EXPLICIT, IMPLICIT AND PARAMETRIC INVARIANT MANIFOLDS FOR MODEL REDUCTION IN CHEMICAL KINETICS

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Explicit, implicit and parametric invariant manifolds for model reduction in chemical kinetics

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Abstract

Many systems studied in chemical kinetics can be posed as a high order nonlinear differential systems with slow and fast variables. This have given impetus to the development of methods that reduce the order of differential systems but retain a desired degree of accuracy. The importance of research of this sort leads to the extremely fast increasing of papers devoted to reduction methods. All these methods are connected with the integral manifolds method in one way or another. We use a geometric singular perturbations method for reducing the model order in chemical kinetics problems. The method relies on the theory of integral manifolds, which essentially replaces the original system by another system on an integral manifold with dimension equal to that of the slow subsystem. Explicit, implicit and parametric representations of a slow invariant manifolds are used.

Keywords: integral manifolds, invariant manifolds, singular perturbations, model reduction, chemical kinetics.

MSC 2000: 34C45, 34D15, 37D10, 80A30

Chapter 1

Introduction

It is common knowledge that a wide range of chemical processes are characterized by extreme differences in the rates of change of variables, so singularly perturbed ordinary differential systems are used as models of such processes [25, 40, 41, 43, 44]). The Bodenstein – Semenov *quasi-steady state* approximation has long been the basis for the reduction chemical systems. More recently, an array of computational approaches have been proposed [2, 3, 17, 18, 19, 21, 27, 29, 30]

A mathematical justification of that method can be given by means of the theory of integral manifolds for singularly perturbed systems (2.2) (see e.g. [4, 11, 12, 14, 15, 20, 24, 31, 33, 40, 45, 46, 48, 47])

The integral manifolds method has been applied to a wide range of problems (see e. g. [1, 5, 7, 10, 15, 23, 31, 32, 35, 36, 39, 38, 42]), and in particular, to some applications in chemical kinetics problems [3, 6, 7, 8, 9, 12, 13, 21, 28, 31, 30, 49].

The technique of applying integral (invariant) manifold methods to singularly perturbed non-linear differential equations was first recognized by Zadiraka in [48] where he showed the existence of a local integral manifold. In a later paper [47], he proved the existence of a global integral manifold. Geometric methods were used by Fenichel in [4], see also [11]. A common feature in the invariant manifold method is that the integral manifolds were constructed by extrapolating the slow or degenerate manifold (i.e. the manifold obtained when the small parameter tends to zero). More techniques and results are also available for analyzing and constructing integral manifolds. Note that asymptotic expansions of slow integral manifolds were first used in [35, 38, 39].

Chapter 2

Slow Integral Manifolds

2.1 Existence, stability and asymptotic expansions

2.1.1 Introduction

In the present chapter we use a method for the qualitative asymptotic analysis of singular differential equations by reducing the order of the differential system under consideration. The method relies on the theory of integral manifolds, which essentially replaces the original system by another system on an integral manifold with dimension equal to that of the slow subsystem.

A smooth surface $y = h(x,\varepsilon)$, $(x \in \mathbb{R}^m, y \in \mathbb{R}^n)$ in $\mathbb{R}^m \times \mathbb{R}^n$ is a slow invariant manifold of the autonomous system

$$\begin{aligned} \dot{x} &= f(x,y,\varepsilon), \\ \varepsilon\dot{y} &= g(x,y,\varepsilon). \end{aligned} \tag{2.1}$$

if any trajectory $x = x(t,\varepsilon)$, $y = y(t,\varepsilon)$ of the system (2.1) that has at least one point $x = x_0$, $y = y_0$ in common with the surface $y = h(x,\varepsilon)$, i.e. $y_0 = h(x_0,\varepsilon)$, it lies entirely in this surface, i.e. $y(t,\varepsilon) = h(x(t,\varepsilon),\varepsilon)$.

Analogously, in the case of non–autonomous system, a smooth surface $y = h(x,t,\varepsilon)$ in $\mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^n$ is a slow integral manifold of

$$\begin{aligned} \frac{dx}{dt} &= f(x,y,t,\varepsilon), \\ \varepsilon\,\frac{dy}{dt} &= g(x,y,t,\varepsilon), \end{aligned} \tag{2.2}$$

if any trajectory $\Big(t, x(t,\varepsilon), y(t,\varepsilon)\Big)$ of solution $x = x(t,\varepsilon)$, $y = y(t,\varepsilon)$ to the system (2.2) that has at least one point $x = x_0$, $y = y_0$ in common with the surface $y = h(x,t,\varepsilon)$, i.e.

$y_0 = h(x_0, t_0, \varepsilon)$, it lies entirely in this surface, i.e. $y(t,\varepsilon) = h(x(t,\varepsilon), t, \varepsilon)$.

The motion along an invariant manifold of the system (2.1) is governed by the equation

$$\dot{x} = f(x, h(x,\varepsilon), \varepsilon). \tag{2.3}$$

If $x(t,\varepsilon)$ is a solution of this equation, then the pair $\Big(x(t,\varepsilon), y(t,\varepsilon)\Big)$, where $y(t,\varepsilon) = h(x(t,\varepsilon),\varepsilon)$, is a solution of the original system (2.1), since it defines a trajectory on the invariant manifold.

The motion along an integral manifold of the non–autonomous system (2.2) is governed by the equation

$$\dot{x} = f(x, h(x,t,\varepsilon), t, \varepsilon).$$

Note that the formal substitution the function $h(x,\varepsilon)$ instead y into the system (2.1) gives the first order PDE (*invariance equation*)

$$\varepsilon \frac{\partial h}{\partial x} f(x, h(x,\varepsilon), \varepsilon) = g(x, h, \varepsilon) \tag{2.4}$$

for $h(x,\varepsilon)$.

In the non–autonomous case *the invariance equation* for $h(x,t,\varepsilon)$ looks as follows

$$\varepsilon \frac{\partial h}{\partial t} + \varepsilon \frac{\partial h}{\partial x} f(x, h(x,t,\varepsilon), t, \varepsilon) = g(x, h, \varepsilon). \tag{2.5}$$

Consider now the *the boundary layer* subsystem of (2.1), that is,

$$\frac{dy}{d\tau} = g(x, y, 0), \quad \tau = t/\varepsilon,$$

treating x as a vector parameter. We shall assume that some of the steady states $y^0 = y^0(x)$ of this subsystem are asymptotically stable and that a trajectory starting at any point of the domain approaches one of these states as closely as desired as $t \to \infty$. This assumption will hold, for example, if the matrix

$$(\partial g/\partial y)(x, y^0(x), 0)$$

is stable for some of the stationary states and the domain can be represented as the union of the domains of attraction of the asymptotically stable steady states. We recall that a matrix is stable if its spectrum is located in the left open complex halfplane, i.e. all eigenvalues of this matrix have negative real parts.

Notwithstanding the fact that we are interested primarily in autonomous systems, all statements will be formulated in the more general case of non–autonomous systems.

It is assumed that

(I) The functions f, g and h are uniformly continuous and bounded, together with their partial derivatives with respect to all variables up to the $(k+2)-$order $(k \geq 0)$.

(II) The eigenvalues $\lambda_i(x,t)(i = 1,\ldots,n)$ of the matrix $B(x,t) = g_y(x,\phi(x,t),t,0)$ satisfy the inequality

$$Re\lambda_i(x,t) \leq -2\gamma < 0, \tag{2.6}$$

for some $\gamma > 0$.

