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A Versatile Algorithm for Computing Invariant Manifolds

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Summary. This paper deals with the numerical computation of invariant manifolds using a method of discretizing global manifolds. It provides a geometrically natural algorithm that converges regardless of the restricted dynamics. Common examples of such manifolds include limit sets, co-dimension 1 manifolds separating basins of attraction (separatrices), stable/unstable/center manifolds, nested hierarchies of attracting manifolds in dissipative systems and manifolds appearing in bifurcations. The approach is based on the general principle of normal hyperbolicity, where the graph transform leads to the numerical algorithms. This gives a highly multiple purpose method. The algorithm fits into a continuation context, where the graph transform computes the perturbed manifold. Similarly, the linear graph transform computes the perturbed hyperbolic splitting. To discretize the graph transform, a discrete tubular neighborhood and discrete sections of the associated vector bundle are constructed. To discretize the linear graph transform, a discrete (un)stable bundle is constructed. Convergence and contractivity of these discrete graph transforms are discussed, along with numerical issues. A specific numerical implementation is proposed. An application to the computation of the ‘slow–transient’ surface of an enzyme reaction is demonstrated.

1 Introduction

Invariant manifolds of dynamical systems typically determine the skeleton of the dynamics, around which a further analysis may be in order. This is true whether the system is dissipative or conservative. For dissipative systems, the phase space often contains a nested hierarchy of attracting manifolds $V_i \subset V_{i+1}$, $i = 0, \dots, n$. The manifold V_i is composed of initial data which evolves slowly compared to initial data in the rest of V_{i+1} . The manifold V_0 contains the global attractor, which may be an equilibrium point or more complicated set. The long-time (medium-time) dynamics is described by the system restricted to V_0 (V_1). By restricting the system to a lower dimensional

manifold, fast transients are removed from consideration. Thus, the dimension of the model is reduced while retaining the essential features of the dynamics.

Analytical formulae for the lower dimensional manifolds and the corresponding reduced systems are only obtainable in special cases. Hence, methods of approximating these manifolds are desirable. For example, in applied bifurcation theory, the center manifold of an equilibrium is approximated locally by polynomials, using a recursive algebraic procedure [23]. This allows the local approximation of the system restricted to the center manifold, up to sufficiently high-order terms. An analysis of the bifurcation is then performed on the approximate center manifold.

In the present paper, we focus on a numerical algorithm which computes global invariant manifolds. This allows a global approximation of the system restricted to the invariant manifold, in principle to arbitrary accuracy. This may aid further analysis of long-time non-local dynamics.

The algorithmic approach is based on the principle of normal hyperbolicity. According to the Invariant Manifold Theorem, normally hyperbolic invariant manifolds persist smoothly under small perturbations of the system. To be specific, the Invariant Manifold Theorem is concerned with the following setup. Given a diffeomorphism F and an F -invariant submanifold V , the invariant manifold \tilde{V} for a nearby diffeomorphism \tilde{F} is constructed. Based on this, an invariant manifold \tilde{V} for the system of interest, \tilde{F} , may be computed given an analytically known initial manifold V for a nearby system F . It turns out that a rough estimate of an initial manifold V is often enough. In addition, the algorithm may be repeated with computed initial data, allowing the potential to compute invariant manifolds of systems not necessarily near a system with a known manifold.

The algorithm is adapted from one of the classical approaches to the proof of the Invariant Manifold Theorem, the graph transform. The theory of invariant manifolds using the graph transform is well developed [21]. In particular the convergence properties of the graph transform are inherited by the algorithm. This complete theory of convergence is one thing that distinguishes this approach from many other approaches to computing invariant manifolds in the literature.

The implementation of methods for computing (non-local) manifolds of dimension ≥ 2 is fairly recent. Some of the related work in this category concerns quasiperiodic (for example [17]) or attracting (for example [10]) tori, parts of global attractors [9] or global (un)stable manifolds [22]. The computations of tori use global parametrizations of the tori where simplicial complexes are used in the present paper. The computations of parts of global attractors use successive subdivisions of a covering of part of the global attractor. This approach computes global attractors which are smooth or non-smooth. The computations of global (un)stable manifolds are concerned with extending a given piece of the manifold, to fill out the global (un)stable manifold. The present paper has the antecedents [2, 3, 5, 27]. In [5, 27] a method to compute saddle-type manifolds is presented. The graph transform and simplicial com-

plexes are used to approximate manifolds. The present paper, starting with a simplicial complex, uses a piecewise polynomial approximation. To do this, a discrete tubular neighborhood is constructed. An approximation of arbitrary order for any manifold is obtained. A tubular neighborhood of V is the geometrical setting of the graph transform. Thus, a discrete tubular neighborhood is a natural approach which allows an analogous development of a discrete graph transform. In addition, the construction of a discrete (un)stable bundle allows a natural derivation of the discrete linear graph transform.

Compared to related work, the present approach gives a general purpose algorithm. It applies to manifolds of arbitrary topological type, attracting or saddle-type, regardless of the restricted dynamics. There is a satisfactory theory of convergence in this general setting. If the manifold is not normally hyperbolic, however, a different approach should be used, see for example [17]. Other novel features of the present paper include the following. In Section 5, a practical approach to solving the global equations associated with the discrete graph transform is proposed. In Section 6, the graph transform approach is used to compute a part of the ‘slow-transient’ surface of an enzyme reaction model. This is the first time this approach has been used to compute this type of surface. For numerical methods designed specifically for this type of problem, see [15, 16, 30].

To repeatedly apply the algorithm, both the perturbed manifold \tilde{V} and its hyperbolic splitting must be approximated. This is done by first using the graph transform Γ to obtain \tilde{V} and then the linear graph transform \mathcal{L} to compute the hyperbolic splitting of \tilde{V} . Thus, in Section 2, Γ and \mathcal{L} are formulated. This includes a discussion of normal hyperbolicity, the Invariant Manifold Theorem, tubular neighborhoods and hyperbolic splittings. In Section 3, the discretizations of the domains of Γ and \mathcal{L} are formulated. To do this, a discrete tubular neighborhood along with a space of discrete sections of the associated vector bundle are constructed. In Section 4, discrete versions Γ_D of Γ and \mathcal{L}_D of \mathcal{L} are formulated, based on the discrete approximating sections of Section 3. Analyses of the convergence and contractivity of Γ_D and \mathcal{L}_D are given. In Section 5, an outline of a computer implementation of the algorithm is given. Some auxiliary numerical techniques, along with numerical conditioning and error, are also discussed. Section 6 contains an application to an enzyme reaction model. For more examples, see [2, 3] or the DISC project website, <http://home.nethere.net/hagen>.

2 Invariant Manifolds

In this section, the basic theory of normally hyperbolic invariant manifolds is introduced. An overview of some definitions and results from [21] is given. For locating a perturbed manifold, the graph transform is formulated. The linear graph transform is formulated to locate the hyperbolic splitting of this perturbed manifold. In later sections, discrete versions of these graph trans-

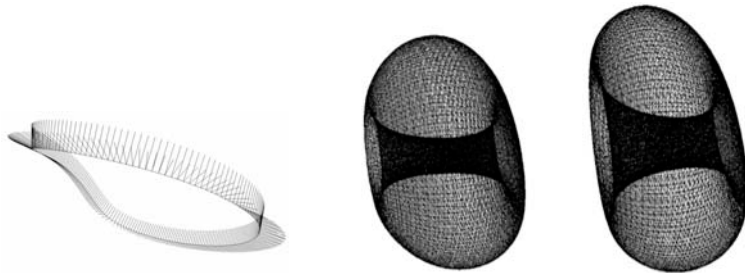


Fig. 1: Lorenz system orbit and hyperbolic splitting; two tori in the Lorenz-84 system, moving away from a Hopf saddle–node bifurcation [23].

forms, suitable for a numerical implementation, will be given. This will be done by replacing the basic elements, like tubular neighborhoods and sections of vector bundles, with discrete constructions.

2.1 Normal Hyperbolicity

The starting point is a C^r diffeomorphism F on a C^∞ Riemannian manifold M , with an invariant submanifold $V \subset M$. Here, V is a compact, C^r , r -normally hyperbolic submanifold of M , $r \geq 1$. The submanifold V is r -normally hyperbolic for F if there is a DF -invariant splitting

$$T_V(M) = N^u(V) \oplus T(V) \oplus N^s(V), \quad (1)$$

and a Riemann structure on the tangent bundle $T_V(M)$, such that, for $y \in V$, $i \geq 0$, and $0 \leq k \leq r$:

$$\begin{aligned} \|DF^i|N_y^s(V)\| \cdot \|(DF^i|T_y(V))^{-1}\|^k &\leq c\mu^i, \\ \|(DF^i|N_y^u(V))^{-1}\| \cdot \|DF^i|T_y(V)\|^k &\leq c(1/\lambda)^i, \end{aligned} \quad (2)$$

for some $0 < \mu < 1 < \lambda < \infty$ and $0 < c < \infty$. Here the operator norms are associated with the Riemann structure on $T_V(M)$. For example, consider the attracting case, $N_y^u(V) = \{0\}$, $y \in V$ and $r = 1$. Condition (2) concerns the linearization of F at V , in other words DF on $T_V(M)$. It states that under the action of the linearization, vectors normal to V are asymptotically contracted more than vectors tangent to V . This means that under the action of the dynamical system F , a neighborhood of a point in V is flattened in the direction of the manifold.

