Reduced Manifolds and Trajectory Curvature

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***Abstract*— It is shown by counter-example that slow invariant manifolds are not associated with points of vanishing solution trajectory curvature. However, vanishing trajectory curvature may be associated with an intrinsic low-dimensional manifold, which approaches a slow invariant manifold as stiffness increases.**

I. Introduction

The identification of slow invariant manifolds associated with nonlinear dynamical systems that describe spatially homogeneous chemical kinetics is a key problem of model reduction for reactive systems. See [1], [2] and references therein for background. In short, the phase space in which non-reduced reactive systems evolves is typically of high dimension, and manifold methods identify manifolds of lower dimension to which the system is attracted at long time. Projection of high-dimensional trajectories onto lower dimensional manifolds can potentially reduce the stiffness of the system while maintaining high fidelity to the underlying high-dimensional system. This can enable more computationally efficient calculation of reaction dynamics.

Ginoux and co-workers [3], [4] have stated that one can identify slow invariant manifolds (SIMs) of two-dimensional dynamical systems by identifying zero-curvature manifolds (ZCMs): those points within the phase space where the curvature of solution trajectories vanishes. Additional development is in [5]. It will be shown here that this criterion fails for the well known Davis-Skodje (DS) [6] system. Instead, the ZCM is found to identify the so-called intrinsic low-dimensional manifold (ILDM) [7].

II. General analysis

We summarize some concepts discussed in detail in [1]-[7]. Spatially homogeneous chemical kinetics can be cast as dynamical system of the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}). \tag{1}$$

Here, we consider $\mathbf{x}$ to be related to the species concentration and think of it as a position in phase space. We consider $\mathbf{v}$ to be the constitutive equation for chemical kinetics, and think of it as a velocity in phase space. Local dynamics may often be analyzed with the aid of the Jacobian matrix $\mathbf{J}$ which is the Fréchet derivative of $\mathbf{v}$ with respect to $\mathbf{x}$:

$$\mathbf{J} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}}. \tag{2}$$

It is the reciprocals of the real parts of the eigenvalues of $\mathbf{J}$ that give the local time scales of reaction. The acceleration $\mathbf{a}$ in phase space is given by

$$\mathbf{a}(\mathbf{x}) = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \frac{d\mathbf{x}}{dt} = \mathbf{J} \cdot \mathbf{v}. \tag{3}$$

The curvature κ of any trajectory is given by

$$\kappa = \frac{||\mathbf{a} \times \mathbf{v}||}{||\mathbf{v}||^3}. \tag{4}$$

The curvature κ vanishes at points $\mathbf{x}$ for which the velocity $\mathbf{v}$ is aligned with the acceleration $\mathbf{a}$.

III. Analysis of the DS System

A. Exact Solution

Consider the DS system, taking $x > 0$, $\gamma > 1$:

$$\frac{dx}{dt} = -x, \qquad x(0) = x_0, \tag{5}$$

$$\frac{dy}{dt} = -\gamma y + \frac{(\gamma-1)x + \gamma x^2}{(1+x)^2}, \qquad y(0) = y_0. \tag{6}$$

The exact solution is

$$x(t) = x_0 e^{-t}, \tag{7}$$

$$y(t) = \frac{x_0 e^{-t}}{1 + x_0 e^{-t}} + \left(y_0 - \frac{x_0}{1+x_0} \right) e^{-\gamma t}. \tag{8}$$

Eliminating t, the exact solution in the phase plane is

$$y(x) = \frac{x}{1+x} + \left(y_0 - \frac{x_0}{1+x_0} \right) \left(\frac{x}{x_0} \right)^{\gamma}. \tag{9}$$

As $\gamma > 1$, the curve approached from arbitrary initial conditions is

$$y_{SIM} = \frac{x}{1+x}. \tag{10}$$

Thus, y_{SIM} captures the slow dynamics of the system. Moreover, if the initial conditions are such that they lie on $y_{SIM}(x)$: $y_0 = x_0/(1+x_0)$, then y_{SIM} is itself a solution trajectory, and thus an invariant manifold.

The exact expressions for $\mathbf{J}$ and $\mathbf{a}$ are

$$\mathbf{J} = \begin{pmatrix} -1 & 0 \\ \frac{\gamma - 1 + (\gamma+1)x}{(1+x)^3} & -\gamma \end{pmatrix}, \tag{11}$$

$$\mathbf{a} = \begin{pmatrix} x \\ \gamma^2 y - \frac{x\left(\gamma^2 (x+1)^2 + x - 1\right)}{(x+1)^3} \end{pmatrix}. \tag{12}$$

The eigenvalues of $\mathbf{J}$ are $\lambda_1 = -1$, $\lambda_2 = -\gamma$. The stiffness ratio is $|\lambda_2/\lambda_1| = \gamma$. Stiffness increases as γ increases. The unique finite fixed point $(0, 0)$ is guaranteed stable because both eigenvalues are everywhere negative, including in the neighborhood of the fixed point.

B. ILDM

As derived in [7] and shown in [2], [6], the ILDM is found by projecting Eqs. (5,6) onto a basis formed from fast and slow eigenmodes of $\mathbf{J}$ and equilibrating the differential equation associated with the fastest time scale. This yields an algebraic equation for the ILDM; solving this for y and simplifying, the ILDM for the DS system is given by

$$y_{ILDM} = \underbrace{\frac{x}{x+1}}_{y_{SIM}} + \frac{2x^2}{\gamma(\gamma-1)(1+x)^3}. \tag{13}$$

Obviously the ILDM and SIM are different, but approach each other as stiffness γ increases.