Then the following result holds (see e.g. [33, 47]):

Proposition 1.1. *Under the assumptions* (I) *and* (II) *there is a sufficiently small positive* ε_1, $\varepsilon_1 \leq \varepsilon_0$, *such that, for* $\varepsilon \in I_1 := \{\varepsilon \in \mathbb{R} : 0 < \varepsilon < \varepsilon_1\}$, *the system* (2.2) *has a smooth integral manifold* $\mathcal{M}_\varepsilon$ *with the representation*

$$\mathcal{M}_\varepsilon := \{(x,y,t) \in \mathbb{R}^{m+n+1} : y = h(x,t,\varepsilon),\ (x,t) \in G \times \mathbb{R}\},$$

for some domain $G \in \mathbb{R}^m$

Proposition 1.1 guarantees that the equation (2.5) can yield $y = h(x,t,\varepsilon)$ which is the slow integral manifold.

Remark. The global boundedness assumption in (I) with respect to (x,y) can be relaxed by modifying f and g outside some bounded region of $\mathbb{R}^n \times \mathbb{R}^m$.

We will present the proof of this Proposition in the Appendix.

2.1.2 Stability of slow integral manifolds

In applications it is often assumed that the spectrum of the Jacobian matrix

$$g_y(x,\phi(x,t),t,0)$$

is located in the left half plane. Under this additional hypothesis the manifold $\mathcal{M}_\varepsilon$ is exponentially attracting for $\varepsilon \in I_1$. This means: the solution $x = x(t,\varepsilon)$, $y = y(t,\varepsilon)$ of the original system (2.2) that satisfied the initial condition $x(t_0,\varepsilon) = x^0$, $y(t_0,\varepsilon) = y^0$ can be represented as

$$\begin{aligned} x(t,\varepsilon) &= v(t,\varepsilon) + \varepsilon\varphi_1(t,\varepsilon), \\ y(t,\varepsilon) &= h(v(t,\varepsilon),t,\varepsilon) + \varphi_2(t,\varepsilon). \end{aligned} \tag{2.7}$$

There exists a point v^0 which is the initial value for a solution $v(t,\varepsilon)$ of the equation $\dot{v} = f(v,h(v,t,\varepsilon),t,\varepsilon)$; the functions $\varphi_1(t,\varepsilon)$, $\varphi_2(t,\varepsilon)$ are corrections that determine the degree to which trajectories passing near the manifold tend asymptotically to the corresponding trajectories on the manifold as t increases. They satisfy the following inequalities:

$$|\varphi_i(t,\varepsilon)| \leq N|y^0 - h(x^0,t_0,\varepsilon)| \exp[-\beta(t-t_0)/\varepsilon], \quad i = 1,2, \tag{2.8}$$

for $t \geq t_0$.

From (2.7) and (2.8) we obtain the following *Reduction Principle* for a stable integral manifold defined by a function $y = h(x,t,\varepsilon)$: a solution $x = x(t,\varepsilon)$, $y = h(x(t,\varepsilon),t,\varepsilon)$

of the original non–autonomous system (2.2) is stable (asymptotically stable, unstable) if and only if the corresponding solution of the system of equations

$$\dot{v} = F(v, t, \varepsilon) = f(v, h(v, t, \varepsilon), t, \varepsilon)$$

on the integral manifold is stable (asymptotically stable, unstable). The Lyapunov Reduction Principle was extended to ordinary differential systems with Lipschitz right–hand sides by Pliss [26], and to singularly perturbed systems in [40]. Thanks to the reduction principle and the representation (2.7), the qualitative behavior of trajectories of the original system near the integral manifold may be investigated by analyzing the equation on the manifold.

2.1.3 Unstable manifolds

Consider system (2.2) and suppose that hypothesis I, II hold, but inequality (2.6) is replaced by

$$Re\lambda_i(x, t) \geq 2\gamma > 0. \tag{2.9}$$

If in system (2.2) we use the new "reverse" time $t \to -t$, then we obtain a system that satisfies hypotheses (I) and (II). Consequently (2.2) has the slow integral manifold $y = h(x, t, \varepsilon)$, and for this manifold all propositions from the previous section are true, with the exception of stability.

But this manifold is stable (and the Reduction Principle applies) with respect to $t \to -\infty$. This means that for increasing t, the trajectories of solutions with initial points near the slow integral manifold move away from this manifold very rapidly.

2.1.4 Conditionally stable manifolds

A rather complicated situation arises if the system (2.2) satisfies hypotheses (I) and (II), but inequality (2.6) is replaced by

$$Re\lambda_i(x, t) \geq 2\gamma_1 > 0, i = 1, \ldots, n_1, \tag{2.10}$$

$$Re\lambda_i(x, t) \leq -2\gamma_2 < 0, i = n_1 + 1, \ldots, n. \tag{2.11}$$

The slow integral manifold $y = h(x, t, \varepsilon)$ is then conditionally stable, i.e. in the space $\mathbb{R}^m \times \mathbb{R}^n$ there exists an n_2–dimensional manifold ($n_2 = n - n_1$), which has the following property. All trajectories, with initial points that belong to this manifold, tend to the slow integral manifold as $t \to \infty$. Besides, in $\mathbb{R}^m \times \mathbb{R}^n$ there exists an n_1–dimensional manifold, such that all trajectories, with initial points that belong to this manifold, tend to the slow integral manifold as $t \to -\infty$.

2.1.5 Asymptotic representation of integral manifolds

When the method of integral manifolds is being used to solve a specific problem, a central question is the calculation of the function $h(x,t,\varepsilon)$ in terms of the manifold described. An exact calculation is generally impossible, and various approximations are necessary. One possibility is the asymptotic expansion of $h(x,t,\varepsilon)$ in integer powers of the small parameter:

$$h(x,t,\varepsilon) = \phi(x,t) + \varepsilon h_1(x,t) + \cdots + \varepsilon^k h_k(x,t) + \dots . \tag{2.12}$$

Substituting this formal expansion into invariance equation

$$\varepsilon \frac{\partial h}{\partial t} + \varepsilon \frac{\partial h}{\partial x} f(x, h(x,t,\varepsilon), t, \varepsilon) = g(x,h,\varepsilon), \tag{2.13}$$

we obtain the relationship

$$\varepsilon \sum_{k\ge 0} \varepsilon^k \frac{\partial h_k}{\partial t} + \varepsilon \sum_{k\ge 0} \varepsilon^k \frac{\partial h_k}{\partial x} f(x, \sum_{k\ge 0} \varepsilon^k h_k, t, \varepsilon)$$

$$= g(x, \sum_{k\ge 0} \varepsilon^k h_k, t, \varepsilon). \tag{2.14}$$

We use the formal asymptotic representations

$$f(x, \sum_{k\ge 0} \varepsilon^k h_k, t, \varepsilon) = \sum_{k\ge 0} \varepsilon^k f_k(x, \phi, h_1, \dots, h_k, t)$$

$$= f_0(x,\phi,t) + \varepsilon f_1(x,\phi,h_1,t) + \cdots + \varepsilon^k f_k(x,\phi,\dots,h_k,t) + \dots,$$

and

$$g(x, \sum_{k\ge 0} \varepsilon^k h_k, t, \varepsilon) = B(x,t) \sum_{k\ge 1} \varepsilon^k h_k + \sum_{k\ge 1} \varepsilon^k g_k(x,\phi,h_1,...,h_{k-1},t)$$

$$= B(x,t)(\varepsilon h_1 + \varepsilon^2 h_2 + \cdots + \varepsilon^k h_k) + \dots$$

$$+\varepsilon g_1(x,\phi,t) + \varepsilon^2 g_2(x,\phi,h_1,t) + \cdots + \varepsilon^k g_k(x,\phi,\dots,h_{k-1},t) + \dots,$$

where the matrix $B(x,t) \equiv (\partial g/\partial y)(x,\phi,t,0)$, and where

$$g(x,\phi(x,t),t,0) = 0.$$

Substituting these formal expansions into (2.14)

