The Slowness of Invariant Manifolds Constructed by Connection of Heteroclinic Orbits

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***Abstract*— It is demonstrated that a common technique in reaction dynamics for construction of Slow Invariant Manifolds, connection of equilibria by heteroclinic orbits, can fail. While the method is guaranteed to generate an invariant manifold, the local dynamics far from equilibrium may be such that nearby trajectories are in fact carried away from the identified invariant manifold, thus rendering it to be of limited utility in capturing slow dynamics far from equilibrium. An eigenvalue-based method is described to characterize the local behavior of such invariant manifolds.**

I. Introduction

Spatially homogeneous chemical reactions are described by dynamical systems of the form

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}), \qquad \mathbf{z}(0) = \mathbf{z}_o, \qquad \mathbf{z}, \mathbf{z}_o, \mathbf{f} \in \mathbb{R}^N. \quad (1)$$

Here, $\mathbf{z}$ is a vector of length N containing the species concentrations, assuming that linear constraints representing element conservation have been removed, t is time, and $\mathbf{f}$ is a non-linear function of $\mathbf{z}$ representing the law of mass action with Arrhenius kinetics.

We take a Slow Invariant Manifold (SIM) to be an invariant manifold (IM) on which slow dynamics are confined and to which nearby trajectories are attracted. The identification of one-dimensional SIMs by constructing heteroclinic orbits connecting equilibria has gained attention since its introduction [1] and extension by others, *e.g.* [2], [3], [4]. The essence of the fundamental hypothesis is illustrated in Fig. 1. That hypothesis is that SIMs may be constructed by 1) identifying equilibria of Eq. (1), *i.e.* points $\mathbf{z}$ where $\mathbf{f}(\mathbf{z}) = \mathbf{0}$, and 2) connecting by trajectories from appropriate

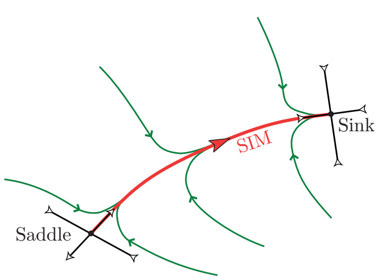

Fig. 1. Sketch of SIM envisioned as the invariant manifold connecting equilibria.

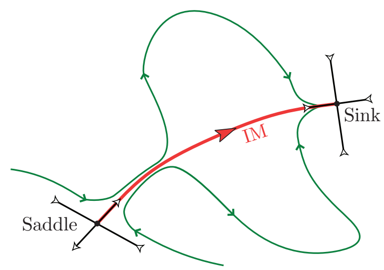

Fig. 2. Sketch of failure of the method of heteroclinic orbit construction for SIM identifcation.

non-physical saddle equilibria (those with at most one positive eigenvalue) to the unique physical equilibrium, which is a sink. Near the equilibria, the IM is guaranteed to be attractive; moreover, for many reactive systems the IM appears to be attractive in regions far from equilibrium.

However, nothing in the SIM construction algorithm precludes the scenario sketched in Fig. 2. Certainly, equilibria can be identified and connected via heteroclinic orbits to construct a canonical IM. But for a generic $\mathbf{f}(\mathbf{z})$, one has no guarantee that trajectories near the canonical IM are in fact attracted to it. In this study, we summarize analyses and an example given by Mengers [5] for attractiveness criteria for an IM; additional background is to be found in [6].

II. Summary of Analysis

With the local Jacobian $\mathbf{J} = \partial\mathbf{f}/\partial\mathbf{z}$, defined throughout the entire phase space, one can analyze $\mathbf{J}$ in the neighborhood of any IM, such as an IM connecting equilibria. At the physical equilibrium, all of the eigenvalues of $\mathbf{J}$ are guaranteed to be negative and real, and all nearby points will be drawn to the physical equilibrium. Away from the physical equilibrium, it is possible for some eigenvalues to be positive, and this can lead to certain trajectories being drawn away from an IM. It is well known that $\mathrm{tr}(\mathbf{J})$ is proportional to the rate of change of a local volume in phase space. However, even if $\mathrm{tr}(\mathbf{J}) < 0$, the existence of a positive eigenvalue can induce a local repulsion of an individual trajectory from an IM.

It is possible [2], [5] to identify a unit tangent vector to the IM, $\boldsymbol{\alpha}_t$, and a set of unit normal vectors, $\boldsymbol{\alpha}_{ni}, i = 1, \ldots, N-1$. These vectors can be used to identify the tangential and normal stretching rates, σ_t and σ_{ni}:

$$\sigma_t = \boldsymbol{\alpha}_t^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_t, \;\; \sigma_{ni} = \boldsymbol{\alpha}_{ni}^T \cdot \mathbf{J}_s \cdot \boldsymbol{\alpha}_{ni}, \;\; i = 1, \dots, N-1. \tag{2}$$

Here $\mathbf{J}_s = (\mathbf{J} + \mathbf{J}^T)/2$, the symmetric part of $\mathbf{J}$. Along the IM, $\boldsymbol{\alpha}_t$ is uniquely defined, up to its sign. However, there are an infinite set of $\boldsymbol{\alpha}_{ni}$ when $N > 2$. Certainly if all possible $\sigma_{ni} < 0$ and $\min_i |\sigma_{ni}| \gg |\sigma_t|$, the IM will be a SIM; however, it is easy to construct cases for which these criteria are not met.

