y}(x,y) = \frac{1}{(x-\varepsilon y)^2} > \left(\frac{1}{x} + \varepsilon\right)^2 > \varepsilon^2.$$

Hence, we can apply the Alternate Antifunnel Theorem (Theorem A.5 on page 310) with $r(x) := \varepsilon^2$. To see why, consider that

$$\int_0^\infty r(x)\,dx = \infty \quad \text{and} \quad \lim_{x\to\infty} [\alpha(x) - H(x)] = \frac{1}{\varepsilon^2\,(1+\varepsilon)}$$

and thus

$$\lim_{x\to\infty} \frac{\alpha(x) - H(x)}{\exp\left(\int_0^x r(s)\,ds\right)} = 0.$$

We can therefore conclude that there is a unique solution $y = \mathcal{M}(x)$ to (11.2) that lies in Γ_1 for all $x > 0$.

(b) Let y be a solution in Γ_0 lying below $\mathcal{M}$. Since $\mathcal{M}$ is the only solution contained in Γ_1, y must leave Γ_1 through the horizontal isocline.

Now, let y be a solution in Γ_0 lying above $\mathcal{M}$. Suppose on the contrary that y never leaves Γ_0 and thus $\mathcal{M}(x) < y(x) < V(x)$ for all $x > 0$. Consider the isocline $w(x) := F\left(x, 2\varepsilon^{-1}\right)$. Since w is a strong lower fence, the proof of the first part of the theorem can be adapted to show that $\mathcal{M}$ is the only solution contained in the region between the isoclines H and w. Thus, there is an $a > 0$ such that $y(a) = w(a)$. Now, $w'(x) < \varepsilon^{-1}$ for all $x > 0$ and $y'(x) \geq 2\varepsilon^{-1}$ if

$y(x) \geq w(x)$. It follows from a simple comparison argument that $w(x) < y(x) < V(x)$ for all $x > a$. So, $y(x) > y(a) + 2\varepsilon^{-1}(x - a)$ for all $x > a$. This is a contradiction since $y(x) > V(x)$ for sufficiently large x.

□

Remarks 11.8:

(i) We are referring to the unique solution between the isoclines as *the* slow manifold. However, all scalar solutions in Γ_0 are technically slow manifolds (and, as it turns out, centre manifolds). This is because, as functions of time, the solutions approach the origin in the slow direction.

(ii) If $w_1(x) < \mathcal{M}(x) < w_2(x)$ for all $x > 0$, where w_1 and w_2 are isoclines, then $w_1(x) \leq H(x)$ and $w_2(x) \geq \alpha(x)$ for all $x > 0$. This follows from the isocline structure and the fact (which we will show later) that $\lim_{x \to 0^+} \mathcal{M}'(x) = 0$ and $\lim_{x \to \infty} \mathcal{M}'(x) = \varepsilon^{-1}$.

11.4.3 Nested Antifunnels

We have seen that the region between the horizontal isocline and the w isocline, where $w(x) := F(x, c)$ for $c \geq \varepsilon^{-1}$, is an antifunnel (containing unique solution $y = \mathcal{M}(x)$) for all $x > 0$. We can find thinner antifunnels than Γ_1. However, these antifunnels will not be valid for all $x > 0$.

For an isocline $w(x) := F(x, c)$, where $0 < c < \varepsilon^{-1}$, to be a strong lower fence on an interval, we need $w'(x) < f(x, w(x))$. Solving the equation $w'(x) = f(x, w(x))$, as we shall see, gives $x = \xi(c)$, where

$$\xi(c) := \left[\frac{K(c)}{\varepsilon}\right]\left[\frac{1}{\sqrt{1 - \varepsilon c}} - 1\right], \quad c \in \left(0, \varepsilon^{-1}\right). \tag{11.10}$$

Note that $1 - \varepsilon c > 0$. We will quickly establish a few properties of $\xi(c)$. See Figure 11.3 for a sketch of the function.

Claim 11.9: *The function $\xi(c)$ satisfies*

$$\lim_{c \to 0^+} \xi(c) = 0, \qquad \lim_{c \to (\varepsilon^{-1})^-} \xi(c) = \infty, \quad \textit{and} \quad \xi'(c) > 0 \quad \textit{for all} \quad c \in \left(0, \varepsilon^{-1}\right). \tag{11.11}$$

Proof: The proof is routine, tedious, and omitted. □

Claim 11.10: *The function $\xi(c)$ is analytic for all $c \in \left(0, \varepsilon^{-1}\right)$. Furthermore, $\xi(c)$ has analytic inverse $\xi^{-1}(x)$ defined for all $x > 0$.*

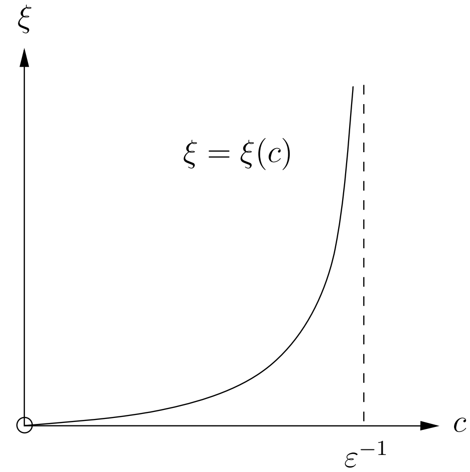

Figure 11.3: Graph of the function $\xi(c)$ for arbitrary $\varepsilon > 0$.

Proof: It is clear from the definition (11.10) that $\xi(c)$ is analytic for all $c \in \left(0, \varepsilon^{-1}\right)$. Using (11.11) in conjunction with the Real Analytic Inverse Function Theorem, we know that $\xi(c)$ is invertible for all $c \in \left(0, \varepsilon^{-1}\right)$ and that $\xi^{-1}(x)$ is analytic for all $x > 0$. $\square$

We are now in a position to establish on what interval a given isocline is a strong fence. Observe that no isocline between the horizontal isocline and the α isocline is strong fence for all $x > 0$. As a consequence, this gives us infinitely many nested antifunnels. These nested antifunnels are formed by altering the strong upper fence (lower boundary) and leaving the strong lower fence (upper boundary) alone. The opposite was the case for the Michaelis-Menten mechanism which required us to alter the strong lower fence (upper boundary) and leave the strong upper fence (lower boundary) alone.

Proposition 11.11: *Let $c \in \left(0, \varepsilon^{-1}\right)$ be fixed and let $w(x) := F(x, c)$ be the isocline for slope c.*

(a) The isocline w satisfies

$$w'(x) \begin{cases} < f(x, w(x)), & \textit{if} \quad 0 < x < \xi(c) \\ = f(x, w(x)), & \textit{if} \quad x = \xi(c) \\ > f(x, w(x)), & \textit{if} \quad x > \xi(c) \end{cases}.$$

(b) The slow manifold satisfies

$$w(x) < \mathcal{M}(x) < \alpha(x) \quad \textit{for all} \quad x > \xi(c).$$

Proof:

(a) We know that

$$f(x, w(x)) = c \quad \text{and} \quad w'(x) = \frac{x\,[2K(c) + \varepsilon x]}{[K(c) + \varepsilon x]^2} \quad \text{for all} \quad x > 0.$$

First, we will solve the equation $w'(x) = f(x, w(x))$ for x. Set

$$\frac{x\,[2K(c) + \varepsilon x]}{[K(c) + \varepsilon x]^2} = c.$$

This leads to the equation

$$\varepsilon\,(1 - \varepsilon c)\,x^2 + 2K(c)\,(1 - \varepsilon c)\,x - cK(c)^2 = 0.$$

Solving,

$$x = \left[\frac{K(c)}{\varepsilon}\right]\left[-1 \pm \frac{1}{\sqrt{1 - \varepsilon c}}\right].$$

Since $x > 0$, the only solution is $x = \xi(c)$. It follows that $w'(x) = f(x, w(x))$ when $x = \xi(c)$. By adapting the above calculation, it can easily be shown $w'(x) < f(x, w(x))$ when $0 < x < \xi(c)$ and $w'(x) > f(x, w(x))$ when $x > \xi(c)$.

(b) It follows from the Alternate Antifunnel Theorem.

□

11.5 Behaviour Near $x = 0$: Introduction

We will eventually show that each solution inside the trapping region Γ_0 can be represented as a Taylor series as $x \to 0^+$. First, we need to establish a basic result.

Proposition 11.12: *Let y be a solution to* (11.2) *lying inside Γ_1 for $x \in (0, a)$, where $a > 0$. Then, we can extend $y(x)$ and $y'(x)$ to say $y(0) = 0$ and $y'(0) = 0$.*

Proof: Observe that

$$\lim_{x \to 0^+} \alpha(x) = 0 \quad \text{and} \quad \lim_{x \to 0^+} \frac{\alpha(x)}{x} = 0.$$

Since

$$0 < y(x) < \alpha(x) \quad \text{for all} \quad x \in (0, a)\,,$$

the Squeeze Theorem establishes $y(0) = 0$. Now,

$$0 < \frac{y(x) - y(0)}{x - 0} < \frac{\alpha(x)}{x} \quad \text{for all} \quad x \in (0, a) .$$

Thus, by the Squeeze Theorem again as well as the definition of (right) derivative, we can say $y'(0) = 0$. □

11.6 Concavity

In this section, we will establish the concavity of all scalar solutions, except for the slow manifold, in the non-negative quadrant. The concavity of the slow manifold will be established later. These results will be obtained, like with the Michaelis-Menten mechanism, by using an auxiliary function.

11.6.1 Introduction

Let y be a solution to (11.2) and consider the function f given in (11.3). If we differentiate the equation $y'(x) = f(x, y(x))$ and apply the Chain Rule, we get

$$y''(x) = \frac{\partial f}{\partial x}(x, y(x)) + \frac{\partial f}{\partial y}(x, y(x)) f(x, y(x)).$$

It is easy to verify that

$$y''(x) = p(x, y(x)) h(x, y(x)), \tag{11.12}$$

where

$$p(x, y) := \frac{1}{x^2 \left(\varepsilon y - x\right)^2} \quad \text{and} \quad h(x, y) := x^2 f(x, y) + y \left(\varepsilon y - 2x\right) . \tag{11.13}$$

The function $p(x, y)$ is positive everywhere except along the vertical isocline and for $x = 0$, where it is undefined. For a given solution, we can overload the functions h and p and consider them defined with respect to y:

$$h(x) := h(x, y(x)) \quad \text{and} \quad p(x) := p(x, y(x)).$$

Claim 11.13: *For a given $x > 0$ with $y(x) \neq V(x)$, the sign of $h(x)$ is the same as the sign of $y''(x)$. Furthermore, the function h has derivative*

$$h'(x) = x^2 p(x) h(x) + 2y(x) \left[\varepsilon y'(x) - 1\right] . \tag{11.14}$$

Region	Concavity of Solutions
$0 \leq y \leq H$	concave down
$H < y < \mathcal{M}$	concave up, then inflection point, then concave down
$\mathcal{M} < y < V$	concave up
$y > V$	concave up, then inflection point, then concave down

Table 11.1: This table gives a summary of the concavity of solutions of (11.2) in the non-negative quadrant.

Proof: The first part of the claim follows from (11.12) and the fact that $p(x) > 0$. To show the second part of the claim, write

$$h(x) = x^2 y' + \varepsilon y^2 - 2xy.$$

Differentiating with respect to x and applying (11.12),

$$h'(x) = 2xy'(x) + x^2 y''(x) + 2\varepsilon y(x) y'(x) - 2\left[y(x) + xy'(x)\right] = x^2 p(x) h(x) + 2y(x)\left[\varepsilon y'(x) - 1\right].$$

$\square$

Remark 11.14: The function h cannot tell us anything about the concavity of solutions at $x = 0$, not even by taking a limit.

Claim 11.15: *Let y be a solution to* (11.2) *and let $x_0 > 0$ with $y(x_0) \neq V(x_0)$. Consider the isocline through the point $(x_0, y(x_0))$, which is given by $w(x) := F(x, y'(x_0))$. Then,*

$$h(x_0) = x_0\left[y'(x_0) - w'(x_0)\right].$$

Furthermore, $y''(x_0) > 0$ if and only if $y'(x_0) > w'(x_0)$ and $y''(x_0) < 0$ if and only if $y'(x_0) < w'(x_0)$.

Proof: The first part follows from (11.8) and (11.13). The second part follows from the first. $\square$

The concavity of all solutions in all regions of the non-negative quadrant can be deduced using the auxiliary function h and Lemma 7.22 on page 177. Table 11.1 summarizes what we will develop in this section. They are all suggested by the phase portraits in Figures 10.1 and 10.2 from Chapter 10.

11.6.2 Establishing the Results

Concavity Below H

Proposition 11.16: *Let y be a solution to (11.2) lying below H with domain $[a, b]$, where $a > b > 0$, $y(a) = H(a)$, and $y(b) = 0$. Then, y is concave down on $[a, b]$.*

Proof: We know $y'(a) = 0$ and $y'(b) = -1$. Also, $y(x) > 0$ and $y'(x) < 0$ for all $x \in (a, b)$. Note that $y < V(x)$ which implies $\varepsilon y - 2x < 0$ for all $x \in [a, b]$. Let h be as in (11.13) defined with respect to the solution y. Observe that

$$h(a) = H(a)\,[\varepsilon H(a) - 2a] < 0 \quad \text{and} \quad h(b) = -b^2 < 0.$$

Observe also that

$$h(x) = x^2 y'(x) + y(x)\,[\varepsilon y(x) - 2x] < 0 \quad \text{for all} \quad x \in (a, b).$$

Therefore, y is concave down on $[a, b]$. $\square$

Concavity Between H and $\mathcal{M}$

Proposition 11.17: *Let y be a solution to (11.2) lying above H and below $\mathcal{M}$ with domain $(0, a]$, where $a > 0$ and $y(a) = H(a)$. Then, there is a unique $x_1 \in (0, a)$ such that $y''(x_1) = 0$. Moreover, y is concave up on $(0, x_1)$ and concave down on $(x_1, a]$.*

Proof: Let h be as in (11.13) defined with respect to the solution y. Now, we know $y'(a) = 0$ and, by Proposition 11.12, we can extend $y'(x)$ continuously and write $y'(0) = 0$. By Rolle's Theorem, there is an $x_1 \in (0, a)$ such that $y''(x_1) = 0$ and hence $h(x_1) = 0$. To show the uniqueness of x_1, suppose that $x_2 \in (0, a)$ is such that $h(x_2) = 0$. Now, since $H(x_2) < y(x_2) < \alpha(x_2)$, by virtue of the isocline structure $0 < y'(x_2) < \varepsilon^{-1}$. Moreover, we see from (11.14) that $h'(x_2) < 0$. By Lemma 7.22, we can conclude $x_2 = x_1$. Finally, by continuity we can conclude that $h(x) > 0$ on $(0, x_1)$ and $h(x) < 0$ on $(x_1, a]$ since $h(a) = y(a)\,[\varepsilon y(a) - 2a] < 0$. $\square$

Concavity Between $\mathcal{M}$ and V

Proposition 11.18: *Let y be a solution to (11.2) strictly between $\mathcal{M}$ and V with domain $(0, a)$, where $a > 0$ and $\lim_{x \to a^-} y(x) = V(a)$. Then, y is concave up on $(0, a)$.*

Proof: Let h be as in (11.13) defined with respect to the solution y. Define the sets

$$I := \{\ x \in (0,a)\ :\ \mathcal{M}(x) < y(x) < \alpha(x)\ \} \quad \text{and} \quad J := \{\ x \in (0,a)\ :\ \alpha(x) \leq y(x) < V(x)\ \}\,.$$

Since since $\lim_{x\to a^-} y(x) = V(a)$, we know that $J \neq \emptyset$. We will show separately that $h(x) > 0$ for each $x \in I$ and for each $x \in J$.

Suppose that $x \in J$. By virtue of the isocline structure, $y'(x) \geq \varepsilon^{-1}$. However, any isocline w satisfies $w'(x) < \varepsilon^{-1}$. Appealing to Claim 11.15, $h(x) > 0$.

If $I = \emptyset$ then we are done. Suppose that $I \neq \emptyset$ and let $x_3 \in J$ be fixed. We have already shown that $h(x_3) > 0$. We need to show that $h(x) > 0$ for all $x \in I$. By continuity, it suffices to show that h has no zeros in I. Suppose, on the contrary, that this is not the case. By Lemma 7.22, h has a right-most zero $x_1 \in I \subset (0, x_3]$. Observe that $y'(x_1) < \varepsilon^{-1}$, which follows from the fact that $y(x_1) < \alpha(x_1)$. Since $h(x_1) = 0$ and $y(x_1) > 0$, (11.14) informs us $h'(x_1) < 0$. Consequently, there is an $x_2 \in (x_1, x_3)$ such that $h(x_2) < 0$. Since $h(x_3) > 0$, the Intermediate Value Theorem implies that h has a zero in (x_2, x_3), which is a contradiction since x_1 is the right-most zero. $\square$

Concavity Above V

Proposition 11.19: *Let y be a solution to* (11.2) *lying above V with domain $(0,a)$, where $a > 0$, $\lim_{x\to 0^+} y(x) = \infty$, and $\lim_{x\to a^-} y(x) = V(a)$. Then, there is a unique $x_1 \in (0,a)$ such that $y''(x_1) = 0$. Moreover, y is concave up on $(0, x_1)$ and concave down on (x_1, a).*

Proof: We know that

$$\lim_{x\to 0^+} y'(x) = -\infty \quad \text{and} \quad \lim_{x\to a^-} y'(x) = -\infty.$$

By continuity, there are $b_1, b_2 \in \mathbb{R}$ such that $0 < b_1 < b_2 < a$ and $y'(b_1) = y'(b_2)$. Thus by Rolle's Theorem, there is an $x_1 \in (0,a)$ such that $y''(x_1) = 0$.

To prove uniqueness, suppose that $x_2 \in (0,a)$ is such that $h(x_2) = 0$, where h is as in (11.13) defined with respect to the solution y. Now, we know from Table 10.1 that $y(x_2) < \varepsilon^{-1}$. Using (11.14), $h(x_2) < 0$. Since x_2 was an arbitrary zero of h, we can conclude using Lemma 7.22 that $x_2 = x_1$. Furthermore, since $h'(x_1) < 0$, we can say that y is concave up on $(0, x_1)$ and concave down on (x_1, a). $\square$

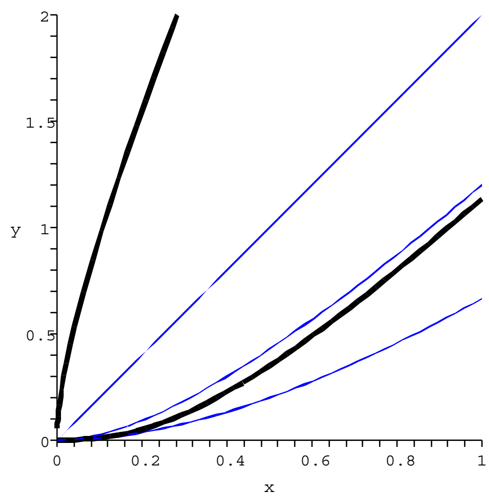

Figure 11.4: The two thick curves are curves along which solutions of (11.2) have inflection points, for parameter value $\varepsilon = 0.5$. The thin curves are the horizontal, α, and vertical isoclines.

11.6.3 Curves of Inflection Points

We know from Table 11.1 that solutions to the scalar differential equation (11.2) can only have inflection points between H and $\mathcal{M}$ or above V. Just like with the Michaelis-Menten mechanism, we can construct a curve of inflection points which is close to the slow manifold.

It is easily verified that

$$h(x,y) = \frac{\varepsilon^2 y^3 - (3\varepsilon x)\, y^2 + \left(2x^2 - \varepsilon x^2 - x\right) y + x^3}{\varepsilon y - x},$$

where h is as in (11.13). Thus, there are three curves along which solutions have zero second derivative, given implicitly by

$$\varepsilon^2 y^3 - (3\varepsilon x)\, y^2 + \left(2x^2 - \varepsilon x^2 - x\right) y + x^3 = 0.$$

One curve lies below the x-axis and is discarded. The other two curves, as expected, are in the positive quadrant. See Figure 11.4.

Recall that, for a fixed $c \in \left(0, \varepsilon^{-1}\right)$, the isocline $w(x) := F(x,c)$ switches from being a strong lower fence to being a strong upper fence at $x = \xi(c)$ and $y = F(\xi(c), c)$, where F is defined in (11.6) and ξ is defined in (11.10). As was the case for the Michaelis-Menten mechanism (see §7.6.3 on page 181),

$$\mathcal{Y}(x) := F\left(x, \xi^{-1}(x)\right), \quad x > 0 \tag{11.15}$$

will be a curve of inflection points between H and $\mathcal{M}$. Note that $H(x) < F(x,c) < \alpha(x)$ for all $x > 0$ and $c \in \left(0, \varepsilon^{-1}\right)$, which follows from the isocline structure. Moreover, $0 < \xi^{-1}(x) < \varepsilon^{-1}$ for all $x > 0$. Thus, $H(x) < \mathcal{Y}(x) < \alpha(x)$ for all $x > 0$.

Claim 11.20: *Suppose that $x_0 > 0$ and $H(x_0) < y_0 < \alpha(x_0)$. Define the slope $c := f(x_0, y_0)$ and isocline $w(x) := F(x,c)$. Then, the isocline w satisfies*

$$w'(x_0) \begin{cases} > f(x_0,y_0), & \text{if} \quad H(x_0) < y_0 < \mathcal{Y}(x_0) \\ = f(x_0,y_0), & \text{if} \quad y_0 = \mathcal{Y}(x_0) \\ < f(x_0,y_0), & \text{if} \quad \mathcal{Y}(x_0) < y_0 < \alpha(x_0) \end{cases} .$$

Proof: Note that $0 < c < \varepsilon^{-1}$ and $y_0 = w(x_0)$. We will only show the third case since the other two cases are similar. Assume that $\mathcal{Y}(x_0) < y_0 < \alpha(x_0)$. Appealing to the isocline structure, we know $\frac{\partial f}{\partial y}(x,y) > 0$ if $x > 0$ and $H(x) < y < \alpha(x)$. Thus, $f(x_0,y_0) > f(x_0, \mathcal{Y}(x_0))$. Since $c = f(x_0,y_0)$ and $\xi^{-1}(x_0) = f(x_0, \mathcal{Y}(x_0))$, we have $c > \xi^{-1}(x_0)$. Since ξ is strictly increasing, $x_0 < \xi(c)$. By virtue of Proposition 11.11, we can conclude $w'(x_0) < f(x_0,y_0)$. □

Claim 11.21: *The curve $y = \mathcal{Y}(x)$ is analytic for all $x > 0$.*

Proof: We know that $\xi^{-1}(x)$ is analytic and $0 < \xi^{-1}(x) < \varepsilon^{-1}$ for all $x > 0$. Since $F(x,c)$ is analytic if $x > 0$ and $0 < c < \varepsilon^{-1}$, we see from the definition (11.15) that $\mathcal{Y}(x)$ is analytic for all $x > 0$. □

Proposition 11.22: *The function h, defined in* (11.13)*, satisfies*

$$h(x,y) \begin{cases} < 0, & \text{if} \quad x > 0,\ H(x) < y < \mathcal{Y}(x) \\ = 0, & \text{if} \quad x > 0,\ y = \mathcal{Y}(x) \\ > 0, & \text{if} \quad x > 0,\ \mathcal{Y}(x) < y < \alpha(x) \end{cases} .$$

Proof: Let $x_0 > 0$ and $H(x_0) < y_0 < \alpha(x_0)$ be fixed. Consider the slope $c := f(x_0,y_0)$ and isocline $w(x) := F(x,c)$. We know from Claim 11.15 that

$$h(x_0,y_0) = x_0 \left[f(x_0,y_0) - w'(x_0) \right].$$

The result follows from Claim 11.20. □

Proposition 11.23: *The curve $y = \mathcal{Y}(x)$ satisfies*

$$H(x) < \mathcal{Y}(x) < \mathcal{M}(x) \quad \textit{for all} \quad x > 0.$$

Proof: We know already that $H(x) < \mathcal{Y}(x) < \alpha(x)$ for all $x > 0$. We know from our results on concavity (see Table 11.1) that $h(x, y) > 0$ if $x > 0$ and $\mathcal{M}(x) < y < \alpha(x)$, where h is the function defined in (11.13). By continuity, we can conclude $h(x, \mathcal{M}(x)) \geq 0$ for all $x > 0$. It follows from Proposition 11.22 that $\mathcal{Y}(x) \leq \mathcal{M}(x)$ for all $x > 0$.