$$\varepsilon \frac{\partial \phi}{\partial t} + \varepsilon^2 \frac{\partial h_1}{\partial t} + \cdots + \varepsilon^k \frac{\partial h_{k-1}}{\partial t} + \dots$$

$$+ \left(\varepsilon \frac{\partial \phi}{\partial x} + \varepsilon^2 \frac{\partial h_1}{\partial x} + \cdots + \varepsilon^k \frac{\partial h_{k-1}}{\partial x} + \dots \right) (f_0(x,\phi,t) +$$

$$+\varepsilon f_1(x,\phi,h_1,t)+\cdots+\varepsilon^k f_k(x,\phi,\dots,h_k,t)+\dots)$$
$$=B(x,t)(\varepsilon h_1+\varepsilon^2 h_2+\cdots+\varepsilon^k h_k)+\dots$$
$$+\varepsilon g_1(x,\phi,t)+\varepsilon^2 g_2(x,\phi,h_1,t)+\cdots+\varepsilon^k g_k(x,\phi,\dots,h_{k-1},t)+\dots,$$

and equating powers of ε, we obtain

$$\frac{\partial\phi}{\partial t}+\frac{\partial\phi}{\partial x}f_0(x,\phi,t)=Bh_1+g_1,$$
$$\frac{\partial h_1}{\partial t}+\frac{\partial\phi}{\partial x}f_1+\frac{\partial h_1}{\partial x}f_0=Bh_2+g_2,$$
$$\cdots$$
$$\frac{\partial h_{k-1}}{\partial t}+\sum_{0\le p\le k-1}\frac{\partial h_p}{\partial x}f_{k-1-p}=Bh_k+g_k,\quad k=2,3,\dots\ .$$

Since B is invertible

$$h_1=B^{-1}\left[\frac{\partial\phi}{\partial t}+\frac{\partial\phi}{\partial x}f_0(x,\phi,t)-g_1\right],$$
$$h_2=B^{-1}\left[\frac{\partial h_1}{\partial t}+\frac{\partial\phi}{\partial x}f_1+\frac{\partial h_1}{\partial x}f_0-g_2\right],$$
$$\cdots$$
$$h_k=B^{-1}\left[\frac{\partial h_{k-1}}{\partial t}+\sum_{0\le p\le k-1}\frac{\partial h_p}{\partial x}f_{k-1-p}-g_k\right]. \tag{2.15}$$

Chapter 3

Explicit representation

Consider now the autonomous singularly perturbed system

$$\dot{x} = f(x, y, \varepsilon), \quad \varepsilon \dot{y} = g(x, y, \varepsilon).$$

The usual approach in the qualitative study of this system is to consider first the degenerate system ($\varepsilon = 0$)

$$\frac{dx}{dt} = f(x, y, 0), \quad 0 = g(x, y, 0),$$

and then to draw conclusions about the qualitative behavior of the full system for sufficiently small ε. The equation $0 = g(x, y, 0)$ describes the slow manifold A smooth surface $y = h(x, \varepsilon)$ in $\mathbb{R}^m \times \mathbb{R}^n$ is a slow invariant manifold of this system if any trajectory $x = x(t, \varepsilon), \quad y = y(t, \varepsilon)$ of the system that has at least one point $x = x_0, \quad y = y_0$ in common with the surface $y = h(x, \varepsilon)$, i.e. $y_0 = h(x_0, \varepsilon)$, it lies entirely in this surface, i.e. $y(t, \varepsilon) = h(x(t, \varepsilon), \varepsilon)$. We also stipulate that $h(x, 0) = \phi(x)$, where $\phi(x)$ is a function whose graph is a sheet of the *slow surface*

$$g(x, y, 0) = 0,$$

The motion along an invariant manifold of the system is governed by the equation

$$\dot{x} = f(x, h(x, \varepsilon), \varepsilon).$$

In applications it is often assumed that the spectrum of the Jacobian matrix

$$g_y(x, \phi(x), 0)$$

is located in the left half plane. Under this additional hypothesis the manifold exists [1] and it is exponentially attracting. If the slow invariant manifold is attractive, the original system may be reduced to this equation.

When the method of integral manifolds is being used to solve a specific problem, a central question is the calculation of the function $h(x, t, \varepsilon)$ in terms of the manifold described. An exact calculation is generally impossible, and various approximations are necessary. One possibility is the asymptotic expansion in integer powers of the small parameter:

$$h(x, t, \varepsilon) = \phi(x) + \varepsilon h_1(x) + \cdots + \varepsilon^k h_k(x) + \dots . \tag{3.1}$$

The coefficients $h_k(x)$ can be found from the invariance equation

$$\varepsilon \frac{\partial h}{\partial x} f(x, h(x, \varepsilon), \varepsilon) = g(x, h, \varepsilon)$$

for $h(x, \varepsilon)$.

3.1 Cooperative phenomenon

Consider now an example of so called *cooperative phenomenon* [22]. A model for this consists of an enzyme molecule E which binds a substrate molecule S to form a single bound substrate-enzyme complex C_1. This complex C_1 not only breaks down to form a product P and enzyme E again, it also combine with another substrate molecule to form a dual bound substrate-enzyme complex C_2. This C_2 complex breaks down to form a product P and the single bound complex C_1. A reaction mechanism for this model is

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C_1 \overset{k_2}{\rightarrow} E + P, \tag{3.2}$$

$$S + C_1 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} C_2 \overset{k_4}{\rightarrow} C_1 + P, \tag{3.3}$$

where k's are the rate constants as indicated.

With lower case letters denoting concentrations, the mass action low applied to (3.2), (3.3) gives

$$\frac{ds}{dt} = -k_1\, s\, e + (k_{-1} - \ k_3 s)c_1 + k_{-3}c_2, \tag{3.4}$$

$$\frac{dc_1}{dt} = k_1\, s\, e - (k_{-1} + k_2 + k_3 s)c_1 + (k_{-3} + k_4)c_2, \tag{3.5}$$

$$\frac{dc_2}{dt} = k_3\, s\, c_1 - (k_{-3} + k_4)c_2 \tag{3.6}$$

$$\frac{de}{dt} = -k_1\, s\, e + (k_{-1} + k_2)c_1, \tag{3.7}$$

$$\frac{dp}{dt} = k_2\, c_1 + k_4\, c_2. \tag{3.8}$$

Appropriate initial conditions are

$$s(0) = s_0, \quad e(0) = e_0, \quad c_1(0) = c_2(0) = p(0) = 0. \tag{3.9}$$

The conservation of the enzyme is obtained by adding the 2nd, 3rd, and 4th equations in (3.4)–(3.8) and using the initial conditions; it is

$$\frac{d}{dt}(c_1 + c_2 + e) = 0 \;\Rightarrow\; c_1 + c_2 + e = e_0. \tag{3.10}$$

The equation for the product $p(t)$ is again uncoupled and given, by integration, once c_1 and c_2 have been found. Thus, by using (3.10), the resulting system is

$$\begin{aligned} \frac{ds}{dt} &= -k_1\, s\, e_0 + (k_{-1} + k_1 s - k_3 s)c_1 + (k_1 s + k_{-3})c_2, & (3.11)\\ \frac{dc_1}{dt} &= k_1\, s\, e_0 - (k_{-1} + k_2 + k_1 s + k_3 s)c_1 + (k_{-3} + k_4 - k_1 s)c_2, & (3.12)\\ \frac{dc_2}{dt} &= k_3\, s\, c_1 - (k_{-3} + k_4)c_2. & (3.13) \end{aligned}$$

