Diffusion Maps and the Discrete Exterior Calculus

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Abstract

Nonlinear dimensionality reduction techniques work by imposing assumptions on the structure of the data, and good results require adaptation to the particular data structure. In this paper we adapt a class of data driven dimensionality reduction techniques to the analysis of Spatiotemporal Dynamics. Our technique finds low-dimensional dynamics for a model of meandering spiral waves and for video recordings of thin liquid-crystal dynamics. Moreover, the low-dimensional dynamics are split by time-scale allowing the extraction of dynamics which are active on the time-scale of interest.

1 Overview

Inexpensive storage and sensors have increased availability of data, however raw data often contains many redundant channels making analysis difficult due to the curse of dimensionality. Recently, new techniques have emerged for Non-Linear Dimensionality Reduction (NLDR) which remove these redundancies and produce a low-dimensional representation of the data. We have adapted a class of NLDR techniques for analysis of spatiotemporal dynamics. Simulations of complex spatiotemporal models, such as Raleigh-Benard convection, indicate that there may be a low-dimensional representation of the process [10]. However, conventional techniques of dimensionality reductions such as the Karhunen-Loeve Decomposition have been unable to recover a low dimensional process even for low drivings levels [10, 11].

The low dimensional representation of a complex system may have a nonlinear relationship to easily measurable macroscopic variables. Consider the example of spatiotemporal patterns produced by electroconvection in a liquid crystal as shown in Figure **??**. The patterns a produced by applying a sinusoidal voltage to the system, however we would not expect to recover the voltage drop across the crystal by a simple linear combination of the pixels in an image of the crystal. State-of-the-art distance preserving NLDR can

unwind the nonlinear relationship between these quantities. Moreover, since the voltage drop is a coarse length scale variable, we can expect to recover this variable using the natural ordering of the coordinates produced by these NLDR techniques.

Recently, a nonlinear dimensionality reduction technique called Diffusion Maps has been developed [4], which can be thought of as a robust nonlinear extension of Principle Component Analysis (equivalently, the Karhunen-Loeve Decomposition). Diffusion Maps can be applied to generic data, however in the case of data generated by Brownian motion in a potential field, Diffusion Maps has a natural dynamical interpretation [3–7]. In particular, the results of [7] show that Diffusion Maps applied to Brownian motion in a potential field produces variables that are dynamically independent. This is made formal in [7] with the notion of *approximately Markovian* sets of variables which, on a coarse time-scale, do not require information about higher order variables to determine their evolution.

1.1 Diffusion Maps

For the analysis of complex systems, Diffusion Maps, introduced by Coifman and Lafon in [4, 5], is a revolutionary dimensionality reduction technique that provides rigorous assumptions and convergence results. Diffusion Maps constructs the transition matrix for a random walk on the data set where the transition probabilities are based on the distance between data points. Under the appropriate renormalizations, this transition matrix will be a discrete approximation to the Laplace-Beltrami operator or the Fokker-Plank operator on a manifold . The eigenfunctions of these operators are shown to give a low dimensional representation of the manifold [4] or a stochastic system on the manifold [5, 7].

In this section we give an alternative construction of Diffusion Maps which reveals the renormalization to be equivalent to a choice of Riemannian Metric. This allows us to interpret each operator as a Laplace operator with respect to a specific metric. We show that when Diffusion Maps is applied to time-delay embeddings of dynamical data, the resulting metric will approximate the Lyapunov Metric for a diffusion operator. For isotropic diffusions in a potential field, the Lyapunov Metric is shown to be equivalent to the metric induced by Diffusion Maps which explains the success of the Diffusion Maps for systems of this type.

1.1.1 Review of Diffusion Maps Construction

Diffusion Maps starts with a symmetric kernel $K_\epsilon(x, y) = h_\epsilon(|x - y|)$, with fast decay; a common choice being a Gaussian $h_\epsilon(z) = e^{-z^2/(2\epsilon)}$. This kernel is first used to interpolate

the distribution $p(x)$ of the data as

$$p_\epsilon(x) = \int_\Omega K_\epsilon(x,y)p(y)dy \cong \sum_i K_\epsilon(x,x_i) \tag{1}$$

