

Explicit, Implicit and Parametric Invariant Manifolds for Model Reduction in Chemical Kinetics

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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.

Explicit representation

We consider the singularly perturbed system

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

The usual approach in the qualitative study of (1) is to consider first the degenerate system ($\varepsilon = 0$)

$$\dot{x} = f(x, y, 0), \quad 0 = g(x, y, 0), \quad (2)$$

and then to draw conclusions about the qualitative behavior of (1) 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 (1) if any trajectory $x = x(t, \varepsilon)$, $y = y(t, \varepsilon)$ of (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. $y(t, \varepsilon) = h(x(t, \varepsilon), \varepsilon)$. We also stipulate that $h(x, 0) = \phi(x)$, $g(x, \phi(x), 0) \equiv 0$.

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.

Note that the formal substitution the function $h(x, \varepsilon)$ instead y into the system (1) gives the first order PDE (invariance equation) for $h(x, \varepsilon)$:

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

When the method of integral manifolds is being used to solve a specific problem, a central question is the calculation of the function $h(x, \varepsilon)$ in terms of the manifold described.

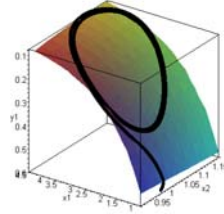


Fig. 1.

An exact calculation is generally impossible, and various approximations are necessary. One possibility is the asymptotic expansion in integer powers of the small parameter:

$$h(x, \varepsilon) = \phi(x) + \varepsilon h_1(x) + \dots + \varepsilon^k h_k(x) + \dots$$

The coefficients $h_k(x)$ can be found from the invariance equation [2,3].

Universal oscillator

Consider a model for universal oscillator with substrate inhibition [4]. It is based on substrate inhibition which is particularly common in many enzyme reactions. This model in the dimensionless form is

$$\begin{aligned} \dot{x}_1 &= J_1 - x_1 + \beta\delta - \beta(x_1 + \delta)y_1 + \beta(1 - \alpha x_1 - \delta)y_2, \\ \dot{x}_2 &= J_2 - \gamma x_2 y_2, \\ \varepsilon \dot{y}_1 &= -x_1 y_1 + (1 + x_2)y_2, \\ \varepsilon \dot{y}_2 &= \delta + (x_1 - \delta)y_1 - (1 + \alpha x_1 + \delta + x_2)y_2. \end{aligned}$$

The limit cycle on the slow invariant manifold depicts in Fig. 1

Parametric representation

For numerous problems it is impossible to find a solution of $g(x, y, 0) = 0$ in the explicit form $y = \varphi(x)$. However, sometimes the solution of $g(x, y, 0) = 0$ can be found as a parametric function

$$x = \chi_0(v), \quad y = \varphi_0(v),$$

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

$$g(\chi_0(v, t), \varphi_0(v, t), t) \equiv 0,$$

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

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

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

$$\dot{v} = F(v, \varepsilon).$$

The functions χ , φ , F can be found as asymptotic expansions [5].

Implicit slow integral manifolds

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

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

In this case the slow integral manifold can be obtained in an implicit form [5]. The flow on the slow integral manifold as a zero approximation is governed by the differential-algebraic system (2). To obtain the first approximation, it is necessary to differentiate $g(x, y, \varepsilon)$ with respect to system (1)

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

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

$$\dot{x} = f(x, y, \varepsilon), \quad g_y g + \varepsilon g_x f = 0,$$

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

$$g + \varepsilon g_y^{-1} g_x f = 0$$

or $g + \varepsilon N = 0$, where $N = g_y^{-1} g_x f$.

To obtain the second order approximation, it is necessary to differentiate $g(x, y, \varepsilon)$ twice. 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

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

To obtain the k -th order approximation, it is necessary to differentiate $g(x, y, \varepsilon)$ k times with respect to system (1).

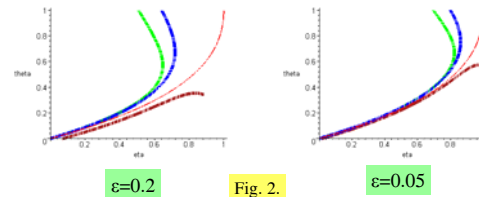


Fig. 2.

Figures 2-3 show the slow curve (red), first (blue) and second order (green) approximation for the examples. Brown lines corresponds to approximations due to the method of intrinsic low-dimensional manifolds (ILDM Method), which was supposed by U. Maas and S. B. Pope in [6].

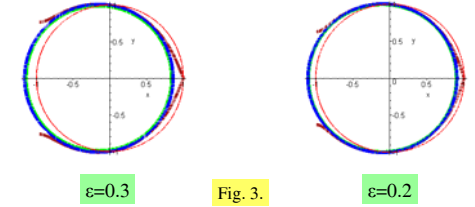


Fig. 3.

Examples

Example 1. Consider the mathematical example

$$\dot{x} = y, \quad \varepsilon \dot{y} = x^2 + y^2 - 1.$$

The first approximation of the slow invariant manifold is

$$y^2 + x^2 - 1 + \varepsilon x = 0.$$

It is easy to check that the second order approximation

$$y^2 + (x + \varepsilon/2)^2 = 1 - \varepsilon^2/4$$

gives the exact equation for this manifold. These approximations are shown in Fig. 2.

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

$$\begin{aligned} \varepsilon \frac{d\theta}{d\tau} &= \eta e^\theta - \alpha \theta := g, \\ \frac{d\eta}{d\tau} &= -\eta e^\theta := f \end{aligned}$$

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

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

These approximations are shown in Fig. 3.

References

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