Diffusion Mapped Delay Coordinates and the Geometry of Dynamical Data

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Motivating Example: High Dimensional Dynamics

Spatiotemporal dynamics of liquid crystals:

- Each image $\approx 1,000,000$ dimensional
- Order of $\approx 100,000$ images
- Latent dimension between 10 and 100
- Find latent variables
- Find slow variables

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Video provided by Rob Cressman and Zrinka Gregurić Ferenček, Physics Dept., GMU

Low Dimensional Dynamics
High Dimensional Observations

Starting point:

- Each image $\approx 10,000$ dimensional
- Order of $\approx 10,000$ images
- Latent dimension between 1 and 10
- Find latent variables
- Find slow variables

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Video provided by Rob Cressman and Zrinka Gregurić Ferenček, Physics Dept., GMU

Model Free Techniques

- Use nothing but these video data sets; ultimate goal:
  - Identify a ‘small’ set of state variables
  - Sort state variables by importance
  - Represent the vector field describing the dynamics
  - Decompose, predict, and control the dynamics
- Assume that parametric modeling has been exhausted
- Use nonparametric modeling
- Notion of *importance* is fundamental

Example of Time Scale Separation with DMDC

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Experiment by Rob Cressman and Zrinka Gregurić Ferenček, Physics Dept., GMU.

Embedology: A Topological Nonparametric Model

- Implicit model: There exists a smooth dynamical system $x'(t) = f(x(t))$ evolving on an m-dimensional manifold $\mathcal{M}$
- Data: A time series of generic observations $y_i = h(x(t_i))$
- **Reconstruction (Takens):** For M sufficiently large, $H(y_i) = (y_i, y_{i-1}, ..., y_{i-M})$ is an embedding of $\mathcal{M} \to \mathbb{R}^{M+1}$
- **Reduction:** Standard approach is to use linear projections, for example Broomhead/King suggest principal components

Diffusion Mapped Delay Coordinates (DMDC)

- DMDC is the geometric extension of Embedology
- Improves on Embedology by preserving geometry instead of chasing variance
- Identifies variables important to the evolution
- **Reconstruction (Berry/Sauer):** Build an embedding of the data which respects the intrinsic geometry of the dynamics
- **Reduction (Coifman/Lafon):** Find a low-dimensional set of variables which preserves the reconstructed geometry

See also: Giannakis, D. and Majda, A. J. Nonlinear Laplacian spectral analysis for time series with intermittency and low-frequency variability. *PNAS vol. 109 num. 7 (2012) pp. 2222-2227.*

DMDC: Example of Time Scale Separation

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Variance Slow Mode

DMDC: Reconstruction

- For time series $\{y_i = h(x_{t_i})\}$ define the κ-weighted *delay coordinates*

$$Y_i = H_\kappa(y_i) = [y_i, e^{-\kappa} y_{i-1}, e^{-2\kappa} y_{i-2}, \ldots, e^{-s\kappa} y_{i-s}]^T$$

- For $0 < \kappa < -\sigma_1$, the embedding H_κ projects onto the most stable Lyapunov component of the dynamics
- For a special choice of κ, the embedding approximates the Lyapunov metric on the most stable component
- The Lyapunov metric represents the *natural* geometry for a dynamical system

The Biased Geometry of Delays

The point of this weighting is to kill off all but the most stable Lyapunov components:

$$Y_i = H_\kappa(y_i) = [y_i, e^{-\kappa} y_{i-1}, e^{-2\kappa} y_{i-2}, \dots, e^{-s\kappa} y_{i-s}]^T$$

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 $i \neq 1$,

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

DMDC: Embedding Geometry of the Cat Map

- Visualize the geometry via eigenfunction of Laplacian on the state space of the Cat Map
- As κ decreases below $-\sigma_1 \approx .962$, geometry becomes localized on stable manifold

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DMDC: Reduction

- Reconstruction requires embedding into a high dimensional ambient space
- Reduction is needed to achieve a manageable embedding
- The reduction must map to a low dimensional Euclidean space while preserving the reconstructed geometry
- A diffusion map is a nonlinear reduction that:
  - preserves the induced geometry
  - can match the invariant measure
  - minimizes the distortion of the geometry
  - has a natural time-series interpretation

