Forced-convergence iterative schemes for the approximation of invariant manifolds

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In many dynamical systems, an invariant manifold attracts the phase-space flow. These manifolds can be approximated by an iterative method based on a functional equation treatment. However, a convergent mapping is not automatically generated from the functional equation. Nevertheless, it is possible to construct a convergent mapping by a simple modification of the original functional equation. As an example, a convergent sequence of approximations to the slow manifold of the Michaelis–Menten system is constructed.

1. Introduction

In many dynamical systems, an invariant manifold attracts the phase-space flow so that the eventual dynamics is shadowed by a trajectory contained in a manifold of lower dimensionality than the full phase-space. This fact is of immense practical utility [10]: If the manifold can be constructed, the original system can be reduced to a lower-dimensional system which, at least after the decay of transients, is completely equivalent to the original. The lower-dimensional system is frequently more convenient to study: If the original system of differential equations was stiff, the reduced system frequently is not [6]. Smaller systems of equations are also far easier to handle so that a more thorough analysis of the system's behavior is often possible on the manifold than in the full phase-space [3].

Chemical kinetics is a rich source of invariant manifold (and inertial manifold [20]) problems ranging in size from small [2] to large [7,19]. Fraser has proposed a relatively simple method for approximating attracting invariant manifolds of systems of ordinary differential equations (ODEs) [2]. The method is also applicable to initial-value partial differential equation (PDE) problems [8,14]. An invariant manifold is so called because it is mapped into itself under the action of the propagator of the dynamical system. Fraser used this invariance to derive a functional iterative scheme directly from a system of ODEs which, under favorable conditions, converges to the manifold. In principle, Fraser's method can be applied to a broad range of manifold approximation problems either analytically or numerically.

It has been known for a few years that Fraser's method can diverge when the curvature of the manifold being approximated is too high [13] although, until recently [11], no concrete example of divergence was known. A method for producing a convergent functional iteration scheme has been developed [11,12]. This method is now being presented to a broader audience because it may have widespread applications, both in manifold approximation and more generally in any problem where fixed-point iteration is used to solve a functional equation.

2. The Michaelis–Menten system and its slow invariant manifold

The Michaelis–Menten mechanism is the basic building block for all enzymological modeling [5]. The evolution of this system is governed by the ODEs [8]

$$\frac{\mathrm{d}s}{\mathrm{d}t} = -k_1 s(e_T - c) + k_{-1}c,$$
$$\frac{\mathrm{d}c}{\mathrm{d}t} = k_1 s(e_T - c) - (k_{-1} + k_{-2})c,$$

where s is the concentration of a reactant (normally called a substrate), c is the concentration of an enzyme-substrate complex, e_T is a constant of the motion arising from enzyme mass conservation and the k_i's are rate constants. Defining

$$x = k_1 s/(k_{-1} + k_{-2}),$$
$$y = c/e_T,$$
$$\tau = k_1 e_T t,$$
$$\alpha = k_{-1}/(k_{-1} + k_{-2}),$$
$$\varepsilon = k_1 e_T/(k_{-1} + k_{-2})$$

and letting overdots denote differentiation with respect to the scaled time τ, we obtain the dimensionless equations

$$\dot{x} = -x(1 - y) + \alpha y, \tag{1a}$$
$$\dot{y} = \big[x(1 - y) - y\big]/\varepsilon. \tag{1b}$$

Throughout this paper, our attention will remain focused on the physically realizable part of phase-space, namely, $\Gamma^+ \equiv (x \geqslant 0) \cup (0 \leqslant y \leqslant 1)$, with physically sensible values of the parameters, i.e., $0 < \alpha < 1$ and $\varepsilon > 0$.