To establish a strict inequality, let h be defined along the solution $y = \mathcal{M}(x)$. Assume, on the contrary, that there is an $x_0 > 0$ such that $h(x_0) = 0$. Using (11.14), $h'(x_0) < 0$. This contradicts the fact that $h(x) \geq 0$ for all $x > 0$. □

11.6.4 The Slow Tangent Manifold

The two curves of inflection points (the one between H and $\mathcal{M}$ given by $y = \mathcal{Y}(x)$ as well as the one above V) are tangent manifolds. To justify this statement, we will use the results of §7.6.4 on page 183.

The Jacobian of the vector field $\mathbf{g}$, given in (11.3), is

$$\begin{pmatrix} -2x + \varepsilon y & \varepsilon x \\ 2x - \varepsilon y & -\varepsilon x - 1 \end{pmatrix}.$$

This matrix has trace and determinant given, respectively, by

$$\tau := -(\varepsilon + 2)\, x + \varepsilon y - 1 \quad \text{and} \quad \Delta := 2x - \varepsilon y.$$

To apply Proposition 7.36, we need to verify that $g_1 \neq 0$, $\frac{\partial g_1}{\partial y} \neq 0$, and $\tau^2 > 4\Delta$ in the relevant regions. Trivially, $g_1 \neq 0$ (except along the vertical isocline) and $g_{12} > 0$ for $x > 0$. To show that $\tau^2 > 4\Delta$ for $x > 0$, observe

$$\tau^2 - 4\Delta = \varepsilon^2 \left[y - \frac{(\varepsilon + 2)\, x - 1}{\varepsilon} \right]^2 + 4\varepsilon x \geq 4\varepsilon x > 0.$$

Remark 11.24: For the Michaelis-Menten mechanism, it is possible to write down the slow tangent manifold explicitly in the form $x = \mathcal{T}(y)$ with the expression for $\mathcal{T}$ being simple. However, for the Lindemann mechanism, the slow tangent manifold is given implicitly by the equation

$$\varepsilon^2 y^3 - (3\varepsilon x)\, y^2 + \left(2x^2 - \varepsilon x^2 - x\right) y + x^3 = 0.$$

Thus, to write down an expression for the slow tangent manifold, either in the form $y = \mathcal{Y}(x)$ or $x = \mathcal{T}(y)$, we need to find the roots of a cubic polynomial. The resulting expressions, in both cases, are quite messy.

11.7 Behaviour Near $x = 0$: Conclusion

In this section, we establish the full asymptotic behaviour of scalar solutions $y(x)$ as $x \to 0^+$. We will begin by attempting to find a Taylor series solution. Consider the differential equation (11.2), which can be re-written

$$\varepsilon xyy' - x^2y' - x^2 + y + \varepsilon xy = 0. \tag{11.16}$$

Assume that $y(x)$ is a solution in Γ_0 of the form

$$y(x) = \sum_{n=0}^{\infty} b_n x^n \tag{11.17}$$

for undetermined coefficients $\{b_n\}_{n=0}^{\infty}$.

Calculate

$$xy(x)y'(x) = \sum_{n=1}^{\infty} c_n x^n, \quad xy(x) = \sum_{n=1}^{\infty} b_{n-1} x^n, \quad \text{and} \quad x^2y'(x) = \sum_{n=2}^{\infty} (n-1)\, b_{n-1} x^n, \tag{11.18}$$

where

$$c_n := \sum_{m=0}^{n-1} (n-m)\, b_m b_{n-m} \quad \text{for} \quad n \geq 1.$$

If we substitute (11.17) and (11.18) into (11.16), we get

$$b_0 + [\varepsilon c_1 + b_1 + \varepsilon b_0]\, x + [\varepsilon c_2 + b_2 + (\varepsilon - 1)\, b_1 - 1]\, x^2 + \sum_{n=3}^{\infty} [\varepsilon c_n + b_n + (\varepsilon + 1 - n)\, b_{n-1}]\, x^n = 0.$$

We must have $b_0 = 0$ from which it follows that $c_1 = 0$. In turn, this means $b_1 = 0$, $c_2 = 0$, $b_2 = 1$, $c_3 = 0$, and $b_3 = 2 - \varepsilon$. Thus, the coefficients $\{b_n\}_{n=0}^{\infty}$ in (11.17) must be given by

$$b_0 = 0, \quad b_1 = 0, \quad b_2 = 1, \quad b_3 = 2 - \varepsilon,$$

$$\text{and} \quad b_n = (n - 1 - \varepsilon)\, b_{n-1} - \varepsilon \sum_{m=2}^{n-2} (n-m)\, b_m b_{n-m} \quad \text{for} \quad n \geq 4. \tag{11.19}$$

We will use centre manifold theory to show that the series (11.17) is fully correct for each solution inside the trapping region Γ_0. However, we must first show that each solution is a centre manifold. That is, we must show that each solution $y(x)$ satisfies $y(0) = 0$ and $y'(0) = 0$. Proposition 11.12 already established that this is true for $y(x)$ inside Γ_1. Note that for the Michaelis-Menten mechanism, solutions generally were not given by a Taylor series at the origin.

Proposition 11.25: *Let y be a solution to* (11.2) *lying inside Γ_0 for $x \in (0, a)$, where $a > 0$. Then, we can extend $y(x)$ and $y'(x)$ to say $y(0) = 0$ and $y'(0) = 0$.*

Proof: These limits have already been established if y is the slow manifold or if y lies below the slow manifold $\mathcal{M}$. Hence, we will assume that

$$\mathcal{M}(x) < y(x) < V(x) \quad \text{for all} \quad x \in (0, a).$$

Let $c := y'\left(\frac{a}{2}\right)$. We know from Table 11.1 that y is concave up on $\left(0, \frac{a}{2}\right)$. Since $\mathcal{M}(x) > 0$ for $x \in \left(0, \frac{a}{2}\right)$, we thus have

$$0 < y(x) < F(x, c) \quad \text{for all} \quad x \in \left(0, \frac{a}{2}\right),$$

where F is the function given in (11.6). Note that

$$\lim_{x \to 0^+} F(x, c) = 0 \quad \text{and} \quad \lim_{x \to 0^+} \frac{F(x, c)}{x} = 0.$$

It follows from the Squeeze Theorem that we can take $y(0) = 0$. Now, observe that

$$0 < \frac{y(x) - y(0)}{x - 0} < \frac{F(x, c)}{x}.$$

Again by the Squeeze Theorem, we see that we can take $y'(0) = 0$. □

Theorem 11.26: *Let $y(x)$ be a scalar solution to* (11.2) *lying inside Γ_0 and consider the coefficients $\{b_n\}_{n=2}^{\infty}$ given in* (11.19)*. Then,*

$$y(x) \sim \sum_{n=2}^{\infty} b_n x^n \quad \textit{as} \quad x \to 0^+.$$

Proof: The Centre Manifold Theorem guarantees that there is a solution $u(x)$ to (11.2) such that

$$u(x) \sim \sum_{n=2}^{\infty} b_n x^n \quad \text{as} \quad x \to 0^+.$$

Since $y(x)$ is a centre manifold, it follows from centre manifold theory that

$$y(x) - u(x) = \mathcal{O}\Big(x^k\Big) \quad \text{as} \quad x \to 0^+$$

for any $k \in \{2, 3, \ldots\}$. See, for example, Theorem 1 on page 16, Theorem 3 on page 25, and properties (1) and (2) on page 28 of [23]. Alternatively, see §A.10 of Appendix A. Therefore,

$$y(x) \sim \sum_{n=2}^{\infty} b_n x^n \quad \text{as} \quad x \to 0^+.$$

□

Remark 11.27: For analytic systems of ordinary differential equations for which the Centre Manifold Theorem applies, if the Taylor series for a centre manifold has a non-zero radius of convergence, then the centre manifold is unique. Since all solutions y to (11.2) lying inside Γ_0 are centre manifolds, we can conclude that the Taylor series $\sum_{n=2}^{\infty} b_n x^n$ has radius of convergence zero.

11.8 All Solutions Must Enter Γ_1

Earlier, in Theorem 11.4, we showed that all solutions $\mathbf{x}(t)$ to the planar system (11.1), except for the trivial solution, eventually enter the trapping region Γ_0. Here, we show that Γ_1 is itself a trapping region. Note that for the Michaelis-Menten mechanism, there were values of the parameters ε and η which prevented Γ_1 from being a true trapping region.

Theorem 11.28: *Let $\boldsymbol{x}(t)$ be the solution to (11.1) with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}_0$, where $\boldsymbol{x}_0 \in S \setminus \{\boldsymbol{0}\}$.*

(a) There is a $t^* > 0$ such that $\boldsymbol{x}(t) \in \Gamma_1$ for all $t \geq t^*$.

(b) Define the region

$$\Gamma_2 := \{\ (x, y)\ :\ x > 0,\ \mathcal{Y}(x) \leq y \leq \alpha(x)\ \}.$$

Then, there is a $t^* > 0$ such that $\boldsymbol{x}(t) \in \Gamma_2$ for all $t \geq t^*$.

Proof:

(a) We know from Theorem 11.4 that $\mathbf{x}(t)$ eventually enters and stays in Γ_0. Let $y(x)$ be the corresponding scalar solution to (11.2). Then, we can say $y'(0) = 0$. Appealing to the isocline structure, this means that $\mathbf{x}(t)$ has entered Γ_1. Furthermore, since $\mathbf{g} \bullet \boldsymbol{\nu} < 0$ along the horizontal and α isoclines which form the boundaries of the region in question, we see that Γ_1 is positively invariant.

(b) It follows from Table 11.1, Proposition 11.22, and the previous part of the theorem.

□

11.9 Bounds on $y(x)$

Let $y(x)$ be the solution to the scalar differential equation (11.2) with initial condition $y(x_0) = y_0$, where $x_0 > 0$ and $y_0 \geq 0$. Our goal is to obtain simple bounds on $y(x)$ over $(0, x_0]$ for three cases. In particular, we will consider $y_0 = 0$, $y_0 = H(x_0)$, and $y_0 = \alpha(x_0)$, where $H(x)$ is the horizontal isocline which is given in (11.4) and $\alpha(x)$ is the isocline for slope ε^{-1} which is given in (11.9). Moreover, we will use these bounds to state bounds on the slow manifold. To these ends, we will use Chaplygin's method (see §A.5 of Appendix A).

If $x > 0$ and $0 \leq y < V(x)$ then

$$\frac{\partial f}{\partial y}(x, y) = \frac{1}{(x - \varepsilon y)^2} > 0 \quad \text{and} \quad \frac{\partial^2 f}{\partial y^2}(x, y) = \frac{2\varepsilon}{(x - \varepsilon y)^3} > 0,$$

where f is the function given in (11.3) and $V(x)$ is the vertical isocline given in (11.4). Note also that

$$f(x, 0) = -1, \quad f(x, H(x)) = 0, \quad \text{and} \quad f(x, \alpha(x)) = \varepsilon^{-1} \quad \text{for all} \quad x > 0.$$

Moreover, note

$$\frac{\partial f}{\partial y}(x, 0) = \frac{1}{x^2}, \quad \frac{\partial f}{\partial y}(x, H(x)) = \frac{(1 + \varepsilon x)^2}{x^2}, \quad \text{and} \quad \frac{\partial f}{\partial y}(x, \alpha(x)) = \frac{[1 + (1 + \varepsilon)\, x]^2}{x^2} \quad \text{for all} \quad x > 0.$$

Consider $x \in (0, x_0]$ to be fixed. Then, the curve $z = f(x, y)$ is concave up on the interval $[0, \alpha(x)]$. See Figure 11.5. This fact enables us to state bounds on $f(x, y)$ using secants and tangents.

- The tangent to $z = f(x, y)$ at $y = 0$ is $z = T_1(x, y)$, where

$$T_1(x, y) := -1 + \frac{1}{x^2}\, y. \tag{11.20a}$$

- The tangent to $z = f(x, y)$ at $y = H(x)$ is $z = T_2(x, y)$, where

$$T_2(x, y) := \frac{(1 + \varepsilon x)^2}{x^2} \left(y - \frac{x^2}{1 + \varepsilon x} \right). \tag{11.20b}$$

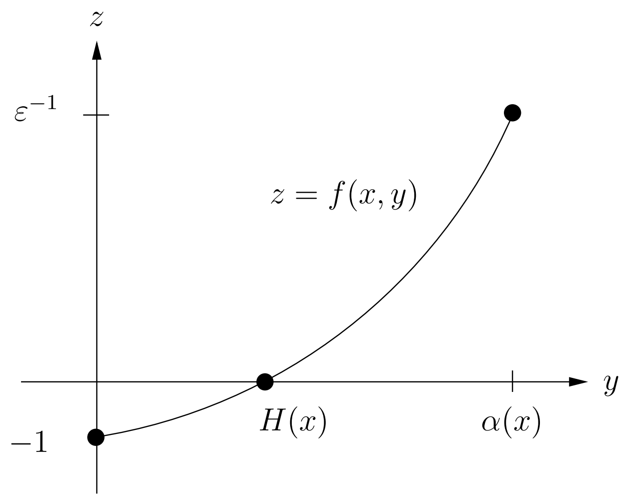

Figure 11.5: For a fixed $x \in (0, x_0]$, the curve $z = f(x, y)$ is concave up on the interval $[0, \alpha(x)]$. This allows us to obtain bounds on $f(x, y)$ over the interval $[0, \alpha(x)]$ using secants and tangents.

- The tangent to $z = f(x, y)$ at $y = \alpha(x)$ is $z = T_3(x, y)$, where

$$T_3(x, y) := \frac{1}{\varepsilon} + \frac{[1 + (1 + \varepsilon)\, x]^2}{x^2} \left\{ y - \frac{(1 + \varepsilon)\, x^2}{\varepsilon\, [1 + (1 + \varepsilon)\, x]} \right\}. \tag{11.20c}$$

- The secant line through $(0, -1)$ and $\left(\alpha(x), \varepsilon^{-1}\right)$ is $z = S_1(x, y)$, where

$$S_1(x, y) := -1 + \frac{1 + (1 + \varepsilon)\, x}{x^2}\, y. \tag{11.20d}$$

- The secant line through $(H(x), 0)$ and $\left(\alpha(x), \varepsilon^{-1}\right)$ is $z = S_2(x, y)$, where

$$S_2(x, y) := \frac{[1 + \varepsilon x]\, [1 + (1 + \varepsilon)\, x]}{x^2} \left(y - \frac{x^2}{1 + \varepsilon x} \right). \tag{11.20e}$$

11.9.1 Case 1: $x_0 > 0$ and $y_0 = 0$

Suppose that $y_0 = 0$ and so $y(x)$ is a solution which terminates on the x-axis at $x = x_0$. Since $y(x)$ is a solution lying below the slow manifold which in turn lies below the isocline $\alpha(x)$, we know that

$$0 \le y(x) \le \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Now, it is apparent from Figure 11.5 that

$$T_3(x, y) \le f(x, y) \le S_1(x, y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,,$$

where $T_3(x, y)$ is as in (11.20c) and $S_1(x, y)$ is as in (11.20d).

Define, for $x \in (0, x_0]$, the functions

$$a_1(x) := -1, \quad b_1(x) := \frac{1 + (1+\varepsilon)\,x}{x^2}, \quad \mu_1(x) := \exp\left(\int_x^{x_0} b_1(z)\,dz\right)$$

along with

$$a_2(x) := -\frac{\varepsilon + (1+\varepsilon)^2\,x}{\varepsilon}, \quad b_2(x) := \frac{[1 + (1+\varepsilon)\,x]^2}{x^2}, \quad \text{and} \quad \mu_2(x) := \exp\left(\int_x^{x_0} b_2(z)\,dz\right).$$

Note that

$$\mu_i(x_0) = 1, \quad \mu_i(x) > 0, \quad \text{and} \quad \mu_i'(x) = -b_i(x)\mu_i(x) \quad (i = 1, 2)\,.$$

Thus, we can write

$$a_2(x) + b_2(x)y(x) \le y'(x) \le a_1(x) + b_1(x)y(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Re-arranging and replacing x with z,

$$\frac{d}{dz}\left(\mu_2(z)y(z)\right) \ge \mu_2(z)a_2(z) \quad \text{and} \quad \frac{d}{dz}\left(\mu_1(z)y(z)\right) \le \mu_1(z)a_1(z) \quad \text{for all} \quad z \in (0, x_0]\,.$$

If we integrate with respect to z from x to x_0, where $x \in (0, x_0]$, apply the initial condition $y(x_0) = 0$, and re-arrange, we obtain

$$-\frac{1}{\mu_1(x)}\int_x^{x_0} \mu_1(z)a_1(z)\,ds \le y(x) \le -\frac{1}{\mu_2(x)}\int_x^{x_0} \mu_2(z)a_2(z)\,ds \quad \text{for all} \quad x \in (0, x_0]\,. \qquad (11.21)$$

Figure 11.6 gives two numerical examples of the bounds given in (11.21).

Remarks 11.29:

(i) The lower bound in (11.21) is a very good approximation to $y(x)$ when x is close to x_0. Moreover, the upper bound in (11.21) is a very good approximation when x is close to 0.

(ii) To get a better upper bound for $y(x)$ when x is close to x_0, we should use the tangent $T_1(x, y)$ in the calculation instead of $T_3(x, y)$. This is evident from Figure 11.6.

11.9.2 Case 2: $x_0 > 0$ and $y_0 = H(x_0)$

Suppose now that $y_0 = H(x_0)$. Thus, $y(x)$ is the solution to (11.2) which terminates on the horizontal isocline at $x = x_0$. We know that

$$H(x) \le y(x) \le \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

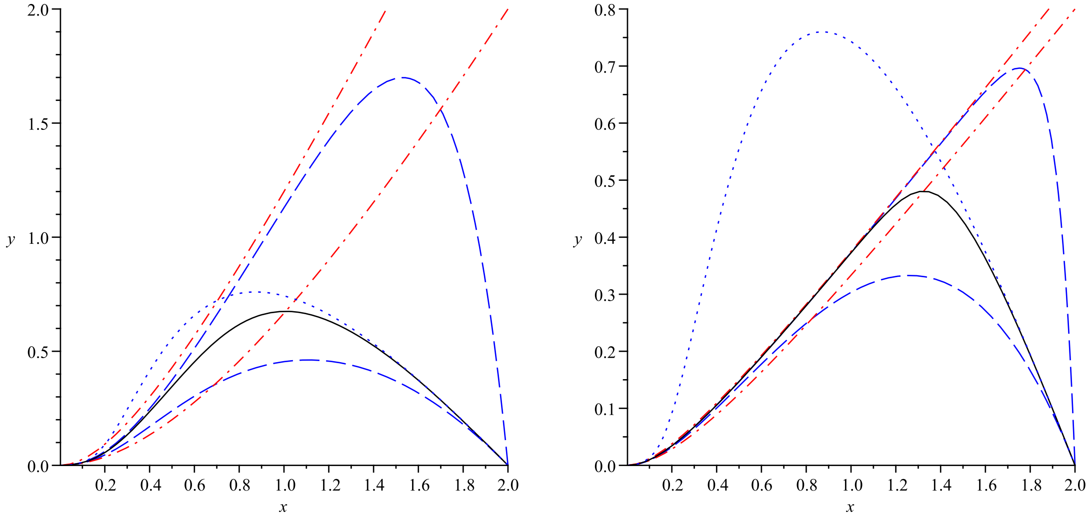

Figure 11.6: For the first picture, suppose $\varepsilon = 0.5$ and $x_0 = 2.0$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (11.21). The solid curve represents the actual solution (found numerically) with $y(x_0) = 0$. The dash-dot curves are the horizontal and α isoclines. The dotted curve represents the upper bound for $y(x)$ which results from using the tangent $T_1(x,y)$ instead of $T_3(x,y)$. The second picture is the same as the first except with $\varepsilon = 2.0$ and $x_0 = 2.0$.

Appealing to Figure 11.5,

$$T_3(x,y) \le f(x,y) \le S_2(x,y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,,$$

where $T_3(x,y)$ is as in (11.20c) and $S_2(x,y)$ is as in (11.20e).

Define, for $x \in (0, x_0]$, the functions

$$a_1(x) := -\left[1 + (1+\varepsilon)\,x\right], \quad b_1(x) := \frac{[1+\varepsilon x]\,[1+(1+\varepsilon)\,x]}{x^2}, \quad \mu_1(x) := \mathsf{exp}\left(\int_x^{x_0} b_1(z)\,dz\right) \tag{11.22}$$

along with

$$a_2(x) := -\frac{\varepsilon + (1+\varepsilon)^2\,x}{\varepsilon}, \quad b_2(x) := \frac{[1+(1+\varepsilon)\,x]^2}{x^2}, \quad \text{and} \quad \mu_2(x) := \mathsf{exp}\left(\int_x^{x_0} b_2(z)\,dz\right). \tag{11.23}$$

Proceeding as we did above, we get

$$\frac{H(x_0) - \int_x^{x_0} \mu_1(z) a_1(z)\,ds}{\mu_1(x)} \le y(x) \le \frac{H(x_0) - \int_x^{x_0} \mu_2(z) a_2(z)\,ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,. \tag{11.24}$$

Figure 11.7 gives two numerical examples of the bounds given in (11.24).

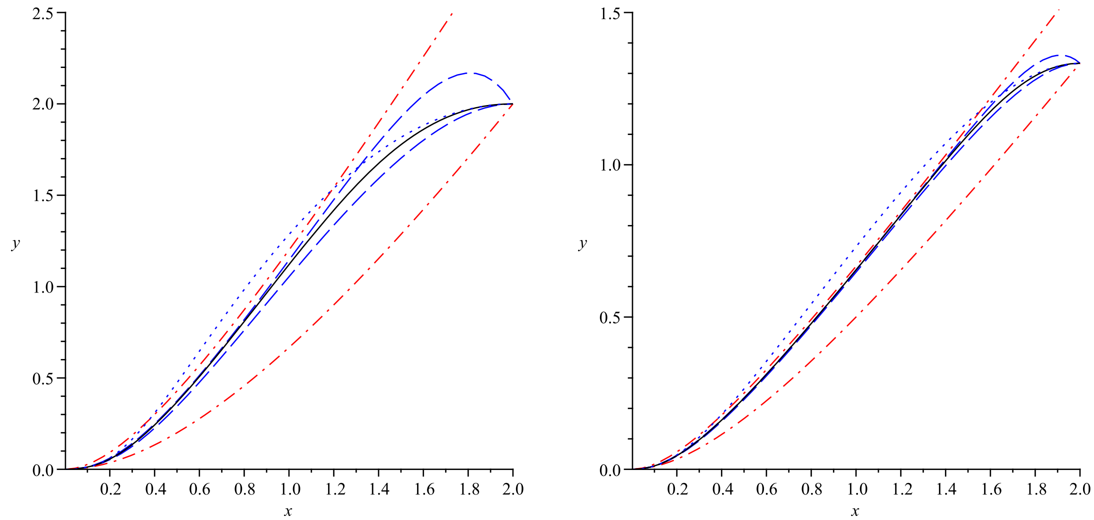

Figure 11.7: For the first picture, suppose $\varepsilon = 0.5$ and $x_0 = 2.0$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (11.24). The solid curve represents the actual solution (found numerically) with $y(x_0) = H(x_0)$. The two dash-dot curves are the horizontal and α isoclines. The dotted curve represents the upper bound for $y(x)$ which results from using the tangent $T_2(x, y)$ instead of $T_3(x, y)$. The second picture is the same as the first except with $\varepsilon = 1.0$ and $x_0 = 2.0$.

11.9.3 Case 3: $x_0 > 0$ and $y_0 = \alpha(x_0)$

Suppose now that $y_0 = \alpha(x_0)$. Thus, $y(x)$ is the scalar solution which terminates on the α isocline at $x = x_0$. We know that

$$H(x) \leq y(x) \leq \alpha(x) \quad \text{for all} \quad x \in (0, x_0]\,.$$

Furthermore, we can see from Figure 11.5 that

$$T_3(x, y) \leq f(x, y) \leq S_2(x, y) \quad \text{for all} \quad x > 0 \quad \text{and} \quad y \in [0, \alpha(x)]\,.$$

Proceeding as before, we obtain

$$\frac{\alpha(x_0) - \int_x^{x_0} \mu_1(z) a_1(z)\, ds}{\mu_1(x)} \leq y(x) \leq \frac{\alpha(x_0) - \int_x^{x_0} \mu_2(z) a_2(z)\, ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,, \qquad (11.25)$$

where $a_i(x)$, $b_i(x)$, and $\mu_i(x)$ for $i = 1, 2$ are as in (11.22) and (11.23). Figure 11.8 gives two numerical examples of the bounds given in (11.25).

