Time-Scale Separation and Complex Systems Reduction from Diffusion-Mapped Delay Coordinates (DMDC)

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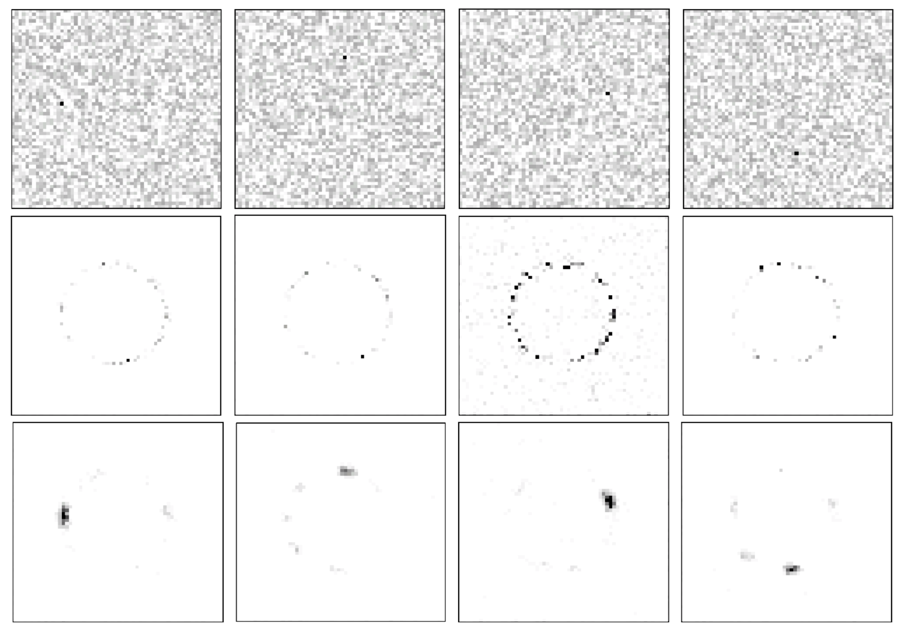
Overview

Nonlinear dimensionality reduction has been successfully applied to very high dimensional observations such as images [5]. However, these methods are typically designed for data that have no dynamics. Dynamical data, meaning data with a time ordering, is a unique problem with different goals than generic dimensionality reduction. Whereas the goal of generic dimensionality reduction is typically to minimize the reconstruction error, such a representation *may not contain dynamically interesting information*.

DMDC Algorithm

Diffusion-Mapped Delay Coordinates (DMDC) is a new data-driven algorithm for time series analysis based on a novel theory of attractor reconstruction. The approach of DMDC can be broken down into two steps, reconstruction and reduction. In the reconstruction step, we show that the classical technique of time-delay embeddings, with appropriate weights, effectively approximates the Lyapunov metric in the most stable Lyapunov direction. Our reconstruction technique necessitates embedding into a high dimensional ambient space, given by the delay coordinates. Thus a second step, reduction, is required to achieve a manageable embedding. However, the reduction step must be carefully designed to preserve the structure reconstructed via the delay coordinates.