We nondimensionalize the system by introducing

$$\begin{gathered} x(\tau) = \frac{s(t)}{s_0}, \quad y_1(\tau) = \frac{c_1(t)}{e_0}, \quad y_2(\tau) = \frac{c_2(t)}{e_0}, \\ \tau = k_1\, e_0\, t, \quad \varepsilon = \frac{e_0}{s_0}, \\ a_1 = \frac{k_{-1}}{k_1 s_0}, \quad a_2 = \frac{k_2}{k_1 s_0}, \quad a_3 = \frac{k_3}{k_1}, \quad a_4 = \frac{k_{-3}}{k_1 s_0}, \quad a_5 = \frac{k_4}{k_1 s_0}, \end{gathered} \tag{3.14}$$

and (3.11)–(3.13) becomes

$$\begin{aligned} \frac{dx}{dt} &= -x + (x - a_3 x + a_1)y_1 + (a_4 + x)y_2 = f(x, y_1, y_2), & (3.15)\\ \varepsilon\,\frac{dy_1}{dt} &= x - (x + a_3 x + a_1 + a_2)y_1 + (a_4 + a_5 - x)y_2 = g_1(x, y_1, y_2), & (3.16)\\ \varepsilon\,\frac{dy_2}{dt} &= a_3 x y_1 - (a_4 + a_5)y_2 = g_2(x, y_1, y_2), & (3.17) \end{aligned}$$

with initial conditions

$$x(0) = 1, \quad y_1(0) = y_2(0) = 0. \tag{3.18}$$

This problem, as the Michaelis-Menten problem, is singularly perturbed for $0 < \varepsilon \ll 1$. Note, that the origin $x = y_1 = y_2 = 0$ is the unique equilibrium of (3.15)–(3.17) with nonnegative x, y_1 and y_2.

Now we use the results of previous section to calculate the approximation of one–dimensional slow invariant manifold and the equation which describes the flow on this manifold.

The corresponding degenerate system is

$$\begin{aligned}\frac{dx}{dt} &= -x+(x-a_3x+a_1)y_1+(a_4+x)y_2,\\ 0 &= x-(x+a_3x+a_1+a_2)y_1+(a_4+a_5-x)y_2,\\ 0 &= a_3xy_1-(a_4+a_5)y_2.\end{aligned}$$

Two last equations give the unique solution

$$\begin{aligned}y_1 &= \bar{\phi}(x)=x/\Delta,\\ y_2 &= \bar{\bar{\phi}}(x)=a_3ax^2/\Delta.\end{aligned}$$

Here Δ/a is the determinant of the Jacobian matrix

$$B=\begin{pmatrix}\frac{\partial g_1}{\partial y_1} & \frac{\partial g_1}{\partial y_2}\\ \frac{\partial g_2}{\partial y_1} & \frac{\partial g_2}{\partial y_2}\end{pmatrix}=\begin{pmatrix}-x-a_3x-a_1-a_2 & a_4+a_5-x\\ a_3x & -a_4-a_5\end{pmatrix},$$

where $\Delta=x+a_1+a_2+a_3ax^2$ and $a=(a_4+a_5)^{-1}$. The slow curve is stable since the $-\operatorname{tr}B(x)$ and $\det B(x)$ are positive.

To calculate the approximation to one-dimensional slow invariant manifold

$$y_1=\bar{h}(x,\varepsilon)=\bar{\phi}(x)+\varepsilon\bar{h}_1(x)+O(\varepsilon^2),$$

$$y_2=\bar{\bar{h}}(x,\varepsilon)=\bar{\bar{\phi}}(x)+\varepsilon\bar{\bar{h}}_1(x)+O(\varepsilon^2),$$

we rewrite invariance equations for system (3.15)-(3.17):

$$\varepsilon\frac{d\bar{\phi}(x)}{dx}\left[-x+(x-a_3x+a_1)(\bar{\phi}(x)+\varepsilon\bar{h}_1(x)+\varepsilon^2...)+(a_4+x)(\bar{\bar{\phi}}(x)+\varepsilon\bar{\bar{h}}_1(x)+\varepsilon^2...)\right]$$

$$=x-(x+a_3x+a_1+a_2)(\bar{\phi}(x)+\varepsilon\bar{h}_1(x)+\varepsilon^2...)+(a_4+a_5-x)(\bar{\bar{\phi}}(x)+\varepsilon\bar{\bar{h}}_1(x)+\varepsilon^2...),$$

$$\varepsilon\frac{d\bar{\bar{\phi}}(x)}{dx}\left[-x+(x-a_3x+a_1)(\bar{\phi}(x)+\varepsilon\bar{h}_1(x)+\varepsilon^2...)+(a_4+x)(\bar{\bar{\phi}}(x)+\varepsilon\bar{\bar{h}}_1(x)+\varepsilon^2...)\right]$$

$$=a_3x(\bar{\phi}(x)+\varepsilon\bar{h}_1(x)+\varepsilon^2...)-(a_4+a_5)(\bar{\bar{\phi}}(x)+\varepsilon\bar{\bar{h}}_1(x)+\varepsilon^2...).$$

Using the formulae

$$\frac{d\bar{\phi}(x)}{dx}=(a_1+a_2-a_3ax^2)/\Delta^2,$$

$$\frac{d\bar{\bar{\phi}}(x)}{dx}=aa_3x[2(a_1+a_2)+x]/\Delta^2,$$

we solve for $\bar{h}_1(x), \bar{\bar{h}}_1(x)$ to get

$$\bar{h}_1(x) = -\frac{(a_2 + a_3a_5ax)ax}{\Delta^4}\Big[a_3ax^3 - (a_1 + a_2)(a_4 + a_5 + 2a_3x - 2a_3ax^2)\Big],$$

$$\bar{\bar{h}}_1(x) = -\frac{(a_2 + a_3a_5ax)ax}{\Delta^4}\Big[-a_3ax^3 - (a_1 + a_2)a_3x\big(1 + 2a(a_1 + a_2) + (3 + 2a_3)ax\big)\Big].$$

The flow on the stable slow invariant manifold

$$y_1 = \frac{x}{\Delta} - \varepsilon\frac{(a_2 + a_3a_5ax)ax}{\Delta^4}\left[a_3ax^3 - (a_1 + a_2)\big(a_4 + a_5 + 2a_3x - 2a_3ax^2\big)\right] + O(\varepsilon^2),$$

$$y_2 = \frac{a_3ax^2}{\Delta} - \varepsilon\frac{(a_2 + a_3a_5ax)ax}{\Delta^4}$$
$$\times\Big[-a_3ax^3 - (a_1 + a_2)a_3x\big(1 + 2a(a_1 + a_2) + (3 + 2a_3)ax\big)\Big] + O(\varepsilon^2)$$

is described by

$$\frac{dx}{dt} = -x + (x - a_3x + a_1)\big(\bar{\phi}(x) + \varepsilon\bar{h}_1(x) + \dots\big) + (a_4 + x)\big(\bar{\bar{\phi}}(x) + \varepsilon\bar{\bar{h}}_1(x) + \dots\big)$$

or

$$\frac{dx}{dt} = -\frac{x(a_2 + a_3a_5ax)}{\Delta} + \varepsilon\big[(x - a_3x + a_1)\bar{h}_1(x) + (a_4 + x)\bar{\bar{h}}_1(x)\big] + O(\varepsilon^2).$$

This last equation implies that the origin is a stable equilibrium.

On Fig. 3.1 we can see that the trajectory approaches the slow invariant manifold very fast and then follows along it as $t \to \infty$.

If we return to the dimension variables, we obtain the generalized Michaelis-Menten law in the case of the two enzyme–substrate complexes.