where $\{x_i\} \in \Omega$ are the discrete observations which are assumed to be sampled from the true density $p(x)$. This implies that in the limit of large data the discrete approximation becomes equality. The idea is to use a kernel density estimate to approximate the Heat kernel as a discrete linear operator, however [4] shows that a subtle renormalization is required to recover the correct operator. Thus, setting

$$\begin{aligned}
K_{\epsilon,\alpha}(x,y) &= \frac{K_\epsilon(x,y)}{p_\epsilon(x)^\alpha p_\epsilon(y)^\alpha} \\
p_{\epsilon,\alpha}(x) &= \int_\Omega K_{\epsilon,\alpha}(x,y)p(y)dy \cong \sum_i K_{\epsilon,\alpha}(x,x_i) \\
F_{\epsilon,\alpha}(f)(x) &= \int_\Omega \frac{K_{\epsilon,\alpha}(x,y)}{p_{\epsilon,\alpha}(x)} f(y)p(y)dy \cong \sum_i \frac{K_{\epsilon,\alpha}(x,x_i)}{p_{\epsilon,\alpha}(x_i)} f(x_i) \\
T_{ji} &= \frac{K_{\epsilon,\alpha}(x_j,x_i)}{p_{\epsilon,\alpha}(x_j)} = \left\langle e^{\epsilon\triangle}\delta_{x_i}, \delta_{x_j} \right\rangle
\end{aligned} \tag{2}$$

they show in [4] that $F_{\epsilon,1}^{t/\epsilon} \to e^{t\triangle}$ and $(I - F_{\epsilon,1})/\epsilon \to \triangle$ as $\epsilon \to 0$, where $\triangle$ is the Laplace-Beltrami operator, and that in the limit of large data the discrete approximations converge as well. Thus we will define the discrete Laplacian of Diffusion Maps as $\overline{\triangle} = (I - T)/\epsilon$ which we will compare with an alternative construction in the next section. Diffusion Maps assumes that the data are sampled from an n-dimensional manifold Σ which is embedded in an ambient euclidean space $\mathbb{R}^N$. Thus the Laplace-Beltrami operator constructed under the renormalization $\alpha = 1$ is in fact the Laplacian with respect to the Riemannian Metric on Σ induced from the ambient space.

Now consider the case when the discrete observations are generated by a stochastic differential equation of the form

$$dx = -\nabla V(x)dt + \sqrt{2}dB_t$$

which corresponds to a Brownian particle in a potential ∇V. Given a prior distribution $\psi_0(x)$ on the location of the Brownian particle, the time evolution of this distribution is governed by the forward Fokker-Planck equation

$$\frac{\partial \psi(x,t)}{\partial t} = \mathcal{O}(\psi(x,t)) = \nabla \cdot (\nabla\psi + \psi\nabla V).$$

In [4, 5] it is shown that $F_{\epsilon,1/2}^{t/\epsilon} \to e^{t\mathcal{O}}$ which means we can approximate the evolution of a distribution ψ_0 on the discrete set $\{x_i\}$ by applying the discrete operator $F_{\epsilon,1/2}^{t/\epsilon}$ to the

vector of samples $\psi_0(x_i)$. In the next section we show that the α parameter corresponds to a choice of Riemannian Metric which will allow us to interpret $\mathcal{O}$ as a Laplacian with respect to the metric induced by ∇V.

The diffusion coordinates give a low-dimensional representation of the system and they are defined for a time scale s by the projection of the data onto the eigenfunctions of the operator $F_{\epsilon,\alpha}^{s/\epsilon}$. Thus letting $F_{\epsilon,\alpha}^{1/\epsilon}\nu_l = \lambda_l\nu_l$ where $1 = \lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_l \geq 0$ the diffusion coordinates are given by

$$\mathcal{P}_{\alpha,s}(x_i) = (\lambda_1^s\nu_1(x_i)/\nu_0(x_i), ..., \lambda_l^s\nu_l(x_i)/\nu_0(x_i)).$$

In the case of a Brownian particle in a potential, it was shown in [7] that the presence of a spectral gap $\lambda_k >> \lambda_{k+1}$ implies that the first k diffusion coordinates at time scale $1/\lambda_{k+1}$ are approximately Markov, meaning that no other coordinates are needed to describe the system at that time scale. This is the notion of *approximately Markovian* which we wish to extend to more general dynamical systems.