One can pose the following optimization problem to identify the maximum σ_n and its associated $\boldsymbol{\alpha}_n$. First, we can recast $\mathbf{J}_s = \mathbf{Q} \cdot \boldsymbol{\Lambda} \cdot \mathbf{Q}^T$, where $\mathbf{Q}$ is a rotation matrix with normalized eigenvectors of $\mathbf{J}_s$ in its columns, and $\boldsymbol{\Lambda}$ is a diagonal matrix with the eigenvalues of $\mathbf{J}_s$ on its diagonal. Then we seek $\boldsymbol{\alpha}_n$ to maximize

$$\sigma_n = (\mathbf{Q}^T \cdot \boldsymbol{\alpha}_n)^T \cdot \boldsymbol{\Lambda} \cdot (\mathbf{Q}^T \cdot \boldsymbol{\alpha}_n), \tag{3}$$

subject to

$$\boldsymbol{\alpha}_n^T \cdot \boldsymbol{\alpha}_n = 1, \qquad \boldsymbol{\alpha}_n^T \cdot \boldsymbol{\alpha}_t = 0. \tag{4}$$

Because $\mathbf{Q}$ and $\boldsymbol{\alpha}_n$ both have unit norms, it is obvious that $|\sigma_n| \le |\lambda_{max}|$, where $|\lambda_{max}|$ is the magnitude of the largest eigenvalue of $\mathbf{J}_s$.

III. Example

Consider the system, of the form of Eq. (1), with $N = 3$:

$$\frac{dz_1}{dt} = \frac{1}{20}(1 - z_1^2), \tag{5a}$$

$$\frac{dz_2}{dt} = -2z_2 - \frac{35}{16}z_3 + 2(1 - z_1^2)z_3, \tag{5b}$$

$$\frac{dz_3}{dt} = z_2 + z_3. \tag{5c}$$

This system has two finite roots, R_1 at $\mathbf{z} = (-1, 0, 0)^T$ and R_2 at $\mathbf{z} = (1, 0, 0)^T$. The Jacobian $\mathbf{J}$ has eigenvalues of $\lambda = \{1/10, -1/4, -3/4\}$ at R_1 and $\lambda = \{-1/10, -1/4, -3/4\}$ at R_2. Thus, R_1 is a saddle with one unstable mode, and R_2 is a sink, analogous to a physical equilibrium in a reactive system. There is a canonical IM defined by the heteroclinic orbit that connects R_1 to R_2 along the $z_2 = z_3 = 0$ axis; however, we find this branch does not attract neighboring trajectories along the entire IM, as is obvious by inspecting Fig. 3, which shows a projection of the IM and nearby trajectories in the (z_1, z_3) plane. The unit tangent to the canonical IM is $\boldsymbol{\alpha}_t = (1, 0, 0)^T$, yielding a tangential stretching rate of $\sigma_t = -z_1/10$. On the canonical IM, we thus find that $\sigma_t \sim 1/10$ near R_1 and $\sigma_t \sim -1/10$ near the physical equilibrium R_2. There exist points all along the canonical IM with $\sigma_n > 0$. For example, at $\mathbf{z} = (0, 0, 0)^T$, the maximum normal stretching rate is $\sigma_{n,max} = -1/2 + \sqrt{2473}/32 = 1.05$ for $\boldsymbol{\alpha}_n = (0, -0.132, -0.991)^T$. Near the physical equilibrium at $\mathbf{z} = (1, 0, 0)^T$, one still finds $\sigma_{n,max} = -1/2 + \sqrt{2665}/32 = 1.11$ for $\boldsymbol{\alpha}_n = (0, -0.187, 0.982)^T$, but the real negative eigenvalues of $\mathbf{J}$ itself render all trajectories to be attracted to the equilibrium. It is likely that non-normality effects [7] need to be further analyzed to better explain the behavior.

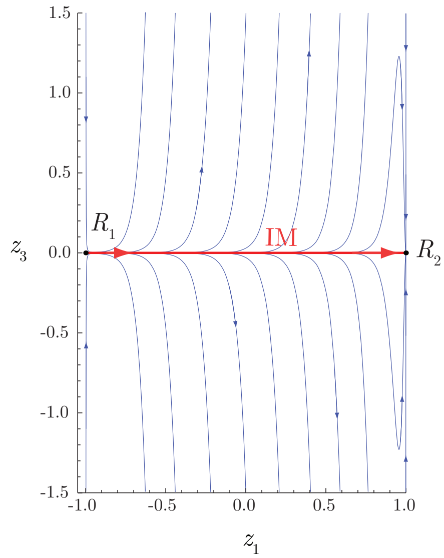

Fig. 3. Projection of the IM connecting equilibria along with nearby trajectories illustrating the non-attractive regions of the IM.

IV. Conclusion

Construction of invariant manifolds via connection of equilibria by heteroclinic orbits offers no guarantee that one has found a slow invariant manifold.

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