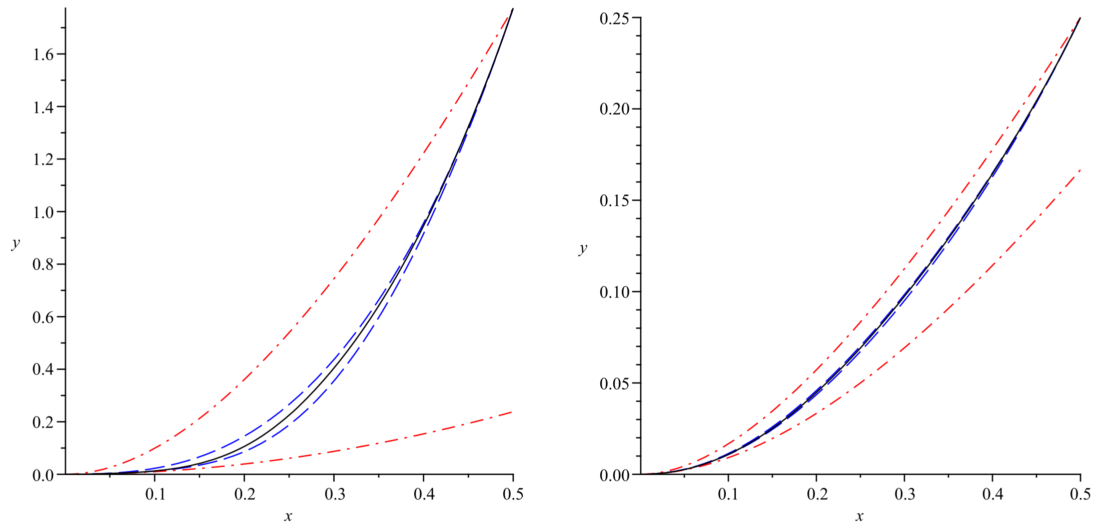

Figure 11.8: For the first picture, suppose $\varepsilon = 0.1$ and $x_0 = 0.5$. The two dashed curves represent the lower and upper bounds for $y(x)$ given in (11.25). The solid curve represents the actual solution (found numerically) with $y(x_0) = \alpha(x_0)$. The two dash-dot curves are the horizontal and α isoclines. The second picture is the same as the first except with $\varepsilon = 1.0$ and $x_0 = 0.5$.

11.9.4 Bounds on the Slow Manifold

We can use the material from the previous two subsections to state bounds on the slow manifold. Suppose that $y_1(x)$ is the solution of (11.2) with initial condition $y(x_0) = H(x_0)$. Suppose also that $y_2(x)$ is the solution of (11.2) with initial condition $y(x_0) = \alpha(x_0)$. It follows that the slow manifold satisfies $y_1(x) \le \mathcal{M}(x) \le y_2(x)$ for all $x \in (0, x_0]$. If we combine (11.24), which gives bounds for $y_1(x)$, and (11.25), which gives bounds for $y_2(x)$, we can conclude that

$$\frac{H(x_0) - \int_x^{x_0} \mu_1(z)a_1(z)\,ds}{\mu_1(x)} \le \mathcal{M}(x) \le \frac{\alpha(x_0) - \int_x^{x_0} \mu_2(z)a_2(z)\,ds}{\mu_2(x)} \quad \text{for all} \quad x \in (0, x_0]\,,$$

where $a_i(x)$, $b_i(x)$, and $\mu_i(x)$ for $i = 1, 2$ (which all depend on x_0) are as in (11.22) and (11.23). It is worth reiterating the fact that $x_0 > 0$ is arbitrary.

11.10 Properties of the Slow Manifold

The purpose of this section is to single out some important properties of the slow manifold.

11.10.1 Bounds on the Slow Manifold

Proposition 11.30: *The slow manifold $y = \mathcal{M}(x)$ satisfies, for all $x > 0$,*

$$0 < H(x) < \mathcal{Y}(x) < \mathcal{M}(x) < \alpha(x).$$

Furthermore,

$$\lim_{x \to 0^+} \mathcal{M}(x) = 0.$$

Proof: The first part follows from Theorem 11.7 and Proposition 11.23. The second part follows from the Squeeze Theorem. □

11.10.2 Concavity of the Slow Manifold

Proposition 11.31: *The slow manifold $y = \mathcal{M}(x)$ is concave up for all $x > 0$.*

Proof: It follows from Propositions 11.22 and 11.30 that $h(x, \mathcal{M}(x)) > 0$ for all $x > 0$, where h is the function defined in (11.13). Since $\mathsf{sgn}(\mathcal{M}''(x)) = \mathsf{sgn}(h(x, \mathcal{M}(x)))$, it must be that the slow manifold is concave up for all $x > 0$. □

11.10.3 The Slope of the Slow Manifold

Proposition 11.32: *The slope of the slow manifold $y = \mathcal{M}(x)$ satisfies*

$$0 < \mathcal{M}'(x) < \varepsilon^{-1} \quad \textit{for all} \quad x > 0.$$

Furthermore,

$$\lim_{x \to 0^+} \mathcal{M}'(x) = 0 \quad \textit{and} \quad \lim_{x \to \infty} \mathcal{M}'(x) = \varepsilon^{-1}.$$

Proof: The first part is a consequence of Proposition 11.30 and the isocline structure. The first limit is a special case of Proposition 11.25. To prove the second limit, let $c \in \left(0, \varepsilon^{-1}\right)$. It follows from Proposition 11.11 and the isocline structure that

$$c < \mathcal{M}'(x) < \varepsilon^{-1} \quad \text{for all} \quad x > \xi(c),$$

where ξ is the function defined in (11.10). Applying (11.11) and the Squeeze Theorem gives the second limit. □

Remark 11.33: The justification which Fraser provides in [43] (just before Theorem 1) that $\lim_{x\to\infty} \mathcal{M}'(x) = \varepsilon^{-1}$ is incorrect. The error is that the distance between the horizontal and vertical isoclines does not tend to zero as x tends to infinity. Thus, the asymptotic behaviour of $\mathcal{M}'(x)$ need not be the same as the asymptotic behaviour of $H'(x)$ and $V'(x)$.

11.10.4 Asymptotic Series for the Slow Manifold at the Origin

Proposition 11.34: *Asymptotically, the slow manifold can be written*

$$\mathcal{M}(x) \sim \sum_{n=2}^{\infty} b_n x^n \quad \textit{as} \quad x \to 0^+,$$

where the coefficients $\{b_n\}_{n=2}^{\infty}$ *are as in* (11.19).

Proof: Since the slow manifold is contained entirely in Γ_0, we can apply Theorem 11.26. □

Corollary 11.35: *The slow manifold satisfies*

$$\mathcal{M}(x) = H(x) + \mathcal{O}\big(x^3\big) \quad \textit{as} \quad x \to 0^+.$$

Moreover, this statement would not be true if we replace $H(x)$ *with any other isocline* $F(x,c)$.

Proof: It follows from a comparison of the asymptotic expansions for $\mathcal{M}(x)$, $H(x)$, and $F(x,c)$. □

11.10.5 Asymptotic Series for the Slow Manifold at Infinity

Here, we will establish the full asymptotic behaviour of the slow manifold at infinity. First, we will extract as much information as possible from the isoclines. Second, we will attempt to find a series in integer powers of x. Third, we will prove definitely that the resulting series is indeed fully correct.

Let $c \in \big(0, \varepsilon^{-1}\big)$. We know from Proposition 11.11 that

$$F(x,c) < \mathcal{M}(x) < \alpha(x) \quad \text{for all} \quad x > \xi(c),$$

where F is defined in (11.6) and ξ is defined in (11.10). Note that

$$F(x,c) = \frac{x}{\varepsilon} - \frac{K(c)}{\varepsilon^2} + \mathcal{O}\left(\frac{1}{x}\right) \quad \text{and} \quad \alpha(x) = \frac{x}{\varepsilon} - \frac{1}{\varepsilon\,(1+\varepsilon)} + \mathcal{O}\left(\frac{1}{x}\right) \quad \text{as} \quad x \to \infty.$$

Since

$$F(x,c) - \frac{x}{\varepsilon} < \mathcal{M}(x) - \frac{x}{\varepsilon} < \alpha(x) - \frac{x}{\varepsilon} \quad \text{for all} \quad x > \xi(c),$$

we can conclude

$$\liminf_{x\to\infty}\left[\mathcal{M}(x) - \frac{x}{\varepsilon}\right] \geq -\frac{K(c)}{\varepsilon^2} \quad \text{and} \quad \limsup_{x\to\infty}\left[\mathcal{M}(x) - \frac{x}{\varepsilon}\right] \leq -\frac{1}{\varepsilon\,(1+\varepsilon)}.$$

Since $c \in \left(0, \varepsilon^{-1}\right)$ is arbitrary and

$$\lim_{c\to(\varepsilon^{-1})^-} -\frac{K(c)}{\varepsilon^2} = -\frac{1}{\varepsilon\,(1+\varepsilon)},$$

we have

$$\lim_{x\to\infty}\left[\mathcal{M}(x) - \frac{x}{\varepsilon}\right] = -\frac{1}{\varepsilon\,(1+\varepsilon)} \quad \text{and} \quad \mathcal{M}(x) = \frac{x}{\varepsilon} - \frac{1}{\varepsilon\,(1+\varepsilon)} + \mathsf{o}(1) \quad \text{as} \quad x \to \infty.$$

Assume that we can write

$$\mathcal{M}(x) = \sum_{n=-1}^{\infty} \rho_n x^{-n} \tag{11.26}$$

for undetermined coefficients $\{\rho_n\}_{n=-1}^{\infty}$. Of course, we expect $\rho_{-1} = \varepsilon^{-1}$. Write the differential equation (11.2) as

$$\varepsilon x y y' - x^2 y' - x^2 + y + \varepsilon x y = 0. \tag{11.27}$$

Substitution of (11.26) in to (11.27) yields

$$\left[\varepsilon c_{-1} + (\varepsilon - 1)\,\rho_{-1} - 1\right] x^2 + \sum_{n=-1}^{\infty}\left[\varepsilon c_{n+1} + (n+1+\varepsilon)\,\rho_{n+1} + \rho_n\right] x^{-n} = 0, \tag{11.28}$$

where

$$c_n := -\sum_{m=0}^{n+1} (n-m)\,\rho_{m-1}\rho_{n-m} \quad \text{for} \quad n \geq -1.$$

Observe that

$$c_{-1} = \rho_{-1}^2, \quad c_0 = \rho_{-1}\rho_0,$$

$$\text{and} \quad c_{n+1} = -n\rho_{-1}\rho_{n+1} - \sum_{m=1}^{n+1} (n-m+1)\,\rho_{m-1}\rho_{n-m+1} \quad \text{for} \quad n \geq 0. \tag{11.29}$$

In order for the coefficient of x^2 in (11.28) to be 0, ρ_{-1} needs to be either -1 or ε^{-1}. Since $\mathcal{M}(x) > 0$ for all $x > 0$, we must have $\rho_{-1} = \varepsilon^{-1}$. Furthermore, in order for the coefficient of x^{-n} for $n \geq -1$ to be 0, we need

$$\varepsilon c_{n+1} + (n+1+\varepsilon)\,\rho_{n+1} + \rho_n = 0 \quad \text{for} \quad n \geq -1.$$

Using (11.29), we see that the coefficients $\{\rho_n\}_{n=-1}^{\infty}$ are given by

$$\rho_{-1} = \frac{1}{\varepsilon}, \quad \rho_0 = -\frac{1}{\varepsilon\,(1+\varepsilon)},$$

$$\text{and} \quad \rho_n = -\frac{1}{1+\varepsilon}\left[\rho_{n-1} - \varepsilon \sum_{m=1}^{n} (n-m)\,\rho_{m-1}\rho_{n-m}\right] \quad \text{for} \quad n \geq 1. \tag{11.30}$$

Proposition 11.36: *Asymptotically, the slow manifold can be written*

$$\mathcal{M}(x) \sim \sum_{n=-1}^{\infty} \rho_n x^{-n} \quad \textit{as} \quad x \to \infty,$$

where the coefficients $\{\rho_n\}_{n=-1}^{\infty}$ *are as in* (11.30).

Proof: To prove the result, we will apply the Centre Manifold Theorem to a fixed point at infinity. Consider the change of variables

$$X := x^{-1} \quad \text{and} \quad Y := y - r(x), \quad \text{where} \quad r(x) := \rho_{-1}x + \rho_0 + \rho_1 x^{-1},$$

with the coefficients ρ_{-1}, ρ_0, and ρ_1 being given in (11.30). Differentiate the new variables with respect to time and use the differential equation (11.1) to obtain the system

$$\begin{aligned}
\dot{X} &= -X^2 g_1\left(X^{-1}, r\left(X^{-1}\right) + Y\right), \\
\dot{Y} &= -r'\left(X^{-1}\right) g_1\left(X^{-1}, r\left(X^{-1}\right) + Y\right) + g_2\left(X^{-1}, r\left(X^{-1}\right) + Y\right),
\end{aligned}$$

where g_1 and g_2 are as in (11.3). This system is not polynomial but there is no harm in considering the system

$$\begin{aligned}
\dot{X} &= -X^3 g_1\left(X^{-1}, r\left(X^{-1}\right) + Y\right), \\
\dot{Y} &= X\left[-r'\left(X^{-1}\right) g_1\left(X^{-1}, r\left(X^{-1}\right) + Y\right) + g_2\left(X^{-1}, r\left(X^{-1}\right) + Y\right)\right],
\end{aligned} \tag{11.31}$$

which is polynomial. This is because the resulting scalar differential equation will be the same. The system at hand, while messy, is in the canonical form for the Centre Manifold Theorem. Note that the eigenvalues of the matrix for the linear part of this system are 0 and $-(1+\varepsilon)$. We know from centre manifold theory that there is a C^∞ centre manifold $Y = \mathcal{C}(X)$ which, we claim, must be the slow manifold.

For the scalar differential equation in the original coordinates, all other solutions except for the slow manifold leave the antifunnel Γ_1. To establish that the slow manifold in the original

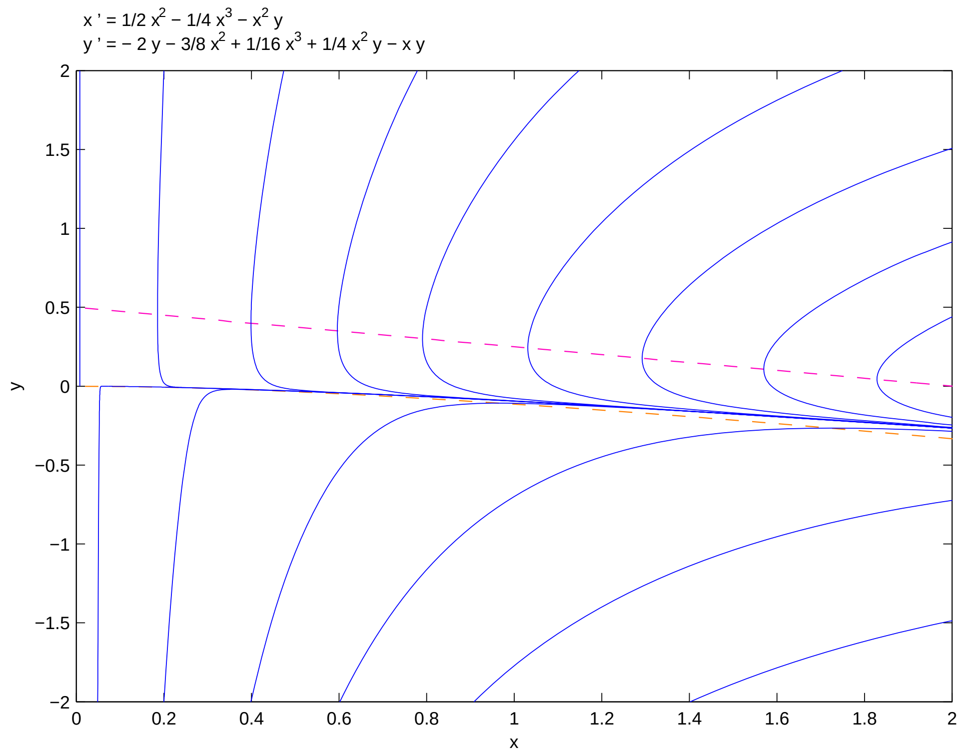

Figure 11.9: A phase portrait for (11.31) for $\varepsilon = 1.0$.

coordinates is the same as the centre manifold in the new coordinates, we need only show that $Y = \mathcal{C}(X)$ is the only scalar solution in the new coordinates which is $\mathsf{o}(1)$ as $X \to 0^+$.

Observe that the Y-axis is invariant. Moreover, the fixed point $(X, Y) = (0, 0)$ is a saddle node (or a degenerate saddle). The physically relevant portion of the phase portrait, namely $X \geq 0$, consists of two hyperbolic sectors, one with the positive Y-axis and the centre manifold as boundaries and the other with the negative Y-axis and the centre manifold as boundaries. See Figure 11.9. This can be shown using techniques in §9.21 of [2] (in particular Theorem 65 on page 340) and §2.11 of [100]. Therefore, $\mathcal{C}(X)$ is the only scalar solution in the new coordinates which is $\mathsf{o}(1)$ as $X \to 0^+$. It follows that the centre manifold is indeed the slow manifold.

By the Centre Manifold Theorem, in the new coordinates the slow manifold can be written

$$\mathcal{M}(X) \sim \sum_{n=2}^{\infty} \widehat{\rho}_n X^n \quad \text{as} \quad X \to 0^+,$$

for some coefficients $\{\widehat{\rho}_n\}_{n=2}^{\infty}$. Upon reverting back to original coordinates and observing that the coefficients in (11.30) are generated uniquely from the differential equation, the conclusion follows.

□

Corollary 11.37: *The slow manifold satisfies*

$$\mathcal{M}(x) = \alpha(x) + \mathcal{O}\left(\frac{1}{x^2}\right) \quad \textit{as} \quad x \to \infty.$$

Moreover, this statement would not be true if we replace $\alpha(x)$ with any other isocline $F(x, c)$.

Proof: It follows from a comparison of the asymptotic expansions for $\mathcal{M}(x)$, $\alpha(x)$, and $F(x, c)$. □

11.10.6 Final Remarks on the Slow Manifold

For the Michaelis-Menten mechanism, α is the optimal isocline near $x = 0$ (see Corollary 7.47). Consequently, α is the best approximation (in terms of isoclines) to planar solutions for large time. The horizontal isocline, on the other hand, is optimal at $x = \infty$ (see Corollary 7.50). For the Lindemann mechanism, however, α is the optimal isocline at $x = \infty$ (see Corollary 11.37) and H is the optimal isocline at $x = 0$ (see Corollary 11.35). Consequently, the QSSA is the best approximation (in terms of isoclines) to planar solutions for large time.

11.11 Summary

Recall that the nonlinear Lindemann mechanism for unimolecular decay is

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \overset{k_2}{\to} P,$$

where A is the molecule that decays, B is the activated complex, and P is the product of the decay. In this chapter, we explored the resulting planar reduction

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = x^2 - y - \varepsilon xy, \quad \dot{} = \frac{d}{dt}$$

in phase space. Equivalently, we studied the scalar differential equation

$$y' = \frac{x^2 - y - \varepsilon xy}{-x^2 + \varepsilon xy}, \quad ' = \frac{d}{dx}.$$

Note that the origin for the planar system is a non-hyperbolic fixed point. In the next chapter, we explore properties of time-dependent solutions.

The isoclines for the planar system are all of the form

$$w(x) = \frac{x^2}{r + \varepsilon x}.$$

Three of these isoclines are especially important, namely the horizontal, vertical, and alpha isoclines:

$$H(x) = \frac{x^2}{1 + \varepsilon x}, \quad V(x) = \frac{x}{\varepsilon}, \quad \text{and} \quad \alpha(x) = \frac{x^2}{\frac{\varepsilon}{1+\varepsilon} + \varepsilon x}.$$

Note that the horizontal isocline corresponds to the QSSA, the vertical isocline corresponds to the EA, and the α isocline corresponds to the slope of the isoclines at infinity. These three isoclines define two important regions in the non-negative quadrant given by

$$\Gamma_0 = \{\ (x, y)\ :\ x > 0,\ H(x) \le y \le V(x)\ \} \quad \text{and} \quad \Gamma_1 = \{\ (x, y)\ :\ x > 0,\ H(x) \le y \le \alpha(x)\ \}.$$

As we showed, both regions are positively invariant and all solutions eventually enter both Γ_0 and Γ_1. Note that $\Gamma_1 \subset \Gamma_0$. Furthermore, we showed that the origin is globally asymptotically stable.

The region Γ_1 is an antifunnel but it is not narrowing. Using the Alternate Antifunnel Theorem allowed us to prove the existence and uniqueness of a solution $y = \mathcal{M}(x)$, called the slow manifold, contained entirely inside Γ_1.

We determined the concavity of all solutions of the scalar differential equation in all regions of the non-negative quadrant. To achieve this, we used the auxiliary function

$$h(x) = x^2 y'(x) + y(x)\left[\varepsilon y'(x) - 2x\right],$$

where y is a solution of the scalar system, which has the same sign as $y''(x)$. Table 11.1 summarizes the results. Furthermore, we constructed a curve $y = \mathcal{Y}(x)$ between H and $\mathcal{M}$ along which solutions have inflection points. This curve can be considered a slow tangent manifold.

All solutions $y(x)$ inside Γ_0 can be written as a Taylor series with radius of convergence zero. To show this, we used centre manifold theory. Furthermore, the leading-order term is quadratic and thus all solutions are centre manifolds.

For a given $x_0 > 0$, the scalar solution $y(x)$ with initial condition $y(x_0) = y_0$, with $0 \leq y_0 \leq \alpha(x_0)$, satisfies $0 \leq y(x) \leq \alpha(x)$ for all $x \in (0, x_0]$. Using Chaplygin's method, we derived tighter bounds on $y(x)$ valid over the interval $x \in (0, x_0]$ for the three cases $y_0 = 0$, $y_0 = H(x_0)$, and $y_0 = \alpha(x_0)$. Furthermore, we used these bounds to state bounds on the slow manifold over the interval $x \in (0, x_0]$.

The chapter was concluded with a summary of properties of the slow manifold. For example, the slow manifold is concave up, strictly increasing, and for large x has an asymptotic series of the form $\mathcal{M}(x) \sim \sum_{n=-1}^{\infty} \rho_n x^{-n}$ as $x \to \infty$.

Chapter 12

Time Estimates

The goal of this chapter is to briefly discuss a few properties of solutions to the planar system for the Lindemann mechanism which fundamentally involve time. In particular, we will construct a low-order asymptotic approximation for $\mathbf{x}(t)$ as $t \to \infty$. Furthermore, we will obtain bounds on $\mathbf{x}(t)$ during the steady-state period and bounds on the length of the pre-steady-state period.

Recall that the Lindemann mechanism for unimolecular decay gives rise to the planar system of differential equations

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = -y + x^2 - \varepsilon xy, \tag{12.1}$$

where $\dot{} = \frac{d}{dt}$ and $\varepsilon > 0$. The horizontal and vertical isoclines, along with the α isocline (which corresponds to the slope ε^{-1} of the slow manifold at infinity), are given by

$$H(x) = \frac{x^2}{1+\varepsilon x}, \quad V(x) = \frac{x}{\varepsilon}, \quad \text{and} \quad \alpha(x) = \frac{x^2}{\frac{\varepsilon}{1+\varepsilon} + \varepsilon x}. \tag{12.2}$$

We showed in Chapter 11 that all non-trivial solutions to (12.1) eventually enter both of the regions Γ_0 and Γ_1, where

$$\Gamma_0 = \{\ (x,y)\ :\ x>0,\ H(x) \le y \le V(x)\ \} \quad \text{and} \quad \Gamma_1 = \{\ (x,y)\ :\ x>0,\ H(x) \le y \le \alpha(x)\ \}.$$

12.1 Behaviour as $t \to \infty$

Let $\mathbf{x}(t)$ be the solution of (12.1) with initial condition $\mathbf{x}(0) = \mathbf{x}_0$, where $\mathbf{x}_0 \in \Gamma_0$. Since the origin is not a sink, the material of Part I does not apply here. However, we can extract information using other techniques.

