Stretching-Based Diagnostics in a Differential Geometry Setting

Johannes Poppe*, Dirk Lebiedz*

*Institute for Numerical Mathematics, Ulm University, Germany

Abstract—It is a prominent challenge to analytically characterize slow invariant manifolds for dynamical systems with multiple time-scales. To this end, we transfer the system into a differential-geometric framework. This setting enables to formulate stretching-based diagnostics in a new context, coinciding with the intrinsic differential-geometric property of sectional curvature.

I. INTRODUCTION

The identification of slow invariant manifolds (SIMs) is an essential part in model-order reduction for reactive systems. The mathematical definition of the SIM by Fenichel can be considered unsatisfactory, because it is only applicable to so-called slow-fast system and does not provide the uniqueness of the SIM. Observing the phase space of the dynamical system (not necessarily a slow-fast system), the SIM becomes a geometric object which attracts trajectories, resulting in a bundling behavior. We aim to find a more general definition of the SIM, guided by the prior observations in phase space within the field of differential geometry. This setting provides one major benefit: All quantities are formulated covariantly, i.e. they are independent of the coordinate choice. A recent work by Heiter and Lebiedz [1] translates the invariance property to multiple time-scales. To this end, we transfer the system to formulate stretching-based diagnostics in a new context, coinciding with the intrinsic differential-geometric property of sectional curvature.

II. GEODESICS IN SPACETIME

Let \( \dot{x} = f(x) \) with \( x \in \mathbb{R}^n \) and \( f: \mathbb{R}^n \to \mathbb{R}^n \) be sufficiently smooth. We consider the extended state space, i.e., the original state space is extended by an additional time-axis \( \tau \). In order to clarify that \( \tau \) is part of the extended state space, we call \( \tau \) "explicit time". In contrast, \( t \) is called implicit time. The resulting curves in the extended system are the solutions of

\[
\frac{d}{dt} \begin{pmatrix} x \\ \tau \end{pmatrix} = \begin{pmatrix} f(x) \\ 1 \end{pmatrix} \in \mathbb{R}^{n+1}.
\]

(1)

Bundling behavior of trajectories of the original system corresponds to bundling of the solutions of (1). The space \( M := \mathbb{R}^{n+1} \) is trivially a manifold. By defining a metric tensor \( g \) (a family of inner products that varies smoothly from point to point), the tuple \((M, g)\) becomes a Riemannian manifold. The core idea is to couple the dynamics of (1) with a metric such that every trajectory becomes a geodesic - a shortest connection path for each tuple of points on the trajectory with regard to the chosen metric. An evident choice for the connection is the so-called Levi-Civita connection. In this setting, solutions of the extended system can be interpreted in analogy to free falling particles in a gravitational field within the framework of general relativity. In the context of chemical reaction mechanisms, the gravitational field correlates to an abstract chemical force. A suitable choice for a metric \( g \) can be derived and expressed by its components regarding the standard coordinates \( x_1, \ldots, x_n, \tau \):

\[
g_{ij} = \begin{pmatrix} \text{Id}_n & -f(x) \\ -f(x)^T & 1 + f(x)^T f(x) \end{pmatrix}.
\]

The bundling trajectories of the extended system (1) becomes a set of geodesics which bundle alongside a specific subset/submanifold of geodesics - the SIM in space time. Hence, the SIM is supposed to be characterized by some differential geometric property representing this bundling behavior.

III. GEODESIC STRETCHING

In general relativity, bundling behavior is related to geodesic deviation, neighboring geodesics experience relative accelerations towards each other.

A. Geodesic Deviation

For \( p \in M \), each geodesic \( \ell: (-\varepsilon, \varepsilon) \to M \) passing through \( p \) at \( t = 0 \) defines the tangent vector

\[
T := \frac{d\ell}{dt}(0) \in T_p M, \quad \text{here:} \quad T = \begin{pmatrix} f(x) \\ 1 \end{pmatrix},
\]

because we plug-in solution trajectories of (1). Geodesic deviation is formally defined as the endomorphism \( R_{\text{dev},p} : T_p M \to T_p M \) formed by inserting the tangent vector \( T \)
into the first and third argument of the Riemann curvature tensor $R_p : (T_p M)^3 \to T_p M$,

$$R_{dev,p}(s) := R_p(T, s)T.$$  \hfill (2)

The intuitive concept of geodesic deviation is shown in Fig. 1. The input vector $s$ is the so-called "separation vector" representing a small difference between two points on the paths of two neighboring geodesics. The output vector represents the relative acceleration between both geodesics.