1.1.2 Alternative Geometric Construction

In [23, 24] an alternative discrete construction of Laplacian operators is defined via a simplicial complex on a data set. In this section we unify the two constructions by interpreting the normalized transition matrix of Diffusion Maps as a weighted simplicial complex corresponding to a Riemannian Metric on the underlying manifold. This new interpretation will be give a new geometric insight into the Diffusion Maps construction and will be important in correctly interpreting the results of Diffusion Maps applied to complex dynamical data. We will define a simplicial complex on our data set by simply taking the complete graph of the data set and including every possible simplex. While this seems excessive, we will use a probabilistic metric to insure that almost all these simplices are given a negligible weight. This reveals the power of Diffusion Maps as a probabilistic approach to geometry, Diffusion Maps weights simplices continuously instead of making a binary decision for each simplex.

Let $\{x_i\}_{i=1}^S$ be our discrete observations, following [23] we let the basic k-simplices be given by ordered collections of $k+1$ data points. Thus there are S^{k+1} k-simplices, and we represent k-chains as column vectors of length S^{k+1} with each entry giving the weight of the corresponding simplex. We now construct the discrete boundary operator on 1-simplices following [23] as

$$\partial\{x_ix_j\} = \{x_j\} - \{x_i\}$$

which extends linearly to a sparse operator taking 1-chains to 0-chains. We represent k-forms as row vectors of length S^{k+1} and define the discrete exterior derivative $d = \partial^t$

to be the transpose of the discrete boundary operator. Note that

$$d\{x_i\} = \sum_{j \neq i} \{x_j x_i\} - \{x_i x_j\}.$$

The operators ∂ and d are purely topological in nature, however to construct the Laplacian we will need a Riemannian Metric. Again, following [23] we define the Riemannian Metric through the Hodge star and the equation

$$\left\langle \gamma^k, \beta^k \right\rangle = \gamma^T \star_k \beta$$

but instead of the Hodge star in [23] we set

$$\begin{aligned} \star_0\{x_i\} &= \frac{1}{p_{\epsilon,\alpha}(x_i)}\{x_i\} && (3) \\ \star_1\{x_i x_j\} &= K_{\epsilon,\alpha}(x_i, x_j)\{x_i x_j\} && (4) \end{aligned}$$

using $p_{\epsilon,\alpha}$ and $K_{\epsilon,\alpha}$ from Equation 2. This allows us to define the codifferential δ as the adjoint of the exterior derivative d under the Riemannian Metric. Thus δ is defined through the formula

$$\begin{aligned} \delta\{x_i x_j\} &= - \star_0 d^T \star_1 \{x_i x_j\} = - \star_0 \partial \star_1 \{x_i x_j\} \\ &= -K_{\epsilon,\alpha}(x_i, x_j)\left(\frac{\{x_j\}}{p_{\epsilon,\alpha}(x_j)} - \frac{\{x_i\}}{p_{\epsilon,\alpha}(x_i)}\right). \end{aligned} \quad (5)$$

So finally we define the discrete Laplacian on 0-forms by $\triangle_0 = (\delta + d)^2 = \delta d$ and a simple computation confirms that

$$\triangle_0 = 2(T - I) = -2\epsilon\overline{\triangle}$$

which differs from the Diffusion Maps discrete Laplacian by a constant multiple (including the well known sign difference). This confirms that for each α the operator given by $\lim_{\epsilon \to 0} \frac{I - F_{\epsilon,\alpha}}{\epsilon}$ is the Laplacian with respect the Riemannian metric defined by Equation 3.

To make the connection to the Riemannian metric explicit, note that each tangent space is represented by discrete 1-chains. The Riemannian metric, which is locally an inner product, is related to the Hodge star, $\star_1$, simply by choosing local bases of 1-chains. For each vertex $\{x_l\}$ we can form n 1-chains $\{\gamma_{ls}\}_{s=1}^n$ such that the Euclidean vectors $\overline{\gamma_{ls}} = \sum_k \gamma_{ls}(k)(x_k - x_l)$ are linearly independent. Thus $\{\gamma_{ls}\}$ define local coordinates on the tangent space at $\{x_l\}$ and the metric is given by

$$g_{ij}(x_l) = \langle \gamma_{li}, \gamma_{lj} \rangle = \gamma_{li}^T \star_1 \gamma_{lj} = \sum_k \gamma_{li}(k)\gamma_{lj}(k) K_{\epsilon,\alpha}(x_l, x_k).$$