12.1.1 A Method using the Integration of Asymptotic Expressions

A First Estimate

Since the origin is globally asymptotically stable (see Theorem 11.4), a first estimate for the components of the solution is

$$x(t) = \mathsf{o}(1) \quad \text{and} \quad y(t) = \mathsf{o}(1) \quad \text{as} \quad t \to \infty. \tag{12.3}$$

Note that Theorem 11.26 in conjunction with (12.3) implies

$$y(t) = x(t)^2 + \mathsf{o}\big(x(t)^2\big) \quad \text{and} \quad \frac{y(t)}{x(t)} = \mathsf{o}(1) \quad \text{as} \quad t \to \infty. \tag{12.4}$$

To obtain further estimates, first we need a lemma.

A Lemma

Lemma 12.1: *Let $a \in \mathbb{R}$ be a constant and let $f, g : [a, \infty) \to \mathbb{R}$ be non-negative, integrable functions such that*

$$f(t) = g(t) + \mathsf{o}(g(t)) \quad \textit{as} \quad t \to \infty.$$

If $G(t)$ is an antiderivative of $g(t)$ such that $\lim\limits_{t\to\infty} G(t) = \infty$, then

$$\int_a^t f(s)\, ds = G(t) + \mathsf{o}(G(t)) \quad \textit{as} \quad t \to \infty.$$

Proof: For any $\delta \in (0, 1)$ there exists a $T \geq a$ such that

$$(1-\delta)\, g(t) \leq f(t) \leq (1+\delta)\, g(t) \quad \text{for all} \quad t \geq T.$$

Then, for $t \geq T$ we have

$$(1-\delta) \int_T^t g(s)\, ds \leq \int_T^t f(s)\, ds \leq (1+\delta) \int_T^t g(s)\, ds.$$

That is,

$$(1-\delta)\, [G(t) - G(T)] \leq \int_T^t f(s)\, ds \leq (1+\delta)\, [G(t) - G(T)]\,.$$

It follows that

$$\liminf_{t\to\infty} \frac{\int_T^t f(s)\, ds}{G(t)} \geq 1 - \delta \quad \text{and} \quad \limsup_{t\to\infty} \frac{\int_T^t f(s)\, ds}{G(t)} \leq 1 + \delta.$$

Since $\delta \in (0, 1)$ was arbitrary,

$$\lim_{t\to\infty} \frac{\int_T^t f(s)\,ds}{G(t)} = 1 \quad \text{and} \quad \int_T^t f(s)\,ds = G(t) + \mathsf{o}(G(t)) \quad \text{as} \quad t \to \infty.$$

Hence,

$$\int_a^t f(s)\,ds = \int_a^T f(s)\,ds + G(t) + \mathsf{o}(G(t)) = G(t) + \mathsf{o}(G(t)) \quad \text{as} \quad t \to \infty.$$

□

Remark 12.2: Suppose, for example, that f is non-negative and integrable on $[0, \infty)$ with

$$f(t) = \frac{1}{t} + \mathsf{o}\left(\frac{1}{t}\right) \quad \text{as} \quad t \to \infty.$$

We cannot immediately apply Lemma 12.1 since t^{-1} is not integrable on $[0, \infty)$. However, for any $a > 0$, Lemma 12.1 says

$$\int_0^t f(t)\,dt = \int_0^a f(t)\,dt + \ln(t) + \mathsf{o}(\ln(t)) = \ln(t) + \mathsf{o}(\ln(t)) \quad \text{as} \quad t \to \infty.$$

A Second Estimate

With the lemma, we can improve the estimate (12.3). First, we will write the differential equation (12.1) as

$$-\frac{\dot{x}(s)}{x(s)^2} = 1 - \varepsilon\,\frac{y(s)}{x(s)}, \quad s \geq 0.$$

If we integrate with respect to s from 0 to t, where $t \geq 0$, we get

$$\frac{1}{x(t)} - \frac{1}{x_0} = t - \varepsilon \int_0^t \frac{y(s)}{x(s)}\,ds. \tag{12.5}$$

We know that

$$\frac{y(t)}{x(t)} > 0 \quad \text{for all} \quad t \geq 0 \quad \text{and} \quad \frac{y(t)}{x(t)} + 1 = 1 + \mathsf{o}(1) \quad \text{as} \quad t \to \infty.$$

By Lemma 12.1,

$$\int_0^t \left[\frac{y(s)}{x(s)} + 1\right] ds = t + \mathsf{o}(t) \quad \text{as} \quad t \to \infty.$$

It follows that

$$\int_0^t \frac{y(s)}{x(s)}\,ds = \mathsf{o}(t) \quad \text{as} \quad t \to \infty. \tag{12.6}$$

Using (12.6) in (12.5) and simplifying,

$$\frac{1}{x(t)} = t\,[1 + \mathsf{o}(1)] \quad \text{as} \quad t \to \infty.$$

Solving for $x(t)$ and utilizing (12.4), we have our second estimate

$$x(t) = \frac{1}{t} + \mathsf{o}\left(\frac{1}{t}\right) \quad \text{and} \quad y(t) = \frac{1}{t^2} + \mathsf{o}\left(\frac{1}{t^2}\right) \quad \text{as} \quad t \to \infty. \tag{12.7}$$

A Third Estimate

We will make use of our second estimate to obtain our third estimate. Now, it follows from (12.7) that

$$\frac{y(t)}{x(t)} = \frac{1}{t} + \mathsf{o}\left(\frac{1}{t}\right) \quad \text{as} \quad t \to \infty.$$

By Lemma 12.1,

$$\int_0^t \frac{y(s)}{x(s)}\, ds = \mathsf{ln}(t) + \mathsf{o}(\mathsf{ln}(t)) \quad \text{as} \quad t \to \infty.$$

Using this in (12.5) and re-arranging, we obtain

$$\frac{1}{x(t)} = t\left[1 - \varepsilon\,\frac{\mathsf{ln}(t)}{t} + \mathsf{o}\left(\frac{\mathsf{ln}(t)}{t}\right)\right] \quad \text{as} \quad t \to \infty.$$

Solving for $x(t)$ and utilizing (12.4), we have the following for our third estimate.

Proposition 12.3: *Let* $\boldsymbol{x}(t)$ *be the solution to* (12.1) *with initial condition* $\boldsymbol{x}(0) = \boldsymbol{x}_0$*, where* $\boldsymbol{x}_0 \in \Gamma_0$*. Then,*

$$x(t) = \frac{1}{t} + \varepsilon\,\frac{\mathsf{ln}(t)}{t^2} + \mathsf{o}\left(\frac{\mathsf{ln}(t)}{t^2}\right) \quad \textit{and} \quad y(t) = \frac{1}{t^2} + 2\varepsilon\,\frac{\mathsf{ln}(t)}{t^3} + \mathsf{o}\left(\frac{\mathsf{ln}(t)}{t^3}\right) \quad \textit{as} \quad t \to \infty.$$

Remark 12.4: We will not attempt to obtain more terms to the asymptotic expansions for $x(t)$ for $y(t)$. Note that if we use the expressions in Proposition 12.3 along with Lemma 12.1 in the differential equation for $x(t)$, we will get no new asymptotic information for $x(t)$. Note also that the asymptotic expressions for $x(t)$ and $y(t)$ do not contain the initial conditions $x(0) = x_0$ and $y(0) = y_0$.

12.1.2 A Method using the Isoclines and Differential Inequalities

Proposition 12.3 can be established using differential inequalities and the isocline structure. Let $c > 0$ be fixed and arbitrary. We know from (12.3), Proposition 11.25, and the isocline structure that there exists a $T \geq 0$ such that

$$H(x(t)) \leq y(t) \leq F(x(t), c) \quad \text{for all} \quad t \geq T, \tag{12.8}$$

where F is given in (11.6). Using (11.6), (12.1), (12.2), and (12.8), we can see that $x(t)$ satisfies

$$-\frac{x(t)^2}{1+\varepsilon x(t)} \le \dot{x}(t) \le -\frac{x(t)^2}{1+bx(t)} \quad \text{for all} \quad t \ge T,$$

where $b := \frac{\varepsilon}{K(c)}$ and K is the function defined in (11.5). It follows from the Initial-Value Comparison Theorem (see Theorem A.6 in Appendix A on page 310) in conjunction with Claim A.26 (which is in Appendix A on page 324) that

$$\chi_\varepsilon(t) \le x(t) \le \chi_b(t) \quad \text{for all} \quad t \ge T, \tag{12.9}$$

where

$$\chi_a(t) := \frac{1}{a\,W\Big(\Big[\frac{1}{ax_0}\,\mathsf{exp}\Big(\frac{1}{ax_0}\Big)\Big]\,\mathsf{exp}\big(\frac{1}{a}\,t\big)\Big)} \quad \text{for} \quad a > 0. \tag{12.10}$$

A standard property of the Lambert W function is

$$W(t) = \mathsf{ln}(t) - \mathsf{ln}(\mathsf{ln}(t)) + \mathsf{o}(\mathsf{ln}(\mathsf{ln}(t))) \quad \text{as} \quad t \to \infty.$$

Consequently, it can be shown

$$W\big(\mathsf{e}^t\big) = t - \mathsf{ln}(t) + \mathsf{o}(\mathsf{ln}(t)) \quad \text{and} \quad \frac{1}{W(\mathsf{e}^t)} = \frac{1}{t} + \frac{\mathsf{ln}(t)}{t^2} + \mathsf{o}\bigg(\frac{\mathsf{ln}(t)}{t^2}\bigg) \quad \text{as} \quad t \to \infty.$$

Hence,

$$\chi_a(t) = \frac{1}{t} + a\,\frac{\mathsf{ln}(t)}{t^2} + \mathsf{o}\bigg(\frac{\mathsf{ln}(t)}{t^2}\bigg) \quad \text{as} \quad t \to \infty.$$

It follows from (12.9) that

$$\liminf_{t\to\infty}\left[x(t) - \frac{1}{t}\right]\left[\frac{t^2}{\mathsf{ln}(t)}\right] \ge \varepsilon \quad \text{and} \quad \limsup_{t\to\infty}\left[x(t) - \frac{1}{t}\right]\left[\frac{t^2}{\mathsf{ln}(t)}\right] \le b.$$

Since c was arbitrary with $\lim\limits_{c\to 0^+} K(c) = 1$ and $\lim\limits_{c\to 0^+} b = \varepsilon$,

$$\lim_{t\to\infty}\left[x(t) - \frac{1}{t}\right]\left[\frac{t^2}{\mathsf{ln}(t)}\right] = \varepsilon.$$

This, once again, gives us Proposition 12.3.

12.2 Bounds on Solutions while in Γ_1

Let $\mathbf{x}(t)$ be the solution of (12.1) with initial condition $\mathbf{x}(0) = \mathbf{x}_0$, where $\mathbf{x}_0 \in \Gamma_1$. We will use differential inequalities to obtain simple bounds on the components of the solution which will be valid for all $t \ge 0$.

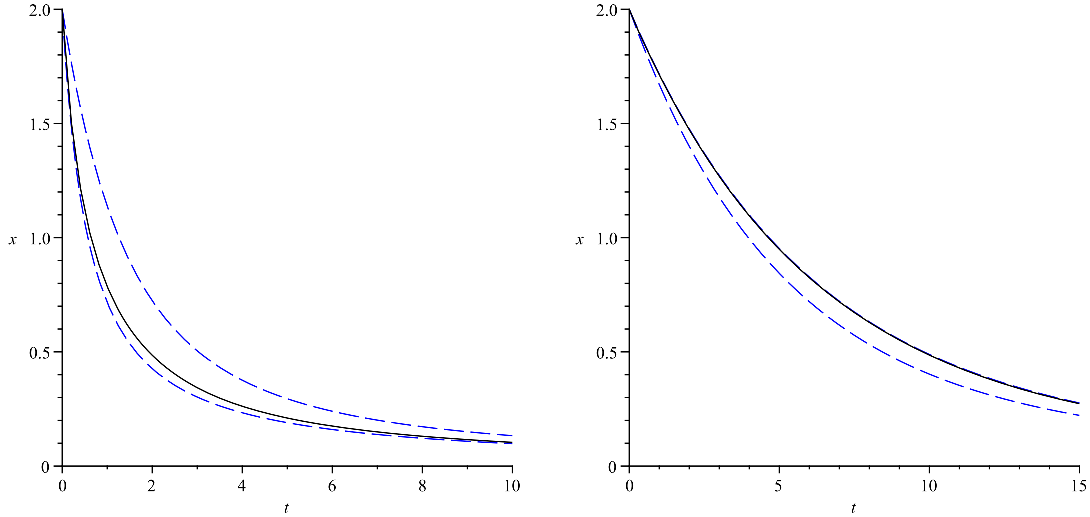

Figure 12.1: For the first picture, suppose $\varepsilon = 0.1$ and $x_0 = 2.0$. The two dashed curves represent the lower and upper bounds for $x(t)$, given in Equation (12.13), while inside Γ_1. The solid curve represents the actual solution (found numerically) with $x(0) = x_0$ and $y(0) = H(x_0)$. The second picture is the same as the first except with $\varepsilon = 5.0$ and $x_0 = 2.0$.

We know from Theorem 11.4 that Γ_1 is positively invariant. Thus,

$$H(x(t)) \leq y(t) \leq \alpha(x(t)) \quad \text{for all} \quad t \geq 0. \tag{12.11}$$

The period of time while a solution is inside Γ_1 (or Γ_0) may be referred to as the "steady-state period" since the solution roughly obeys the QSSA. Using (12.1), (12.2), and (12.11), we see that $x(t)$ satisfies

$$-\frac{x(t)^2}{1+\varepsilon x(t)} \leq \dot{x}(t) \leq -\frac{x(t)^2}{1+(1+\varepsilon)\,x(t)} \quad \text{for all} \quad t \geq 0. \tag{12.12}$$

It follows from the Initial-Value Comparison Theorem in conjunction with Claim A.26 that

$$\chi_\varepsilon(t) \leq x(t) \leq \chi_{1+\varepsilon}(t) \quad \text{for all} \quad t \geq 0,$$

where $\chi_a(t)$ was defined in (12.10). Figure 12.1 demonstrates the bounds on $x(t)$. Furthermore, since both H and α are strictly increasing functions and $y(t)$ satisfies (12.11), we have thus proven the following.

Proposition 12.5: *Let* $\boldsymbol{x}(t)$ *be the solution of* (12.1) *with initial condition* $\boldsymbol{x}(0) = \boldsymbol{x}_0$*, where* $\boldsymbol{x}_0 \in \Gamma_1$*. Then,*

$$\chi_\varepsilon(t) \leq x(t) \leq \chi_{1+\varepsilon}(t) \quad \textit{and} \quad H\left(\chi_\varepsilon(t)\right) \leq y(t) \leq \alpha\left(\chi_{1+\varepsilon}(t)\right) \quad \textit{for all} \quad t \geq 0. \tag{12.13}$$

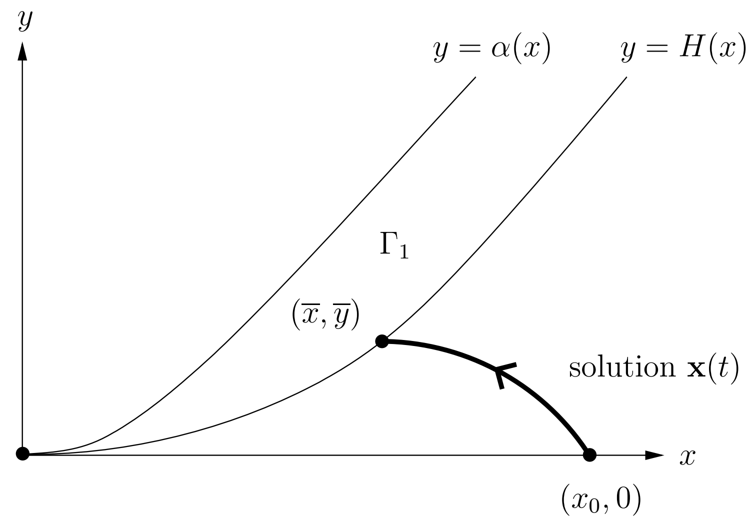

Figure 12.2: Estimating the time it takes for a solution starting at $x(0) = x_0$ and $y(0) = 0$ to enter the antifunnel Γ_1. The solution enters Γ_1 through $(\overline{x}, \overline{y})$ at time $\overline{t}$.

Remark 12.6: Since $0 < x(t) \leq x_0$ for all $t \geq 0$, we can take the inequalities in (12.12) one step further to obtain

$$-x(t)^2 \leq \dot{x}(t) \leq -\frac{x(t)^2}{1 + (1+\varepsilon)\, x_0} \quad \text{for all} \quad t \geq 0.$$

Solving these gives the nicer-looking (yet weaker) bounds

$$\frac{x_0}{1 + x_0 t} \leq x(t) \leq \frac{x_0}{1 + \left[\frac{x_0}{1+(1+\varepsilon)x_0}\right] t} \quad \text{for all} \quad t \geq 0.$$

12.3 Time to Enter Γ_1

Suppose that $x_0 > 0$. Let $\mathbf{x}(t)$ be the solution of (12.1) with $x(0) = x_0$ and $y(0) = 0$. See Figure 12.2. Let $\overline{t} > 0$ be the time it takes for $\mathbf{x}(t)$ to enter Γ_1. Moreover, let $(\overline{x}, \overline{y})$ be the point at which $\mathbf{x}(t)$ enters Γ_1. We want to estimate $\overline{t}$, which equals the length of the "pre-steady-state period," with easily computable bounds.

12.3.1 Bounds on $\overline{t}$ in terms of $\overline{x}$

Since $\mathbf{x}(t)$ starts on the positive x-axis and enters Γ_1 at time $\overline{t}$, we have

$$0 \leq y(t) \leq H(x(t)) \quad \text{for all} \quad t \in \left[0, \overline{t}\right].$$

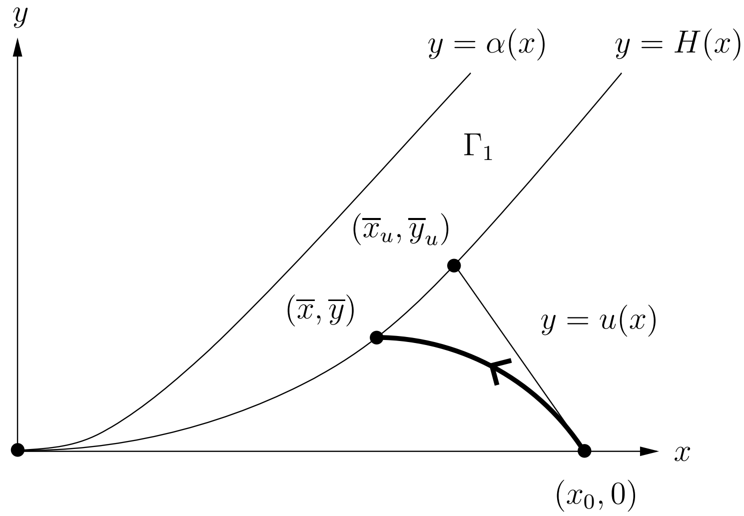

Figure 12.3: The point of intersection $(\overline{x}_u, \overline{y}_u)$ of $y = u(x)$ and $y = H(x)$, where $u(x)$ is the tangent to the scalar solution $y(x)$ at $x = x_0$ and H is the horizontal isocline. Obviously, $\overline{x}_u$ is an upper bound for $\overline{x}$.

Using this in conjunction with (12.1) and (12.2) gives us the differential inequalities

$$-x(t)^2 \leq \dot{x}(t) \leq -\frac{x(t)^2}{1 + \varepsilon x(t)} \quad \text{for all} \qquad \text{for all} \quad t \in \left[0, \overline{t}\right].$$

By inspection,

$$\frac{x_0}{1 + x_0 t} \leq x(t) \leq \chi_\varepsilon(t) \quad \text{for all} \quad t \in \left[0, \overline{t}\right],$$

where $\chi_a(t)$ is given in (12.10). If we set $t = \overline{t}$ and $x(t) = \overline{x}$ then solve for $\overline{t}$, we get

$$\frac{1}{\overline{x}} - \frac{1}{x_0} \leq \overline{t} \leq \left(\frac{1}{\overline{x}} - \frac{1}{x_0}\right) - \varepsilon \ln\left(\frac{\overline{x}}{x_0}\right). \tag{12.14}$$

Since we do not know $\overline{x}$, we need to find bounds on $\overline{x}$ which depend only on ε and x_0.

12.3.2 Upper Bound $\overline{x}_u$ for $\overline{x}$

Let $y(x)$ be the corresponding scalar solution. We will use the tangent line at $x = x_0$ to give us an upper bound for $\overline{x}$. Now, $y(x_0) = 0$ and $y'(x_0) = -1$, the second of which follows from Table 10.1. So, the tangent line to $y(x)$ at $x = x_0$ is

$$u(x) := x_0 - x.$$

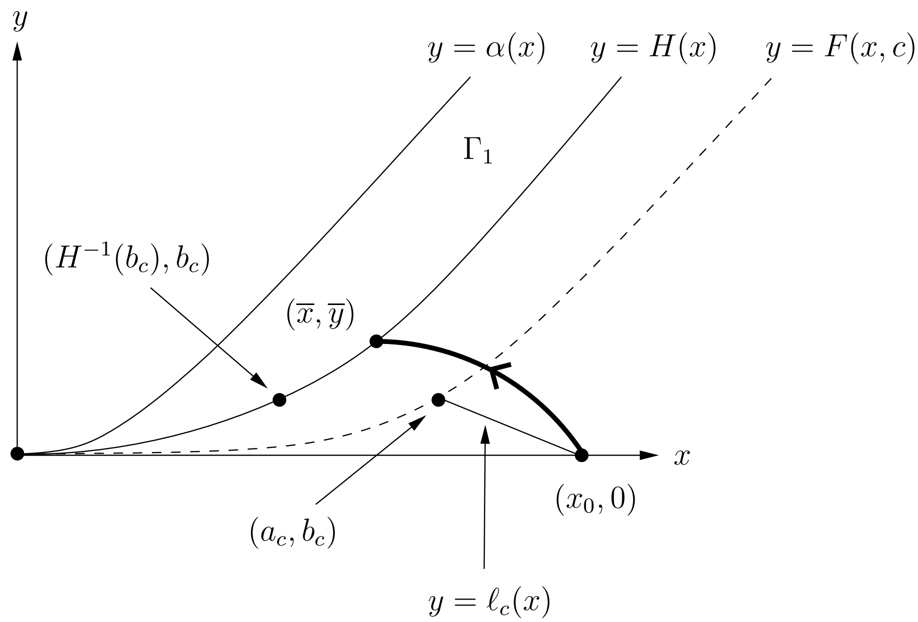

Figure 12.4: This figure depicts a straight-line lower bound $y = \ell_c(x)$, for any $c \in (-1, 0)$, for the solution curve $y = y(x)$. The point (a_c, b_c), where $b_c = \ell_c(a_c)$, is found using the Comparison Theorem and allows us to find lower bounds on $\overline{x}$ and $\overline{y}$. In particular, $\overline{y} \geq b_c$ and $\overline{x} \geq H^{-1}(b_c)$.

This tangent line intersects the horizontal isocline twice (once to the left of the y-axis and once to the right). Let $(\overline{x}_u, \overline{y}_u)$ be the point of intersection which occurs to the right of the y-axis. See Figure 12.3. Thus,

$$\frac{(\overline{x}_u)^2}{1 + \varepsilon \overline{x}_u} = x_0 - \overline{x}_u \quad \text{and} \quad (1 + \varepsilon)(\overline{x}_u)^2 + (1 - x_0\varepsilon)\,\overline{x}_u - x_0 = 0.$$

Solving for the positive root,

$$\overline{x}_u = \frac{(x_0\varepsilon - 1) + \sqrt{(x_0\varepsilon + 1)^2 + 4x_0}}{2(1 + \varepsilon)}. \tag{12.15}$$

We know from Table 11.1 that $y(x)$ is concave down on $[\overline{x}, x_0]$. Thus, $y(x) \leq u(x)$ on $[\overline{x}, x_0]$. Furthermore, the horizontal isocline is strictly increasing. Therefore, we indeed have $\overline{x} \leq \overline{x}_u$ and $\overline{y} \leq \overline{y}_u$.

12.3.3 Lower Bound $\overline{x}_\ell$ for $\overline{x}$

Finding an easily-computable lower bound $\overline{x}_\ell$ for $\overline{x}$ will not be as easy as for the upper bound $\overline{x}_u$. Furthermore, our explicit value of $\overline{x}_\ell$ will not be as pretty as for the Michaelis-Menten mechanism.