B. Stretching-Based Diagnostics

In [2], Adrover et al. study SIMs by comparing so-called stretching ratios $\omega_v(x)$ of solution trajectories of a given dynamic system $\dot{x} = F(x)$ for different vectors $v(x) \in \mathbb{R}^n = T_p \mathbb{R}^n$. Each stretching rate is defined by

$$\omega_v(x) := \frac{\langle J_F v, v \rangle}{\langle v, v \rangle},$$

where $J_F$ represents the Jacobian matrix of $F$. For a given sub-manifold $U \subset \mathbb{R}^n$ and $p \in U$, the tangent space $T_p \mathbb{R}^n$ is decomposed into the direct sum of tangent space $T_p U$ and normal space $N_p U$. Adrover et al. argue that on the SIM, stretching in normal directions is supposed to dominate tangent directions. Hence - in case of a one-dimensional SIM in a two-dimensional system, with $v_t$ and $v_0$ being tangent and normal to the trajectory respectively - the so-called stretching ratio

$$r(x) := \frac{\omega_{v_0}(x)}{\omega_{v_t}(x)}$$

is supposed to be larger than one at the SIM. Bundling of trajectories is directly correlated to the stretching ratio. It appears evident that $r(x)$ is particularly large on the SIM, making its maximization on the phase space for a fixed choice of reaction progress variables (RPVs) a viable option to approximate the SIM.

C. Adapting the Stretching-Based Approach

We integrate this stretching-based approach within the framework from subsection III-A in the following way: We replace the euclidean metric $\langle \cdot, \cdot \rangle$ with the metric $g$ defined above and expand each $v \in T_p \mathbb{R}^n$ by an additional explicit time component (which is set to 0): $\mathbb{R}^n \ni v \mapsto \begin{pmatrix} v \\ 0 \end{pmatrix} := \tilde{v} \in \mathbb{R}^{n+1}$.

Instead of the Jacobian matrix acting on each tangent vector representing an infinitesimal acceleration, we apply the geodesic deviation endomorphism defined in (2). The result is the notion of so-called geodesic stretching

$$\omega_{g,v} := \frac{g(R_{dev,p}(\tilde{v}), \tilde{v})}{g(\tilde{v}, \tilde{v})}.$$  

D. Geometrical Interpretation

One can show that $\omega_{g,v}$ has an intrinsic differential geometric meaning: It represents the sectional curvature $K(\tilde{v}, \tilde{v})$ of the expanded vector $\tilde{v}$ with tangent vector $T$ of each space time trajectory from above:

$$\frac{g(R(\tilde{v}, \tilde{v}) T, \tilde{v})}{g(\tilde{v}, \tilde{v})} - g(\tilde{v}, T)^2 := K(\tilde{v}, T).$$

Sectional curvature depends on the given metric $g$. Hence, there is no direct connection to the utilized sectional curvature in [1] which is based on a different metric.

E. Results

We test our ansatz by considering the well-known nonlinear Davis-Skodje (DS) system:

$$\frac{dx}{dt} = -x$$

$$\frac{dy}{dt} = -\gamma y + \left(\gamma - 1\right) x + \gamma x^2$$

where $\gamma > 1$ is a fixed parameter and $x > 0$. This system has a one-dimensional SIM given by the graph representation $y = h(x) = \frac{x}{1+x}$. Fig. 2 shows geodesic stretching ratios near the SIM for system (3) with $\gamma = 3$. Setting $x$ as RPV and maximizing the ratio with respect to $y$ yields points near the SIM.

**ACKNOWLEDGEMENT**

Special thanks goes to the Klaus-Tschira foundation for financial funding of the project.

**REFERENCES**

[1] P. Heiter and D. Lebiedz, “Towards Differential Geometric Characterization of Slow Invariant Manifolds in Extended Phase Space: Sectional Curvature and Flow Invariance”, in SIAM J. Applied Dynamical Systems Vol. 17 (2018), No. 1, pp. 732–753

[2] A. Adrover, F. Creta, M. Giona, M. Valorani, “Stretching-based diagnostics and reduction of chemical kinetic models with diffusion”, in Journal of Computational Physics 225 (2007) 1442–1471