

# Learning manifolds from data

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Mathematics Colloquium  
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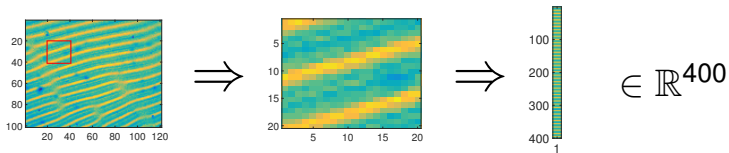
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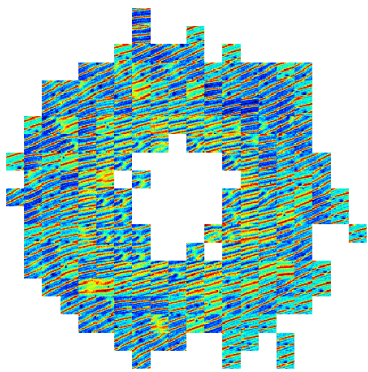
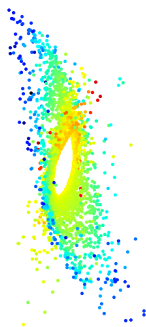
# MOTIVATING EXAMPLE: NEMATIC LIQUID CRYSTAL



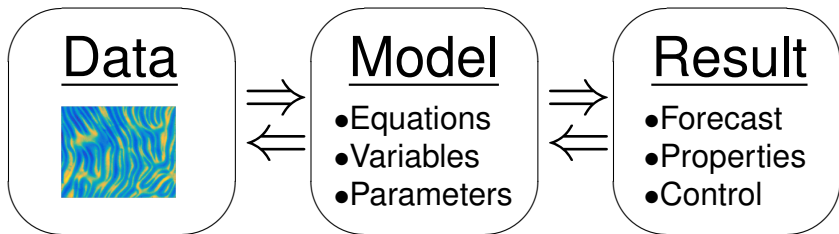
# FINDING HIDDEN STRUCTURE IN DATA



The sub-image geometry:



# PARAMETRIC MODELING



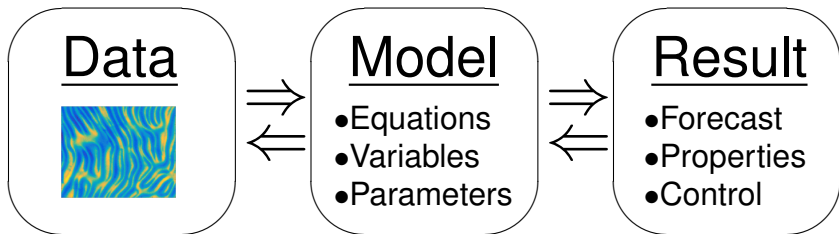
## ▶ Model error:

- ▶ Trade off **resolution** and **complexity**
- ▶ Stationarity/Homogeneity of parameters

## ▶ Assimilate Data: Fit Parameters/Variables

- ▶ Lumps together **noise** and **model error**

# PARAMETRIC MODELING



## ▶ Model error:

- ▶ Trade off **resolution** and **complexity**
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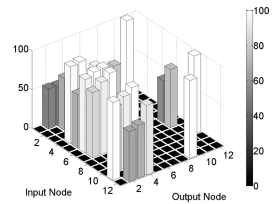
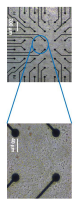
## ▶ **Assimilate Data:** Fit Parameters/Variables

- ▶ Lumps together **noise** and **model error**

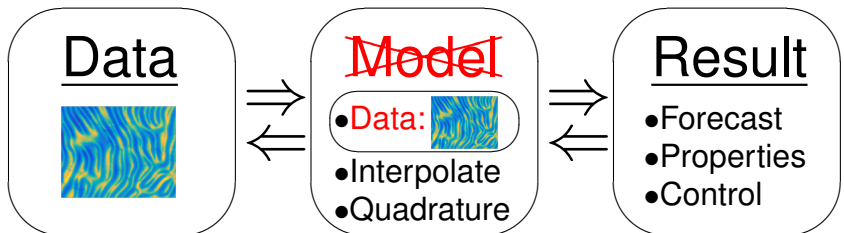
# DATA ASSIMILATION

- ▶ Estimate state/parameters from noisy observations
- ▶ EnKF requires noise covariances (unknown)
- ▶ **Adaptive** data assimilation
  - ▶ Estimates covariances, compensates for model error
  - ▶ Extends (Mehra 1970,1972) to nonlinear systems