Let $y(x)$ be the corresponding scalar solution. We know that $y(x_0) = 0$ and $y'(x_0) = -1$. Now, we want to find a function $\ell(x)$ for which $y(x) \geq \ell(x)$ in some left neighbourhood of x_0. For the Michaelis-Menten mechanism (see §8.3.3), we used a hyperbola. Unfortunately, we will not be able to use a hyperbola here for computational reasons in order to obtain an explicit lower bound on $\overline{x}$. Instead, consider the straight line

$$\ell_c(x) := c\,(x - x_0) \quad \text{for} \quad c \in (-1, 0)\,.$$

Note that $\ell_c(x_0) = 0$ and $\ell_c'(x) = c$ for all $x \in \mathbb{R}$. We would like to find $a_c \in (0, x_0)$ such that $f(x, \ell_c(x)) \leq \ell_c'(x)$ on $[a_c, x_0]$ which, by virtue of the Final-Value Comparison Theorem (see Theorem A.7), implies that $y(x) \geq \ell_c(x)$ on $[a_c, x_0]$.

Consider the isocline for slope c, namely $y = F(x, c)$. Appealing to the isocline structure, $f(x, \ell_c(x)) \leq c$ provided $0 \leq \ell_c(x) \leq F(x, c)$. Thus, we need to solve $F(x, c) = \ell_c(x)$ for x. Specifically, we need to solve

$$\frac{x^2}{K(c) + \varepsilon x} = c\,(x - x_0)\,.$$

Solving for the positive root gives us

$$a_c = \frac{c\,[K(c) - \varepsilon x_0] + \sqrt{c^2\,[K(c) + \varepsilon x_0]^2 - 4cK(c)x_0}}{2\,[1 - \varepsilon c]}.$$

Let $b_c := \ell_c(a_c) = c\,(a_c - x_0)$.

As we can see from Figure 12.4, $\overline{y} \geq b_c$ and $\overline{x} \geq H^{-1}(b_c)$ for any $c \in (-1, 0)$. Note that

$$H^{-1}(y) = \tfrac{1}{2}\left[\varepsilon y + \sqrt{\varepsilon^2 y^2 + 4y}\right].$$

Ideally, we would find the value of c which maximizes b_c. However, we cannot find an explicit, tangible value for c to accomplish this. Note that $\lim\limits_{c \to -1^+} b_c = 0$ and $\lim\limits_{c \to 0^-} b_c = 0$ with $b_c > 0$ for $c \in (-1, 0)$. To obtain a reasonable approximation for the optimal choice of c, consider the tangent lines to b_c at $c = -1$ and $c = 0$. These tangents are given, respectively, by $y = x_0^2\,(c + 1)$ and $y = -x_0 c$. We will take the c-value of the point of intersection of these two tangents, which is

$$c := -\frac{x_0}{1 + x_0}, \tag{12.16}$$

as the value of c to define $\overline{x}_\ell$ and $\overline{y}_\ell$. Figure 12.5 demonstrates two examples of this method. The corresponding straight-line lower bound is given by

$$\ell(x) := -\left(\frac{x_0}{1 + x_0}\right)(x - x_0)\,.$$

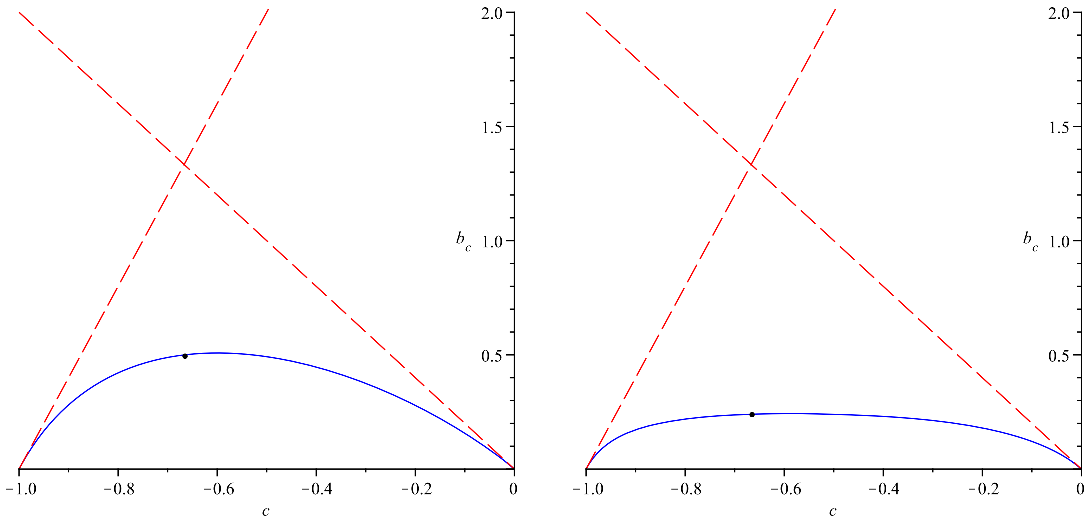

Figure 12.5: For the first picture, suppose $\varepsilon = 0.1$ and $x_0 = 2.0$. The value of b_c is plotted versus c over $(-1, 0)$. The c-value of the intersection point of the tangent lines at $c = -1$ and $c = 0$ gives an approximation of the location of the maximum value of b_c over the interval. The second picture is the same as the first except with $\varepsilon = 5.0$, and $x_0 = 2.0$.

Take

$$a := \frac{c\left[K(c) - \varepsilon x_0\right] + \sqrt{c^2\left[K(c) + \varepsilon x_0\right]^2 - 4cK(c)x_0}}{2\left[1 - \varepsilon c\right]} \quad \text{and} \quad b := \ell(a), \tag{12.17}$$

where c is as in (12.16). Note that, with the value of c given in (12.16), we have $K(c) = 1 + x_0$ and $cK(c) = -x_0$. Therefore, with a and b as in (12.17) we will take

$$\overline{x}_\ell := H^{-1}(b) \quad \text{and} \quad \overline{y}_\ell := b \tag{12.18}$$

as our lower bounds, respectively, for $\overline{x}$ and $\overline{y}$. Figure 12.6 gives two examples of locating the points $(\overline{x}_\ell, \overline{y}_\ell)$ and $(\overline{x}_u, \overline{y}_u)$.

12.3.4 Bounds on $\bar{t}$ in terms of $\overline{x}_\ell$ and $\overline{x}_u$

The goal of this section was to obtain non-trivial bounds on the time $\bar{t}$ it takes for the solution $\mathbf{x}(t)$ to enter the antifunnel Γ_1. In (12.14), we stated bounds on $\bar{t}$ in terms of $\overline{x}$, which is the x-value of the point of entry of $\mathbf{x}(t)$ into Γ_1. Observe that the expressions on the left and right of (12.14) are both strictly decreasing functions of $\overline{x}$. Since we have bounds on $\overline{x}$, namely $\overline{x}_\ell \leq \overline{x} \leq \overline{x}_u$, we have thus proven the following.

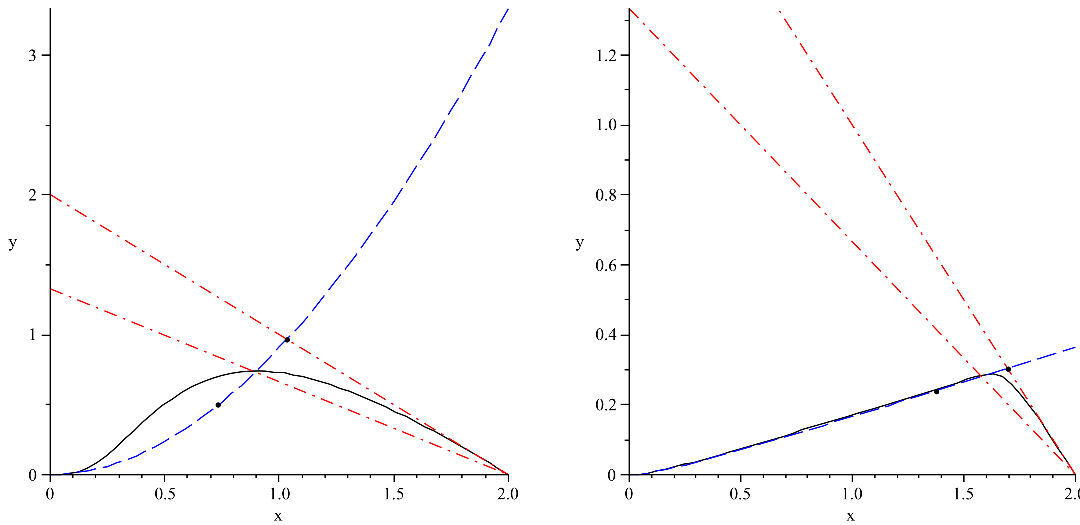

Figure 12.6: For the first picture, suppose $\varepsilon = 0.1$ and $x_0 = 2.0$. The actual solution (solid line) and horizontal isocline (dashed line, the quasi-steady-state approximation) are shown. Also shown are the straight line $y = \ell(x)$ (left dash-dot line) and tangent line $y = x_0 - x$ (right dash-dot line). The points $(\overline{x}_\ell, \overline{y}_\ell)$ and $(\overline{x}_u, \overline{y}_u)$ are indicated by the solid circles. The second picture is the same as the first except with $\varepsilon = 5.0$, and $x_0 = 2.0$.

Proposition 12.7: *Suppose that $x_0 > 0$. Let $\boldsymbol{x}(t)$ be the solution of* (12.1) *with $x(0) = x_0$ and $y(0) = 0$. If $\overline{t}$ is the time it takes for $\boldsymbol{x}(t)$ to enter Γ_1, then*

$$\frac{1}{\overline{x}_u} - \frac{1}{x_0} \leq \overline{t} \leq \frac{1}{\overline{x}_\ell} - \frac{1}{x_0} - \varepsilon \, ln\left(\frac{\overline{x}_\ell}{x_0}\right), \tag{12.19}$$

where $\overline{x}_\ell$ is given in (12.18) *and $\overline{x}_u$ is given in* (12.15).

Define

$$\overline{t}_\ell := \frac{1}{\overline{x}_u} - \frac{1}{x_0} \quad \text{and} \quad \overline{t}_u := \frac{1}{\overline{x}_\ell} - \frac{1}{x_0} - \varepsilon \ln\left(\frac{\overline{x}_\ell}{x_0}\right) \tag{12.20}$$

which are the lower and upper bounds for $\overline{t}$. Figure 12.7 gives two examples of using (12.19) to find bounds on $\overline{t}$.

Remark 12.8: If we choose $\varepsilon = 0$ and $x_0 = 2.0$ then (12.20) gives us $\overline{t}_\ell = 0.5$ and $\overline{t}_u \approx 0.901$. That is, $\lim\limits_{\varepsilon \to 0^+} \overline{t} \neq 0$. Recall that the limit was always zero for the Michaelis-Menten mechanism.

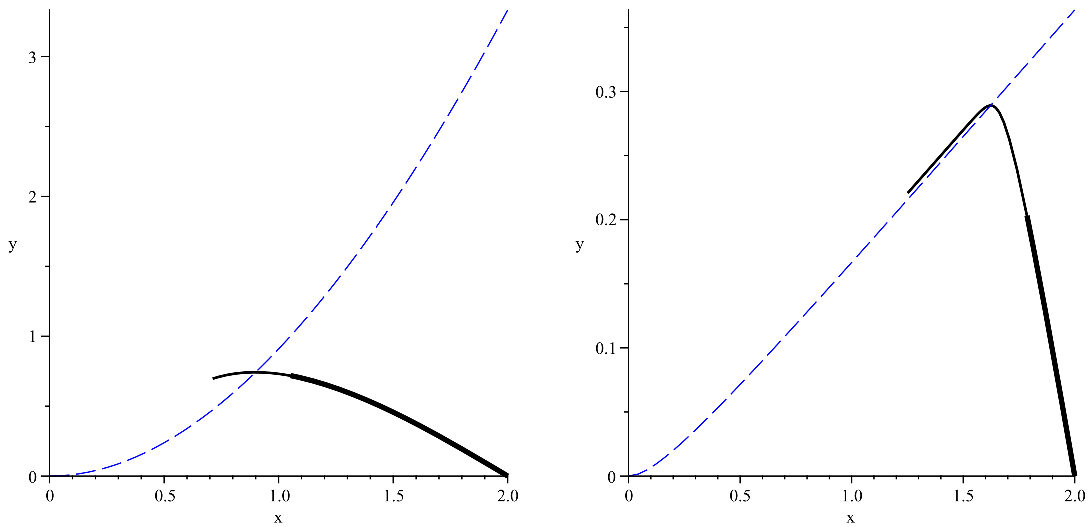

Figure 12.7: For the first picture, suppose $\varepsilon = 0.1$ and $x_0 = 2.0$. With these values, we can calculate the bounds on $\bar{t}$ (the time it takes for the solution to cross the horizontal isocline) to be $\bar{t}_\ell \approx 0.468$ and $\bar{t}_u \approx 0.966$ using (12.15), (12.18), and (12.20). The actual solution (solid line) and horizontal isocline (dashed line) are shown. The thick portion of the solution corresponds to $t \in [0, \bar{t}_\ell]$ and the thin portion of the solution corresponds to $t \in [\bar{t}_\ell, \bar{t}_u]$. Indeed, $\bar{t} \in [\bar{t}_\ell, \bar{t}_u]$. The second picture is the same as the first except with $\varepsilon = 5.0$, and $x_0 = 2.0$. The lower and upper bounds for $\bar{t}$ respectively are $\bar{t}_\ell \approx 0.0895$ and $\bar{t}_u \approx 2.10$.

12.4 Summary

The purpose of this chapter was to develop some basic time estimates for solutions $\mathbf{x}(t)$, with initial condition $\mathbf{x}_0$, to the planar system which arises from the Lindemann mechanism. This system, recall, is given by

$$\dot{x} = -x^2 + \varepsilon xy, \quad \dot{y} = -y + x^2 - \varepsilon xy.$$

First, we used two methods (integration of asymptotic expansions and differential inequalities) in conjunction with properties we have developed in this thesis to establish the long-term asymptotic behaviour of $\mathbf{x}(t)$ when $\mathbf{x}_0 \in \Gamma_0$, where

$$\Gamma_0 = \{\ (x, y)\ :\ x > 0,\ H(x) \le y \le V(x)\ \}$$

with H being the horizontal isocline and V being the vertical isocline. In particular, we showed

$$x(t) = \frac{1}{t} + \varepsilon\,\frac{\ln(t)}{t^2} + \mathsf{o}\left(\frac{\ln(t)}{t^2}\right) \quad \text{and} \quad y(t) = \frac{1}{t^2} + 2\varepsilon\,\frac{\ln(t)}{t^3} + \mathsf{o}\left(\frac{\ln(t)}{t^3}\right) \quad \text{as} \quad t \to \infty.$$

Second, we obtained bounds on the solution if $\mathbf{x}_0 \in \Gamma_1$, where

$$\Gamma_1 = \{\ (x, y)\ :\ x > 0,\ H(x) \le y \le \alpha(x)\ \}$$

with α being the isocline for slope ε^{-1} (the slope of the slow manifold at infinity). Specifically,

$$\chi_\varepsilon(t) \le x(t) \le \chi_{1+\varepsilon}(t) \quad \text{and} \quad H\left(\chi_\varepsilon(t)\right) \le y(t) \le \alpha\left(\chi_{1+\varepsilon}(t)\right) \quad \text{for all} \quad t \ge 0,$$

where

$$\chi_a(t) = \frac{1}{a\, W\left(\left[\frac{1}{ax_0}\,\mathsf{exp}\left(\frac{1}{ax_0}\right)\right]\mathsf{exp}\left(\frac{1}{a}\,t\right)\right)} \quad \text{for} \quad a > 0.$$

Note that $W(x)$ is the Lambert W function. Alternatively, we showed that

$$\frac{x_0}{1 + x_0 t} \le x(t) \le \frac{x_0}{1 + \left[\frac{x_0}{1+(1+\varepsilon)x_0}\right] t} \quad \text{for all} \quad t \ge 0.$$

Finally, we found lower and upper bounds on the time $\overline{t}$ for the solution to enter Γ_1 (which it does through the point $(\overline{x}, \overline{y})$) when the initial condition is on the positive x-axis. In particular, using the Comparison Theorem and other tricks we showed that

$$\frac{1}{\overline{x}_u} - \frac{1}{x_0} \le \overline{t} \le \frac{1}{\overline{x}_\ell} - \frac{1}{x_0} - \varepsilon\,\mathsf{ln}\left(\frac{\overline{x}_\ell}{x_0}\right)$$

are lower and upper bounds on $\overline{t}$, where

$$\overline{x}_\ell = H^{-1}(b) \quad \text{and} \quad \overline{x}_u = \frac{(x_0\varepsilon - 1) + \sqrt{(x_0\varepsilon + 1)^2 + 4x_0}}{2\,(1+\varepsilon)}$$

and b is defined in (12.17).

Chapter 13

Modifications to the Lindemann Mechanism

The standard (nonlinear) Lindemann mechanism of unimolecular decay is

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \xrightarrow{k_2} P, \tag{13.1}$$

where A is the molecule that decays, B is the activated complex, and P is the product of the decay. In this chapter, we mention some possible alterations to this basic scheme. The techniques we have employed throughout this thesis can be adapted to these alterations.

13.1 Linear Lindemann Mechanism

13.1.1 The Model and Differential Equations

In the Linear Lindemann mechanism, the decaying molecule is activated by a collision with a different chemical species. Symbolically,

$$A + M \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B + M, \quad B \xrightarrow{k_2} P,$$

where M is the other chemical species. The Law of Mass Action gives us the ordinary differential equations

$$\begin{aligned}
\dot{a} &= k_{-1}bm - k_1 am, \\
\dot{m} &= 0, \\
\dot{b} &= k_1 am - k_{-1}bm - k_2 b, \\
\dot{p} &= k_2 b,
\end{aligned}$$

where $\dot{} = \frac{d}{dt}$. The traditional initial conditions are $a(0) = a_0$, $m(0) = m_0$, $b(0) = 0$, and $p(0) = 0$. However, we will consider the initial conditions to be arbitrary. It is apparent from the differential equations that

$$m(t) \equiv m_0 \quad \text{and} \quad a(t) + b(t) + p(t) \equiv a_0,$$

the second of which is the conservation law (10.3) for the standard Lindemann mechanism. Note that we use the constant a_0 since, traditionally, B and P are not initially present.

13.1.2 Reduction and Re-scaling

Since $m(t)$ is constant and $p(t)$ does not affect $a(t)$ and $b(t)$, we are left with the linear planar system

$$\dot{a} = -\left(k_1 m_0\right) a + \left(k_{-1} m_0\right) b, \quad \dot{b} = \left(k_1 m_0\right) a - \left(k_{-1} m_0 + k_2\right) b.$$

The dimensions of the quantities in the planar system are

$$[a, b, m_0] = \frac{Q}{L^3}, \quad \left[\dot{a}, \dot{b}\right] = \frac{Q}{L^3 T}, \quad [k_2] = \frac{1}{T}, \quad \text{and} \quad [k_{-1}, k_1] = \frac{L^3}{QT}.$$

If we define

$$\tau := k_1 m_0 t, \quad x := \left(\frac{k_1}{k_2}\right) a, \quad y := \left(\frac{k_1}{k_2}\right) b, \quad \varepsilon := \frac{k_{-1}}{k_1}, \quad \text{and} \quad \eta := \frac{k_2}{k_1 m_0},$$

which are all dimensionless, we obtain the system

$$x' = -x + \varepsilon y, \quad y' = x - (\varepsilon + \eta)\, y, \tag{13.2}$$

where $' = \frac{d}{d\tau}$. See Figure 13.1, which clearly suggests the existence of a trapping region and a slow manifold.

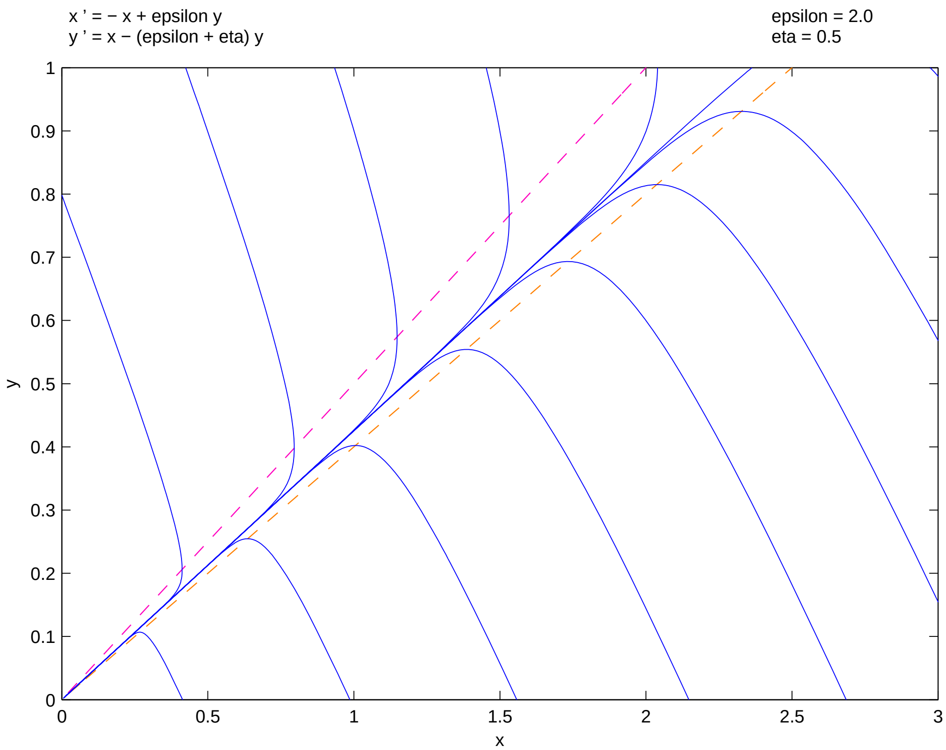

Figure 13.1: A phase portrait for (13.2) for $\varepsilon = 2.0$ and $\eta = 0.5$.

13.1.3 The Slow Manifold

Define the matrix

$$\mathbf{A} := \begin{pmatrix} -1 & \varepsilon \\ 1 & -\varepsilon - \eta \end{pmatrix}.$$

Then, the system (13.2) can be written $\mathbf{x}' = \mathbf{A}\mathbf{x}$. It is easy to show that $\mathbf{A}$ has eigenvalues and associated eigenvectors given by

$$\lambda_\pm := \tfrac{1}{2}\left[-(\varepsilon + \eta + 1) \pm \sqrt{(\varepsilon + \eta + 1)^2 - 4\eta}\right] \quad \text{and} \quad \mathbf{v}_\pm := \begin{pmatrix} \varepsilon \\ \lambda_\pm + 1 \end{pmatrix}.$$

Observe that the eigenvalues are both negative and distinct. If we let

$$\sigma := \frac{\lambda_+ + 1}{\varepsilon}$$

denote the slope of the slow eigenvector $\mathbf{v}_+$, we see that $\mathcal{M}(x) := \sigma x$ is the slow manifold. Moreover, for initial conditions $x(0) = x_0$ and $y(0) = \sigma x_0$ (that is, the initial condition is on the slow manifold), (13.2) can be easily solved to give

$$x(\tau) = x_0 \mathrm{e}^{\lambda_+ \tau} \quad \text{and} \quad y(\tau) = \sigma x_0 \mathrm{e}^{\lambda_+ \tau}.$$

13.2 Continuous Removal of the Decaying Molecule

13.2.1 The Model and Differential Equations

Suppose that, in (13.1), the decaying molecule is continuously removed from the reaction (perhaps to save as much of it as possible before it all decays). Symbolically,

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A + B, \quad B \overset{k_2}{\to} P, \quad A \overset{k_3}{\to} 0.$$

The Law of Mass Action gives us the system

$$\begin{aligned}
\dot{a} &= k_{-1}ab - k_1 a^2 - k_3 a, \\
\dot{b} &= k_1 a^2 - k_{-1}ab - k_2 b, \\
\dot{p} &= k_2 b.
\end{aligned}$$

13.2.2 Reduction and Re-scaling

Note that the reaction-rate constant k_3 has dimensions $[k_3] = T^{-1}$. Note also that the third differential equation has no bearing on the first two. Define the dimensionless variables

$$\tau := k_2 t, \quad x := \left(\frac{k_1}{k_2}\right) a, \quad y := \left(\frac{k_1}{k_2}\right) b, \quad \varepsilon := \frac{k_{-1}}{k_1}, \quad \text{and} \quad \delta := \frac{k_3}{k_2}.$$

All of these, except for δ, are exactly the ones we used for the standard Lindemann mechanism (13.1). It is easy to verify that we are left with the planar system

$$x' = -\delta x - x^2 + \varepsilon xy, \quad y' = x^2 - y - \varepsilon xy, \tag{13.3}$$

where $' = \frac{d}{d\tau}$. See Figure 13.2, which clearly suggests the existence of a trapping region and a slow manifold. Observe that the vertical isocline of (13.3) does not pass through the origin.