The Michaelis–Menten system (1) has been extensively studied: Since this system represents a closed, isothermal chemical system, its equilibrium point ($x = y = 0$) is globally stable [4,17]. The equilibrium point is always approached along a one-dimensional (slow) invariant manifold $\mathcal{M}$ which attracts the phase-space flow [8,9,13, 14] (figure 1). This slow manifold is a solution of the trajectory equation

$$y' = \frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\dot{y}}{\dot{x}} = \frac{x(1 - y) - y}{\varepsilon[-x(1 - y) + \alpha y]}. \tag{2}$$

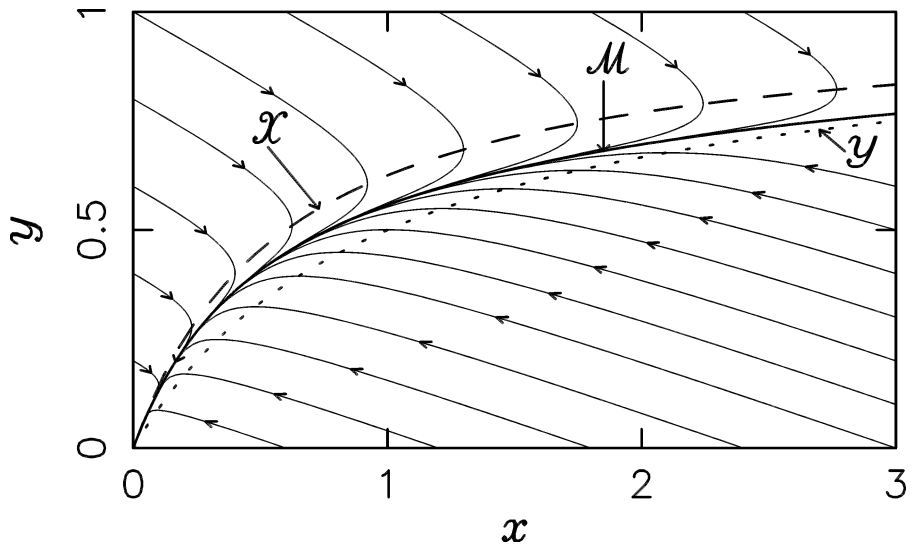

Figure 1. Trajectories for the Michaelis–Menten system with $\alpha = 0.6$ and $\varepsilon = 5$. Note that nearly all trajectories approach the equilibrium point along a one-dimensional manifold $\mathcal{M}$. This manifold lies between the x and y nullclines ($\mathcal{X}$ and $\mathcal{Y}$).

In order to prove the theorems of the next section, we need to establish some facts about the geometry of the slow manifold of this system. We first prove that the slow manifold exists and has a positive slope everywhere in the physically realizable part of phase-space Γ^+. To prove this, we first note that the eigenvalues of the Jacobian of equations (1) are negative everywhere in Γ^+. (The proof of this proposition is easy but tedious since the characteristic polynomial can be solved analytically.) This means that the flow always contracts distances between nearby coevolving points. Furthermore, the flow is into the region bounded by the two nullclines (the curves $\mathcal{X} \equiv (\dot{x} = 0)$ and $\mathcal{Y} \equiv (\dot{y} = 0)$). (See figure 1. The proof of this fact is also elementary.) Thus $y_{\mathcal{M}}$ must lie within this region. The equations of these nullclines are

$$y_{\mathcal{X}}(x) = x/(x + \alpha), \tag{3a}$$

$$y_{\mathcal{Y}}(x) = x/(x + 1). \tag{3b}$$

$\mathcal{X}$ always lies above $\mathcal{Y}$ since $0 < \alpha < 1$. However, in the limit of large x, both $y_{\mathcal{X}} \to 1$ and $y_{\mathcal{Y}} \to 1$. Since nearby trajectories cannot diverge from one another and since the flow is into the region bounded by $\mathcal{X}$ and $\mathcal{Y}$, there is a unique trajectory which attracts the flow in this region. Furthermore, since between the two nullclines $\dot{x} < 0$ and $\dot{y} < 0$, $y' > 0$ for all trajectories in this region and, in particular, $y'_{\mathcal{M}} > 0$.

Near the equilibrium point, the equation of the slow manifold $\mathcal{M}$ can be expanded in a Taylor series [8]:

$$y_{\mathcal{M}}(x) = \sigma_1 x + \sigma_2 x^2 + \cdots$$

($\sigma_0 = 0$ because $y_{\mathcal{M}}(0) = 0$). Substituting this functional form into equation (2) and keeping only leading-order terms, we obtain a quadratic equation for σ_1. The two roots have opposite signs but we know that $\mathcal{M}$ must have a positive slope so

$$\sigma_1 = \frac{\varepsilon - 1 + \sqrt{(\varepsilon - 1)^2 + 4\alpha\varepsilon}}{2\alpha\varepsilon}.$$