The *Invariant Manifold Theorem* [21, Theorem 4.1] states that a C^r diffeomorphism \tilde{F} , that is C^r -near F , has an r -normally hyperbolic invariant manifold \tilde{V} , that is C^r and C^r -near V . This theorem and its proof suggests

that it may be possible to compute an approximation to \tilde{V} from a given V . To implement this idea, we look more closely at a proof of the invariant manifold theorem.

First, we focus on a tubular neighborhood of V [20, 24]. A tubular neighborhood of V in M is a vector bundle E with base space V , an open neighborhood U of V in M , an open neighborhood Z of the zero section in E and a homeomorphism $\phi : Z \rightarrow U$. Here, ϕ must satisfy $\phi \circ \sigma_0 = i$, where $\sigma_0 : V \rightarrow E$ is the zero section and $i : V \rightarrow M$ is the inclusion. For example, the normal bundle $E = \bigcup_{p \in V} T_p(V)^\perp$ of V in M gives a tubular neighborhood of V , at least if $r \geq 2$. In fact, any Lipschitz vector bundle $N(V)$, transverse to $T(V)$ in $T_V(M)$, gives a tubular neighborhood of V in M . In the following, \tilde{V} is constructed in the neighborhood U in M , or equivalently in the neighborhood Z in $N(V)$. A slight technical adjustment is made here. Namely, below, Z is the closure of a neighborhood, $Z = Z(\epsilon) = \{(p, v) \in N(V) : |v|_p \leq \epsilon\}$.

For any Lipschitz transverse vector bundle $N(V)$, the invariant splitting (1) induces a splitting $N(V) = N^u(V) \oplus N^s(V)$ into stable and unstable parts. The hyperbolic splitting $T_V(M) = N^u(V) \oplus T(V) \oplus N^s(V)$ has the same growth properties (2) as the invariant splitting. Sections of Z may now be written $\sigma(p) = (p, v^s(p), v^u(p))$, where $v^s(p) \in Z_p^s = N_p^s(V) \cap Z$, $v^u(p) \in Z_p^u = N_p^u(V) \cap Z$.

2.2 The Graph Transform

The graph transform uses the \tilde{F} -dynamics near V to locate \tilde{V} . The domain of the graph transform is a certain space of sections of the vector bundle $Z = Z(\epsilon)$. The graphs of the sections in the domain are the Lipschitz manifolds near V in Lipschitz norm. In fact, the graph transform is a contraction on a space of Lipschitz sections $\sigma : V \rightarrow Z$. To define the Lipschitz constant of a section, a C^0 connection in $T_V(M)$ is used [25]. A connection gives a way to compare points in different fibers of $T_V(M)$. It does this using a continuous family of horizontal subspaces $H(y)$, $y \in T_V(M)$, which extend the tangent spaces of V . More precisely, a C^0 connection in the vector bundle $\pi : T_V(M) \rightarrow V$ is a C^0 distribution $H : T_V(M) \rightarrow T(T_V(M))$ with $T_y(T_V(M)) = H(y) \oplus V(y)$, $y \in T_V(M)$, where $V(y)$ is the kernel of $D\pi$. Here, it is also required that the horizontal subspace of the associated frame bundle corresponding to $H(y)$ be invariant under the structure group. This implies, in particular, that if $\sigma_0 : V \rightarrow T_V(M)$ is the zero section, then $H(\sigma_0(p)) = D\sigma_0(T_p(V))$.

To define the slope of a section $\sigma : V \rightarrow T_V(M)$ at $p \in V$, let $\theta : V \rightarrow T_V(M)$ be a C^1 section with $\theta(p) = \sigma(p)$ and $D\theta(T_p(V)) = H(\sigma(p))$. Then the slope of σ at p is

$$\text{slope}_p(\sigma) = \limsup_{x \rightarrow p} \frac{|\sigma(x) - \theta(x)|_x}{d_V(x, p)},$$

[21]. Since Z^s and Z^u are subbundles of $T_V(M)$, this also gives a natural definition of the slope of sections $\sigma^s : V \rightarrow Z^s$ and $\sigma^u : V \rightarrow Z^u$. From this,

the Lipschitz constant of σ^s is $\text{Lip}(\sigma^s) = \sup_{p \in V} \text{slope}_p(\sigma^s)$, and similarly for σ^u . Now, the Lipschitz constant of a section $\sigma(p) = (p, v^s(p), v^u(p))$ of Z is $\text{Lip}(\sigma) = \max\{\text{Lip}(\sigma^s), \text{Lip}(\sigma^u)\}$, where $\sigma^s(p) = (p, v^s(p))$ and $\sigma^u(p) = (p, v^u(p))$. The domain of the graph transform is $\mathcal{S}_{\epsilon, \delta} = \{\sigma : V \rightarrow Z : \text{Lip}(\sigma) \leq \delta\}$. The norm on $\mathcal{S}_{\epsilon, \delta}$ is $\|\sigma\| = \max\{|\sigma^s|_s, |\sigma^u|_u\}$, where $|\cdot|_s$ and $|\cdot|_u$ are the natural C^0 norms on sections of Z^s and Z^u , respectively. With this norm, $\mathcal{S}_{\epsilon, \delta}$ is complete.

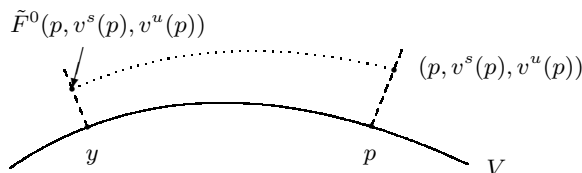


Fig. 2: Invariance condition (3).

To formulate the graph transform, the starting point is the \tilde{F} -invariance condition $\phi \circ \sigma(V) = \tilde{F} \circ \phi \circ \sigma(V)$. This is split into two coupled equations, a part on V and a part normal to V . We put $\tilde{F}^0 = \phi^{-1} \circ \tilde{F} \circ \phi$ and work in $N(V)$. The image of $\phi \circ \sigma$ is \tilde{F} -invariant if and only if

$$\begin{aligned} (y, v^s(y), v^u(y)) &= \tilde{F}^0(p, v^s(p), v^u(p)), \\ y &= \pi \circ \tilde{F}^0(p, v^s(p), v^u(p)), \end{aligned} \quad (3)$$

for $p \in V$, where $\pi : N(V) \rightarrow V$ is the vector bundle projection. See Figure 2. Under our hypotheses, $y = \pi \circ \tilde{F}^0(p, v^s(p), v^u(p))$ may be solved for a unique $p \in V$ given $y \in V$ and $\sigma \in \mathcal{S}_{\epsilon, \delta}$ for small ϵ, δ and $\theta = \|F - \tilde{F}\|_{C^1}$. Denote this solution by $p = p(y, v^s, v^u)$. Now, given $\sigma \in \mathcal{S}_{\epsilon, \delta}$, $\sigma(p) = (p, v^s(p), v^u(p))$, the *graph transform* of σ is the section $\Gamma(\sigma)(p) = (p, w^s(p), w^u(p))$. Here, w^s is defined by

$$w^s(y) = P_y^s \circ \tilde{F}^0(p, v^s(p), v^u(p)), \quad p = p(y, v^s, v^u), \quad (4)$$

for $y \in V$, where $P_y^s : N_y(V) \rightarrow N_y(V)$ is the linear projection with range $N_y^s(V)$ and nullspace $N_y^u(V)$. The unstable part w^u is defined implicitly by

$$\begin{aligned} w^u(y) &= P_y^u \circ \tilde{F}^0(p, v^s(p), w^u(p)), \\ y &= \pi \circ \tilde{F}^0(p, v^s(p), w^u(p)), \end{aligned} \quad (5)$$

for $p \in V$, where $P_y^u : N_y(V) \rightarrow N_y(V)$ is the linear projection with range $N_y^u(V)$ and nullspace $N_y^s(V)$. In (5), there is a unique solution for $w^u(p)$ for small θ, ϵ , and δ .

If $\sigma = \Gamma(\sigma)$, then (4) and (5) imply (3). Hence σ is a fixed point of Γ if and only if the graph of σ is \tilde{F} -invariant. By replacing \tilde{F} with \tilde{F}^N above, for some large integer N , Γ becomes a contraction on $\mathcal{S}_{\epsilon, \delta}$ whose fixed point σ^* satisfies $\phi \circ \sigma^*(V) = \tilde{V}$.