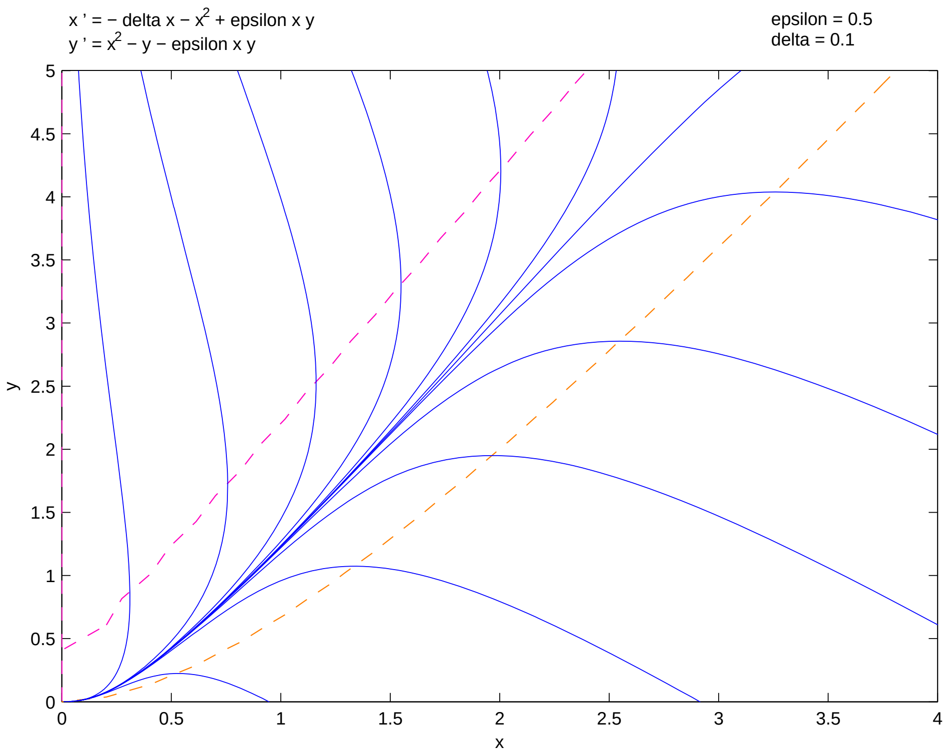

Figure 13.2: A phase portrait for (13.3) for $\varepsilon = 0.5$ and $\delta = 0.1$.

Remark 13.1: The origin is a sink for the system (13.3) and thus the material of Part I can be applied. This model, which the author of this thesis has not seen in the literature, was proposed merely as a potential means of proving Theorem 11.26. To be more specific, the ratio of the eigenvalues for the system (13.3) is $\kappa = \frac{1}{\delta}$. Thus, as $\delta \to 0^+$ we have $\kappa \to \infty$ and the system (13.3) reduces to the standard planar system for the Lindemann mechanism. It is suggested by Theorems 2.16 and 5.28 that, as $\kappa \to \infty$, we obtain a Taylor series for any scalar solution $y(x)$ at the origin for the standard Lindemann mechanism.

Part IV

Open Questions and Appendices

Chapter 14

Open Questions

In this final chapter, we will mention some open problems. To be more specific, these open problems include results that could be improved, areas that could be explored further, and questions that have arisen which have not be fully answered. References to the appropriate location in the thesis, when applicable, will be given to serve as a setup of the issue at hand.

- In Chapter 4, which dealt with the case of closely-spaced eigenvalues, we proved two smoothness results for the transformation $\boldsymbol{\psi}$ (see Propositions 4.17 and 4.19). Suppose that $\mathbf{b}$ is C^r in a neighbourhood of the origin. It seems plausible, with modest additional assumptions on $\mathbf{b}$, that $\boldsymbol{\psi}$ is C^r in a neighbourhood of the origin.

- In Chapter 4, which dealt with the case of closely-spaced eigenvalues, we derived a simple conjugacy result (Theorem 4.15) for the function $\boldsymbol{\psi}(\mathbf{x}_0)$. Moreover, the iterates (of the first type) had a nice semi-group property (Lemma 4.22) which allowed us to construct iterates (of the third type) which were flows. Unfortunately, the iterates for the case of widely-spaced eigenvalues, covered in Chapter 5, resisted all attempts at similar results (which are desired).

- For Chapter 5, the general case of widely-spaced eigenvalues when $\mathbf{A} \in \mathbb{R}^n$ is Hurwitz with Jordan canonical form $\mathbf{J}$ has not yet been worked out in detail. See §5.8.

- A result of Segel and Slemrod, in [112], could be improved. There, they only have bounds on the QSSA for finite time intervals. It should be possible to extend this to include time intervals of infinite length.

- In his book [62], Hoppensteadt uses a so-called QSSA Theorem that gives an error bound between a solution of the planar system for the Michaelis-Menten mechanism and the quasi-steady-state approximation which results from a matched asymptotic expansion. This error is $\mathcal{O}(\varepsilon)$ for time intervals of infinite length. It should be possible to improve this to include errors of the form $\mathcal{O}\big(\varepsilon\, \mathsf{e}^{-\mu t}\big)$ for some $\mu > 0$.

- The use of Padé approximants (see for example [6]) may yield a useful approximation of the slow manifold $\mathcal{M}(x)$. For the Michaelis-Menten mechanism, Proposition 7.45 gives us the asymptotic expression

$$\mathcal{M}(x) = \sum_{n=1}^{\ell} \sigma_n x^n + \mathsf{o}\Big(x^{\ell}\Big) \quad \text{as} \quad x \to 0^+,$$

  where ℓ is the largest integer strictly less than κ. We could then construct a Padé approximant $p_{[m/n]}(x)$, where $m, n \in \mathbb{N}_0$ and $m + n = \ell$. It would interesting to see how well $p_{[m/n]}(x)$ approximates $\mathcal{M}(x)$ over the semi-infinite interval $[0, \infty)$ in the different regimes ε small, ε large, and ε intermediate.

- Consider the Michaelis-Menten mechanism. For sufficiently small $\varepsilon > 0$, geometric singular perturbation theory (in particular Fenichel's Theorem) has been applied to give a slow invariant manifold $\mathcal{M}_\varepsilon$ within distance $\mathcal{O}(\varepsilon)$ of the quasi-steady-state manifold $\mathcal{M}_0$ (which is normally hyperbolic). See, for example, [40, 67, 126]. Moreover, there are perturbed local stable and unstable manifolds of $\mathcal{M}_\varepsilon$ which are the unions of invariant families of, respectively, stable and unstable fibers. It would be nice to have similar results which are valid for intermediate and large ε.

- In §8.3 which begins on page 213, we obtained crude but non-trivial bounds on the length $\bar{t}$ of the pre-steady-state period for the Michaelis-Menten mechanism. We showed that $\lim\limits_{\varepsilon \to 0^+} \bar{t} = 0$. However, it would be nice to have the leading-order behaviour in ε of $\bar{t}$.

- In §9.1, we noted that the Michaelis-Menten and Henri mechanisms yield the same planar reduction. There are a number of techniques in the literature for the kinetic distinguishing of these mechanisms. It would be nice if we could distinguish the mechanisms using a result or technique from this thesis.

- We concluded §9.3 with a conjecture. In particular, we claim that the three-dimensional reduction of the Michaelis-Menten mechanism with competitive inhibition has a trapping region, with boundaries given by the isoclines, containing a unique solution.

- In Proposition 12.3, which is in §12.1 that begins on page 281, we give asymptotic expressions for $x(t)$ and $y(t)$ as $t \to \infty$. Here, $(x(t), y(t))$ is a solution of the planar system for the Lindemann mechanism. It would be nice to add more terms to these asymptotic expressions. More specifically, we would like to obtain the lowest-order term which depends on the initial conditions.

- In §12.3 which begins on page 287, we obtained crude but non-trivial bounds on the length $\overline{t}$ of the pre-steady-state period for the Lindemann mechanism. We did not, however, give a value of $\lim\limits_{\varepsilon \to 0^+} \overline{t}$. (The limit, if it exists, would be strictly positive and would likely be messy or impossible to give explicitly.) Moreover, it would be nice to have the leading-order behaviour in ε of $\overline{t}$.

  When $\varepsilon = 0$, the dimensionless planar system for the Lindemann mechanism is

  $$\dot{x} = -x^2, \quad \dot{y} = -y + x^2,$$

  where $\dot{} = \frac{d}{dt}$. With initial conditions $x(0) = x_0$ and $y(0) = 0$, this can be solved yielding

  $$x(t) = \frac{x_0}{1 + x_0 t}, \quad y(t) = x_0^2 \, \mathsf{e}^{-t} \int_0^t \frac{\mathsf{e}^{-s}}{(1 + x_0 s)^2} \, ds.$$

  Note that $y(t)$ can be written in terms of exponential integrals. Finding the length of the pre-steady-state period amounts to solving $y(\overline{t}) = x(\overline{t})^2$ for $\overline{t}$ (which is unique and strictly positive).

Appendix A

Review Material

This chapter consists of a review of important results and concepts that are employed throughout this thesis. The presentation is cold and concise with the goal being to mention only what is needed.

A.1 Law of Mass Action

Suppose that a sequence of m simultaneous chemical reactions involving n chemical species is occurring. Symbolically,

$$\sum_{j=1}^{n} a_{ij} X_j \xrightarrow{k_i} \sum_{j=1}^{n} b_{ij} X_j \quad (i \in I)\,,$$

where $I := \{1, \ldots, m\}$. If we let $J := \{1, \ldots, n\}$, then $\{X_j\}_{j \in J}$ are the chemical species involved in the reactions, $\{k_i\}_{i \in I}$ are the reaction-rate constants, and $\{a_{ij}, b_{ij}\}_{(i,j) \in I \times J}$ are the stoichiometric coefficients. If we denote the concentration of X_j at time t by $x_j(t)$, the Law of Mass Action says that

$$\dot{x}_j = \sum_{i=1}^{m} (b_{ij} - a_{ij})\, k_i \prod_{\ell=1}^{n} x_\ell^{a_{i\ell}} \quad (j \in J)\,,$$

where $\dot{} = \frac{d}{dt}$. The Law of Mass Action is standard and can be found, for example, in [39] and [122].

This "law" is not generally valid at very high or very low concentrations. It is derived using statistical methods and is based on the idea that reaction rates are determined by the probability of collisions involving reactants.

A.2 Asymptotics

This thesis deals with many asymptotics results. For good references on general asymptotics, see for example [10, 19, 38, 97].

Definition A.1: Let f and g be two functions defined in a neighbourhood of $x = a$. (If $a = \infty$, then f and g are defined for sufficiently large x.)

(a) Suppose that there are $\delta, k > 0$ such that $|f(x)| \leq k\,|g(x)|$ for all $x \in (a - \delta, a + \delta)$. (If $a = \infty$, then suppose that there are $X, k > 0$ such that $|f(x)| \leq k\,|g(x)|$ for all $x > X$.) Then, $f(x)$ is *big-oh* of $g(x)$ as $x \to a$. This is written $f(x) = \mathcal{O}(g(x))$ as $x \to a$.

(b) Suppose that $\lim_{x \to a} \dfrac{f(x)}{g(x)} = 0$. Then, $f(x)$ is *little-oh* of $g(x)$ as $x \to a$. This is written $f(x) = \mathsf{o}(g(x))$ as $x \to a$.

(c) Suppose that $\lim_{x \to a} \dfrac{f(x)}{g(x)} = 1$. Then, $f(x)$ is asymptotic to $g(x)$ as $x \to a$. This is written $f(x) \sim g(x)$ as $x \to a$. Observe that[1] $f(x) = g(x) + \mathsf{o}(g(x))$ as $x \to a$ is equivalent to $f(x) \sim g(x)$ as $x \to a$.

(d) Suppose that there are functions $\{\varphi_n\}_{n=0}^{\infty}$ such that $f(x) = \sum_{n=0}^{m} b_n \varphi_n(x) + \mathsf{o}(\varphi_m(x))$ as $x \to a$ for each m. Then, $f(x)$ has *asymptotic series* (or *asymptotic expansion*) $\sum_{n=0}^{\infty} b_n \varphi_n(x)$. This is written $f(x) \sim \sum_{n=0}^{\infty} b_n \varphi_n(x)$ as $x \to a$.

Remark A.2: There are many interesting and counter-intuitive facts related to asymptotics.

(i) If $f(x) \sim g(x)$ as $x \to a$ it does not follow that $f(x) - g(x) = \mathsf{o}(1)$ as $x \to a$ (that is the difference tends to zero). For a counter-example, consider $f(x) := \mathsf{e}^x$ and $g(x) := \mathsf{e}^x + x$ as $x \to \infty$.

(ii) If $f(x) = \mathsf{o}(x)$ as $x \to 0^+$ it does not follow that $f(x) = \mathcal{O}(x^r)$ as $x \to 0^+$ for some $r > 1$. For a counter-example, consider $f(x) := \dfrac{x}{\ln x}$.

(iii) Using $\varphi_n(x) := x^{-n}$, the asymptotic series for e^{-x} as $x \to \infty$ is the zero series. Note that, in general, if f has an asymptotic series as $x \to a$ in terms of $\{\varphi_n\}_{n=0}^{\infty}$, then it is unique.

[1] By $f(x) = g(x) + \mathsf{o}(g(x))$ as $x \to a$ we mean $f(x) - g(x) = \mathsf{o}(g(x))$ as $x \to a$.

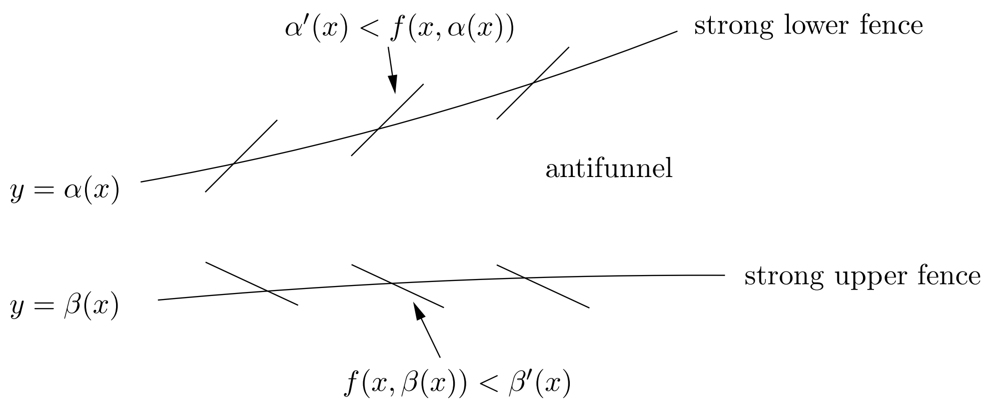

Figure A.1: An antifunnel. The defining characteristic is that solutions have greater slope along α than α itself and smaller slope along β than β itself.

A.3 Antifunnel Theorem

A good reference for antifunnels (as well as funnels) is Chapter 1 and 4 of [64]. The standard Antifunnel Theorem can be found on pages 31–33 and an Alternate Antifunnel Theorem can be found on page 196. The Ważewski method, which is covered for example in the survey article [119], can be viewed as a generalization of the funnel/antifunnel method.

Definition A.3: Let I be an interval with end points a and b (with $a < b$) and consider the scalar differential equation $y' = f(x, y)$ over I.

(a) The curve $\alpha \in C^1(I)$ is a *lower fence* if $\alpha'(x) \le f(x, \alpha(x))$ for all $x \in I$. If there is always a strict inequality, the fence is *strong*. Otherwise, the fence is *weak*.

(b) The curve $\beta \in C^1(I)$ is an *upper fence* if $f(x, \beta(x)) \le \beta'(x)$ for all $x \in I$. If there is always a strict inequality, the fence is *strong*. Otherwise, the fence is *weak*.

(c) Let α and β be, respectively, strong lower and upper fences. If $\beta(x) < \alpha(x)$ on I, then the set

$$\Gamma := \{ \ (x, y) \ : \ x \in I, \ \beta(x) \le y \le \alpha(x) \ \}$$

is called an *antifunnel*. Moreover, if $\lim_{x \to b^-} |\alpha(x) - \beta(x)| = 0$ then Γ is *narrowing*.

Theorem A.4 (Antifunnel Theorem): *Let Γ be an antifunnel with strong lower and upper fences α and β, respectively, for the differential equation $y' = f(x, y)$ over the interval I. Then,* *there exists a solution $y(x)$ to the differential equation such that $(x, y(x)) \in \Gamma$ for all $x \in I$. If, in addition, Γ is narrowing and $\frac{\partial f}{\partial y}(x, y) \geq 0$ in Γ, then the solution $y(x)$ is unique.*

Theorem A.5 (Alternate Antifunnel Theorem): *Let Γ be an antifunnel with strong lower and upper fences α and β, respectively, for the differential equation $y' = f(x, y)$ over the interval I, where $I = [a, \infty)$ or $I = (a, \infty)$. Suppose that there is a function r such that*

$$r(x) < \frac{\partial f}{\partial y}(x, y) \quad \text{for all} \quad (x, y) \in \Gamma \quad \text{and} \quad \lim_{x \to \infty} \frac{\alpha(x) - \beta(x)}{\exp\left(\int_a^x r(s)\, ds\right)} = 0.$$

Then, there exists a unique solution $y(x)$ to the differential equation such that $(x, y(x)) \in \Gamma$ for all $x \in I$.

Proof: This result was presented as an exercise in [64] and so we will provide an abbreviated proof for the case $I = [a, \infty)$. Note that if $I = (a, \infty)$ then we could consider the interval $I = [c, \infty)$, where $c > a$, and let $c \to a^+$. Existence is guaranteed by the first Antifunnel Theorem. To prove uniqueness, suppose on the contrary that $y_1(x)$ and $y_2(x)$ are distinct solutions with $y_2(x) > y_1(x)$ for all $x \in I$. Let $u(x) := y_2(x) - y_1(x)$ which, in particular, satisfies $u(a) > 0$. Now, for any $x \in I$ we have

$$u'(x) = f(x, y_2(x)) - f(x, y_1(x)) = \int_{y_1(x)}^{y_2(x)} \frac{\partial f}{\partial y}(x, s)\, ds \geq r(x)u(x).$$

Solving the differential inequality $u'(x) \geq r(x)u(x)$ yields

$$u(x) \geq u(a) \exp\left(\int_a^x r(s)\, ds\right) \quad \text{for all} \quad x \in I.$$

Observe that

$$u(a) \leq \frac{u(x)}{\exp\left(\int_a^x r(s)\, ds\right)} \leq \frac{\alpha(x) - \beta(x)}{\exp\left(\int_a^x r(s)\, ds\right)} \quad \text{for all} \quad x \in I.$$

Using the limit in the statement of the theorem gives us the contradiction $u(a) \leq 0$. ☐

A.4 Comparison Theorems

The comparison method, which is covered for example in Chapter 1 of [74], Chapter II of [123], and §II.9 of [124], has obvious similarities to the material we discussed regarding antifunnels. Certain versions, perhaps the simplest, of standard comparison results are given below.

Theorem A.6 (Initial-Value Comparison Theorem): *Let $I := [a, b]$ be a given interval, where $b > a$, and let $f \in C^1(I \times \mathbb{R}, \mathbb{R})$ be a given function. Let $y \in C^1(I, \mathbb{R})$ satisfy $y' = f(x, y)$ on I and $y(a) = y_0$.*

(a) Let $\ell \in C^1(I \times \mathbb{R}, \mathbb{R})$ *satisfy* $\ell'(x) \leq f(x, \ell(x))$ *on* I *and* $\ell(a) = y_0$*. Then,* $y(x) \geq \ell(x)$ *on* I*.*

(b) Let $u \in C^1(I \times \mathbb{R}, \mathbb{R})$ *satisfy* $u'(x) \geq f(x, u(x))$ *on* I *and* $u(a) = y_0$*. Then,* $y(x) \leq u(x)$ *on* I*.*

Theorem A.7 (Final-Value Comparison Theorem): *Let* $I := [a, b]$ *be a given interval, where* $b > a$*, and let* $f \in C^1(I \times \mathbb{R}, \mathbb{R})$ *be a given function. Let* $y \in C^1(I, \mathbb{R})$ *satisfy* $y' = f(x, y)$ *on* I *and* $y(b) = y_0$*.*

(a) Let $\ell \in C^1(I \times \mathbb{R}, \mathbb{R})$ *satisfy* $\ell'(x) \geq f(x, \ell(x))$ *on* I *and* $\ell(b) = y_0$*. Then,* $y(x) \geq \ell(x)$ *on* I*.*

(b) Let $u \in C^1(I \times \mathbb{R}, \mathbb{R})$ *satisfy* $u'(x) \leq f(x, u(x))$ *on* I *and* $u(b) = y_0$*. Then,* $y(x) \leq u(x)$ *on* I*.*

A.5 Chaplygin's Method

Chaplygin's method, which can be found for example in §1.3 of [89], is very useful in conjunction with the Comparison Theorem. Let $I := [a, b]$ be an interval and let $f \in C^2\big(\mathbb{R}^2, \mathbb{R}\big)$ be a function. Let $\ell, u \in C(I, \mathbb{R})$ be two further functions that satisfy $\ell(x) \leq u(x)$ on I. Suppose that $x \in I$ is fixed and consider the curve $z = f(x, y)$ over the interval $J_x := [\ell(x), u(x)]$. If $\frac{\partial^2 f}{\partial y^2}(x, y) \geq 0$ on J_x then the curve $z = f(x, y)$ over J_x is below the secant through the points $(\ell(x), f(x, \ell(x)))$ and $(u(x), f(x, u(x)))$. Furthermore, the curve $z = f(x, y)$ over J_x is above the tangent line at the point $(\ell(x), f(x, \ell(x)))$. Therefore, for any $y \in J_x$ we have[2]

$$f(x, \ell(x)) + \frac{\partial f}{\partial y}(x, \ell(x))\,[y - \ell(x)] \leq f(x, y) \leq f(x, \ell(x)) + \left[\frac{f(x, u(x)) - f(x, \ell(x))}{u(x) - \ell(x)}\right][y - \ell(x)]\,.$$

Similarly, if $\frac{\partial^2 f}{\partial y^2}(x, y) \leq 0$ on J_x then

$$f(x, \ell(x)) + \left[\frac{f(x, u(x)) - f(x, \ell(x))}{u(x) - \ell(x)}\right][y - \ell(x)] \leq f(x, y) \leq f(x, \ell(x)) + \frac{\partial f}{\partial y}(x, \ell(x))\,[y - \ell(x)]$$

for any $y \in J_x$.

[2] Alternatively, we could use $(u(x), f(x, u(x)))$ as the point of tangency and replace

$$f(x, \ell(x)) + \frac{\partial f}{\partial y}(x, \ell(x))\,[y - \ell(x)] \quad \text{with} \quad f(x, u(x)) + \frac{\partial f}{\partial y}(x, u(x))\,[y - u(x)]\,.$$

A.6 Gronwall's Inequality

Gronwall's Inequality, and its generalization Bihari's Inequality, are very important in differential equations. See, for example, [12, 51, 100].

Lemma A.8 (Gronwall's Inequality): *Let $c \geq 0$ be a constant and let $f, g \in [a,b] \to \mathbb{R}$ be continuous, non-negative functions. If*

$$f(x) \leq c + \int_a^x f(s)g(s)\,ds \quad \textit{for all} \quad x \in [a,b]$$

then

$$f(x) \leq c\,\mathsf{exp}\left(\int_a^x g(s)\,ds\right) \quad \textit{for all} \quad x \in [a,b].$$

Remark A.9: Suppose instead that

$$f(x) \leq c + \int_a^x \omega\left(f(s)\right)g(s)\,ds \quad \text{for all} \quad x \in [a,b],$$

where ω is a continuous and strictly increasing function with $\omega(0) = 0$. If $\Omega(u)$ is an antiderivative of $\dfrac{1}{\omega(u)}$, then it is easy to show that

$$\Omega(f(x)) \leq \Omega(c) + \int_a^x g(s)\,ds \quad \text{for all} \quad x \in [a,b].$$

This is Bihari's Inequality. There are tedious details to worry about regarding $\Omega(0)$ and the domain of Ω^{-1}.

A.7 Barbălat's Lemma

Barbălat's Lemma is useful in stability theory of ordinary (and delay) differential equations. See, for example, page 323 of [70].