Asymptotically (at large x), the slow manifold can be expanded in the form

$$y_{\mathcal{M}}(x) = \rho_0 + \rho_1/x + \rho_2/x^2 + \cdots.$$

By substitution into the trajectory equation, we find

$$\rho_0 = 1, \tag{4a}$$

$$\rho_1 = -1, \tag{4b}$$

$$\rho_2 = 1, \tag{4c}$$

$$\rho_i = -\rho_{i-1} + \varepsilon \sum_{j=1}^{i-2} j\rho_j(\rho_{i-j-1} + \alpha\rho_{i-j-2}), \tag{4d}$$

where equation (4d) is used for $i > 2$.

3. The Fraser iterated functional mapping

A method for obtaining analytic approximations to the slow manifold has been proposed [2] and studied [13]. The slow manifold is a solution of equation (2) and thus is a fixed point of the functional equation

$$y = F(x, y') = \frac{x(1 + \varepsilon y')}{(x + \alpha)(1 + \varepsilon y') + 1 - \alpha} \tag{5}$$

obtained from the trajectory equation by simple inversion. This functional equation is used as the basis of an iterative scheme

$$y_{n+1} = F(x, y_n'). \tag{6}$$

A suitable starting function $y_0(x)$ must be chosen.

We now prove that this mapping always converges near the origin and for $x \to \infty$ under mild assumptions about the initial function. Suppose that the initial function y_0 has a Taylor expansion near the origin with $y_0'(0) \geqslant 0$. Then clearly

$$\lim_{x \to 0} y_n = 0 \quad \forall n > 0.$$

We may therefore assume that $y_n = \sigma_1^{(n)} x + \mathrm{O}(x^2)$ without loss of generality. To lowest order, the mapping (6) becomes

$$\sigma_1^{(n+1)} = \frac{1 + \varepsilon\sigma_1^{(n)}}{1 + \alpha\varepsilon\sigma_1^{(n)}}.$$

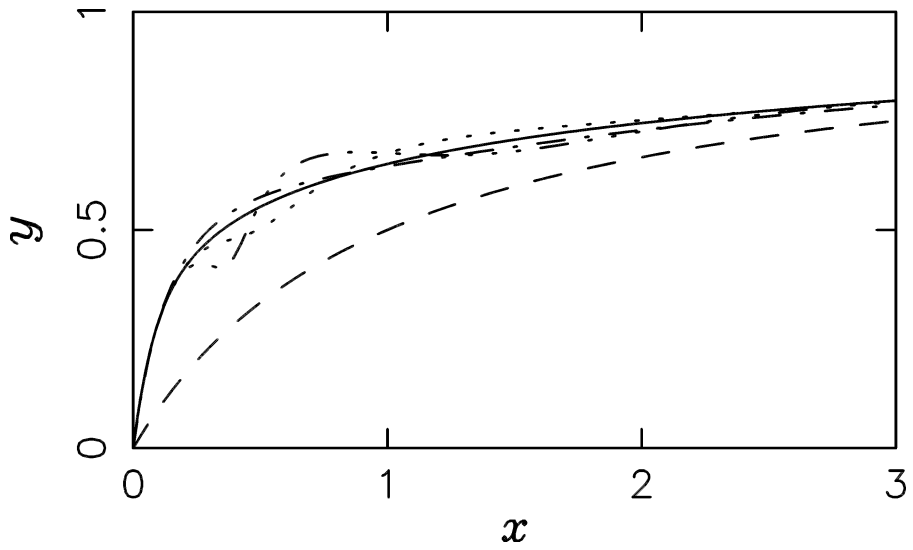

Figure 2. Slow manifold (solid line) and approximations generated by the Fraser iterative method for $\alpha = 0.2$ and $\varepsilon = 10$. Iteration is started from the y nullcline (– – – –). The second (– · – ·), fourth (· · · ·) and fifth (– · · ·) iterates are shown.

By a standard method [16], it can be shown that the sequence $\sigma_1^{(n)}$ converges to σ_1 for every $\sigma_1^{(0)} \geqslant 0$.