3.2 Enzyme-substrate-inhibitor system

In this section a enzyme-substrate reaction is considered [22]. The reaction consists of an enzyme E with a single reaction site (many enzymes have several such sites) for which two substrates compete and form one of two complexes. These break down to give two products and the original enzyme. When one substrate combines with the enzyme it means, in effect, that it is inhibiting the other substrate's reaction with that enzyme. The reactions can be written schematically as

$$S + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \overset{k_2}{\to} P_S + E, \tag{3.19}$$

$$I + E \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} EI \overset{k_4}{\to} P_I + E, \tag{3.20}$$

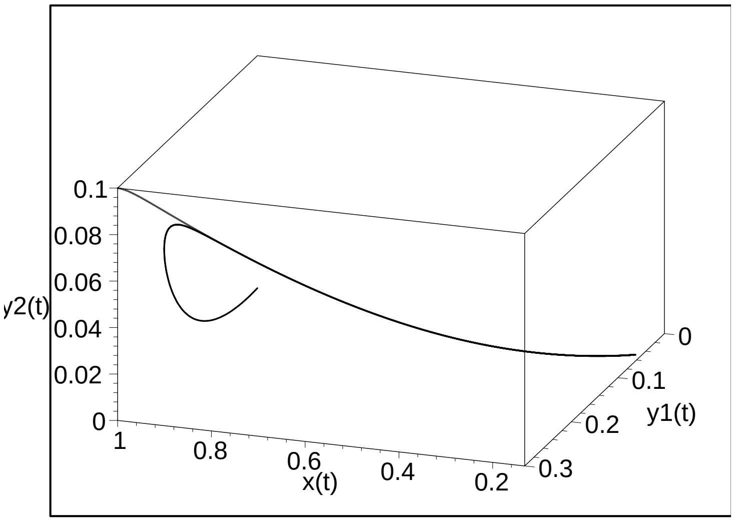

Figure 3.1: The trajectory and slow invariant manifold of (3.15)-(3.17) for $a_1 = 1$, $a_2 = 1$, $a_3 = 1$,$a_4 = 1$, $a_5 = 2$, and $\varepsilon = 0.01$.

where S and I are the two substrates, which compete for the same enzyme, and P_S and P_I are the products of two enzyme-substrate reactions.

When two substrates are competing for the same enzyme site the reaction system, (3.19) and (3.20) is said to be *fully competitive*. In such reactions one or other of the substrates can be singled out for its reaction rate to be measured in an experiment. The one so singled out is called the substrate and the other the *inhibitor*. We chose the inhibitor to be I and its reaction to be (3.20).

Applying the law mass action to (3.19), (3.20) gives the kinetic equations for the concentrations of the reactants. Since we shall be interested primarily in the rates of the reactions of S and I we do not need the equations for the products: only the rate constants k_2 and k_4 in (3.19), (3.20) are involved. Thus we need only consider the kinetic equations for the substrate, inhibitor, and enzyme complex whose concentrations as functions of time t are denoted by

$$\begin{aligned} s(t) = [S], \quad i(t) = [I], \quad e(t) = [E], \\ c_s(t) = [ES], \quad c_i(t) = [EI]. \end{aligned} \tag{3.21}$$

The kinetic equations for these concentrations for the reactions (3.19), (3.20) are

$$\frac{ds}{dt} = -k_1\, s\, e + k_{-1}\, c_s, \tag{3.22}$$

$$\frac{dc_s}{dt} = k_1\, s\, e - (k_{-1} + k_2)c_s, \tag{3.23}$$

$$\frac{di}{dt} = -k_3\, i\, e + k_{-3}\, c_i, \tag{3.24}$$

$$\frac{dc_i}{dt} = k_3\, i\, e - (k_{-3} + k_4)c_i \tag{3.25}$$

$$\frac{de}{dt} = -k_1\, s\, e - k_3\, i\, e + (k_{-1} + k_2)c_s + (k_{-3} + k_4)c_i. \tag{3.26}$$

Appropriate initial conditions for equations (3.22)–(3.26) are that there are no enzyme complexes initially but s, i, and e are prescribed, that is

$$s(0) = s_0, \quad i(0) = i_0, \quad e(0) = e_0, \quad c_s(0) = c_i(0) = 0. \tag{3.27}$$

The conservation equation for the enzyme e is obtained immediately by adding (3.23), (3.25), (3.26) and using the initial conditions (3.27) to get

$$\frac{d}{dt}(c_s + c_i + e) = 0 \;\Rightarrow\; c_s + c_i + e = e_0. \tag{3.28}$$

Eliminating e from (3.22)–(3.26) by using (3.28) gives four equations for s, i, c_s and c_i. We introduce nondimensional variables by

$$x_1(\tau) = \frac{s(t)}{s_0}, \quad x_2(\tau) = \frac{i(t)}{i_0}, \quad y_1(\tau) = \frac{c_s(t)}{e_0}, \quad y_2(\tau) = \frac{c_i(t)}{e_0},$$

$$\tau = k_1\, e_0\, t, \quad \varepsilon = \frac{e_0}{s_0}, \quad \beta = \frac{i_0}{s_0}, \quad \gamma = \frac{k_3}{k_1}, \tag{3.29}$$

$$K_s = \frac{k_{-1} + k_2}{k_1 s_0}, \quad K_i = \frac{k_{-3} + k_4}{k_3 i_0}, \quad L_s = \frac{k_2}{k_1 s_0}, \quad L_i = \frac{k_4}{k_3 i_0}.$$

Then the four equations for s, i, c_s and c_i become the four nondimensional equations

$$\frac{dx_1}{dt} = -x_1 + (x_1 + K_s - L_s)y_1 + x_1 y_2, \tag{3.30}$$

$$\frac{dx_2}{dt} = \gamma[-x_2 + x_2 y_1 + (x_2 + K_i - L_i)y_2], \tag{3.31}$$

$$\varepsilon\,\frac{dy_1}{dt} = x_1 - (x_1 + K_s)y_1 - x_1 y_2, \tag{3.32}$$

$$\varepsilon\,\frac{dy_2}{dt} = \beta\gamma[x_2 - x_2 y_1 - (x_2 + K_i)y_2], \tag{3.33}$$

with initial conditions

$$x_1(0) = x_2(0) = 1, y_1(0) = y_2(0) = 0. \tag{3.34}$$

We now use the results of the previous section to calculate the approximate two–dimensional slow invariant manifold and the equation that describes the flow on this manifold.

The corresponding degenerate system is

$$\frac{dx_1}{dt} = -x_1 + (x_1 + K_s - L_s)y_1 + x_1 y_2, \tag{3.35}$$

$$\frac{dx_2}{dt} = \gamma[-x_2 + x_2 y_1 + (x_2 + K_i - L_i)y_2], \tag{3.36}$$

$$0 = x_1 - (x_1 + K_s)y_1 - x_1 y_2, \tag{3.37}$$

$$0 = \beta\gamma[x_2 - x_2 y_1 - (x_2 + K_i)y_2], \tag{3.38}$$

The last two equations give the unique solution

$$y_1 = \bar{\phi}(x_1, x_2) = K_i x_1/\Delta,$$
$$y_2 = \bar{\bar{\phi}}(x_1, x_2) = K_s x_2/\Delta.$$

Here $\Delta\beta\gamma$ is the determinant of the Jacobian matrix

$$B(x_1, x_2) = \begin{pmatrix} \dfrac{\partial g_1}{\partial y_1} & \dfrac{\partial g_1}{\partial y_2} \\ \dfrac{\partial g_2}{\partial y_1} & \dfrac{\partial g_2}{\partial y_2} \end{pmatrix} = \begin{pmatrix} -x_1 - K_s & -x_1 \\ -\beta\gamma x_2 & -\beta\gamma(x_2 + K_i) \end{pmatrix},$$

where $\Delta = K_s x_2 + K_i x_1 + K_s K_i$. The slow surface is stable since the $-\mathrm{tr}\, B(x_1, x_2)$ and $\det B(x_1, x_2)$ are positive.