The connection between Diffusion Maps and the geometric construction provides valuable insights into both methods. The geometric formulation reveals that the choice of α

in Diffusion Maps is actually a choice of Riemannian metric, this will allow us to better understand the effect of time-delay coordinates on Diffusion Maps. In particular this reveals that when $\alpha = 1$ the Riemannian metric is chosen to be that inherited from the ambient space (since the input to Diffusion Maps is always given as an embedding in an ambient Euclidean space). Moreover, the results of Diffusion Maps in [4] show that a normalization by $\frac{1}{2\epsilon}$ will be required for the discrete Laplacian $\triangle_0$ to converge to the correct operator in the limit as $\epsilon \to 0$. Finally, the geometric formulation allows natural generalizations to higher order Laplacians which is a subject of ongoing research [23, 24].

1.2 Geometric Interpretation of Diffusion Maps

In Section **??** we have seen that given a finite data set, sampled near a manifold embedded in $\mathbb{R}^N$, a diffusion map constructs a discrete approximation to the heat kernel on the manifold. The diffusion coordinates of Equation (**??**) are given by the eigenfunctions of the heat kernel. In this section we will show that the diffusion coordinates give a mapping (for $l > 2n$ an embedding) of our manifold into $\mathbb{R}^l$ which gives the minimal distortion of the geometry of the manifold.

Note that since the matrix $T^{t/\epsilon}$ is a Grammian matrix, the diffusion coordinates (given by the eigenfunctions of $T^{t/\epsilon}$) are the principal components of the associated inner product space [9]. Thus the diffusion coordinates give an embedding into $\mathbb{R}^L$ which minimizes the distortion of the diffusion distance. Moreover, it is shown in [14] that the diffusion coordinates minimize the functional

$$E[\Phi] = \sum_{l=1}^{L} \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} (\phi_l(x) - \phi_l(y))^2 \frac{K_{\epsilon,\alpha}(x,y)}{p_{\epsilon,\alpha}(x)} p(x)p(y)dxdy$$

over maps $x \mapsto \Phi(x) = (\phi_1(x), ..., \phi_L(x))$ with $\langle \phi_i, \phi_j \rangle = \delta_{ij}$. Note that $K_{\epsilon,\alpha}$ is a localizing kernel with exponential decay. Thus, the diffusion coordinates minimize the local distortion of distance, and since the Riemannian metric is a local feature, the diffusion map will minimize the distortion of the Riemannian metric. This shows that the diffusion map gives the best geometry preservation of any dimensionality reduction technique. Since we wish to preserve the Lyapunov geometry constructed by the time-delay embedding, the diffusion map is the natural choice when reducing the dimensionality of the state space. We next interpret the diffusion map as a time-series.

1.3 Geometric Visualization

We first review the relationship of the geodesic distances on the manifold Ω to the Laplace-Beltrami operator $\triangle$, the heat kernel $e^{t\triangle}$ and the geometry given by the Riemannian

metric g . The choice of Riemannian metric g, Laplace-Beltrami operator $\triangle$, and heat kernel $e^{t\triangle}$ are equivalent, the choice of one uniquely determines the other. The geodesics are defined to be smooth curves $\gamma : [0, 1] \to \mathcal{M}$ which minimize the length functional

$$L[\gamma] = \int_0^1 \sqrt{g_{\gamma(t)}(\dot{\gamma}, \dot{\gamma})} dt$$

where the endpoints of γ are fixed. Geodesics are not necessarily unique, but on a compact manifold the geodesic distance (the minimal value of the length functional) is always defined and is unique [?laplacianBook]. Moreover, the geodesic distance can be written in terms of the heat kernel as

$$d(x, y) = \lim_{t \to 0} -4t \log \left\langle e^{t\triangle}\delta_x, \delta_y \right\rangle_{L^2(\mathcal{M},g)}.$$

Recall from Section **??** that the matrix $T_{ij} = \dfrac{K_{\epsilon,\alpha}(x_j, x_i)}{p_{\epsilon,\alpha}(x_j)}$ is the discrete approximation to the heat kernel for $\alpha = 1$. Thus we can approximate the geodesic distance between sample points x_i and x_j as

$$d_t(x_i, x_j) = -4t \log((T^{t/\epsilon})_{ij}) \cong -4t \log \left(\sum_{l=0}^{L} \lambda_l^t \nu_l(x_i)\nu_l(x_j) \right) = -4t \log \left(\mathcal{P}_{1,t}(x_i) \cdot \mathcal{P}_{1,t}(x_j) \right)$$

for t small. Note that for t small we will need to take L very large to get a good approximation of the geodesic distances; see the Appendix for a practical discussion of how to choose t.