Lemma A.10 (Barbălat's Lemma): *Let $a \in \mathbb{R}$ be a constant.*

(a) Suppose that $f : [a,\infty) \to \mathbb{R}$ is a uniformly continuous function with $\int_a^\infty |f(x)|\,dx < \infty$. Then, $\lim\limits_{x\to\infty} f(x) = 0$.

(b) Suppose that $g : [a,\infty) \to \mathbb{R}$ is a differentiable function such that g' is uniformly continuous and $\lim\limits_{x\to\infty} g(x)$ exists and is finite. Then, $\lim\limits_{x\to\infty} g'(x) = 0$.

A.8 Equilibrium Points

An *equilibrium point* (also known as a *fixed point*, a *zero*, a *critical point*, and a *singular point*) of the differential equation $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$ is a vector $\mathbf{p}$ such that $\mathbf{g}(\mathbf{p}) = \mathbf{0}$. In dynamical systems, it is important to classify an equilibrium point in order to understand how solutions behave near this point. The definitions and pictures in this section are standard. See, for example, Chapters 1 and 2 of [100].

Definition A.11: Let $\mathbf{p}$ be an equilibrium point of the differential equation $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$ and define the matrix $\mathbf{A} := \mathbf{Dg}(\mathbf{p})$.

(a) If no eigenvalue of $\mathbf{A}$ has zero real part then $\mathbf{p}$ is *hyperbolic*.

(b) Suppose that $\mathbf{p}$ is hyperbolic. If all the eigenvalues of $\mathbf{A}$ have strictly negative real parts then $\mathbf{p}$ is a *sink*. If all the eigenvalues of $\mathbf{A}$ have strictly positive real parts then $\mathbf{p}$ is a *source*. If $\mathbf{p}$ is neither a sink nor a source then it is a *saddle*.

Figure A.2 depicts the phase portraits for four sinks encountered in this thesis. Figure A.3 depicts the phase portrait for a non-sink equilibrium point which is encountered in this thesis (a saddle node) along with the phase portrait of a saddle.

A.9 Theorems of Hartman-Grobman, Hartman, and Poincaré

The Hartman-Grobman Theorem, which relates flows of a nonlinear differential equation to the flows of the linearization, is arguably the most fundamental result in the theory of dynamical systems. There are many variations of this result, such as Poincaré's Theorem (which is a very special case and pre-dates the Hartman-Grobman Theorem) and Hartman's Theorem. For Poincaré's Theorem see, for example, page 190 of [4], §IV.4 of [78], and [101]. For the Hartman-Grobman Theorem and Hartman's Theorem, see for example [50, 52, 53, 54, 100]. For Sternberg's Theorem, which is another alternative, see for example [115, 116, 117, 118].

Consider the nonlinear differential equation $\dot{\mathbf{x}} = \mathbf{g}(\mathbf{x})$ along with its linearization at the origin $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$. Here, we have $\dot{} = \frac{d}{dt}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{g}(\mathbf{x}) \in \mathbb{R}^n$, $\mathbf{g}(\mathbf{0}) = \mathbf{0}$, and $\mathbf{A} := \mathbf{Dg}(\mathbf{0})$. Let $\boldsymbol{\phi}_t(\mathbf{x}_0)$ be the flow of the nonlinear system.

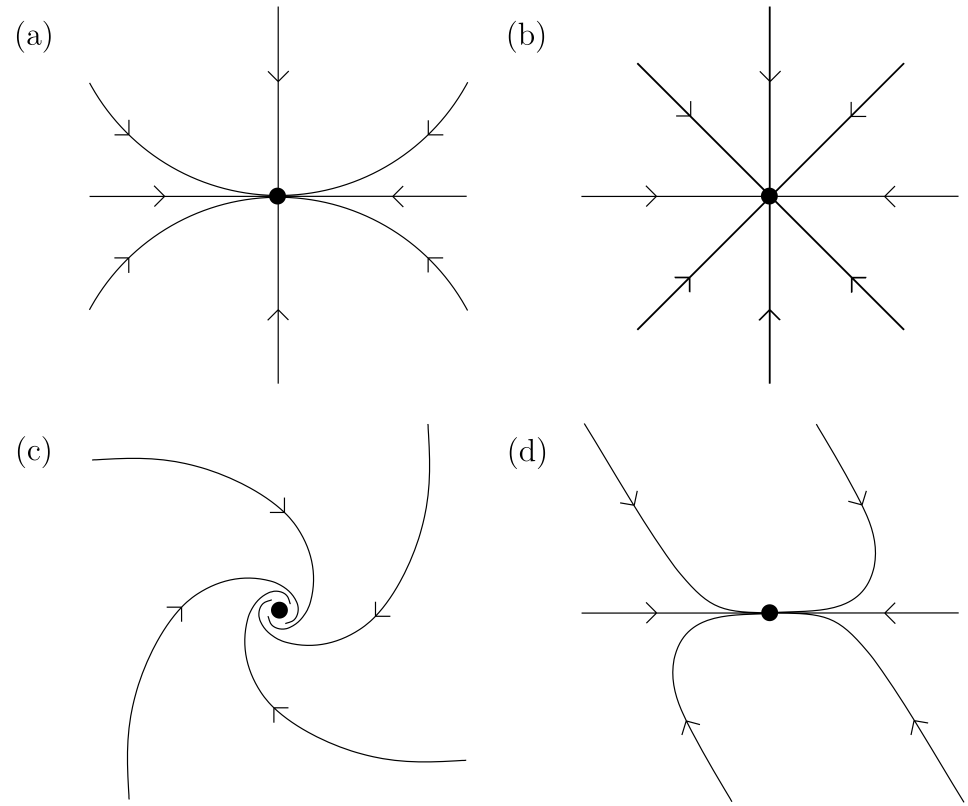

Figure A.2: The phase portraits for four typical sinks. (a) stable node (b) star node (special type of stable node) (c) stable spiral (d) Jordan node

Theorem A.12 (Hartman-Grobman Theorem): *Suppose that the origin is a hyperbolic equilibrium point and $\boldsymbol{g} \in C^1(E)$, where $E \subset \mathbb{R}^n$ is a domain containing the origin. Then, there exist domains $U \subset E$ and V containing the origin and a function $\boldsymbol{\psi}$ such that $\boldsymbol{\psi}$ is a homeomorphism from U to V and, for each $\boldsymbol{x} \in U$, there is an open interval $I(\boldsymbol{x})$ containing 0 such that*

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\boldsymbol{x})\right) = \mathrm{e}^{t\boldsymbol{A}}\boldsymbol{\psi}(\boldsymbol{x}) \quad \textit{for all} \quad t \in I(\boldsymbol{x}).$$

Theorem A.13 (Hartman's Theorem): *Suppose that the origin is either a sink or a source and $\boldsymbol{g} \in C^2(E)$, where $E \subset \mathbb{R}^n$ is a domain containing the origin. Then, there exist domains $U \subset E$ and V containing the origin and a function $\boldsymbol{\psi}$ such that $\boldsymbol{\psi}$ is a C^1-diffeomorphism from U to V and, for each $\boldsymbol{x} \in U$, there is an open interval $I(\boldsymbol{x})$ containing 0 such that*

$$\boldsymbol{\psi}\left(\boldsymbol{\phi}_t(\boldsymbol{x})\right) = \mathrm{e}^{t\boldsymbol{A}}\boldsymbol{\psi}(\boldsymbol{x}) \quad \textit{for all} \quad t \in I(\boldsymbol{x}).$$

Definition A.14: Suppose that the eigenvalues of $\mathbf{A}$ are given by $\{\lambda_k\}_{k=1}^n$.

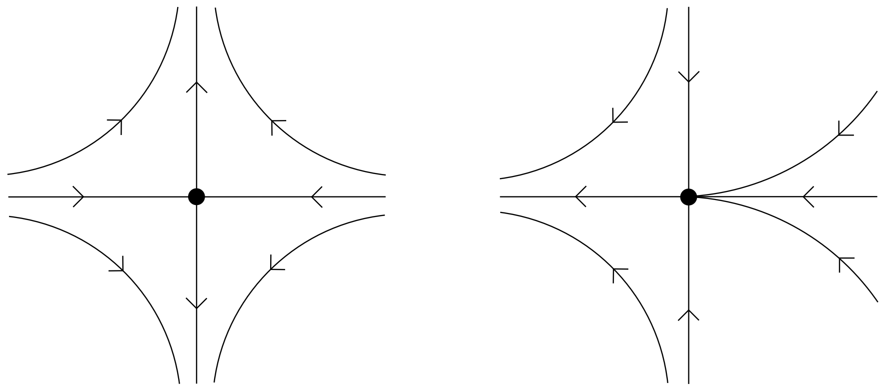

Figure A.3: The phase portraits for two non-sinks. (a) saddle (b) saddle node (half saddle, half node)

(a) The eigenvalues are said to be *resonant* if there exist $\{a_k\}_{k=1}^n \subset \mathbb{N}_0$ and $j \in \{1, \ldots, n\}$ such that $\sum_{k=1}^n a_k \geq 2$ and $\lambda_j = \sum_{k=1}^n a_k \lambda_k$. The number $\sum_{k=1}^n a_k$ is the *order* of the resonance.

(b) The *convex hull* of $\{\lambda_k\}_{k=1}^n$ is the smallest convex set in the complex plane containing all the eigenvalues. The eigenvalues are said to belong to the *Poincaré domain* if this convex hull does not contain zero.

Theorem A.15 (Poincaré's Theorem): *Suppose that $\boldsymbol{g}$ is analytic at the origin. Suppose further that the eigenvalues of $\boldsymbol{A}$ belong to the Poincaré domain and are non-resonant. Then, there are domains U and V containing the origin such that for any $\boldsymbol{x}_0 \in U$ there exists a unique $\boldsymbol{y}_0 \in V$ and interval $I(\boldsymbol{x}_0)$ containing 0 such that*[3]

$$\boldsymbol{\phi}_t(\boldsymbol{x}_0) = e^{t\boldsymbol{A}}\boldsymbol{y}_0 + \boldsymbol{q}\left(e^{t\boldsymbol{A}}\boldsymbol{y}_0\right) \quad \textit{for all} \quad t \in I(\boldsymbol{x}_0)$$

for some analytic function $\boldsymbol{q}$ which satisfies $\boldsymbol{q}(\boldsymbol{0}) = \boldsymbol{0}$ and $\boldsymbol{Dq}(\boldsymbol{0}) = \boldsymbol{0}$.

A.10 The Centre Manifold Theorem

The results in this section on the Centre Manifold Theorem can be found in Chapters 1 and 2 of [23], which is the standard reference for centre manifold theory. In particular, see Theorem 1 on page 16, Theorem 3 on page 25, and properties (1) and (2) on page 28. For the Centre Manifold

[3] Equivalently, for any $\mathbf{y}_0 \in V$ there exists a unique $\mathbf{x}_0 \in U$ and interval $I(\mathbf{x}_0)$ containing 0 such that the remainder of the statement is true.

Theorem, the canonical system is

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{f}(\mathbf{x}, \mathbf{y}), \quad \dot{\mathbf{y}} = \mathbf{B}\mathbf{y} + \mathbf{g}(\mathbf{x}, \mathbf{y}), \tag{A.1}$$

where the first equation corresponds to the centre component and the second equation corresponds to the stable component.[4] In particular, we have $\mathbf{x} \in \mathbb{R}^m$, $\mathbf{y} \in \mathbb{R}^n$, $\mathbf{A} \in \mathbb{R}^{m \times m}$, $\mathbf{B} \in \mathbb{R}^{n \times n}$, $\mathbf{f}(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^m$, $\mathbf{g}(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^n$, and $\dot{} = \frac{d}{dt}$. Moreover, we assume that $\mathbf{A}$ has eigenvalues with zero real part and $\mathbf{B}$ has eigenvalues with negative real part. Finally, we assume that $\mathbf{f}$ and $\mathbf{g}$ are C^r in a neighbourhood of the origin, where $r \geq 2$, with $\mathbf{f}(\mathbf{0}) = \mathbf{0}$, $\mathbf{g}(\mathbf{0}) = \mathbf{0}$, $\mathbf{Df}(\mathbf{0}) = \mathbf{0}$, and $\mathbf{Dg}(\mathbf{0}) = \mathbf{0}$.

Definition A.16: Suppose that $\mathbf{y} = \mathbf{h}(\mathbf{x})$ is an invariant manifold for (A.1) for sufficiently small $\|\mathbf{x}\|$. If $\mathbf{h}$ is C^r in a neighbourhood of the origin, $\mathbf{h}(\mathbf{0}) = \mathbf{0}$, and $\mathbf{Dh}(\mathbf{0}) = \mathbf{0}$, then $\mathbf{y} = \mathbf{h}(\mathbf{x})$ is a (local) C^r *centre manifold* for the system (A.1).

Define the operator $\mathbf{T}$ by

$$\mathbf{T}[\mathbf{h}](\mathbf{x}) := \mathbf{Dh}(\mathbf{x})\left[\mathbf{A}\mathbf{x} + \mathbf{f}(\mathbf{x}, \mathbf{h}(\mathbf{x}))\right] - \left[\mathbf{B}\mathbf{h}(\mathbf{x}) + \mathbf{g}(\mathbf{x}, \mathbf{h}(\mathbf{x}))\right].$$

Observe that if $\mathbf{T}[\mathbf{h}] = \mathbf{0}$ then $\mathbf{y} = \mathbf{h}(\mathbf{x})$ is an invariant manifold for the system (A.1). To see why, just differentiate $\mathbf{y} = \mathbf{h}(\mathbf{x})$ with respect to t and apply (A.1). It follows that if $\mathbf{y} = \mathbf{h}(\mathbf{x})$ is a centre manifold for (A.1) for sufficiently small $\|\mathbf{x}\|$, then $\mathbf{T}[\mathbf{h}](\mathbf{x}) = \mathbf{0}$ for sufficiently small $\|\mathbf{x}\|$. Consider also the differential equation

$$\dot{\mathbf{u}} = \mathbf{A}\mathbf{u} + \mathbf{f}(\mathbf{u}, \mathbf{h}(\mathbf{u})), \tag{A.2}$$

which describes the time evolution along the centre manifold.

Theorem A.17 (Centre Manifold Theorem): *Consider the system* (A.1). *There exists a function* $\boldsymbol{h}$ *such that* $\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{x})$ *is a* C^r *centre manifold for sufficiently small* $\|\boldsymbol{x}\|$.

Theorem A.18:

(a) The zero solution of (A.1) *has the same stability classification as the zero solution of* (A.2).

(b) Suppose that the zero solution of (A.2) *is stable. Let* $\boldsymbol{z}(t) = (\boldsymbol{x}(t), \boldsymbol{y}(t))^T$ *be a solution to* (A.1) *with* $\|\boldsymbol{z}_0\|$ *sufficiently small. Then, there exists a solution* $\boldsymbol{u}(t)$ *of* (A.2) *and a* $\gamma > 0$ *(which depends only on* $\boldsymbol{B}$*) such that*

$$\boldsymbol{x}(t) = \boldsymbol{u}(t) + \mathcal{O}\big(e^{-\gamma t}\big) \quad \textit{and} \quad \boldsymbol{y}(t) = \boldsymbol{h}\left(\boldsymbol{u}(t)\right) + \mathcal{O}\big(e^{-\gamma t}\big) \quad \textit{as} \quad t \to \infty.$$

[4] We could also consider a system with an unstable component.

Theorem A.19: *Let $\boldsymbol{h}$ be the C^r centre manifold guaranteed to exist by the Centre Manifold Theorem. Suppose that the function $\boldsymbol{p}$ satisfies $\boldsymbol{p}(\boldsymbol{0}) = \boldsymbol{0}$ and $\boldsymbol{Dp}(\boldsymbol{0}) = \boldsymbol{0}$. Then, as $\|\boldsymbol{x}\| \to 0$,*

$$\|\boldsymbol{T}[\boldsymbol{p}](\boldsymbol{x})\| = \mathcal{O}\Big(\|\boldsymbol{x}\|^k\Big) \implies \|\boldsymbol{h}(\boldsymbol{x}) - \boldsymbol{p}(\boldsymbol{x})\| = \mathcal{O}\Big(\|\boldsymbol{x}\|^k\Big).$$

Corollary A.20: *If $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$ are two C^r centre manifolds for* (A.1) *for sufficiently small $\|\boldsymbol{x}\|$ then, for any k,*

$$\|\boldsymbol{h}_1(\boldsymbol{x}) - \boldsymbol{h}_2(\boldsymbol{x})\| = \mathcal{O}\Big(\|\boldsymbol{x}\|^k\Big) \quad \textit{as} \quad \|\boldsymbol{x}\| \to 0.$$

A.11 Normal Forms

The theory of normal forms, which originated with Poincaré, yields a method of reducing a nonlinear differential equation to a "simpler" differential equation by means of a near-identity, analytic transformation. See, for example, [16, 27, 100, 127].

Consider the nonlinear differential equation

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{b}(\mathbf{x}),$$

where $\mathbf{x} \in \mathbb{R}^n$, $\dot{} = \frac{d}{dt}$, $\mathbf{A} \in \mathbb{R}^{n\times n}$, $\mathbf{b} \in C^r(\mathcal{N}, \mathbb{R}^n)$ for some $r \in \{3, 4, \ldots\}$ and neighbourhood $\mathcal{N} \subset \mathbb{R}^n$ with $\mathbf{0} \in \mathcal{N}$, $\mathbf{b}(\mathbf{0}) = \mathbf{0}$, and $\mathbf{Db}(\mathbf{0}) = \mathbf{0}$. Denote by $\mathcal{H}_k$ the set of all vectors in $\mathbb{R}^n$ whose components are homogeneous polynomials of degree $k \in \{2, \ldots, r-1\}$. Then, by Taylor's Theorem we can write

$$\mathbf{b}(\mathbf{x}) = \sum_{k=2}^{r-1} \mathbf{b}_k(\mathbf{x}) + \mathcal{O}(\|\mathbf{x}\|^r) \quad \text{as} \quad \|\mathbf{x}\| \to 0,$$

where $\mathbf{b}_k(\mathbf{x}) \in \mathcal{H}_k$ for each $k \in \{2, \ldots, r-1\}$. Define also the set $\mathcal{H} := \bigoplus_{k=2}^{r-1} \mathcal{H}_k$ and the operator

$$\mathcal{L} : \mathcal{H} \to \mathcal{H}, \quad \mathcal{L}(\mathbf{h}(\mathbf{x})) := \mathbf{Dh}(\mathbf{x})\mathbf{A}\mathbf{x} - \mathbf{A}\mathbf{h}(\mathbf{x}).$$

Observe that

$$\mathcal{L}(\mathcal{H}_k) \subset \mathcal{H}_k \quad \text{and} \quad \mathcal{H}_k = \mathcal{L}(\mathcal{H}_k) \oplus \mathcal{G}_k,$$

where $\mathcal{G}_k := \mathcal{H}_k \backslash \mathcal{L}(\mathcal{H}_k)$.

Theorem A.21 (Normal Form Theorem): *By a sequence of near-identity, analytic transformations, the differential equation $\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}(\boldsymbol{x})$ can be transformed to $\dot{\boldsymbol{y}} = \boldsymbol{A}\boldsymbol{y} + \boldsymbol{c}(\boldsymbol{y})$, where*

$$\boldsymbol{c}(\boldsymbol{y}) = \sum_{k=2}^{r-1} \boldsymbol{c}_k(\boldsymbol{y}) + \mathcal{O}(\|\boldsymbol{y}\|^r) \quad \textit{as} \quad \|\boldsymbol{y}\| \to 0$$

and $\boldsymbol{c}_k(\boldsymbol{y}) \in \mathcal{G}_k$ for each $k \in \{2, \ldots, r-1\}$.

Remarks A.22:

(i) The normal form differential equation given in the theorem is not unique.

(ii) The terms $\{\mathbf{c}_k(\mathbf{y})\}_{k=2}^{r-1}$ are called *resonance terms*.

(iii) If $\mathbf{A}$ has no resonances of order k then $\mathcal{L}(\mathcal{H}_k) = \mathcal{H}_k$ and $\mathcal{G}_k = \{\mathbf{0}\}$. Consequently, $\mathbf{c}_k(\mathbf{y}) = \mathbf{0}$.

A.12 Method of Characteristics

The method of characteristics is typically the first technique a student learns to solve a partial differential equation. See, for example, §1.4 of [66] and Chapter 1 of [87]. Consider the quasi-linear partial differential equation

$$a(x,y,u)\,\frac{\partial u}{\partial x}(x,y,u) + b(x,y,u)\,\frac{\partial u}{\partial y}(x,y,u) = c(x,y,u) \tag{A.3}$$

subject to the initial condition $u(x,0) = f(x)$, where $a, b, c, f \in C^1$. Observe that (A.3) can be written

$$(a,b,c) \bullet (u_x, u_y, -1) = 0$$

and thus the vector field (a,b,c) is tangential to the solution surface $z = u(x,y)$. It follows that the solution of the system of ordinary differential equations

$$\frac{dx}{dt} = a(x,y,u), \quad \frac{dy}{dt} = b(x,y,u), \quad \frac{du}{dt} = c(x,y,u) \tag{A.4}$$

gives a curve parameterized by t lying in the solution surface $z = u(x,y)$. Solving (A.4) subject to the initial condition $(x(0), y(0), u(0)) = (s, 0, f(s))$ gives us a solution of the form $(x(t,s), y(t,s), u(t,s))$. Writing (t,s) in terms of (x,y) gives us the solution $u(x,y)$ to (A.3).

A.13 Cauchy Product of Series

For the two series

$$\sum_{n=0}^{\infty} a_n \quad \text{and} \quad \sum_{n=0}^{\infty} b_n,$$

the *Cauchy product* is given by

$$\sum_{n=0}^{\infty} c_n = \left(\sum_{n=0}^{\infty} a_n\right)\left(\sum_{n=0}^{\infty} b_n\right), \quad \text{where} \quad c_n := \sum_{m=0}^{n} a_m b_{n-m}.$$

The product series converges if one of the original two series converges absolutely. See, for example, pages 73–74 of the classic [110]. Two other useful forms which follow from this are the following:

$$\left(\sum_{n=0}^{\infty} a_n x^n\right)\left(\sum_{n=0}^{\infty} b_n x^n\right) = \sum_{n=0}^{\infty} c_n x^n, \quad \text{where} \quad c_n := \sum_{m=0}^{n} a_m b_{n-m}$$

and

$$\left(\sum_{n=0}^{\infty} \frac{a_n}{n!}\, x^n\right)\left(\sum_{n=0}^{\infty} \frac{b_n}{n!}\, x^n\right) = \sum_{n=0}^{\infty} \frac{c_n}{n!}\, x^n, \quad \text{where} \quad c_n := \sum_{m=0}^{n} \binom{n}{m} a_m b_{n-m}.$$

A.14 Left and Right Eigenvectors

For a good reference on left and right eigenvectors, see for example Chapter 1 of [129]. Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be a general matrix with (right) eigenvalues $\{\lambda_i\}_{i=1}^n$ and associated (right) eigenvectors $\{\mathbf{v}_i\}_{i=1}^n$. That is,

$$\mathbf{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i \quad (i = 1, \ldots, n)\,. \tag{A.5}$$

The eigenvectors are always taken to be non-zero. We know that the eigenvalues of $\mathbf{A}^T$ are also $\{\lambda_i\}_{i=1}^n$. Let the (right) eigenvectors of $\mathbf{A}^T$ be $\{\mathbf{w}_i\}_{i=1}^n$. That is,

$$\mathbf{A}^T \mathbf{w}_i = \lambda_i \mathbf{w}_i \quad (i = 1, \ldots, n)\,.$$

If we take the transpose of both sides of this equation, we obtain

$$\mathbf{w}_i^T \mathbf{A} = \lambda_i \mathbf{w}_i^T \quad (i = 1, \ldots, n)\,. \tag{A.6}$$

Since this equation is the same as the eigenvalue equation for $\mathbf{A}$ except with the vector acting on the left of $\mathbf{A}$ instead of on the right, the vectors $\{\mathbf{w}_i\}_{i=1}^n$ are called the left eigenvectors of $\mathbf{A}$. Using (A.5) and (A.6), it is easy to verify the following orthogonality condition.