To calculate the approximate two-dimensional slow invariant manifold

$$y_1 = \bar{h}(x_1, x_2, \varepsilon) = \bar{\phi}(x_1, x_2) + \varepsilon \bar{h}_1(x_1, x_2) + O(\varepsilon^2),$$

and

$$y_2 = \bar{\bar{h}}(x_1, x_2, \varepsilon) = \bar{\bar{\phi}}(x_1, x_2) + \varepsilon \bar{\bar{h}}_1(x_1, x_2) + O(\varepsilon^2)$$

we use the invariance equations for system (3.30)-(3.33):

$$\varepsilon \frac{\partial \bar{\phi}(x_1, x_2)}{\partial x_1} \Big(-x_1 + (x_1 + K_s - L_s)\big(\bar{\phi}(x_1, x_2) + \varepsilon \bar{h}_1(x_1, x_2) + O(\varepsilon^2)\big)$$
$$+ x_1 \big(\bar{\bar{\phi}}(x_1, x_2) + \varepsilon \bar{\bar{h}}_1(x_1, x_2) + O(\varepsilon^2)\big)\Big)$$

$$+\varepsilon\gamma\frac{\partial\bar{\phi}(x_1,x_2)}{\partial x_2}\Big(-x_2+x_2\big(\bar{\phi}(x_1,x_2)+\varepsilon\bar{h}_1(x_1,x_2)+O(\varepsilon^2)\big)$$

$$+(x_2+K_i-L_i)\big(\bar{\bar{\phi}}(x_1,x_2)+\varepsilon\bar{\bar{h}}_1(x_1,x_2)+O(\varepsilon^2)\big)\Big)$$

$$=x_1-(x_1+K_s)\big(\bar{\phi}(x_1,x_2)+\varepsilon\bar{h}_1(x_1,x_2)+O(\varepsilon^2)\big)-x_1\big(\bar{\bar{\phi}}(x_1,x_2)+\varepsilon\bar{\bar{h}}_1(x_1,x_2)+O(\varepsilon^2)\big),$$

$$\varepsilon\frac{\partial\bar{\bar{\phi}}(x_1,x_2)}{\partial x_1}\Big(-x_1+(x_1+K_s-L_s)\big(\bar{\phi}(x_1,x_2)+\varepsilon\bar{h}_1(x_1,x_2)+O(\varepsilon^2)\big)$$

$$+x_1\big(\bar{\bar{\phi}}(x_1,x_2)+\varepsilon\bar{\bar{h}}_1(x_1,x_2)+O(\varepsilon^2)\big)\Big)$$

$$+\varepsilon\gamma\frac{\partial\bar{\bar{\phi}}(x_1,x_2)}{\partial x_2}\Big(-x_2+x_2\big(\bar{\phi}(x_1,x_2)+\varepsilon\bar{h}_1(x_1,x_2)+O(\varepsilon^2)\big)$$

$$+(x_2+K_i-L_i)\big(\bar{\bar{\phi}}(x_1,x_2)+\varepsilon\bar{\bar{h}}_1(x_1,x_2)+O(\varepsilon^2)\big)\Big)$$

$$=\beta\gamma\big[x_2-x_2\big(\bar{\phi}(x_1,x_2)+\varepsilon\bar{h}_1(x_1,x_2)+O(\varepsilon^2)\big)-(x_2+K_i)\big(\bar{\bar{\phi}}(x_1,x_2)+\varepsilon\bar{\bar{h}}_1(x_1,x_2)+O(\varepsilon^2)\big)\big].$$

Using the formulae

$$\frac{\partial\bar{\phi}(x_1,x_2)}{\partial x_1}=K_iK_s(x_2+K_i)/\Delta^2,$$
$$\frac{\partial\bar{\phi}(x_1,x_2)}{\partial x_2}=K_iK_s(-x_1)/\Delta^2,$$
$$\frac{\partial\bar{\bar{\phi}}(x_1,x_2)}{\partial x_1}=K_iK_s(-x_2)/\Delta^2,$$
$$\frac{\partial\bar{\bar{\phi}}(x_1,x_2)}{\partial x_2}=K_iK_s(x_1+K_s)/\Delta^2,$$

we find the expressions for $\bar{h}_1(x),\bar{\bar{h}}_1(x)$:

$$\bar{h}_1(x)=\frac{K_iK_s}{\beta\gamma\Delta^4}\big(\beta\gamma(x_2+K_i)Px_1-x_1x_2Q\big),$$

$$\bar{\bar{h}}_1(x)=\frac{K_iK_s}{\beta\gamma\Delta^4}\big(-\beta\gamma x_1x_2P+(x_1+K_s)x_2Q\big),$$

where

$$P=(K_iL_s-\gamma K_sL_i)x_2+K_i^2L_s,$$
$$Q=-(K_iL_s-\gamma K_sL_i)x_1+\gamma K_s^2L_i.$$

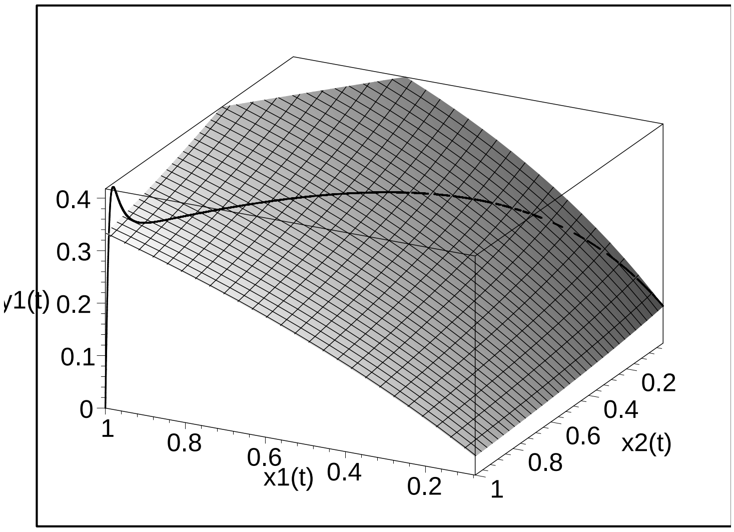

Figure 3.2: The projections of the trajectory and slow invariant manifold of (3.30)–(3.34) on the space $x_1x_2y_1$ for $K_i = K_s = 1$, $L_i = L_s = 1$, $\gamma = 2$, $\beta = 0.1$, and $\varepsilon = 0.01$.

Consequently, the first order approximation is

$$\frac{dx_1}{dt} = \frac{K_i}{\Delta}\left[-L_s x_1 + \frac{\varepsilon K_s}{\beta\gamma\Delta^3}\big(\beta\gamma[K_i x_1 + (K_s - L_s)(x_2 + K_i)]Px_1 + L_s Q x_1 x_2\big)\right] + O(\varepsilon^2),$$

$$\frac{dx_2}{dt} = \frac{\gamma K_s}{\Delta}\left[-L_i x_2 + \frac{\varepsilon K_i}{\beta\gamma\Delta^3}\big(\beta\gamma x_1 x_2 L_i P + [K_s x_2 + (K_i - L_i)(x_1 + K_s)]Qx_2\big)\right] + O(\varepsilon^2),$$

$$y_1 = \frac{K_i x_1}{\Delta} + \varepsilon\frac{K_i K_s}{\beta\gamma\Delta^4}\big[\beta\gamma(x_2 + K_i)Px_1 - x_1x_2Q\big] + O(\varepsilon^2),$$

$$y_2 = \frac{K_s x_2}{\Delta} + \varepsilon\frac{K_i K_s}{\beta\gamma\Delta^4}\big[-\beta\gamma x_1 x_2 P + (x_1 + K_s)x_2 Q\big] + O(\varepsilon^2).$$

The first and the second equations above imply that the origin

$$\begin{cases} x_1 = x_2 = 0 \\ y_1 = y_2 = 0 \end{cases}$$

is a stable equilibrium.