2.3 The Linear Graph Transform

Two linear graph transforms \mathcal{L}^s and \mathcal{L}^u are used to determine the hyperbolic splitting $N^u(\tilde{V}) \oplus T(\tilde{V}) \oplus N^s(\tilde{V})$ of \tilde{V} . Here, \mathcal{L}^s determines $N^s(\tilde{V})$ and \mathcal{L}^u determines $N^u(\tilde{V})$. These two linear graph transforms are contractions on certain spaces of sections. These spaces of sections are determined by the initial data for \mathcal{L}^s and \mathcal{L}^u .

To illustrate the details, here \mathcal{L}^u is formulated. Given a transverse bundle $N(\tilde{V})$, first the initial data for \mathcal{L}^u in $N(\tilde{V})$ is determined. Let $Q : T_{\tilde{V}}(M) \rightarrow T_{\tilde{V}}(M)$, be, on each fiber $T_y(M)$, the linear projection with range $N_y(\tilde{V})$ and nullspace $T_y(\tilde{V})$. Initial data $N(\tilde{V}) = N^{u,0}(\tilde{V}) \oplus N^{s,0}(\tilde{V})$ are then

$$N^{u,0}(\tilde{V}) = Q(N^{u,1}(\tilde{V})), \quad N^{s,0}(\tilde{V}) = Q(N^{s,1}(\tilde{V})),$$

where $N_y^{u,1}(\tilde{V})$, $N_y^{s,1}(\tilde{V})$ are obtained from $N_p^u(V)$, $N_p^s(V)$, $y = \phi \circ \sigma^*(p)$, by parallel translation $T_p(M) \rightarrow T_y(M)$ along ϕ -images of fibers of $N(V)$, [1, 25]. There exists $\alpha > 0$, where $\alpha \rightarrow 0$ as $\epsilon + \delta + \theta \rightarrow 0$, such that, if $\{\angle N(V), T(V)\}$, $\{\angle N(\tilde{V}), T(\tilde{V})\} \geq \alpha > 0$, then this procedure produces non-degenerate initial data $N^{u,0}(\tilde{V}), N^{s,0}(\tilde{V})$.

The domain of \mathcal{L}^u is a space of sections whose graphs are the j -plane bundles near $N^{u,0}(\tilde{V})$ in $N(\tilde{V})$, where j is the dimension of $N^{u,0}(\tilde{V})$. These are sections of the bundle $L(\tilde{V})$ whose fiber at $y \in \tilde{V}$ is the space of linear transformations $N_y^{u,0}(\tilde{V}) \rightarrow N_y^{s,0}(\tilde{V})$, $L(N_y^{u,0}(\tilde{V}), N_y^{s,0}(\tilde{V}))$, [21]. The domain of \mathcal{L}^u is $\mathcal{S}_\eta = \{\sigma : \tilde{V} \rightarrow L(\tilde{V}) : \sup_y \|\sigma(y)\| \leq \eta\}$, where the operator norm $\|\cdot\|$ is associated with the Riemann structure on $T_{\tilde{V}}(M)$. The space \mathcal{S}_η is complete with respect to the norm $|\sigma| = \sup_y \|\sigma(y)\|$.

To formulate \mathcal{L}^u , the starting point is the invariance condition. The linear mapping induced by $D\tilde{F} : T_{\tilde{V}}(M) \rightarrow T_{\tilde{V}}(M)$ on $N(\tilde{V}) \subset T_{\tilde{V}}(M)$ is $\Phi = Q \circ D\tilde{F}|_{N(\tilde{V})} : N(\tilde{V}) \rightarrow N(\tilde{V})$. The graph of $\sigma \in \mathcal{S}_\eta$ is Φ -invariant if and only if $\Phi(\text{graph}\{\sigma(x)\}) = \text{graph}\{\sigma(y)\}$, $y = \tilde{F}(x)$, $x \in \tilde{V}$. This condition is split into a part in $N^{u,0}(\tilde{V})$ and a part in $N^{s,0}(\tilde{V})$. Let $P_y^u : N_y(\tilde{V}) \rightarrow N_y(\tilde{V})$ be the linear projection with range $N_y^{u,0}(\tilde{V})$ and nullspace $N_y^{s,0}(\tilde{V})$. Define P_y^s analogously. Then the graph of $\sigma \in \mathcal{S}_\eta$ is Φ -invariant if and only if

$$\begin{aligned} \sigma(y)(\tilde{\rho}) &= P_y^s \circ \Phi(\rho, \sigma(x)(\rho)), \\ \tilde{\rho} &= P_y^u \circ \Phi(\rho, \sigma(x)(\rho)), \end{aligned} \tag{6}$$

for $\rho \in N_x^{u,0}(\tilde{V})$, $x \in \tilde{V}$, where $y = \tilde{F}(x)$. The second equation in (6) is a linear mapping $N_x^{u,0}(\tilde{V}) \rightarrow N_y^{u,0}(\tilde{V})$, $\rho \rightarrow \tilde{\rho}$, which is invertible for small

ϵ , δ , θ and η . Denote the inverse $B_y(\tilde{\rho}) = \rho$. Then, the graph transform of σ is the section $\mathcal{L}^u(\sigma)(y) = P_y^s \circ \Phi \circ (\text{id}, \sigma(x)) \circ B_y$ for $y \in \tilde{V}$. Here, $(\text{id}, \sigma(x)) : N_x^{u,0}(\tilde{V}) \rightarrow N_x(\tilde{V})$ is $(\text{id}, \sigma(x))(\rho) = (\rho, \sigma(x)(\rho))$.

The graph of σ is Φ -invariant if and only if σ is a fixed point of \mathcal{L}^u . By replacing Φ with Φ^N above, for some large integer N , and for ϵ , δ , θ and η small, \mathcal{L}^u is a contraction on \mathcal{S}_η whose fixed point σ^* gives the Φ -invariant bundle $N^u(\tilde{V})$. The formulation of \mathcal{L}^s is analogous.

To summarize, one step of the proposed continuation algorithm has two parts. The initial data is an F -invariant manifold V with hyperbolic splitting $N^u(V) \oplus T(V) \oplus N^s(V)$. The first step uses the graph transform Γ on V with $N^u(V) \oplus T(V) \oplus N^s(V)$ to determine the \tilde{F} -invariant manifold \tilde{V} . That is, starting with the zero section σ_0 , Γ is iterated, $\Gamma^i(\sigma_0) \rightarrow \sigma^*$ in C^0 norm as $i \rightarrow \infty$. The second step uses linear graph transforms \mathcal{L}^s and \mathcal{L}^u together with initial data determined by \tilde{V} and $N^u(V) \oplus T(V) \oplus N^s(V)$ to determine the hyperbolic splitting $N^u(\tilde{V}) \oplus T(\tilde{V}) \oplus N^s(\tilde{V})$ of \tilde{V} . Now the first and second steps are repeated with initial data \tilde{V} , $N^u(\tilde{V}) \oplus T(\tilde{V}) \oplus N^s(\tilde{V})$.

3 Discrete Sections

In this section, discrete versions of V , its hyperbolic splitting, transverse bundle and sections of the transverse bundle are constructed. From this, the discrete version of the graph transform in Section 4 follows. Here, the manifold $M = \mathbb{R}^n$ with the constant Riemann metric induced by the usual inner product. This is not, in principle, a reduction of the generality of the method, since V may be embedded in \mathbb{R}^n and the property of normal hyperbolicity (2) is independent of the Riemann structure.

The initial manifold V is approximated by a geometric simplicial complex $\mathcal{C} \subset \mathbb{R}^n$ supporting $V \subset \mathbb{R}^n$, [6, 26]. Recall that the polyhedron $P \subset \mathbb{R}^n$ of \mathcal{C} is the set of all points in the simplices of \mathcal{C} with the subspace topology. A simplicial complex \mathcal{C} supports V if the vertices of all simplices are in V and P is homeomorphic to V . If H is the maximal diameter of the simplices of \mathcal{C} then P converges to V in Lipschitz norm as $H \rightarrow 0$. Denote by $\mathcal{C}_1 \dots \mathcal{C}_N$ the d -simplices of \mathcal{C} , $d = \dim V$. For the uniformity of the polynomial approximations on each \mathcal{C}_i as $H \rightarrow 0$, it is required that $\{\mathcal{C}_i\}_{i=1}^N$ be a regular family. This means that, if h_i is the diameter of \mathcal{C}_i and ρ_i the supremum of the diameters of the inscribed spheres of \mathcal{C}_i , then h_i/ρ_i is bounded uniformly for all i and $H \rightarrow 0$, [8].

Next, discrete approximations to the transverse bundle and hyperbolic splitting of V are described. The approximation to the hyperbolic splitting will be given by vector bundles $N^s(P)$ and $N^u(P)$, where $N(P) = N^s(P) \oplus N^u(P)$ is the transverse bundle associated with a tubular neighborhood of P .