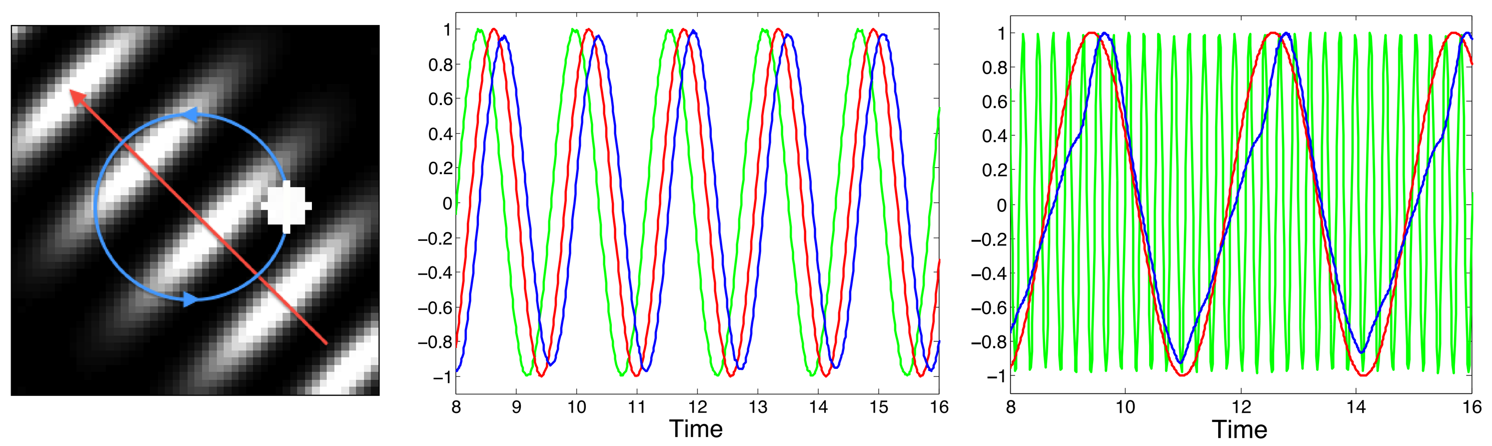


Original Video Frames

SVD Reconstruction

Time-delay Reconstruction

In the example above we show how time-delays help capture the important dynamical information from a noisy video of a black pixel moving in a circle. Below we illustrate the shortcomings of SVD with a video which combines large variance stripes with a low variance defect. While the SVD always picks out the high variance stripes, DMDC separates these features based on time-scale. On the left is a frame from the video, the plots compare SVD (green) with DMDC (blue) when the stripes are moving slower (middle) and when the defect is moving slower (right).



The theory of time-delay coordinates as introduced by Takens [3] shows that by appending delayed values of a generic observation of a dynamical system, one achieves a diffeomorphic copy of the attractor in some Euclidean space. The fact that the embedding is given by a diffeomorphism of the attractor shows that the time-delay embedding is topology-preserving, however crucially it introduces a new geometry to the data set. Assume a multivariate observation of dimension r, given by a smooth nonlinear $h \in C^\infty(\mathcal{M}, \mathbb{R}^r)$. For $\kappa, \tau > 0$ define the κ-weighted *delay coordinate map* $H : \mathcal{M} \to \mathbb{R}^{r(s+1)}$ by

$$H(x) = [h(x), e^{-\kappa} h(F_{-\tau}(x)), e^{-2\kappa} h(F_{-2\tau}(x)), \ldots, e^{-s\kappa} h(F_{-s\tau}(x))]^T.$$

Reconstruction of Attractor Geometry

Let $\mathcal{M}$ be an n-dimensional smooth compact Riemannian manifold which is the attractor of a system denoted $\dot{x} = f(x)$, with invariant measure μ for the induced flow F_t. To accommodate discrete observations of the dynamics we will consider the flow F_τ for a fixed time step $\tau > 0$. According to Oseledets [4], there exist real numbers $\sigma_1 < \ldots < \sigma_k$, with $k \le n$, such that for μ-almost every x there is a splitting $T_x\mathcal{M} = \bigoplus_{i=1}^k E_i(x)$, where $\dim E_i = d_i$, and where $d_1 + \ldots + d_k = n$. For $\epsilon > 0$, the *ϵ-Lyapunov metric* $\langle u, v \rangle_\epsilon$ is defined by

$$\langle u_i, v_i \rangle_\epsilon = \sum_{j \in \mathbb{Z}} e^{-2(\sigma_i j + \epsilon |j|)} \langle DF_{j\tau}(x) u_i, DF_{j\tau}(x) v_i \rangle_{T_x\mathcal{M}}$$

for $u_i, v_i \in E_i(x)$. The Lyapunov metric is intrinsic to the dynamics because, when measured in the Lyapunov metric, the dynamics satisfy uniform bounds and moreover all the Lyapunov spaces are orthogonal.

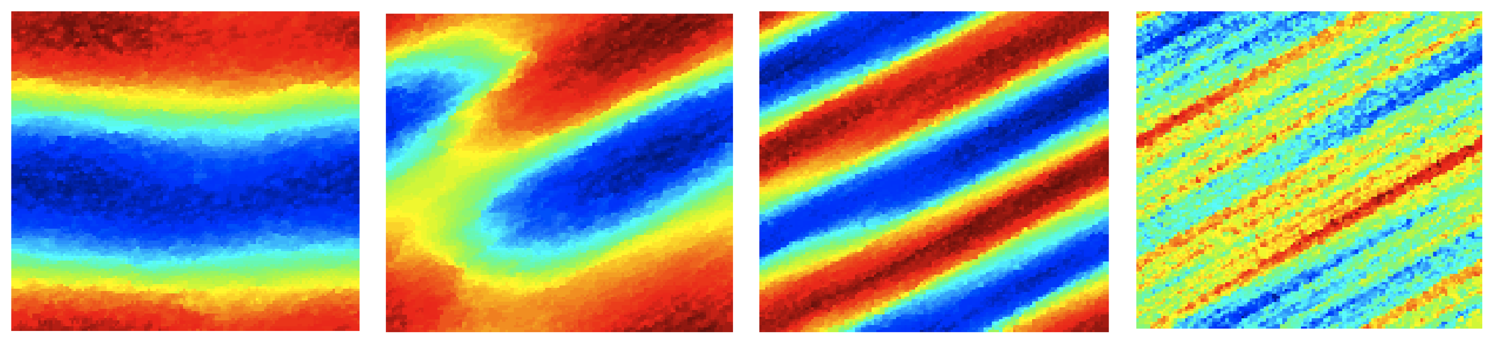
Theorem: Let $\mathcal{M}$ be a compact manifold, $u, v \in T_x\mathcal{M}$ and let $\hat{u} = DH(u)$ and $\hat{v} = DH(v)$ be the images under the time-delay embedding H given above. Let $u_i = \pi_i(u)$ be the projection onto the ith Oseledets space, and assume u_1 and v_1 are nonzero. Let $0 < \kappa < -\sigma_1$. Then for a prevalent choice of h and for all $i \neq 1$,