The proof of convergence in the limit of infinite x is a little more involved and is only sketched here. The complete proof can be seen in the author's thesis [11]. First note that if y_0 is differentiable as $x \to \infty$ and $y_0' \geqslant 0$, then $y_n \to 1$ as $x \to \infty$ for all $n > 0$. Next assume that y_i is an iterate of y_0 whose asymptotic expansion agrees with that of $y_{\mathcal{M}}$ to $\mathrm{O}(x^{-m})$. (The initial function must itself have a regular asymptotic expansion.) Thus

$$y_i = \sum_{i=0}^{m} \rho_i x^{-i} + \mathrm{O}\big(x^{-(m+1)}\big).$$

We subject this function to the mapping (6) and obtain the asymptotic expansion of the result. By a simple inductive argument, we obtain

$$y_{i+1} = \sum_{i=0}^{m+2} \rho_i x^{-i} + \mathrm{O}\big(x^{-(m+3)}\big),$$

i.e., we gain *two* coefficients of the asymptotic expansion for every iteration of the mapping.

At intermediate values of x, we must use linearized stability analysis to determine the behavior of the mapping (6). Elements of this analysis have previously been published [13]. Define

$$\delta y_n(x) = y_n(x) - y_{\mathcal{M}}(x).$$

When the derivative of $\delta y_n(x)$ is sufficiently small,

$$\delta y_{n+1} = \delta y'_n \left.\frac{\mathrm{d}F}{\mathrm{d}y'}\right|_{\mathcal{M}} \tag{7a}$$

with

$$\left.\frac{\mathrm{d}F}{\mathrm{d}y'}\right|_{\mathcal{M}} = \frac{\varepsilon x(1-\alpha)}{[\varepsilon y'_{\mathcal{M}}(x+\alpha)+x+1]^2}. \tag{7b}$$

If x is neither very large nor very small and $\varepsilon(1-\alpha)$ is large, the amplitude can be large. Thus, while the iterative method is unconditionally convergent at large and small x, it is not so everywhere. Figure 2 shows an example in which the Fraser iterative scheme diverges. As predicted, this occurs when $\varepsilon(1-\alpha)$ is large. The scheme continues to converge at large and small x but the iterates buckle at intermediate values of the free variable.

4. Stabilized iteration

Fraser's method generally works extremely well [2,8,13–15]. Of course, as we have shown above, there are excellent reasons for this: It produces a sequence of functions which rapidly converges to the equation of the manifold both near the equilibrium point and very far away from it. It therefore makes an excellent starting point for a globally convergent method.

Thomas et al. [18] have described a method for stabilizing numerical iterative processes. Their method relies on a simple transformation of the equation being solved which leaves the fixed points unaltered. It has long been known that point and functional mappings are related in such a way that methods applicable to one can often be extended to the other [1]. (This property was used in an earlier paper in this series [13] in which Aitken's sequence acceleration method was used to accelerate the convergence of a sequence of functions generated by Fraser's method.) We thus adapt the stabilization method of Thomas, Richelle and d'Ari to our manifold approximation problem.

We start with the functional equation (5) and add $A(x)y$ to both sides, where $A(x)$ is an arbitrary weighting function:

$$y + A(x)y = F(x, y') + A(x)y.$$

Of course, this transformation does not alter the fixed points of the original functional equation. Now rewrite