To be specific, a tubular neighborhood of P is induced by a transverse field of k_0 -planes $\mu : P \rightarrow \mathcal{G}_{n,k_0} =$ the Grassmann manifold of k_0 -planes of \mathbb{R}^n , $k_0 = \text{codim } V$, provided μ is locally Lipschitz with respect to Riemannian

metrics [20, 32]. Note that the approximation to the hyperbolic splitting satisfies $N_x(P) = N_x^s(P) \oplus N_x^u(P) \subset T_x(\mathbb{R}^n)$, $x \in P$. Here, $T_x(\mathbb{R}^n)$, $x \in P$, are as usual identified with the ambient space \mathbb{R}^n containing V and also the underlying space \mathbb{R}^n of the Grassmann manifold via the standard basis. By this identification, the field μ gives a transverse bundle $N(P)$. In fact, the field μ is made up of two parts, $\mu(x) = \mu_1(x) \oplus \mu_2(x)$, $x \in P$, where $\mu_i : P \rightarrow \mathcal{G}_{n,k_i}$ for $i = 1, 2$, $k_1 = \dim N^s(V)$ and $k_2 = \dim N^u(V)$. Here, μ_1 gives $N^s(P)$ and μ_2 gives $N^u(P)$.

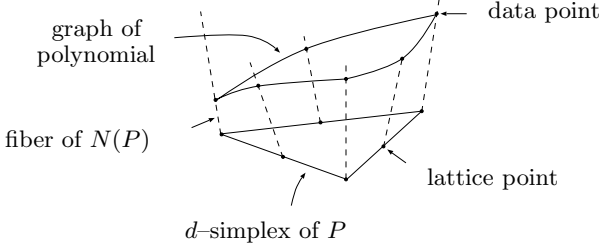
The bundle $N^s(V)$ is approximated by $N^s(P)$ as follows. The given $N(V)$ induces a homeomorphism $\psi : P \rightarrow V$. Let $N^{s,0}(P)$ be the vector bundle over P whose fiber at $y \in P$ is $N_{\psi(y)}^s(V)$. To approximate $N^s(V)$, the Lipschitz field $\vartheta : P \rightarrow \mathcal{G}_{n,k_1}$, $\vartheta(y) = N_y^{s,0}(P)$, is approximated by a field $\mu_1 : P \rightarrow \mathcal{G}_{n,k_1}$.

The field μ_1 is constructed by interpolating a given finite set of data points in \mathcal{G}_{n,k_1} . These data points are the k_1 -planes $\{N_y^s(V) : y \in \mathcal{C}^0\}$, where \mathcal{C}^0 is the set of vertices of \mathcal{C} . The interpolation is performed in the space of frames for the k_1 -planes of \mathcal{G}_{n,k_1} . Since the same procedure is used for μ_2 , in the following we will use k to denote a variable which may be k_1 or k_2 . Recall that $\mathcal{F}_{n,k}$, the space of k -frames in \mathbb{R}^n , $k \leq n$, is given the structure of a smooth manifold by its natural identification with the space of $n \times k$ matrices of rank k . The space of $n \times k$ matrices of rank k is a smooth manifold due to its identification with an open subset of \mathbb{R}^{nk} , [1].

In the case $k = 1$, the following method may be used to interpolate the k -plane fibers at the vertices of a d -simplex \mathcal{C}_i . Given $d+1$ nearby 1-plane fibers at the vertices of \mathcal{C}_i , choose $d+1$ unit vector bases $b_1 \dots b_{d+1}$ for the fibers, all contained in a small neighborhood in the frame manifold. Then a basis for the interpolating 1-plane fiber at the barycentric coordinates (t_1, \dots, t_{d+1}) [7] is obtained by normalizing the vector $v = t_1 \cdot b_1 + \dots + t_{d+1} \cdot b_{d+1}$. This is numerically practical since the nearness of the bases $b_1 \dots b_{d+1}$ implies that $|v|$ is near one.

For the construction of discrete k -plane bundles in the case $k > 1$, see [4]. Here, plane rotation matrices are used to interpolate special orthonormal bases for the k -plane fibers at the vertices of a d -simplex.

Next, a discrete approximation of a section in $\mathcal{S}_{\epsilon,\delta}$ is constructed. The field of k_0 -planes $\mu : P \rightarrow \mathcal{G}_{n,k_0}$ induces a vector bundle $N(P)$ with base space P , whose fiber at $x \in P$ is the k_0 -plane $\mu(x)$. This $N(P)$ gives a tubular neighborhood of P . Analogous to the approach in Section 2, we work in a neighborhood of the zero section in $N(P)$, which is equivalent to a neighborhood of P in \mathbb{R}^n . Any C^r , $r \geq 1$, manifold \tilde{V} Lipschitz-near V corresponds to the graph of a section σ of $N(P)$, for small H . The section σ is C^r on each \mathcal{C}_i . A candidate manifold \tilde{V} is approximated by a section σ_D of $N(P)$ which is polynomial on each \mathcal{C}_i in appropriate coordinates. On each \mathcal{C}_i , σ_D is a polynomial map into the fibers of $N(P)$. In fact, $N(P) = N^s(P) \oplus N^u(P)$, where the fiber of $N^s(P)$ at $x \in P$ is the k_1 -plane $\mu_1(x)$ and the fiber of $N^u(P)$ at $x \in P$ is the k_2 -plane $\mu_2(x)$. The approximating section is $\sigma_D(x) = (x, v^s(x), v^u(x))$,


 Fig. 3: Approximation to \tilde{V} , attracting case, $p = 2$.

where $v^s(x) \in N_x^s(P)$, $v^u(x) \in N_x^u(P)$. In appropriate coordinates, on each \mathcal{C}_i , v^s and v^u are Lagrange polynomials of order $p \geq 1$, [7].

The section σ on \mathcal{C}_i is approximated by interpolating a discrete data set consisting of the values of σ at certain points of \mathcal{C}_i . The discrete data set for σ_D on \mathcal{C}_i consists of the points of intersection of the graph of σ in $N_{\mathcal{C}_i}(P)$ with the fibers $N_x(P)$, for points x in the principal lattice of order p of \mathcal{C}_i . See Figure 3. The principal lattice of order p of \mathcal{C}_i , denoted Σ_i , is the set of points in \mathcal{C}_i with barycentric coordinates $b_1 \dots b_{d+1} \in \{0, 1/p \dots (p-1)/p, 1\}$, [7]. Denote the points of Σ_i by $x_{i,j} \in \mathcal{C}_i \subset P$, $j = 1 \dots m$. Then the points of intersection of the graph of σ in $N_{\mathcal{C}_i}(P)$ with the fibers $N_x(P)$, $x \in \Sigma_i$, are

$$(x_{i,j}, v_{i,j}^s, v_{i,j}^u) \in N_{\mathcal{C}_i}(P), \text{ for some } v_{i,j}^s \in N_{x_{i,j}}^s(P), v_{i,j}^u \in N_{x_{i,j}}^u(P),$$

$j = 1 \dots m$. The discrete section σ_D is composed of stable and unstable parts, $v^s(x)$ and $v^u(x)$. Here, $v^s(x)$, $x \in \mathcal{C}_i$, is fitted to $v_{i,j}^s$, $j = 1 \dots m$, and $v^u(x)$, $x \in \mathcal{C}_i$, is fitted to $v_{i,j}^u$, $j = 1 \dots m$.

Coordinates on $N_{\mathcal{C}_i}^s(P)$, $i = 1 \dots N$, are induced by smooth orthonormal moving frames. Namely, an orthonormal basis of $N_x^s(P)$ is given by the columns of an $n \times k_1$ matrix $E_i(x)$ which depends smoothly on $x \in \mathcal{C}_i$. For each $x \in \mathcal{C}_i$, this matrix induces an invertible linear transformation $\xi_i(x) : \mathbb{R}^{k_1} \rightarrow N_x^s(P)$, $\xi_i(x)(\rho) = E_i(x)\rho$. There is a unique Lagrange polynomial $\eta_i^s : \mathcal{C}_i \rightarrow \mathbb{R}^{k_1}$ of total degree p fitting the data

$$\eta_i^s(x_{i,j}) = \xi_i(x_{i,j})^{-1}(v_{i,j}^s), \quad j = 1 \dots m,$$

[7, 8]. Now put $v^s(x) = \xi_i(x) \circ \eta_i^s(x)$ for $x \in \mathcal{C}_i$.

The construction of v^u is analogous to the construction of v^s . The resulting approximating section $\sigma_D(x) = (x, v^s(x), v^u(x))$ of $N(P)$ is continuous. If \tilde{V} is of smoothness class C^{p+1} , σ_D is an approximation to σ of order p . That is, $\sup\{|v(x) - v_D(x)|_x : x \in P\} = O(H^{p+1})$ as $H \rightarrow 0$, where $\sigma(x) = (x, v(x))$ and $\sigma_D(x) = (x, v_D(x))$.