DMDC: Application to Meandering Spiral Waves

- Barkley's model generates meandering spiral waves
- DMDC captures the slow precession of the meandering spiral

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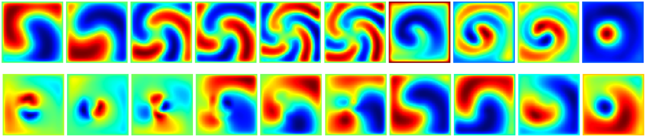
SVD:

DMDC:



DMDC: Application to Liquid Crystals

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Time Scale Separation on the Stable Component

We assume the evolution on the stable component is a small perturbation of $\mathcal{L}$ so that

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

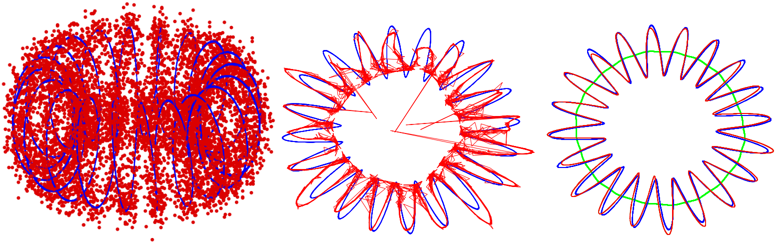
The l-th diffusion map eigenfunction satisfies

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

The eigenvalue γ_l determines the amount of history of $\hat{\mathcal{F}}$ integrated into the mode $\hat{\psi}_l$ For $\hat{\mathcal{F}}$ sufficiently regular the time scale of $\hat{\psi}_l$ will be determined by γ_l

Example of Time Scale Separation

- Spiral (blue) is an attractor, noise is perturbation along the unstable manifold
- Projection onto stable manifold removes noise
- Diffusion Maps finds the correct geometry
- Coarse geometry gives projection onto slow manifold (green)



How does DMDC separate time-scales?

- Time-delay embeddings bias the geometry; weights can influence this bias
- Bias can be leveraged to project onto stable dynamics
- Evolution on stable component more likely to allow time-scale separation
- Current approach requires evolution to be small perturbation of heat equation

The Big Picture: The Geometry of Data

- Nonparametric analysis of smoothly varying data is sensitive to geometry
- It is important to find the intrinsic geometry specific to your goals, meaning one which is invariant to unwanted or incidental features of the data
- We can now give two examples of the intrinsic/extrinsic dichotomy

The Intrinsic Geometry for Generic Data (Diffusion Maps)

- Generic data has no a priori structure except the geometric prior
- The embedding geometry is a desired feature of data (intrinsic)
- The sampling density is an unwanted influence (extrinsic)
- The key feature of diffusion maps is ability to control the sampling bias from the geometry

The Intrinsic Geometry for Dynamical Systems

- Observation may arbitrarily distort the state space geometry
- Dynamically equivalent (diffeomorphic) copies of an attractor can have different geometries
- The observation geometry and Takens' embedding geometry are both *entirely* extrinsic
- Lyapunov geometry is intrinsic since it
  - is independent of observation (generically)
  - makes the Oseledets spaces orthogonal
  - gives uniform bounds on expansion/contraction rates

Program for the Future

- Identify the intrinsic geometry for common data types
  - spatiotemporal
  - networks
  - multiscale
  - hybrid systems
- Develop methods to extract the intrinsic geometry
- Can every geometry be represented with a kernel?
- How do we extract information from the geometry that is relevant to the data?
  - cohomology classes
  - differential forms
  - curvature

References

- T. Berry, R. Cressman, Z. Greguric-Ferencek, T. Sauer, *Time-scale separation from diffusion-mapped delay coordinates.* SIAM J. Appl. Dyn. Syst. 12, 618-649 (2013).
- Giannakis, D. and Majda, A. J. *Nonlinear Laplacian spectral analysis for time series with intermittency and low-frequency variability.* PNAS 109, 2222-2227 (2012).
- Diffusion Maps (Coifman, Lafon, Kevrekidis, Singer, et al.)