$$y = \frac{F(x, y') + A(x)y}{1 + A(x)}$$

and label

$$y_{n+1} = \frac{F(x, y'_n) + A(x)y_n}{1 + A(x)} \tag{8}$$

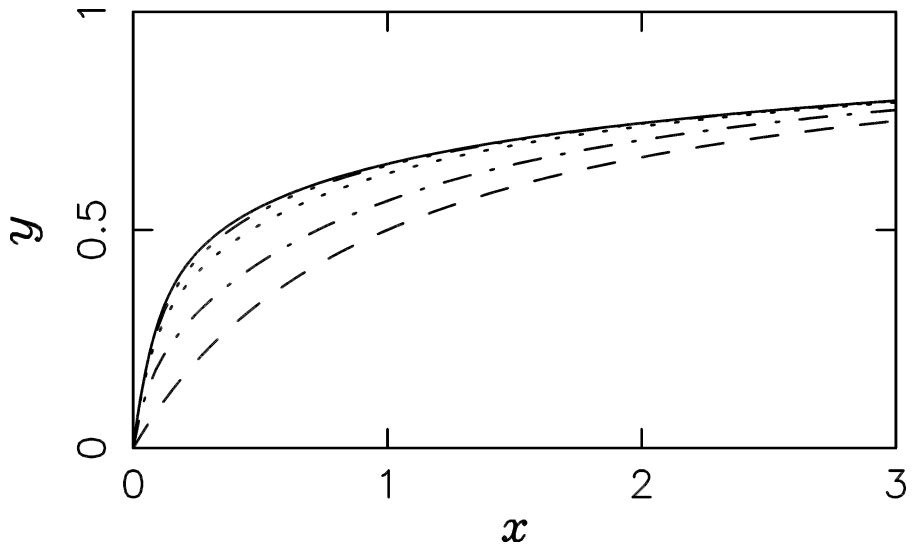

Figure 3. Slow manifold (solid line) and approximations generated by the modified iterated mapping (8) with weighting function (10) for the same parameters as figure 2. Iteration is again started from the y nullcline (– – – –). The first (– · – ·), third (· · · ·) and fifth (– · · ·) iterates are shown.

to obtain a new iterative scheme.

The weighting function $A(x)$ is chosen by performing a linearized stability analysis of scheme (8) about the slow manifold $y_{\mathcal{M}}$ as we did for Fraser's method. In this case, we get

$$\delta y_{n+1} = \frac{\delta y'_n}{1+A}\left.\frac{\mathrm{d}F}{\mathrm{d}y'}\right|_{\mathcal{M}} + \frac{A}{1+A}\delta y_n. \tag{9}$$

We first note that if we choose a function A which is positive everywhere in Γ^+, the effects of this modification to Fraser's method are, first, to decrease the amplitude of the term involving the derivative of δy_n and, second, to introduce a new term in δy_n whose amplitude is fractional. If A is very small we recover Fraser's mapping. When A is very large, the amplitude of the derivative term is annihilated but the new term causes slower convergence. Thus, this method represents a tradeoff: We can dispel divergence due to the derivative but convergence will be slowed. We thus want $A(x)$ to be as small as possible, but sufficient to cause iteration to converge. In particular, if the Fraser scheme converges automatically in some part of phase-space, as it does for the Michaelis–Menten mechanism near the origin and at large x, we want $A(x)$ to be small there in order to preserve this property.

Examining the form of equation (9), we conclude that it should be sufficient to choose

$$A(x) > \left|\frac{\mathrm{d}F}{\mathrm{d}y'}\right|_{\mathcal{M}}$$

and, given equation (7b) and the fact that $y'_{\mathcal{M}} > 0$, we see that the function

$$A(x) = \frac{\varepsilon x(1-\alpha)}{(x+1)^2} \tag{10}$$

satisfies all of our criteria. Note that $A(x)$ vanishes as $x \to 0$ and as $x \to \infty$, preserving the excellent convergence properties of the basic scheme at the extremes. This is a direct consequence of modeling the function A on the amplitude of the linearized error propagator.

Iteration of equation (8) with $A(x)$ given by equation (10) converges almost as quickly as does iteration of the basic scheme when the latter converges. When the Fraser method produces a divergent sequence, the sequence produced by the modified mapping (8) converges, albeit slowly. Figure 3 shows the result of applying the modified mapping using the y nullcline (equation (3b)) as a starting function with the same parameters as were used to produce figure 2. Slow (but reasonable) convergence is observed.

5. Conclusion

The method we have developed here for stabilizing functional iteration requires a few steps, some of which may be difficult in particular cases:

1. As much information as possible is obtained concerning the fixed point under investigation (behavior at extreme values of the arguments, etc.).
2. The mapping is transformed by the method of Thomas, Richelle and d'Ari to an equivalent functional mapping.
3. The modified mapping is linearized about the fixed point of interest.
4. The weighting function is chosen from an analysis of the linearization. This is the most difficult step of the process and, in some cases, there may not exist a weighting function which both adequately suppresses divergence and leads to acceptable rates of convergence. Furthermore, even when good weighting functions exist, it may be very difficult to extract one from the error analysis. However, it may be possible to guess a reasonable form in many cases. If difficulties are encountered here, it may be sensible to go back to step 1 to see if any important geometric information about the function being approximated has been neglected.

In short, either technical or theoretical difficulties may prevent a successful application of the method described in this paper to any given problem. Nevertheless, it is a potentially extremely useful addition to a theoretician's bag of tricks.

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