4 The Discrete Graph Transform

In this section the discrete graph transform Γ_D , used to approximate \tilde{V} , is formulated. This is done in Sections 4.1 and 4.2 by replacing the components of the graph transform described in Section 2 with the discrete counterparts of Section 3. Namely, $N(V) = N^u(V) \oplus N^s(V)$ is replaced by $N(P) = N^u(P) \oplus N^s(P)$ in Section 4.1 and the sections σ of $N(V)$ are replaced by discrete sections σ_D of $N(P)$ in Section 4.2.

In addition, the discrete linear graph transforms \mathcal{L}_D^u and \mathcal{L}_D^s , used to approximate the hyperbolic splitting of \tilde{V} , are formulated. The approximations of the stable and unstable bundles, $N^s(P)$ and $N^u(P)$, lead to \mathcal{L}_D^s and \mathcal{L}_D^u in Section 4.3.

4.1 The Graph Transform of Sections of $N(P)$

In this section, the graph transform is formulated as in Section 2.2, replacing $N(V) = N^u(V) \oplus N^s(V)$ by $N(P) = N^u(P) \oplus N^s(P)$. The difference between this section and Section 2.2 is that here $N(P)$ is Lipschitz rather than smooth.

The Lipschitz constant of a section σ^s of $N^s(P)$ is defined as follows. First, $N(P)$ induces a homeomorphism $\psi : V \rightarrow P$. Suppose $N^s(V)$ is the vector bundle over V whose fiber at $p \in V$ is $N_{\psi(p)}^s(P)$. Since $N^s(V)$ is a subbundle of $T_V(M)$, the Lipschitz constant of the section $\sigma^s \circ \psi$ of $N^s(V)$ is defined in Section 2. Hence, $\text{Lip}\{\sigma^s\} = \text{Lip}\{\sigma^s \circ \psi\}$, and similarly for σ^u . Now, $\text{Lip}\{\sigma\}$ for a section σ of $N(P)$ is defined as in Section 2.2. Suppose $Z = Z(\epsilon) = \{(x, v) \in N(P) : |v|_x \leq \epsilon\}$ and $\mathcal{S}_{\epsilon, \delta} = \{\sigma : P \rightarrow Z : \text{Lip}(\sigma) \leq \delta\}$. The space $\mathcal{S}_{\epsilon, \delta}$ with the C^0 norm $\|\cdot\|$ described in Section 2.2 is complete.

Given $\sigma \in \mathcal{S}_{\epsilon, \delta}$, $\sigma(x) = (x, v^s(x), v^u(x))$, the graph transform of σ is a section $\Gamma(\sigma)(x) = (x, w^s(x), w^u(x))$ of $N(P)$. Here, $w^s(x)$ is the stable part of the intersection of the \tilde{F}^0 -image of the graph of σ with the fiber $N_x(P)$. Thus, to define $w^s(x)$ for a given $x \in P$, first solve

$$x = \pi \circ \tilde{F}^0(p, v^s(p), v^u(p)), \quad (7)$$

for $p \in P$, where $\pi : N(P) \rightarrow P$ is the vector bundle projection. In (7) we are solving for the unique $p \in P$ such that $\tilde{F}^0 \circ \sigma(p)$ is contained in the fiber $Z_x(P)$. Equation (7) has a unique solution for $p \in P$, provided ϵ, δ, θ and H are small. Denote this solution by $p = p(x, v^s, v^u)$. Now, $w^s(x)$ is given by the formula

$$w^s(x) = P_x^s \circ \tilde{F}^0(p, v^s(p), v^u(p)), \quad (8)$$

for $x \in P$, where $P_x^s : N_x(P) \rightarrow N_x(P)$ is the linear projection with range $N_x^s(P)$ and nullspace $N_x^u(P)$.

The unstable part w^u is defined implicitly by eliminating x in

$$v^u(x) = P_x^u \circ \tilde{F}^0(p, v^s(p), w^u(p)), \quad x = \pi \circ \tilde{F}^0(p, v^s(p), w^u(p)), \quad (9)$$

for $p \in P$, where $P_x^u : N_x(P) \rightarrow N_x(P)$ is the linear projection with range $N_x^u(P)$ and nullspace $N_x^s(P)$. In (9) we are solving for the vector $w = w^u(p) \in Z_p^u(P)$ such that the \tilde{F}^0 -image of $(p, v^s(p), w)$ has unstable component in the graph of v^u . There is a unique solution for $w^u(p)$ in (9) for small ϵ , δ , θ and H . The proof that there are unique solutions in (7) and (9) follows from the Lipschitz implicit function theorem [12, page 207]. As in Section 2.2, by replacing \tilde{F} with \tilde{F}^N if necessary, Γ becomes a contraction on $\mathcal{S}_{\epsilon, \delta}$ whose fixed point gives the \tilde{F} -invariant manifold \tilde{V} .

4.2 The Discrete Graph Transform

In this section, the formulation of Γ_D started in Section 4.1 is finished. The domain of Γ from Section 4.1 is restricted to the subset of $\mathcal{S}_{\epsilon, \delta}$ consisting of discrete sections. For $\sigma_D \in \mathcal{S}_{\epsilon, \delta}$, where σ_D is a discrete section of the form constructed in Section 3, $\Gamma(\sigma_D)$ is not a discrete section. Thus, define $\Gamma_D(\sigma_D) = \mathcal{I} \circ \Gamma(\sigma_D)$, where $\mathcal{I} \circ \sigma$ is the discrete section approximating σ described in Section 3. Whether Γ_D leaves $\mathcal{S}_{\epsilon, \delta}$ invariant depends on the effect \mathcal{I} has on both the C^0 norm and the Lipschitz constant of sections in $\mathcal{S}_{\epsilon, \delta}$.

To be precise, a formula for $\mathcal{I}(\sigma)$ is obtained. A section $\sigma \in \mathcal{S}_{\epsilon, \delta}$ is

$$\sigma(x) = (x, \xi_i^s(x) \circ f_i^s(x), \xi_i^u(x) \circ f_i^u(x)), \quad x \in \mathcal{C}_i \quad (10)$$

for some $f_i^s : \mathcal{C}_i \rightarrow \mathbb{R}^{k_1}$ and $f_i^u : \mathcal{C}_i \rightarrow \mathbb{R}^{k_2}$. Here, ξ_i^s and ξ_i^u are defined in Section 3. Recall that $\xi_i^s(x) : \mathbb{R}^{k_1} \rightarrow N_x^s(P)$, $\xi_i^s(x)(\rho) = E_i^s(x)\rho$, where the columns of the $n \times k_1$ matrix $E_i^s(x)$ form an orthonormal basis for $N_x^s(P)$, $x \in \mathcal{C}_i$. The description of $\xi_i^u(x)$ is analogous. Recall that Σ_i , defined in Section 3, is the principal lattice of order $p \geq 1$ of the d -simplex \mathcal{C}_i . Then $\mathcal{I}(\sigma)$ is the discrete section σ_D of $N(P)$ whose data on \mathcal{C}_i consists of the points of intersection of the graph of σ in $N_{\mathcal{C}_i}(P)$ with the fibers $N_x(P)$, $x \in \Sigma_i$. To be specific,

$$\mathcal{I}(\sigma)(x) = (x, \xi_i^s(x) \circ L_i^s \circ f_i^s(x), \xi_i^u(x) \circ L_i^u \circ f_i^u(x))$$

for $x \in \mathcal{C}_i$, where L_i^s and L_i^u are the standard Lagrange interpolation operators on functions on \mathcal{C}_i . Here, the Lagrange interpolation operators are defined as follows. Given $f : \mathcal{C}_i \rightarrow \mathbb{R}^{k_1}$, $L_i^s \circ f : \mathcal{C}_i \rightarrow \mathbb{R}^{k_1}$ is the unique polynomial of total degree p with $L_i^s \circ f(x) = f(x)$ for $x \in \Sigma_i$. The definition of L_i^u is analogous.

The maximum factor of growth of the C^0 norm of a section under \mathcal{I} is $C_p = \sup\{\|\mathcal{I}(\sigma)\|/\|\sigma\| : \sigma \in \mathcal{S}_{\epsilon, \delta}\}$. The maximum factor of growth of the Lipschitz constant of a section under \mathcal{I} is $C'_p = \sup\{\text{Lip}\{\mathcal{I}(\sigma)\}/\text{Lip}\{\sigma\} : \sigma \in \mathcal{S}_{\epsilon, \delta}\}$. Here, C_p and C'_p are bounded as $H \rightarrow 0$. The Lipschitz constant of \mathcal{I} is also bounded by C_p for $p \geq 1$. If $C_p = C'_p = 1$, \mathcal{I} has no deleterious effect on Γ , and Γ_D is a contraction on $\mathcal{S}_{\epsilon, \delta}$ with no adjustments to any parameters. In general, however, $C_p, C'_p > 1$. Note that C_p and C'_p are smaller for smaller $p \geq 1$. Even for $p = 1$, though, $C'_p > 1$.