$$\lim_{s\to\infty} \frac{\langle \hat{u}_i, \hat{v}_i \rangle}{||\hat{u}||\,||\hat{v}||} = 0 \qquad \text{and} \qquad \lim_{s\to\infty} \frac{\langle \hat{u}, \hat{v} \rangle - \langle \hat{u}_1, \hat{v}_1 \rangle}{||\hat{u}||\,||\hat{v}||} = 0.$$

In the example below we illustrate the effect on the geometry of the torus by time-delay embedding via Arnold's cat map, a discrete time map on the torus $S^1 \times S^1$ given by

$$a_{j+1} = 2a_j + b_j \text{ mod } 1 \qquad \text{and} \qquad b_{j+1} = a_j + b_j \text{ mod } 1.$$

We choose a point $(a_0, b_0) \in [0,1]^2$ randomly and apply the cat map for N iterations, producing the points $\{(a_j, b_j)\}_{j=0}^N$. To test Theorem , we then embed the torus into $\mathbb{R}^3$ and observe the dynamics via the weighted delay coordinates given above.



In the above images we show the first nontrivial eigenfunction of the Laplace-Beltrami operator in the (a, b)-plane, with $s = 2048$ delays and $\kappa = 1.2, 0.8, 0.4, 0.01$ from left to right.

Reduction via Diffusion Map

The weighted time-delay embedding introduces a natural geometry on a dynamical system and we wish to preserve this geometry while finding lower-dimensional coordinates. Diffusion Maps is a data-driven technique for dimensionality reduction which preserves geometric features. The components of the diffusion map approximate the eigenfunctions of the Laplace-Beltrami operator, and thus give a nonlinear map $\Psi_{\alpha,t} : \Omega \to \mathbb{R}^L$ which, at the data point x_i, is given by

$$\Psi_{\alpha,t}(x_i) = [\lambda_1^t \psi_1(x_i), ..., \lambda_L^t \psi_L(x_i)]^T$$

In [1] we show that for a time series:

- A diffusion map can match the invariant measure.
- The diffusion map minimizes the distortion of the attractor geometry.
- The coordinates of the diffusion map have a natural time-series interpretation.
- The eigenvalue of a diffusion map coordinate determines the time-scale.
- The α and t parameters control the measure and scale of the map respectively.
- In the limit of large data and $t \to 0$ the geometry is recovered.

Time-Scale Separation

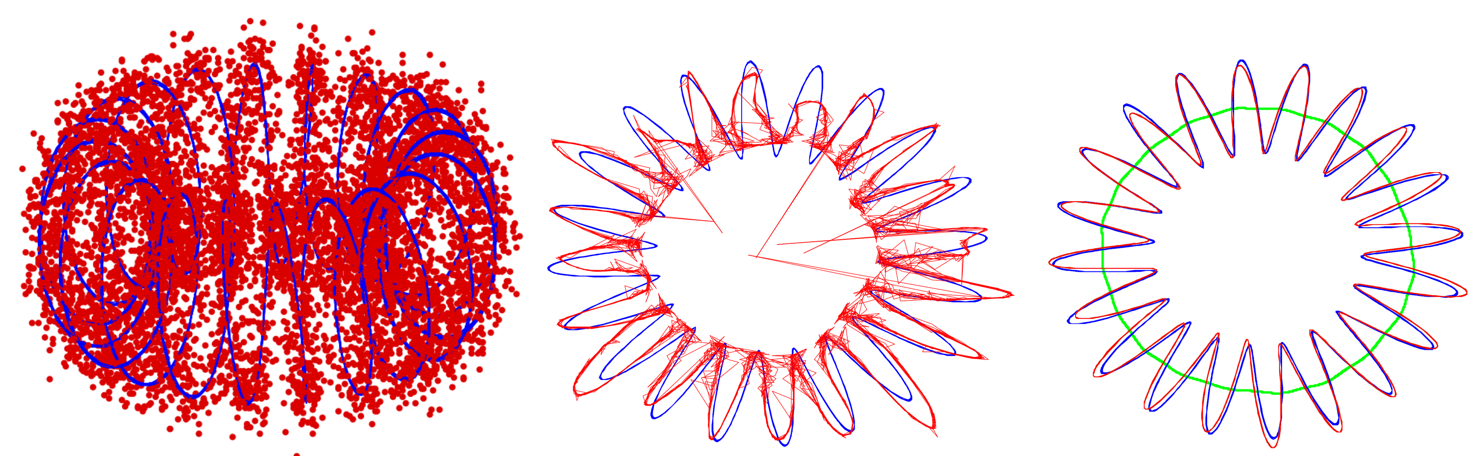
Since diffusion maps can only approximate operators $\mathcal{L}$, which are Laplacians up to a conformal transformation, we now assume that we can write the full evolution as a non-autonomous perturbation of $\mathcal{L}$ so that