Figs. 3.2–3.3 show that the trajectory of (3.30)–(3.34) approaches the slow invariant manifold very fast and then follows along it as $t \to \infty$.

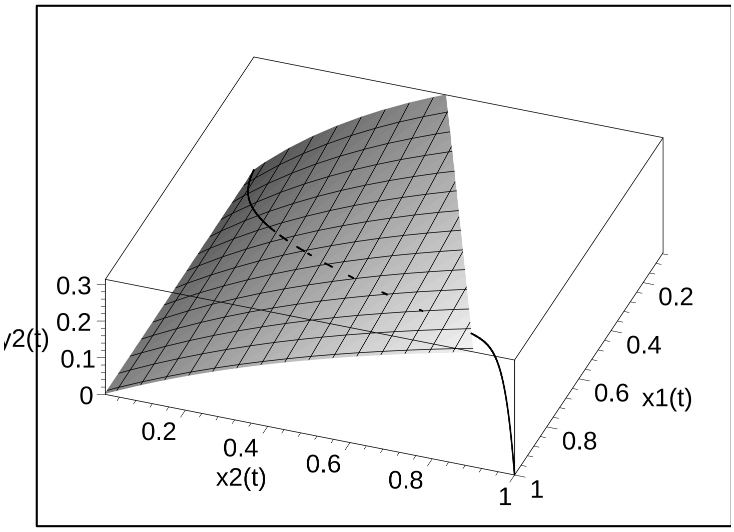

Figure 3.3: The projections of the trajectory and slow invariant manifold of (3.30)–(3.34) on the space $x_1x_2y_2$ for $K_i = K_s = 1$, $L_i = L_s = 1$, $\gamma = 2$, $\beta = 0.1$, and $\varepsilon = 0.01$.

Chapter 4

Implicit slow integral manifolds

To describe slow integral manifolds for systems like (2.2) the explicit representation is usual. In this case the approximation to $h(x, t, \varepsilon)$ may be obtained as an asymptotic expansion in powers of ε.

In general, it is impossible to find the function $y = \phi(x, t) = h(x, t, 0)$ exactly from the equation

$$g(x, y, t, 0) = 0.$$

In this case the slow integral manifold can be obtained in an implicit form. The flow on the slow integral manifold as a zero approximation is governed by the following differential-algebraic system:

$$\dot{x} = f(x, y, t, 0), \tag{4.1}$$

$$0 = g(x, y, t, 0). \tag{4.2}$$

To obtain the first approximation, it is necessary to differentiate $g(x, y, t, \varepsilon)$ with respect to (2.2)

$$\varepsilon \frac{d}{dt} g = g_y g + \varepsilon g_t + \varepsilon g_x f.$$

As a first approximation, the flow on the slow integral manifolds is governed by the differential-algebraic system

$$\dot{x} = f(x, y, t, \varepsilon), \tag{4.3}$$

$$g_y g + \varepsilon g_t + \varepsilon g_x f = 0, \tag{4.4}$$

where terms of order $o(\varepsilon)$ can be neglected. The equation (4.4) may be represented in more convenient form:

$$g + \varepsilon g_y^{-1} g_t + \varepsilon g_y^{-1} g_x f = 0. \tag{4.5}$$

In the case of autonomous system the equation (4.5) takes the form

$$g + \varepsilon N = 0,$$

where

$$N = g_y^{-1} g_x f.$$

To obtain the second order approximation, it is necessary to differentiate $g(x, y, t, \varepsilon)$ twice with respect to (2.2). Unfortunately, the corresponding relationships are too cumbersome. Because of this, we consider the case of autonomous systems. Then the second order approximation takes the form

$$g_y g + \varepsilon g_x f + \varepsilon N_y g + \varepsilon^2 N_x f = 0,$$

or

$$g + \varepsilon N + \varepsilon g_y^{-1} N_y g + \varepsilon^2 g_y^{-1} N_x f = 0$$

and finally

$$g + \varepsilon N + \varepsilon^2 g_y^{-1}(N_x f - N_y N) = 0. \tag{4.6}$$

In (4.3), (4.6) all terms multiplied by ε^3 can be neglected.

To obtain the k–th order approximation, it is necessary to differentiate $g(x, y, t, \varepsilon)$ k times with respect to with respect to (2.2) (or with respect to (2.1) in the case of autonomous system).

To check these formulae it is sufficient to note that in the calculation of the asymptotic expansions of $h(x, t, \varepsilon)$

$$h = \phi + O(\varepsilon), \quad h = \phi + \varepsilon h_1 + O(\varepsilon^2),$$

$$h = \phi + \varepsilon h_1 + \varepsilon^2 h_2 + O(\varepsilon^3),$$

the use of invariance equation gives the same result as an implicit equation.

To illustrate this, consider the example

$$\dot{x} = y, \qquad \varepsilon \dot{y} = x^2 + y^2 - a, \qquad a > 0.$$

The first approximation of the slow integral manifold is

$$y^2 + x^2 - a + \varepsilon x = 0.$$

It is easy to check that the second order approximation

$$y^2 + (x + \varepsilon/2)^2 = a - \varepsilon^2/4$$

gives the exact equation for this manifold.

Example 2. Consider now the following systems (the classical heat explosion model with reactant consumption)

$$\varepsilon \frac{d\theta}{d\tau} = \eta e^{\theta} - \alpha\theta := g,$$

$$\frac{d\eta}{d\tau} = -\eta e^{\theta} := f$$

Here θ is the dimensionless temperature and η is the dimensionless concentration. The first approximation of the slow integral manifold is

$$g_1 := g - \varepsilon\eta e^{2\theta}/g_\theta = 0,$$

where $g_\theta = \eta \exp\theta - \alpha$, and the second order approximation is

$$g_2 := g_1 - \varepsilon^2 \left(\alpha\eta e^{\theta}/g_\theta^3 + \eta^2 e^{4\theta}(\eta e^{\theta} - 2\alpha)/g_\theta^4\right) = 0.$$

4.1 Method of intrinsic manifolds

The method of intrinsic low-dimensional manifolds (ILDM Method) was supposed by U. Maas and S. B. Pope in [19] and developed in many later papers. This method, as applied to the differential system (2.1) in the form

$$\dot{x} = f(x, y, \varepsilon), \quad \dot{y} = \varepsilon^{-1} g(x, y, \varepsilon).$$

is based on a partition of the Jacobian matrix

$$J = J(x, y, \varepsilon) = \begin{pmatrix} \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial y} \\ \varepsilon^{-1}\dfrac{\partial g}{\partial x} & \varepsilon^{-1}\dfrac{\partial g}{\partial y} \end{pmatrix},$$

into a fast and slow components at each point of $(x-y)$–space and a Schur decomposition [37] to generate bases for the corresponding fast and slow subspace. This is a much more elaborate procedure than is necessary for the simplification of (2.1), because the implicit equation for intrinsic low-dimensional manifold results the using of ILDM Method. The asymptotic method of slow integral manifolds in implicit form discussed above, was suggested by V. Sobolev (see, for example, [6] in Russian, or [16, 34] in English), is much more simple and efficient. To illustrate this expression we restrict our attention to the system with scalar variables x and y.