To deal with $C_p > 1$ or $C'_p > 1$, one of the parameters of Γ is modified. For simplicity, consider the attracting case. Suppose that $0 < \alpha < 1$ is the factor of (weakest) normal contraction toward V under F . Also, $0 < \mu < 1$ from (2) is a bound on $\alpha/\{\text{the factor of (strongest) tangential contraction under } F\}$. Given $\sigma \in \mathcal{S}_{\epsilon,\delta}$, the C^0 norm and Lipschitz constant of $\Gamma(\sigma)$ are multiplied by factors $c\alpha^N + o(1)$ and $c\mu^N + o(1)$, respectively, as $\epsilon + \delta + \theta + H \rightarrow 0$. The C^0 norm and Lipschitz constant of $\Gamma_D(\sigma)$ are multiplied by factors $C_p c\alpha^N + o(1)$ and $C'_p c\mu^N + o(1)$, respectively. Thus, by choosing N large enough, we obtain $\Gamma_D : \mathcal{S}_{\epsilon,\delta} \rightarrow \mathcal{S}_{\epsilon,\delta}$. Also, Γ_D is a contraction since

$$\text{Lip}\{\Gamma_D\} \leq \text{Lip}\{\mathcal{I}\}\text{Lip}\{\Gamma\} = C_p c\alpha^N + o(1)$$

as $\epsilon + \delta + \theta + H \rightarrow 0$.

Alternatively, it is possible to estimate $\text{Lip}\{\mathcal{I}(\sigma)\}$ using the constant $C''_p = H \sup\{\text{Lip}\{\mathcal{I}(\sigma)\}/\|\sigma\| : \sigma \in \mathcal{S}_{\epsilon,\delta}\}$, which is bounded as $H \rightarrow 0$. In this case, there exists a constant $c > 0$ and a positive function $\omega(H) \rightarrow 0$ as $H \rightarrow 0$, such that the following holds. If $\epsilon = cH\delta$, $\omega(H) < c\delta$, $\theta < c\epsilon$, δ is sufficiently small and N sufficiently large, then $\Gamma_D : \mathcal{S}_{\epsilon,\delta} \rightarrow \mathcal{S}_{\epsilon,\delta}$ is a contraction [2]. This result does not use the full hypothesis of normal hyperbolicity, but only the existence of a C^1 , 0-normally hyperbolic manifold \tilde{V} , [21]. This explains why Γ_D is a contraction, in practice, for some dynamical systems even in the absence of normal hyperbolicity.

In either of the scenarios in the preceding two paragraphs, Γ_D has a fixed point $\sigma^*_D \in \mathcal{S}_{\epsilon,\delta}$, where $\phi \circ \sigma^*_D(P) \rightarrow \tilde{V}$ in C^0 norm as $H \rightarrow 0$. In fact, $\phi \circ \sigma^*_D(P) \rightarrow \tilde{V}$ in Lipschitz norm as $H \rightarrow 0$ if $p = 1$ or $r \geq 2$. In addition, if \tilde{V} is of smoothness class C^{p+1} , then $\phi \circ \sigma^*_D(P)$ is a C^0 approximation to \tilde{V} of order p .

4.3 The Discrete Linear Graph Transform

This section deals with the computation of the approximate hyperbolic splitting of \tilde{V} . In Section 4.2, an approximation $\phi \circ \sigma^*_D(P)$ to \tilde{V} was obtained for $H \rightarrow 0$. The simplicial complex $\tilde{\mathcal{C}}$ with vertices $\phi \circ \sigma^*_D(\mathcal{C}^0)$, where \mathcal{C}^0 is the set of vertices of P , supports the manifold $\phi \circ \sigma^*_D(P)$. Suppose $\tilde{P} \subset \mathbb{R}^n$ is the polyhedron of $\tilde{\mathcal{C}}$ and $N(\tilde{P})$ is a given transverse bundle. Given such an $N(\tilde{P})$, the approximate hyperbolic splitting of \tilde{V} is given by a splitting $N(\tilde{P}) = N^u(\tilde{P}) \oplus N^s(\tilde{P})$.

In this section, the discrete linear graph transforms \mathcal{L}^u_D and \mathcal{L}^s_D are used to determine $N^u(\tilde{P})$ and $N^s(\tilde{P})$. Here it is assumed that $N(\tilde{P})$ and $N(P)$ are approximately normal in the following sense. Each d -simplex subspace P_i , $i = 1 \dots N$, of P is a manifold with boundary with tangent bundle $T(P_i)$. Then

$$\inf\{\langle N_x(P), T_x(P_i) \rangle : \text{all } P_i \text{ containing } x, x \in P\} \rightarrow \pi/2$$

as $H \rightarrow 0$. Next, \mathcal{L}^u_D is formulated. The formulation of \mathcal{L}^s_D is analogous.

The initial data for \mathcal{L}_D^u is a splitting $N(\tilde{P}) = N^{u,0}(\tilde{P}) \oplus N^{s,0}(\tilde{P})$. This splitting is obtained from $N(P) = N^u(P) \oplus N^s(P)$ by parallel translation followed by projection onto the fibers of $N(\tilde{P}) \subset T_{\tilde{P}}(\mathbb{R}^n)$ using Q , as in Section 2.3. To be specific, suppose π is the vector bundle projection of $N(P)$. Then $N_y^{u,1}(\tilde{P})$, $N_y^{s,1}(\tilde{P})$ are obtained from $N_p^u(P)$, $N_p^s(P)$, $p = \pi \circ \phi^{-1}(y)$, by parallel translation $T_p(\mathbb{R}^n) \rightarrow T_y(\mathbb{R}^n)$ along ϕ -images of fibers of $N(P)$. In the present case, parallel translation is trivially defined by the identification of $T_x(\mathbb{R}^n)$, $x \in \mathbb{R}^n$, with the ambient space \mathbb{R}^n . In the present setting,

$$Q : T_{\tilde{P}}(\mathbb{R}^n) \rightarrow N(\tilde{P}) \subset T_{\tilde{P}}(\mathbb{R}^n),$$

is, on each fiber $T_x(\mathbb{R}^n)$, the linear orthogonal projection with range $N_x(\tilde{P})$. The initial data are then

$$N^{u,0}(\tilde{P}) = Q(N^{u,1}(\tilde{P})), \quad N^{s,0}(\tilde{P}) = Q(N^{s,1}(\tilde{P})).$$

This procedure produces non-degenerate initial data for $\epsilon + \delta + \theta + H \rightarrow 0$.

As in Section 2.3, $L(\tilde{P})$ is the bundle whose fiber at $y \in \tilde{P}$ is the space of linear transformations $N_y^{u,0}(\tilde{P}) \rightarrow N_y^{s,0}(\tilde{P})$. The domain of \mathcal{L}_D^u is a subset of the space of sections $\mathcal{S}_\eta = \{\sigma : \tilde{P} \rightarrow L(\tilde{P}) : \sup_y \|\sigma(y)\| \leq \eta\}$, where the operator norm $\|\cdot\|$ is associated with the Riemann structure on $T_{\tilde{P}}(\mathbb{R}^n)$. The space \mathcal{S}_η is complete with respect to the norm $|\sigma| = \sup_y \|\sigma(y)\|$.

The domain of \mathcal{L}_D^u is the subset of \mathcal{S}_η consisting of discrete sections. A discrete section in \mathcal{S}_η is constructed using the construction of a discrete field of k_2 -planes $\mu : \tilde{P} \rightarrow \mathcal{G}_{n,k_2}$ in Section 3. A discrete section σ_D of $L(\tilde{P})$ is constructed from given data $\{\sigma_D(x) \in L_x(\tilde{P}) : x \in \tilde{\mathcal{C}}^0\}$, where $\tilde{\mathcal{C}}^0$ is the set of vertices of \tilde{P} , as follows. Using the method of Section 3, construct the field $\mu : \tilde{P} \rightarrow \mathcal{G}_{n,k_2}$ of k_2 -planes determined by the set of k_2 -plane data points

$$\left\{ \text{graph}\{\sigma_D(x)\} \subset N(\tilde{P}) \subset T_{\tilde{P}}(\mathbb{R}^n) : x \in \tilde{\mathcal{C}}^0 \right\}.$$

The discrete section σ_D is then uniquely characterized by $\text{graph}\{\sigma_D(x)\} = \mu(x)$, $x \in \tilde{P}$.

To construct \mathcal{L}_D^u , first the linear graph transform \mathcal{L}^u is formulated in the present setting, replacing $N(\tilde{V})$ by $N(\tilde{P})$. Thus, instead of a smooth manifold and transverse bundle, here they are only Lipschitz. In addition, the formulation of \mathcal{L}^u in this section is slightly different from the formulation of \mathcal{L}^u in Section 2.3 because \tilde{P} is not \tilde{F} -invariant. Second, the domain of \mathcal{L}^u is restricted to discrete sections, $\mathcal{L}_D^u(\sigma_D) = \mathcal{I} \circ \mathcal{L}^u(\sigma_D)$, $\sigma_D \in \mathcal{S}_\eta$. Here, for $\sigma \in \mathcal{S}_\eta$, $\mathcal{I}(\sigma)$ is the discrete section of $L(\tilde{P})$ defined by the data $\{\sigma(x) : x \in \tilde{\mathcal{C}}^0\}$.