Since we wish to achieve a low dimensional representation of our data, it is natural to generalize the geodesic distance to the diffusion distance, defined in [4] as

$$d_t(x, y) = \left\langle e^{t\triangle}\delta_x, \delta_y \right\rangle_{L^2(\mathcal{M},g)} \cong \mathcal{P}_{1,t}(x_i) \cdot \mathcal{P}_{1,t}(x_j)$$

Moreover, if we write T in its eigendecomposition $T^{1/\epsilon} = V\Lambda V^{-1}$ then we have

$$-4t \log(T^{t/\epsilon}) = -4t^2 V \log(\Lambda) V^{-1}$$

so we can also approximate the geodesic distance as

$$d_t(x_i, x_j) = -4t \log((T^{t/\epsilon})_{ij}) \cong -4t^2 \sum_{l=0}^{L} \log(\lambda_l)\nu_l(x_i)\nu_l(x_j).$$

Next we define the discrete Laplacian $L = \dfrac{I - T}{\epsilon}$ (note that this is exactly the graph Laplacian for an appropriately weighted graph) and also the pseudo-inverse L^+ of the Laplacian.

If the data points $\{x_i\}_{i=1}^N$ are sampled from a smooth manifold then the Diffusion Maps coordinates can be used to give an efficient embedding of this manifold into a low dimensional space. In [4] it is shown that the Diffusion Maps coordinates given by $\mathcal{P}_{\alpha,s}(x_i)$ in Equation **??** give an embedding into a Euclidean space such that the Euclidean distance in the embedding space approximates the diffusion distance on the original manifold. This gives a continuous hierarchy of embeddings indexed by the parameter s which represents the scale of the diffusion distance. It is also argued in [4] that for small s we can truncate the coordinates of $\mathcal{P}_{\alpha,s}(x_i)$ to achieve a good low dimensional embedding of the data set $\{x_i\}$.

Metric Multi-Dimensional Scaling (MDS) gives a general technique for constructing a low dimensional embedding which minimizes distortion of a given metric. Given a metric d represented by a matrix of squared distances $D_{ij} = d(x_i, x_j)^2$ metric MDS reconstructs the Gram matrix G then uses the first k eigenvectors of the Gram matrix G as an optimal embedding of the data set x_i into $\mathbb{R}^k$. The matrix of inner products can be computed from a matrix of squared distance by double centering the matrix of squared distances

$$G = D - \frac{1}{N} D\mathbf{1}_N - \frac{1}{N}\mathbf{1}_N^T D + \frac{1}{N^2}\mathbf{1}_N^T D\mathbf{1}_N.$$

However, in this case we can compute the Gram matrix directly by considering the Nxl matrix $\mathcal{P}_{i,\cdot} = \mathcal{P}_{\alpha,s}(x_i)$ so that $G = \mathcal{P}\mathcal{P}^T$. Metric MDS gives an optimal low dimensional representation of the data set in the sense of minimizing the distortion of the metric d [9]. Thus for each value of the scale parameter s we can achieve a low dimensional embedding via metric MDS. Moreover, in [`?biharmonicdist`] it is suggested that $s = -1$ gives an optimal representation of the manifold.

In the previous section we showed that Diffusion Maps can recover the geometry (represented by the Riemannian metric or the Laplace operator with respect to that metric) of a data set and can construct a class of conformal transformations of the geometry, indexed by the parameter α. In order to analyze a different geometry, Diffusion Maps requires a isometric embedding of the data with respect to the desired Riemannian metric. In our applications to dynamical systems, this isometric embedding requires a very large dimensional ambient Euclidean space. Thus the procedure in this section can be used to recover low dimensional representations of the new metric which allows us to visualize the changing geometry in a low dimensional state space.

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