Hamilton, Berry, Peixoto, Sauer (PRE, 2013)  
 Berry & Sauer (Tellus A, 2013)  
 Berry & Harlim (Proc. Royal Society A, 2014)  
 Hamilton, Berry, & Sauer (Physical Review X, 2016 )  
 Harlim & Berry (Monthly Weather Review, in review)



# NONPARAMETRIC MODELING



- ▶ **Tools:** For functions  $f \in \mathcal{H}$  determined by values  $\vec{f}_i = f(x_i)$ 
  - ▶ Interpolate:  $f(x) = \sum_j \langle f, \varphi_j \rangle \varphi_j(x)$
  - ▶ Quadrature:  $\langle f, \varphi_i \rangle \approx \sum_j f(x_j) \varphi_j(x_i)$
  - ▶ Operator Representation:  $\mathbf{A}_{jk} = \langle \varphi_j, \mathcal{A}\varphi_k \rangle$
- ▶ All require a **basis**  $\{\varphi_j\}$ !

# ROADMAP

- ▶ What is manifold learning?  $\Rightarrow$  Estimate Laplacian,  $\Delta$
- ▶ How to find the Laplacian?  $\Rightarrow$  Graph Laplacian,  $\mathbf{L}$
- ▶ Convergence  $\mathbf{L} \rightarrow \Delta$  and overcoming limitations
- ▶ **Key result:** Extension to non-compact manifolds
- ▶ New graph construction based on key result (TDA)
- ▶ Applications and future directions

# WHAT IS MANIFOLD LEARNING?

- ▶ **Geometric prior:** Data on Riemannian manifold  $\mathcal{M} \subset \mathbb{R}^m$
- ▶ **Goal:** Represent all the information about a manifold
- ▶ A smooth embedded manifold  $\mathcal{M} \subset \mathbb{R}^m$  **inherits:**
  - ▶ A **metric tensor**  $g_x : T_x\mathcal{M} \times T_x\mathcal{M} \rightarrow \mathbb{R}$  (inner product)
  - ▶  $g$  completely determines the geometry of  $\mathcal{M}$
  - ▶ A **volume form**  $dV(x) = \sqrt{\det(g_x)} dx^1 \wedge \dots \wedge dx^d$
- ▶ Laplace-Beltrami operator,  $\Delta$ , is equivalent to  $g$ 
  - ▶  $\Delta f = \operatorname{div} \circ \nabla = \frac{1}{\sqrt{|g|}} \partial_i g^{ij} \sqrt{|g|} \partial_j f$
  - ▶  $g(\nabla f, \nabla h) = \frac{1}{2}(f\Delta h + h\Delta f - \Delta(fh))$

# WHAT IS MANIFOLD LEARNING?

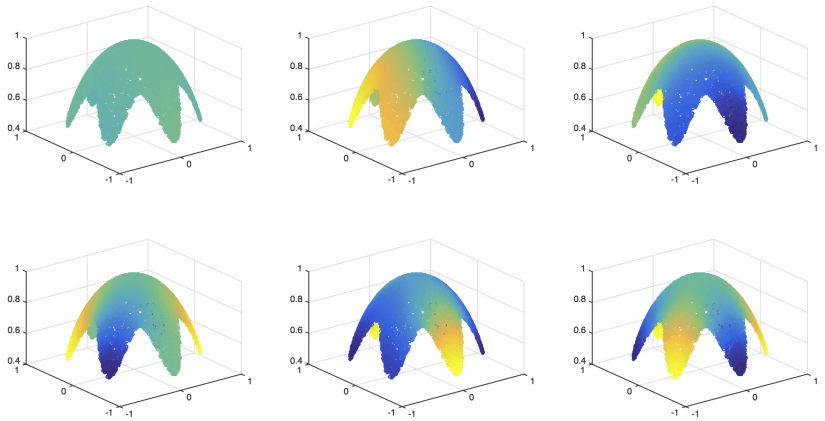
- ▶ **Manifold learning**  $\Leftrightarrow$  **Estimating Laplace-Beltrami**
- ▶ **Hodge theorem:**  
Eigenfunctions  $\Delta\varphi_i = \lambda_i\varphi_i$  orthonormal basis for  $L^2(\mathcal{M}, g)$
- ▶ Smoothest functions:  $\varphi_i$  minimizes the functional

$$\lambda_j = \min_{\substack{f \perp \varphi_k \\ k=1, \dots, j-1}} \left\{ \frac{\int_{\mathcal{M}} \|\nabla f\|^2 dV}{\int_{\mathcal{M}} |f|^2 dV} \right\}$$