To formulate \mathcal{L}^u , the invariance condition is derived. To define the mapping Φ induced by $D\tilde{F}$ on $N(\tilde{P})$, suppose π is the vector bundle projection of $N(\tilde{P})$ and $\phi : Z \rightarrow U$ is the homeomorphism, defined in Section 2.1, associated with the tubular neighborhood of \tilde{P} induced by $N(\tilde{P})$. Then the linear mapping induced by $D\tilde{F}_x : T_x(\mathbb{R}^n) \rightarrow T_y(\mathbb{R}^n)$, $y = \tilde{F}(x)$, $x \in \tilde{P}$, on $N(\tilde{P})$ is

$$\Phi = Q \circ \gamma \circ D\tilde{F}|_{N(\tilde{P})} : N(\tilde{P}) \rightarrow N(\tilde{P}).$$

Here $\gamma : T_y(\mathbb{R}^n) \rightarrow T_p(\mathbb{R}^n)$, $p = \pi \circ \phi^{-1}(y)$, $y \in U$, is parallel translation. Note that $y \in U$ for small H because $\tilde{P} \rightarrow \tilde{V}$ in C^0 norm as $H \rightarrow 0$.

Given a section $\sigma \in \mathcal{S}_\eta$, the linear graph transform $\mathcal{L}^u(\sigma)$ is characterized by the condition $\Phi(\text{graph}\{\sigma(x)\}) = \text{graph}\{\mathcal{L}^u(\sigma)(y)\}$ where $y = \pi \circ \phi^{-1} \circ \tilde{F}(x)$. To calculate $\mathcal{L}^u(\sigma)(y)$ for a given $y \in \tilde{P}$, first solve $y = \pi \circ \phi^{-1} \circ \tilde{F}(x)$ for $x \in \tilde{P}$. Next, given an orthonormal basis $e_1 \dots e_{k_2}$ for $N_y^{u,0}(\tilde{P})$, solve $e_i = P_y^u \circ \Phi(\rho_i, \sigma(x)(\rho_i))$ for $\rho_i \in N_x^{u,0}(\tilde{P})$, $i = 1 \dots k_2$. Then $\mathcal{L}^u(\sigma)(y)$ is given by the formula

$$\mathcal{L}^u(\sigma)(y)(e_i) = P_y^s \circ \Phi(\rho_i, \sigma(x)(\rho_i)),$$

$i = 1 \dots k_2$. If Φ is replaced by Φ^N , then $\mathcal{L}^u : \mathcal{S}_\eta \rightarrow \mathcal{S}_\eta$ is a contraction for $\epsilon + \delta + \theta + \eta + H$ small and N large.

Next, conditions are determined which guarantee $\mathcal{L}_D^u(\sigma_D) \in \mathcal{S}_\eta$ for $\sigma_D \in \mathcal{S}_\eta$ and that $\mathcal{L}_D^u : \mathcal{S}_\eta \rightarrow \mathcal{S}_\eta$ is a contraction. Recall $\mathcal{L}_D^u(\sigma_D) = \mathcal{I} \circ \mathcal{L}^u(\sigma_D)$ for $\sigma_D \in \mathcal{S}_\eta$. Thus, the norm of $\mathcal{I}(\sigma)$, $\sigma \in \mathcal{S}_\eta$ and the Lipschitz constant of \mathcal{I} on \mathcal{S}_η must be estimated. For $\sigma \in \mathcal{S}_\eta$, $|\mathcal{I}(\sigma)| \leq \eta + o(1)$ and $\text{Lip}\{\mathcal{I}\} = 1 + o(1)$ as $H \rightarrow 0$. Thus, $\mathcal{L}_D^u : \mathcal{S}_\eta \rightarrow \mathcal{S}_\eta$ is a contraction for $\epsilon + \delta + \theta + \eta + H$ small and N large.

The fixed point $\sigma_D^* \in \mathcal{S}_\eta$ of \mathcal{L}_D^u gives an approximation to $N^u(\tilde{V})$ in the following sense. Suppose $\gamma : N_x(\tilde{V}) \rightarrow N_y(\tilde{P})$, $y = \pi \circ \phi^{-1}(x)$, is parallel translation and σ is a section of $L(\tilde{P})$ satisfying $\text{graph}\{\sigma(y)\} = \gamma(N_x^u(\tilde{V}))$, $y = \pi \circ \phi^{-1}(x)$, $y \in \tilde{P}$. Then $|\sigma - \sigma_D^*| \rightarrow 0$ as $H \rightarrow 0$.

5 Numerical Implementation

In this section, a specific computer implementation of the discrete graph transform is outlined. In Section 5.1, a practical numerical approach for solving equations (7), (8) and (9) is proposed. The main part is solving (7), as well as the second equation in (9), for a point $p \in V$. Note that this is a global problem. In Section 5.2, numerical conditioning and error for these problems is discussed. Also, some important smoothing techniques are mentioned. These are useful for stabilizing a computation in which non-smooth data appears.

The discrete graph transform/linear graph transform algorithm takes as input an approximation to V and its hyperbolic splitting. It returns as output an approximation to \tilde{V} and its hyperbolic splitting. Then, the algorithm may be repeated taking as input the newly computed data. In practice, the input/output to the algorithm are the following: (i) A polyhedron P Lipschitz-near a C^r F -invariant submanifold $V \subset \mathbb{R}^n$, $r \geq 1$. (ii) Approximately normal fibers $N_x(P)$, $x \in \mathcal{C}^0 =$ the vertices of P , and a splitting $N_x(P) = N_x^u(P) \oplus N_x^s(P)$, $x \in \mathcal{C}^0$, which is near the hyperbolic splitting.

The graph transform algorithm, which returns as output an approximation to \tilde{V} , is the subject of Section 5.1. The linear graph transform algorithm, which returns as output an approximation to the hyperbolic splitting of \tilde{V} , will not be discussed further here. It is less complicated than the graph transform algorithm since it presents no additional nonlinear equations to solve.

5.1 The Discrete Graph Transform Algorithm

The graph transform algorithm starts with the zero section σ_D^0 of $Z(P)$ and for $i \geq 0$ repeats (graph transform step) until the convergence criteria are met. The graph transform step takes as input a discrete section σ_D^i of $Z(P)$ and returns as output a discrete section $\sigma_D^{i+1} = \Gamma_D \circ \sigma_D^i$ of $Z(P)$. Here, $Z(P) = \{(x, v) \in N(P) : |v|_x \leq \epsilon\}$ is from Section 4.1 and Γ_D is from Section 4.2. The convergence criteria for the graph transform are the following. The iteration of (graph transform step) is stopped when $|\sigma_D^{i+1} - \sigma_D^i| < \text{error}$ and the contraction factor $|\sigma_D^{j+2} - \sigma_D^{j+1}| / |\sigma_D^{j+1} - \sigma_D^j| < 1$ is approximately constant for all $j < i$ sufficiently large [5].

The graph transform step consists of the following. Recall that Σ_i , defined in Section 3, is the principal lattice of order $p \geq 1$ of the d -simplex \mathcal{C}_i . A discrete section of $Z(P)$ is determined by a discrete set of data points, one in each fiber $Z_x(P)$, $x \in G = \bigcup\{\Sigma_i : i = 1 \dots N\} \subset P$. Thus for the graph transform step, the *input* is the set of data points $\sigma_D^i(x)$, $x \in G$, and the *output* is the set of data points $\sigma_D^{i+1}(x) = (\Gamma_D \circ \sigma_D^i)(x)$, $x \in G$. The sections have stable and unstable parts, $\sigma_D^i(x) = (x, v^{s,i}(x), v^{u,i}(x))$ and $\sigma_D^{i+1}(x) = (x, v^{s,i+1}(x), v^{u,i+1}(x))$. Hence, the graph transform step has two independent stages, one for determining the stable part $v^{s,i+1}(x)$, $x \in G$ and one for determining the unstable part $v^{u,i+1}(x)$, $x \in G$.

Some notation used below is ϕ , defined in Section 2.1 and $\tilde{F}^0 = \phi^{-1} \circ \tilde{F} \circ \phi$, defined in Section 2.2.