Claim A.23: *If the eigenvalues $\{\lambda_i\}_{i=1}^n$ of $\boldsymbol{A}$ are all non-zero and distinct, then the left eigenvectors $\{\boldsymbol{w}_i\}_{i=1}^n$ and the right eigenvectors $\{\boldsymbol{v}_i\}_{i=1}^n$ satisfy the orthogonality condition*

$$\boldsymbol{w}_i^T \boldsymbol{v}_j = 0 \quad (i \neq j)\,.$$

Suppose we want to find the matrix exponential $\mathsf{e}^{t\mathbf{A}}$. Assume that the eigenvalues $\{\lambda_i\}_{i=1}^n$ are all distinct and non-zero and the eigenvectors $\{\mathbf{v}_i\}_{i=1}^n$ and $\{\mathbf{w}_i\}_{i=1}^n$ are chosen so that $\mathbf{w}_i^T \mathbf{v}_j = \delta_{ij}$ for $i, j = 1, \ldots, n$, where δ_{ij} is the Kronecker delta. Define the matrices

$$\mathbf{P} := (\mathbf{v}_1 \ \cdots \ \mathbf{v}_n) \quad \text{and} \quad \boldsymbol{\Lambda} := \mathsf{diag}\,(\lambda_1, \ldots, \lambda_n)\,.$$

Since $\left\{\mathbf{w}_i^T\mathbf{v}_j\right\}_{i,j=1}^n = \mathbf{I}_n$, we see that

$$\mathbf{P}^{-1} = \begin{pmatrix}\mathbf{w}_1 & \cdots & \mathbf{w}_n\end{pmatrix}^T \quad \text{and} \quad \mathbf{\Lambda} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}.$$

Moreover,

$$\mathbf{A} = \sum_{i=1}^n \lambda_i \left(\mathbf{v}_i\mathbf{w}_i^T\right) \quad \text{and} \quad \mathsf{e}^{t\mathbf{A}} = \sum_{i=1}^n \mathsf{e}^{\lambda_i t}\left(\mathbf{v}_i\mathbf{w}_i^T\right).$$

A.15 Jordan Canonical Form

See, for example, pages 38–39 of [30] and §1.8 of [100]. Let $\mathbf{A} \in \mathbb{R}^{n\times n}$ be a matrix. Suppose that $\mathbf{A}$ has $\ell \in \{1,\ldots,n\}$ distinct eigenvalues $\{\lambda_i\}_{i=1}^\ell \subset \mathbb{C}$ with respective multiplicities $\{m_i\}_{i=1}^\ell \subset \mathbb{N}$ where $\sum_{i=1}^\ell m_i = n$. For $i \in \{1,\ldots,\ell\}$, define the Jordan block $\mathbf{J}_i \in \mathbb{R}^{m_i\times m_i}$ by[5]

$$\mathbf{J}_i := \begin{pmatrix} \lambda_i & 1 & 0 & \cdots & 0 & 0 \\ 0 & \lambda_i & 1 & \cdots & 0 & 0 \\ 0 & 0 & \lambda_i & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_i & 1 \\ 0 & 0 & 0 & \cdots & 0 & \lambda_i \end{pmatrix}.$$

Hence define the Jordan canonical form

$$\mathbf{J} := \bigoplus_{i=1}^\ell \mathbf{J}_i = \begin{pmatrix} \mathbf{J}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{J}_\ell \end{pmatrix}.$$

Then, there exists an invertible matrix $\mathbf{P}$ such that

$$\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{J}.$$

Moreover,

$$\mathsf{e}^{t\mathbf{J}} = \bigoplus_{i=1}^\ell \mathsf{e}^{t\mathbf{J}_i} \quad \text{and} \quad \mathsf{e}^{t\mathbf{A}} = \mathbf{P}\mathsf{e}^{t\mathbf{J}}\mathbf{P}^{-1}.$$

[5] If $m_i = 1$ then $\mathbf{J}_i = (\lambda_i)$.

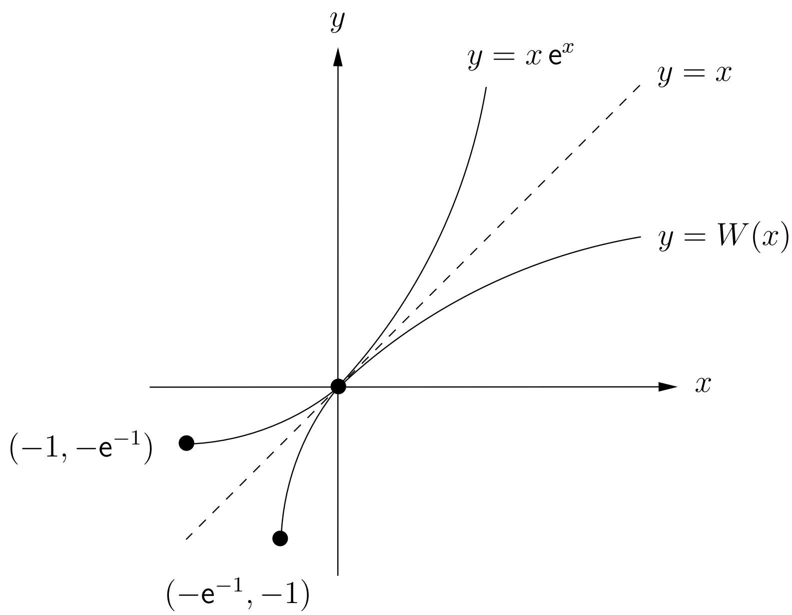

Figure A.4: The Lambert W function and its inverse.

A.16 The Lambert W Function

Perhaps the simplest transcendental equation is

$$x = W\,\mathsf{e}^W,$$

where $x \in \mathbb{R}$ and $W \geq -1$. Solving for W in terms of x gives the Lambert W function.[6] A good reference for the Lambert W function along with its properties is [31], which is also where the function was given its name.

Figure A.4 gives a sketch of $W(x)$ as well as its inverse. We will now mention a few basic properties of the Lambert W function.

- For any $x \in \mathbb{R}$, $W(x\,\mathsf{e}^x) = x$.
- For $x > -\mathsf{e}^{-1}$, $W(x)$ is differentiable with

$$W'(x) = \begin{cases} 1, & \text{if} \quad x = 0 \\ \dfrac{W(x)}{x\,[1 + W(x)]}, & \text{if} \quad x \neq 0 \end{cases}.$$

[6] The Lambert W function is also called the $\mathsf{plog}(x)$ function. Note that there are other branches for solutions W of $x = W\,\mathsf{e}^W$ but we need only concern ourselves with the principal branch.

- The Taylor series for $W(x)$ at $x = 0$ is

$$W(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}\, n^{n-2}}{(n-1)!}\, x^n, \quad |x| < \mathsf{e}^{-1}.$$

- Asymptotically, $W(x)$ satisfies

$$W(x) = \ln(x) - \ln(\ln(x)) + \mathsf{o}(\ln(\ln(x))) \quad \text{as} \quad x \to \infty.$$

- The function $W(x)$ is strictly increasing and concave down for $x \geq -\mathsf{e}^{-1}$. Furthermore, $W(x) \leq x$ for all $x \geq -\mathsf{e}^{-1}$.

A.16.1 Solving an Important Equation

Suppose that $x, y > 0$ satisfy the equation

$$y = x^a \mathsf{e}^{bx},$$

where $a, b > 0$ are constants. We want to find x as a function of y. Now, observe that

$$\frac{b}{a}\, \sqrt[a]{y} = \left(\frac{b}{a}\, x\right) \exp\left(\frac{b}{a}\, x\right).$$

Using the definition of the Lambert W function and multiplying by $\frac{a}{b}$ allows us to solve for x. Therefore, we have proven the following.

Claim A.24: *Let $x, y, a, b > 0$. Then,*

$$y = x^a \mathsf{e}^{bx} \quad \textit{if and only if} \quad x = \frac{a}{b}\, W\left(\frac{b}{a}\, \sqrt[a]{y}\right).$$

A.16.2 Solving an Important Initial Value Problem

Suppose that we want to solve the initial value problem

$$\frac{dx}{dt} = -\frac{ax}{1 + bx}, \quad x(0) = x_0,$$

where $a, b, x_0 > 0$ are constants. Observe that $x = 0$ is a solution of the differential equation and $x' < 0$ for $x > 0$. Hence, we can conclude that

$$0 < x(t) \leq x_0 \quad \text{for all} \quad t \geq 0.$$

First, write the differential equation as

$$\left[\frac{1}{x(s)} + b\right] \frac{dx(s)}{ds} = -a \quad \text{for all} \quad s \geq 0.$$

Now, integrate with respect to s from 0 to t, where $t \geq 0$, to get

$$[\ln(x(t)) - \ln(x_0)] + b\,[x(t) - x_0] = -at.$$

Re-arranging,

$$\ln(x(t)) + bx(t) = \ln(x_0) + bx_0 - at.$$

Taking the exponential of both sides,

$$x(t)\,\mathrm{e}^{bx(t)} = x_0 \mathrm{e}^{bx_0} \mathrm{e}^{-at}.$$

Using the definition of the Lambert W functions enables us to state the following.

Claim A.25: *The solution of the initial value problem*

$$\frac{dx}{dt} = -\frac{ax}{1+bx}, \quad x(0) = x_0,$$

where $a, b, x_0 > 0$ are constants, is

$$x(t) = \frac{1}{b}\, W\left(\left[bx_0 \mathrm{e}^{bx_0}\right] \mathrm{e}^{-at}\right).$$

A.16.3 Solving Another Important Initial Value Problem

Suppose now that we want to solve the initial value problem

$$\frac{dx}{dt} = -\frac{ax^2}{1+bx}, \quad x(0) = x_0,$$

where $a, b, x_0 > 0$ are constants. Like before, we know that

$$0 < x(t) \leq x_0 \quad \text{for all} \quad t \geq 0.$$

If we write the differential equation as

$$\left[-\frac{1}{x(s)^2} - \frac{b}{x(s)}\right] \frac{dx(s)}{ds} = a \quad \text{for all} \quad s \geq 0$$

and integrate with respect to s from 0 to t, where $t \geq 0$, we obtain

$$\left[\frac{1}{x(t)} - \frac{1}{x_0}\right] - b\,[\ln(x(t)) - \ln(x_0)] = at.$$

Re-arranging,

$$\frac{1}{x(t)} + \mathsf{ln}\left(\frac{1}{x(t)^b}\right) = \frac{1}{x_0} + \mathsf{ln}\left(\frac{1}{x_0^b}\right) + at.$$

Taking the exponential of both sides,

$$\left(\frac{1}{x(t)}\right)^b \mathsf{exp}\left(\frac{1}{x(t)}\right) = \left(\frac{1}{x_0}\right)^b \mathsf{exp}\left(\frac{1}{x_0}\right) \mathsf{exp}(at)\,.$$

Appealing to Claim A.24,

$$\frac{1}{x(t)} = b\,W\left(\left[\frac{1}{bx_0}\,\mathsf{exp}\left(\frac{1}{bx_0}\right)\right]\mathsf{exp}\left(\frac{a}{b}\,t\right)\right).$$

Therefore, we have proven the following.

Claim A.26: *The solution of the initial value problem*

$$\frac{dx}{dt} = -\frac{ax^2}{1+bx}, \quad x(0) = x_0,$$

where $a, b, x_0 > 0$ are constants, is

$$x(t) = \frac{1}{b\,W\left(\left[\frac{1}{bx_0}\,\mathsf{exp}\left(\frac{1}{bx_0}\right)\right]\mathsf{exp}\left(\frac{a}{b}\,t\right)\right)}.$$

Appendix B

Other Interesting Things

In this appendix, we will present some interesting results or approaches that were not fully realized and do not fit in anywhere else in the thesis.

B.1 An Interesting Limit

Suppose that the sequence $\{c_n\}_{n=1}^{\infty} \subset \mathbb{R}$ has limit $c \in \mathbb{R}$. A well-known fact is

$$\lim_{n\to\infty} \frac{1}{n} \left(\sum_{m=1}^{n} c_m \right) = c.$$

That is, the sequence of averages also has limit c. We can form a similar result involving two convergent sequences. This result will be utilized later in this chapter.

Proposition B.1: *Consider two sequences $\{a_n\}_{n=0}^{\infty} \subset \mathbb{R}$ and $\{b_n\}_{n=0}^{\infty} \subset \mathbb{R}$ having respective limits $a \in \mathbb{R}$ and $b \in \mathbb{R}$. Then,*

$$\mathit{lim}_{n\to\infty} \frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} a_m b_{n-m} = ab.$$

Proof: Let $\varepsilon > 0$ be arbitrary and fixed. Define

$$M := \sup_{n\in\mathbb{N}_0} \{|a_n|, |b_n|\} < \infty$$

and observe that $|a|, |b| \leq M$. Since $\lim_{n\to\infty} a_n = a$ and $\lim_{n\to\infty} b_n = b$, we know that there is an $N_1 \in \mathbb{N}_0$ such that

$$|a_n - a| < \frac{\varepsilon}{6M} \quad \text{and} \quad |b_n - b| < \frac{\varepsilon}{6M} \quad \text{for all} \quad n > N_1.$$

Since $\sum_{m=0}^{n} \binom{n}{m} = 2^n$,

$$\left| \frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} a_m b_{n-m} - ab \right| \le \frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} \left| a_m b_{n-m} - ab \right| .$$

Let $n > 2N_1 + 1$ be fixed. We will show that

$$\frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} \left| a_m b_{n-m} - ab \right| < \varepsilon \tag{B.1}$$

which will prove the proposition.

Observe that

$$0 < N_1 + 1 \le n - N_1 - 1 < n \quad \text{and} \quad m, n-m > N_1 \quad \text{for} \quad m \in \{N_1 + 1, \ldots, n - N_1 - 1\} .$$

We will break the sum in (B.1) into three separate sums,

$$\frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} \left| a_m b_{n-m} - ab \right| = \frac{1}{2^n} \left[\sum_{m=0}^{N_1} + \sum_{m=N_1+1}^{n-N_1-1} + \sum_{m=n-N_1}^{n} \right] \binom{n}{m} \left| a_m b_{n-m} - ab \right| , \tag{B.2}$$

and look at each separately.

Manipulating the middle sum of (B.2),

$$\begin{aligned} &\frac{1}{2^n} \sum_{m=N_1+1}^{n-N_1-1} \binom{n}{m} \left| a_m b_{n-m} - ab \right| \\ &= \frac{1}{2^n} \sum_{m=N_1+1}^{n-N_1-1} \binom{n}{m} \left| a_m b_{n-m} - a b_{n-m} + a b_{n-m} - ab \right| \\ &= \frac{1}{2^n} \sum_{m=N_1+1}^{n-N_1-1} \binom{n}{m} \left| \left[a_m - a \right] b_{n-m} + a \left[b_{n-m} - b \right] \right| \\ &\le \frac{1}{2^n} \sum_{m=N_1+1}^{n-N_1-1} \binom{n}{m} \left[\frac{\varepsilon}{6M} M + M \frac{\varepsilon}{6M} \right] \\ &< \frac{\varepsilon}{3}. \end{aligned}$$

To analyze the first sum in (B.2), note that $\left| a_m b_{n-m} - ab \right| \le 2M^2$ for all $m, n \in \mathbb{N}_0$. So, the first sum thus satisfies[1]

$$\begin{aligned}\frac{1}{2^n}\sum_{m=0}^{N_1}\binom{n}{m}\left|a_m b_{n-m}-ab\right| &\le \frac{2M^2}{2^n}\sum_{m=0}^{N_1}\binom{n}{m}\\ &\le \frac{2M^2\left(N_1+1\right)}{2^n}\binom{n}{N_1}\\ &= \frac{2M^2\left(N_1+1\right)n\left(n-1\right)\cdots\left(n-N_1+1\right)}{2^n N_1!}\\ &\le 2M^2\left[\frac{N_1+1}{N_1!}\right]\left[\frac{n^{N_1}}{2^n}\right].\end{aligned}$$

Since $\lim\limits_{n\to\infty}\dfrac{n^{N_1}}{2^n}=0$, it follows that there is an $N_2>2N_1+1$ such that if $n>N_2$ then

$$\frac{1}{2^n}\sum_{m=0}^{N_1}\binom{n}{m}\left|a_m b_{n-m}-ab\right|<\frac{\varepsilon}{3}.$$

Similarly for the third sum in (B.2), there is an $N_3>N_2$ such that if $n>N_3$ then

$$\frac{1}{2^n}\sum_{m=n-N_1}^{n}\binom{n}{m}\left|a_m b_{n-m}-ab\right|<\frac{\varepsilon}{3}.$$

$\square$

B.2 The Fraser Iterative Scheme

The (dimensionless) scalar differential equation for the Michaelis-Menten mechanism is

$$y'=\frac{x-\left(1+x\right)y}{\varepsilon\left[-x+\left(1-\eta+x\right)y\right]}, \tag{B.3}$$

where $'=\frac{d}{dx}$. By solving this equation for y, one can form the Fraser iterative scheme

$$y_{n+1}(x):=\frac{x\left[1+\varepsilon y_n'(x)\right]}{1+\varepsilon\left(1-\eta\right)y_n'(x)+x\left[1+\varepsilon y_n'(x)\right]}\qquad\left(n\in\mathbb{N}_0\right), \tag{B.4}$$

where $y_0(x)$ is an appropriately chosen initial function. See, for example, [43, 92, 104, 106, 107, 109].

Assume that the iterates $\{y_n(x)\}_{n=0}^{\infty}$ can be written

$$y_n(x)=\sum_{i=0}^{\infty}\sigma_i^{(n)}x^i\qquad\left(n\in\mathbb{N}_0\right). \tag{B.5}$$

[1]Since $n>2N_1+1$, it must be that $\binom{n}{0},\binom{n}{1},\ldots,\binom{n}{N_1}$ are in ascending order.

It was noted by Roussel in [106] that if $\sigma_1^{(0)} \geq 0$ then $\lim_{n\to\infty} \sigma_1^{(n)} = \sigma$, where $\sigma > 1$ is the slope of the slow eigenvector. We will mention a few convergence properties of both $\left\{\sigma_1^{(n)}\right\}_{n=0}^{\infty}$ and $\left\{\sigma_2^{(n)}\right\}_{n=0}^{\infty}$. In regards to $\left\{\sigma_2^{(n)}\right\}_{n=0}^{\infty}$, we want to know when the sequence converges to σ_2, which is given in (7.27b). The reader may want to see Equation 7.28, which informs us of the sign and existence of σ_2 in relation to the ratio $\kappa > 1$ of the eigenvalues.

Substitution of (B.5) into (B.4) yields

$$y_{n+1}(x) = \left[\frac{1+\varepsilon\sigma_1^{(n)}}{1+\varepsilon(1-\eta)\,\sigma_1^{(n)}}\right] x + \left\{\frac{2\varepsilon\eta\sigma_2^{(n)} - \left[1+\varepsilon\sigma_1^{(n)}\right]^2}{\left[1+\varepsilon(1-\eta)\,\sigma_1^{(n)}\right]^2}\right\} x^2 + \mathcal{O}\big(x^3\big) \quad \text{as} \quad x \to 0^+.$$

Hence, we have the recursive relationships

$$\sigma_0^{(n+1)} = 0, \quad \sigma_1^{(n+1)} = \frac{1+\varepsilon\sigma_1^{(n)}}{1+\varepsilon(1-\eta)\,\sigma_1^{(n)}}, \quad \text{and} \quad \sigma_2^{(n+1)} = \frac{2\varepsilon\eta\sigma_2^{(n)} - \left[1+\varepsilon\sigma_1^{(n)}\right]^2}{\left[1+\varepsilon(1-\eta)\,\sigma_1^{(n)}\right]^2} \quad (n \in \mathbb{N}_0)\,.$$

Observe that if $\sigma_1^{(0)} = \sigma$ then $\sigma_1^{(n)} = \sigma$ for all $n \in \mathbb{N}_0$. Note that if we choose $y_0(x) := \alpha(x)$ (that is, the isocline for slope σ) then $\sigma_0^{(0)} = 0$ and $\sigma_1^{(0)} = \sigma$. We will now state a couple of properties of $\left\{\sigma_1^{(n)}\right\}_{n=0}^{\infty}$ and $\left\{\sigma_2^{(n)}\right\}_{n=0}^{\infty}$. In the interest of space, we omit the proofs.

Claim B.2: *Consider the sequence* $\left\{\sigma_1^{(n)}\right\}_{n=0}^{\infty}$. *If* $\sigma_1^{(0)} \geq 0$ *then* $\left\{\sigma_1^{(n)}\right\}_{n=0}^{\infty}$ *is monotonic with* $\lim_{n\to\infty} \sigma_1^{(n)} = \sigma$.

Claim B.3: *Consider the sequence* $\left\{\sigma_2^{(n)}\right\}$, *where we take* $\sigma_1^{(0)} = \sigma$. *Then,*

$$\lim_{n\to\infty} \sigma_2^{(n)} = \begin{cases} \sigma_2, & \textit{if} \quad \kappa > 2 \\ -\infty, & \textit{if} \quad \kappa = 2 \\ +\infty, & \textit{if} \quad 1 < \kappa < 2 \quad \textit{and} \quad \sigma_2^{(0)} > \sigma_2 \\ -\infty, & \textit{if} \quad 1 < \kappa < 2 \quad \textit{and} \quad \sigma_2^{(0)} < \sigma_2 \end{cases}.$$

B.3 Alternate Fraser Iterative Scheme

Write the differential equation (B.3) as

$$y = \left[\frac{x}{1+x}\right] + \left[\frac{\varepsilon x}{1+x}\right] y' - \left[\frac{\varepsilon(1-\eta+x)}{1+x}\right] yy'.$$

Combining this with Proposition B.1 suggests the iteration scheme

$$y_{n+1}(x) := \left[\frac{x}{1+x}\right] + \left[\frac{\varepsilon x}{1+x}\right] y_n'(x) - \left[\frac{\varepsilon\,(1-\eta+x)}{1+x}\right] \frac{1}{2^n} \sum_{m=0}^{n} \binom{n}{m} y_m(x) y_{n-m}'(x) \quad (n \in \mathbb{N}_0)\,.$$

Define the (exponential) generating function

$$w(x,\tau) := \sum_{n=0}^{\infty} \frac{y_n(x)}{n!}\,\tau^n$$

and observe

$$y_n(x) = \frac{\partial^n w}{\partial \tau^n}(x,0) \quad (n \in \mathbb{N}_0)\,.$$

It is easy to confirm that $w(x,\tau)$ satisfies the delay partial differential equation

$$\frac{\partial w}{\partial \tau}(x,\tau) = \left[\frac{x}{1+x}\right] \mathsf{e}^{\tau} + \left(\frac{\varepsilon x}{1+x}\right) \frac{\partial w}{\partial x}(x,\tau) - \left[\frac{\varepsilon\,(1-\eta+x)}{1+x}\right] w\left(x, \tfrac{1}{2}\tau\right) \frac{\partial w}{\partial x}\left(x, \tfrac{1}{2}\tau\right).$$

Solving this is much easier said than done. See, for example, [56, 130] for references on functional differential equations. Delay differential equations have been considered in chemical kinetics. See, for example, [105].

B.4 A Related Delay Differential Equation

Consider the initial value problem

$$\dot{v}(t) = v(rt), \quad v(0) = 1,$$

where $r \in (0,1)$ is a constant and $\dot{} = \frac{d}{dt}$. This can be written as the integral equation

$$v(t) = 1 + \int_0^t v(rs)\,ds.$$

Define the interval $I := [0,\infty)$, the weighted norm

$$\|f\| := \sup_{t \in I} \left\{ \mathsf{e}^{-\sigma t}\,|f(t)| \right\},$$

where $\sigma > r^{-1}$ is a constant, and the operator

$$T : C^1(I,\mathbb{R}) \to C^1(I,\mathbb{R})\,, \quad Tu(t) := 1 + \int_0^t u(rs)\,ds.$$

It is easy to verify using the Contraction Mapping Theorem, which can be found for example on pages 220–221 of [110], that T has a unique fixed point v which is the unique solution of the initial value problem.

Using the power series method, we can obtain a series solution for the initial value problem. This series is given by

$$v(t) = \sum_{n=0}^{\infty} \frac{r^{\frac{1}{2}n(n-1)}}{n!} t^n.$$

Using the ratio test, we see that the series converges absolutely for all $t \in \mathbb{R}$.

Consider the change of variables $u(\tau) := v(\mathsf{e}^\tau)$. With this, the given initial value problem is converted to

$$u'(\tau) = \mathsf{e}^\tau u(\tau - c), \quad \lim_{\tau \to -\infty} u(\tau) = 1,$$

where $c := -\ln(r)$ and $' = \frac{d}{d\tau}$.

Interestingly, we can solve the initial value problem

$$\frac{\partial w}{\partial t}(x,t) = \phi(x) w(x, rt), \quad w(x,0) = w_0(x)$$

using the function $v(t)$. In particular,

$$w(x,t) = w_0(x) v(t\phi(x)).$$

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