$$\frac{\partial \varphi}{\partial t} = -\mathcal{L}(\varphi) + \mathcal{F}(x, t).$$

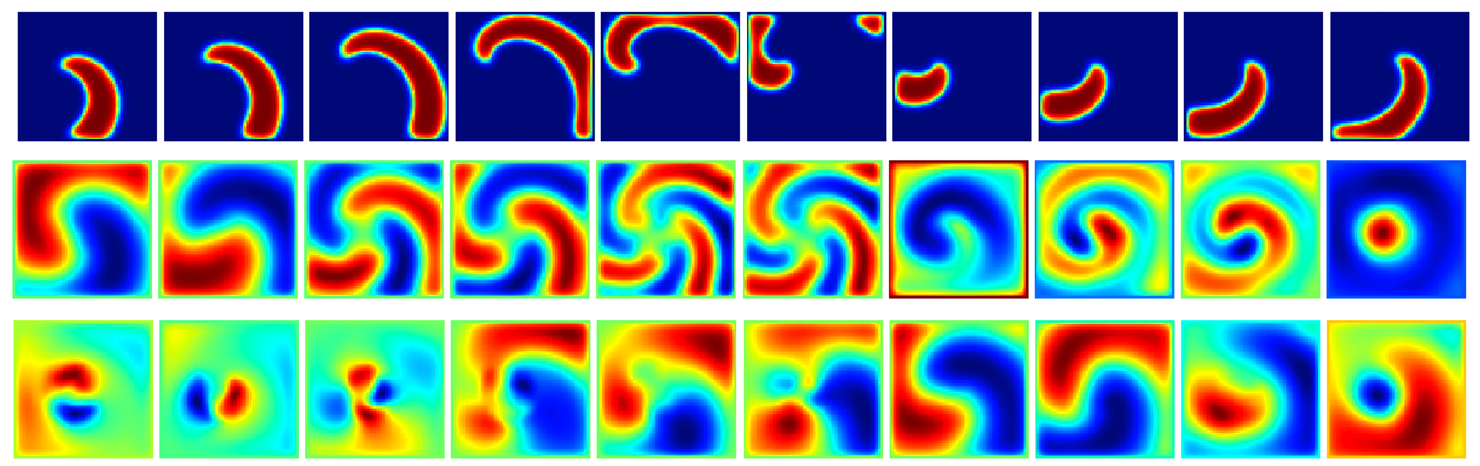
In this case we show in [1] that the l-th diffusion map mode satisfies

$$\hat{\psi}_l(t) = a e^{-\gamma_l t} + b \int_0^t e^{-\gamma_l (t-s)} \hat{\mathcal{F}}(s) ds.$$

Thus, the eigenvalue γ_l will determine the amount of history from the non-autonomous term $\hat{\mathcal{F}}$ is integrated into the mode $\hat{\psi}_l$. Thus, for $\hat{\mathcal{F}}$ sufficiently regular the time scale of $\hat{\psi}_l$ will be determined by γ_l.



In the above example we show the reconstruction of dynamics on a torus from noisy observations using various values of κ. All plots show the x, y-plane dynamics in blue. The noisy observations are shown in red in the leftmost plot. In the middle and right plot, the reconstructed dynamics for $\kappa = 1, 0.02$ are shown in red and the projection onto the slow manifold is shown in green.



In the above example we apply DMDC to video of a meandering spiral wave generated by the Barkley model,

$$\begin{aligned} u_t &= \Delta u + \frac{1}{\rho} u(1-u)\left(u - \frac{v+b}{a}\right) \\ v_t &= u - v \end{aligned}$$

In the top row we show frames from the video. In the middle row we show the spatial modes generated by applying SVD to the weighted attractor reconstruction. In the last row we show the spatial modes generated by DMDC. In [1] we show that DMDC isolates a long period oscillation in the meandering that the SVD analysis ignores.

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