Following to [12, 13], after calculations on the base of Schur decomposition, it is possible represent the equation defines by ILDM Method in the form

$$g_y g + \varepsilon g_x f - \varepsilon\lambda_s g = 0, \tag{4.7}$$

where λ_s is the eigenvalue

$$\lambda_s = \frac{1}{2}(\varepsilon^{-1} g_y + f_x) - \sqrt{\frac{1}{4}(\varepsilon^{-1} g_y + f_x)^2 - \varepsilon^{-1}(g_y f_x - f_y g_x)}$$

of (2×2)–matrix J. When this result is compared with that of equation (4.4) in the autonomous case

$$g_y g + \varepsilon g_x f = 0, \tag{4.8}$$

it is apparent that equation (4.7) includes "unnecessary" term $-\varepsilon\lambda_s g$. As it was shown above, equation (4.8) permits to calculate the slow invariant manifold in the form

$$y = \phi(x) + \varepsilon h_1(x) + O(\varepsilon^2)$$

with error of order $O(\varepsilon^2)$. In the paper [12, 13] it is shown that in general case ILDM equation (4.7) gives the same error, and only in the case $\phi_{xx}(x) \equiv 0$ corresponding error is of order $O(\varepsilon^3)$. However it is more convenient to use the second order approximation equation in form (4.6) or in the form

$$g_y g + \varepsilon g_x f + \varepsilon N_y g + \varepsilon^2 N_x f = 0,$$

where

$$N = g_y^{-1} g_x f,$$

than the ILDM equation. Moreover, equation (4.6) gives the error of order $O(\varepsilon^3)$ in general case not only for planar systems but also in the case of vector variables x and y. Note that the assumption $g_y < 0$ in scalar case or negativeness of real parts of all eigenvalues of matrix g_y in vector case, guarantees as an attractivity of manifolds as solvability implicit equations.

Chapter 5

Parametric representation of integral manifolds

The implicit form of integral manifolds has evident disadvantages, but for numerous problems it is impossible to find a solution of $g(x, y, t, 0) = 0$ in the explicit form $y = \varphi(x, t)$. However, sometimes the solution of $g(x, y, t, 0) = 0$ can be found as a parametric function

$$x = \chi_0(v, t), \qquad y = \varphi_0(v, t),$$

where $v \in R^m$, and the following identity holds

$$g(\chi_0(v, t), \varphi_0(v, t), t, 0) \equiv 0, t \in R, \quad v \in R^m.$$

In this case the slow integral manifold may be found in parametric form

$$x = \chi(v, t, \varepsilon), \qquad y = \varphi(v, t, \varepsilon),$$

where $t \in R$, $v \in R^m$, $\chi(v, t, 0) = \chi_0$, $\varphi(v, t, 0) = \varphi_0$. The flow on the manifold is governed by the equation

$$\dot{v} = F(v, t, \varepsilon), \tag{5.1}$$

and the function $F(v, t, \varepsilon)$ will be determined below. The functions χ, φ, F can be found as asymptotic expansions

$$\begin{aligned}
\chi(v, t, \varepsilon) &= \chi_0(v, t) + \varepsilon\chi_1(v, t) + \ldots + \varepsilon^k\chi_k(v, t) + \ldots, \\
\varphi(v, t, \varepsilon) &= \varphi_0(v, t) + \varepsilon\varphi_1(v, t) + \ldots + \varepsilon^k\varphi_k(v, t) + \ldots, \\
F(v, t, \varepsilon) &= F_0(v, t) + \varepsilon F_1(v, t) + \ldots + \varepsilon^k F_k(v, t) + \ldots,
\end{aligned} \tag{5.2}$$

in agreement with (5.1), from the equations

$$\frac{\partial \chi}{\partial t} + \frac{\partial \chi}{\partial v} F = f(\chi, \varphi, t, \varepsilon), \tag{5.3}$$

$$\varepsilon\frac{\partial\varphi}{\partial t}+\varepsilon\frac{\partial\varphi}{\partial v}F=g(\chi,\varphi,t,\varepsilon). \tag{5.4}$$

Equating coefficients of powers of the small parameter ε we obtain

$$\frac{\partial\chi_0}{\partial t}+\frac{\partial\chi_0}{\partial v}F_0=f(\chi_0,\varphi_0,t,0), \qquad g(\chi_0,\varphi_0,t,0)=0,$$

$$\frac{\partial\chi_1}{\partial t}+\frac{\partial\chi_1}{\partial v}F_0+\frac{\partial\chi_0}{\partial v}F_1=f_x(\chi_0,\varphi_0,t,0)\chi_1$$
$$+f_y(\chi_0,\varphi_0,t,0)\varphi_1+f_1,$$

$$\frac{\partial\varphi_0}{\partial t}+\frac{\partial\varphi_0}{\partial v}F_0=g_x(\chi_0,\varphi_0,t,0)\chi_1+g_y(\chi_0,\varphi_0,t,0)\varphi_1+g_1,$$
$$f_1=f_\varepsilon(\chi_0,\varphi_0,t,0), \qquad g_1=g_\varepsilon(\chi_0,\varphi_0,t,0).$$

The relationships (5.3), (5.4) contain unknown functions χ, φ, F. In a concrete problem it is possible to consider one of these functions or any m scalar components of χ,φ and F as known functions, and all others may be found from (5.3), (5.4). Moreover, it is possible at any step of the calculation of coefficients in (5.2) to choose any m components of these coefficients as given functions. In the case that F is a given function, equations (5.2), (5.3) are used to calculate the coefficients of asymptotic expansions of χ and φ. If it is possible to predetermine the function χ, then these equations allow the calculation of F and φ.

Note that in the case of the explicit form $y=h(x,t,\varepsilon)$,

$$v=x, \quad \chi=v, \quad \varphi=h(v,t,\varepsilon), \quad F=f(v,h(v,t,\varepsilon),t,\varepsilon),$$

(5.4) takes the form

$$\varepsilon\frac{\partial h}{\partial t}+\varepsilon\frac{\partial h}{\partial v}f(v,h,t,\varepsilon)=g(v,h,t,\varepsilon), \qquad h=h(v,t,\varepsilon).$$

If $dim\ x=dim\ y$ and the role of v is that of y, then $\varphi=v$ and

$$\frac{\partial\chi}{\partial t}+\frac{\partial\chi}{\partial v}F=f(\chi,v,t,\varepsilon), \quad \varepsilon F=g(\chi,v,t,\varepsilon). \tag{5.5}$$

The equation for χ follows immediately

$$\varepsilon\frac{\partial\chi}{\partial t}+\frac{\partial\chi}{\partial v}g(\chi,v,t,\varepsilon)=\varepsilon f(\chi,v,t,\varepsilon),$$

whence, under the assumption $\det(\frac{\partial\chi_0}{\partial v})\neq 0$, it is possible to calculate χ as an asymptotic expansion. Note that $g(\chi_0,\varphi_0,t,0)=0$ means that equation (5.1) is regularly perturbed, because the last equation in (5.5) implies, in this case, $F=O(1)$ as $\varepsilon\to 0$.

Consider the examples from the previous section.

In the case of mathematical example the slow curve $x^2+z^2=1$, may be represented in a parametric form

$$x=\cos v, \quad y=\sin v.$$

Let $F(v,\varepsilon)=-1$. Then it is easy to find the slow invariant manifold as an asymptotic expansion

$$x=\cos v-\varepsilon/2-\varepsilon 2\frac{1}{8}\cos v+\ldots,$$

$$y=\sin v-\varepsilon 2\frac{1}{8}\sin v+\ldots.$$

Note that the exact formulae have the following form

$$x=\sqrt{1-\varepsilon^2/4}\cos v-\varepsilon/2,$$

$$y=\sqrt{1-\varepsilon 2/4}\sin v.$$

Returning to the example concerning with a combustion problem, we obtain

$$x=\chi(y,\varepsilon)=\alpha y e^{-y}+\varepsilon\frac{y}{y-1}+\varepsilon^2 e^y\frac{y^2(y-2)}{\alpha(y-1)^4}+O(\varepsilon^3).$$

The role of variable v here plays the fast variable y. This representation is true outside some neighborhood of $y=0$, and it gives the approximation of attractive (repulsive) one-dimensional slow invariant manifold if $0\le y<1$ $(1<y)$.

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