C. ZCM

The ZCM is seen from Eq. (4) to exist when the velocity and acceleration vectors are parallel:

$$\mathbf{a} \times \mathbf{v} = \mathbf{0}. \tag{14}$$

Use Eqs. (5,6) to form $\mathbf{v}$ and Eq. (12) for $\mathbf{a}$, substitute into Eq. (14), and solve to find the ZCM:

$$y_{ZCM} = \underbrace{\frac{x}{x+1}}_{y_{SIM}} + \frac{2x^2}{\gamma(\gamma-1)(1+x)^3}. \tag{15}$$

The ZCM is exactly the ILDM and is not the SIM. The ZCM is not a solution trajectory, so it is not an invariant manifold. Note that the ZCM itself has curvature. Solution trajectories possess no curvature when they intersect the ZCM. The ZCM approaches the SIM as stiffness γ increases.

Figure 1 shows a phase plane for the DS system with moderate stiffness, $\gamma = 3$. Included are the trajectory $y(x)$ corresponding to $x(0) = 1$, $y(0) = 3/5$, $y_{ZCM} = y_{ILDM}$, and y_{SIM}. Also shown are the vector fields of $\mathbf{v}$ and $\mathbf{a}$. The trajectory crosses through y_{ZCM} at a point where the trajectory itself has no curvature, with $\mathbf{v}$ parallel to $\mathbf{a}$. The trajectory then approaches y_{SIM}.

D. Quantification at a point

Still taking $\gamma = 3$, consider the point $x = 1$. At that point the reduction that is Eq. (10) recommends for us to project to the SIM, yielding $y_{SIM} = 1/2$. At this point, the original Eqs. (5,6) tell us $dx/dt = -1$ and $dy/dt = -1/4$. Dividing, we see at that this point Eqs. (5,6) tell us $dy/dx = 1/4$. We can differentiate directly Eq. (10) for the SIM and get

$$\frac{dy_{SIM}}{dx} = \frac{1}{(1+x)^2}, \qquad \left.\frac{dy_{SIM}}{dx}\right|_{x=1} = \frac{1}{4}. \tag{16}$$

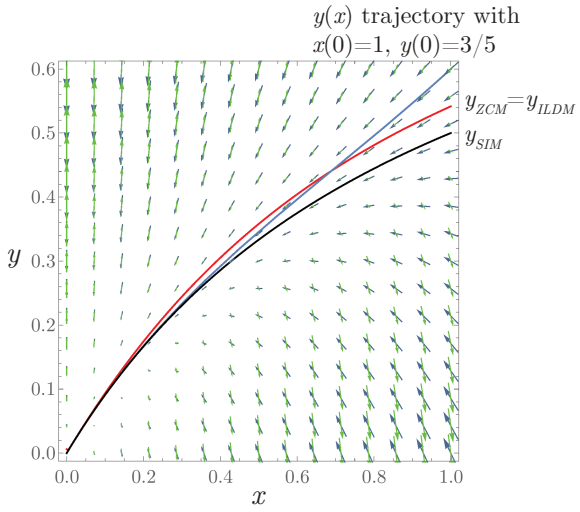

Fig. 1. Trajectory, ZCM, ILDM, SIM, $\mathbf{v}$, and $\mathbf{a}$ for DS system with $\gamma = 3$.

Thus the slope of the SIM is identical to that predicted by Eqs. (5,6). This is consistent with the SIM also being a trajectory, necessary for it to be an invariant manifold.

At the same point $x = 1$, the ZCM, Eq. (15) recommends we project to $y_{ZCM} = 13/24$. At this point, the original Eqs. (5,6) tell us $dx/dt = -1$ and $dy/dt = -3/8$. Dividing, we see at that this point Eqs. (5,6) tell us $dy/dx = 3/8$. We can differentiate directly Eq. (15) for the ZCM and get

$$\frac{dy_{ZCM}}{dx} = \frac{1}{(1+x)^2} + \frac{(x-2)x}{3(1+x)^4}, \qquad \left.\frac{dy_{ZCM}}{dx}\right|_{x=1} = \frac{13}{48}. \tag{17}$$

The slope of the ZCM is not predicted by Eqs. (5,6).

IV. Conclusion

The ZCM is an ILDM but not a SIM. The ZCM and ILDM better approximate the SIM as stiffness increases.

References

[1] J. M. Powers, S. Paolucci, J. D. Mengers, and A. N. Al-Khateeb, "Slow attractive canonical invariant manifolds for reactive systems *J. Math. Chem.*, vol. 53, 2015, pp. 737-766.

[2] S. Singh, J. M. Powers, and S. Paolucci, "On slow manifolds of chemically reactive systems," *J. Chem. Phys.*, vol. 117, 2002, pp. 1482-1496.

[3] J. M. Ginoux and B. Rossetto, "Differential geometry and mechanics: applications to chaotic dynamical systems," *Int. J. Bifurcation Chaos*, vol. 16, 2006, pp. 887-910.

[4] J. M. Ginoux, B. Rossetto, and L. O. Chua, "Slow invariant manifolds as curvature of the flow of dynamical systems," *Int. J. Bifurcation Chaos*, vol. 18, 2008, pp. 3409-3430.

[5] J. M. Ginoux, "The slow invariant manifold of the Lorenz-Krishnamurthy Model," *Quant. Theory Dyn. Syst.*, vol. 13, 2014, pp. 19-37.

[6] M. J. Davis and R. T. Skodje, "Geometric investigation of low-dimensional manifolds in systems approaching equilibrium," *J. Chem. Phys.*, vol. 111, 1999, pp. 859-874.

[7] U. Maas and S. B. Pope, "Simplifying chemical kinetics: intrinsic low-dimensional manifolds in composition space," *Combust. Flame*, vol. 88, 1992, pp. 239-264.