Graph transform step: *Stable part*

For $x \in G$:

1. Put $v^s = v^{s,i}$, $v^u = v^{u,i}$ in (7) and (8).
2. Solve (7) for $p \in P$.
 - 2.1 Determine a neighborhood containing $p \in P$.
 - $A_j \equiv \cup\{\mathcal{C}_k : \mathcal{C}_k \cap \mathcal{C}_j \neq \emptyset\}$ for $j = 1 \dots N$.
 - Find $j^* \in \{1 \dots N\}$ with $\tilde{F}^0 \circ \sigma_D^i(A_{j^*}) \cap Z_x(P) \neq \emptyset$.
 - (a) $\mathcal{C}_j^0 \equiv$ vertices of \mathcal{C}_j , $j = 1 \dots N$.
 - (b) $B_j \equiv d$ -simplex with vertices $\phi \circ \tilde{F}^0 \circ \sigma_D^i(\mathcal{C}_j^0)$, $j = 1 \dots N$.
 - (c) For $j = 1 \dots N$: Test $B_j \cap \phi(Z_x(P)) \neq \emptyset$. If true, return $j = j^*$.
 - 2.2 Locate $p \in A_{j^*}$ to a desired tolerance.
 - (a) Search for p in each $\mathcal{C}_k \subset A_{j^*}$ using a standard root finding method [14].
 - (b) If no root found in (a), search \mathcal{C}_k in successively larger regions around A_{j^*} .

3. Evaluate (8) at p to obtain $v^{s,i+1}(x) = w^s(x)$.

In 2.1, a simple geometrical test is used to find A_{j^*} . This step is typically only necessary for $i = 0$, the same j^* may be used for $i > 0$, since the location of $p \in P$ may not change much as i increases. The approach in 2.1 is justified by the fact that σ_D^i is kept approximately flat over \mathcal{C}_j and \tilde{F}^0 is well approximated by its linearization over the set $\sigma_D^i(\mathcal{C}_j)$ as $H \rightarrow 0$.

Graph transform step: Unstable part

For $p \in G$:

1. Put $v^s = v^{s,i}, v^u = v^{u,i}$ in (9).
2. Solve (9) for $w = w^u(p) \in Z_p^u(P)$.

Comment: Use a standard root finding method [14] with initial guess $w = 0$. Function evaluations in the root finding method require a call to the following subroutine.

2.1 Given $w \in Z_p^u(P)$, solve the second equation in (9) for $x = x(w) \in P$.

(a) $y \equiv \phi \circ \tilde{F}^0(p, v^{s,i}(p), w)$.

(b) $x \in P$ is the point near y with $y - x$ parallel to $\phi(Z_x(P))$. There are two stages to solving for x , similar to *Stable part* step 2.

3. Put $v^{u,i+1}(p) = w$.

5.2 Numerical Conditioning and Smoothing Techniques

The global equations (7), (8) and (9) associated with the graph transform pose a numerically well-conditioned problem. To be specific, solving (7) for $p \in P$ is numerically optimally conditioned for $N(P)$ chosen perpendicular to V , as is evaluation of the second equation of (9). In practice, $N(P)$ is an approximate normal bundle in the sense of Section 4.3. In the evaluation of (8) at p , hyperbolicity damps the numerical discretization and rounding error. Solving (9) for w^u is a well-conditioned problem. This is because the normal hyperbolicity of V implies that small errors in w^u produce large deviations in the right hand side of the first equation of (9).

As discussed in Section 4.2, it may be necessary to control the Lipschitz constant of discrete sections $\sigma_D(x) = (x, v^s(x), v^u(x))$, $x \in P$. The Lipschitz constant of sections is effectively controlled in practice using two techniques. The first is even redistribution of the grid points G . This replaces P with a nearby polyhedron P' with each $\mathcal{C}_i \subset P'$ close to the shape of the standard d -simplex. The second technique is local fairing [11] of the data $v^s(x) \in N_x^s(P)$ and $v^u(x) \in N_x^u(P)$, $x \in \Sigma_i$, which smooths out $\text{graph}\{\sigma_D\}$. Consider for example the attracting case. Here, the data $\sigma_D^i(x) \in Z_x(P)$, $x \in \Sigma_i$, is tested for large deviations. If an undesirable data point $\sigma_D^i(x^*)$ is detected, it is replaced by the average of $\sigma_D^i(x)$, $x \neq x^*$, $x \in \Sigma_i$. To be precise, the average $y \in \mathbb{R}^n$ of $\phi \circ \sigma_D^i(x) \in \mathbb{R}^n$, $x \neq x^*$, $x \in \Sigma_i$, is obtained. Then, y is projected onto the affine k_1 -plane $\phi \circ Z_x^*(P)$ to obtain $z \in \phi \circ Z_x^*(P) \subset \mathbb{R}^n$. The data point $\sigma_D^i(x^*)$ is replaced by $\phi^{-1}(z)$. Prior to these steps, it is important to

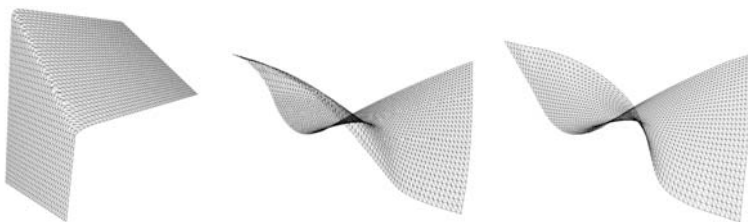


Fig. 4: Enzyme reaction surfaces: left $k_p = 0.1, k_1 = 10^3$; middle $k_p = 0.1, k_1 = 1.0$; right $k_p = 1.0, k_1 = 1.0$.

use local averaging of the fibers of $N(P)$, to make $N_x(P)$, $x \in \mathcal{C}_i$, more nearly parallel. For each $x \in \mathcal{C}^0$, $N_x(P)$ is replaced by the average of the $N_y(P)$ for $y \in \mathcal{C}^0$ near x . This is sometimes necessary because, in practice, small bumps in P can introduce degeneracies in its approximate normal bundle $N(P)$.

6 An Application

This section deals with a problem of chemical kinetics. The ‘slow–transient’ surface of an enzyme reaction is computed for a variety of parameter values. This application requires a modification to the algorithm of Section 5. This modification allows the computation of just a part of an invariant manifold. This is a necessary adaptation in cases where the invariant manifold is so large that its data cannot be held in computer memory.

The ‘slow–transient’ surface, in the phase space of chemical species concentration variables, is useful in chemical kinetics for model reduction. After a short time interval, the n -tuple of chemical species concentrations is restricted to the surface, at least for experimentally measurable tolerances. The dynamics of the reaction after this short time interval is described by the dynamics on the surface. In principle, once this surface is known, the system may be reduced to a 2D system on the surface. In chemical kinetics, the steady state and equilibrium approximations, as well as variations on these, have been used to approximate the slow–transient surface [13]. These approximations are typically valid in limiting cases.

In the enzyme reaction model

$$\begin{aligned} \dot{s} &= -k_1(e_0 - c - q) s + k_{-1} c \\ \dot{c} &= k_1(e_0 - c - q) s - (k_{-1} + k_2) c + k_{-2} q, \quad (s, c, q) \in \mathbb{R}^3, \\ \dot{q} &= k_2 c - (k_{-2} + k_p) q \end{aligned} \quad (11)$$

the variables s, c and q are the concentrations of different chemical species undergoing chemical reaction [30]. Here, $k_1, k_{-1}, k_2, k_{-2}, k_p > 0$ are the rate constants and $e_0 > 0$ is the concentration of the enzyme, taken to be constant. The attracting equilibrium is 0 in the physical region $\{0 \leq s < \infty, c + q \leq e_0, 0 \leq c, q\} \subset \mathbb{R}^3$. In Figure 4, the part of the slow–transient surface in the physical region restricted to $\{0 \leq s \leq 2\}$ is computed for three parameter choices. In every case, $e_0 = 1.0, k_{-1} = 1.0, k_2 = 1.0$ and $k_{-2} = 1.0$. The middle surface is computed by alternate means in [30].

In the present example, the dynamics are described by a nested hierarchy of attracting invariant manifolds in 3D. This is an equilibrium point contained in a curve contained in a surface, the slow–transient surface, which separates the physical region of phase space. The rate of attraction toward the surface is faster than toward the curve in the surface. The rate of attraction toward the curve in the surface is faster than toward the point in the curve. The part of the slow–transient surface in the physical region restricted to $\{0 \leq s \leq 2\}$ is a manifold with boundary S . A technical obstacle here is that S is only part of an invariant surface and is not overflowing invariant. For a diffeomorphism F , a compact manifold with boundary S is overflowing invariant under F if $S \subset F(S^0)$, where $S^0 = S \setminus \partial S$ is the interior of S . For such manifolds, the graph transform works in principle with no modification [12]. For the present example, a modification to the general purpose algorithm presented in Section 5 is required. Namely, local extrapolation of S at its boundary is used after each graph transform step. This means the following. In the present case, the order of approximation is $p = 1$. Thus, the output data of a graph transform step is σ_D^i where $\text{graph}\{\sigma_D^i\} = P$ is a polyhedral manifold with boundary. The d -simplices of P whose points are on the boundary of P are flatly extended to form a slightly larger polyhedron $P' \supset P$. This P' is used as input to the next graph transform step. For other approaches to computing the slow–transient surface in chemical kinetics, see [15, 16, 30].

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