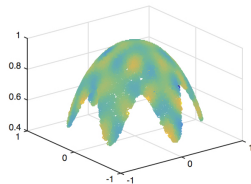
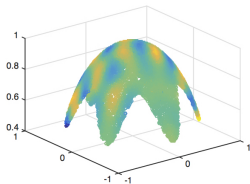
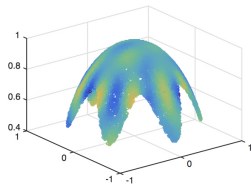
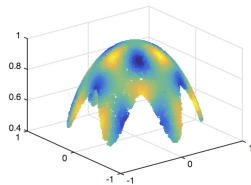
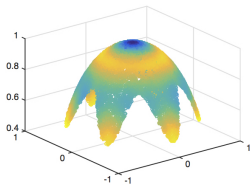
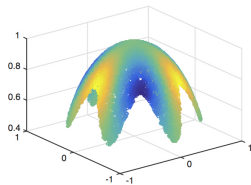
- ▶ Eigenfunctions of  $\Delta$  are custom Fourier basis
  - ▶ Smoothest orthonormal basis for  $L^2(\mathcal{M}, g)$
  - ▶ Can be used to define wavelet frame
  - ▶ Define the Sobolev spaces on  $\mathcal{M}$



# HARMONIC ANALYSIS ON MANIFOLDS

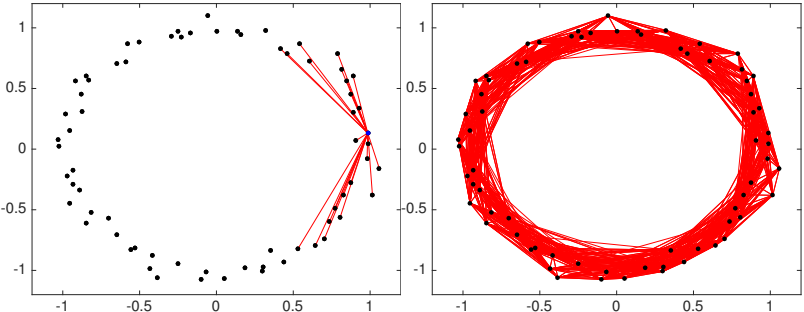


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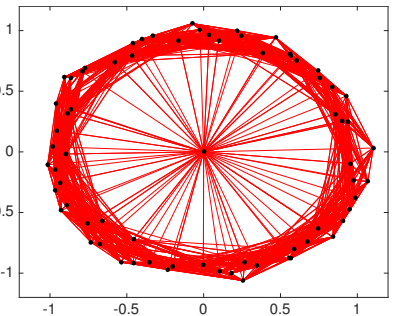
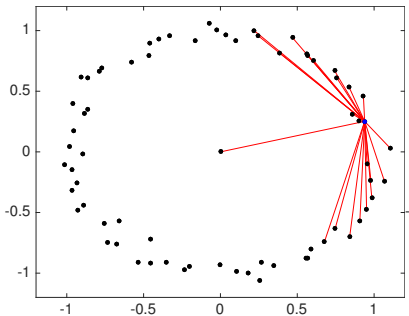
# SO HOW DO WE FIND THE LAPLACIAN FROM DATA?

- ▶ Assume data lies on (or at least near) a manifold
- ▶ Approximate manifold with graph  $\Rightarrow$  Connect nearby points



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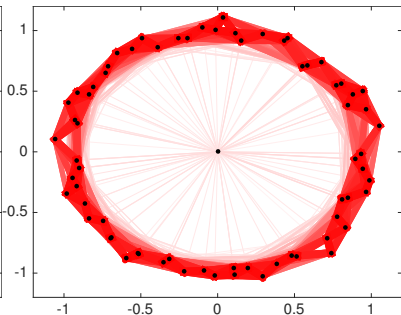
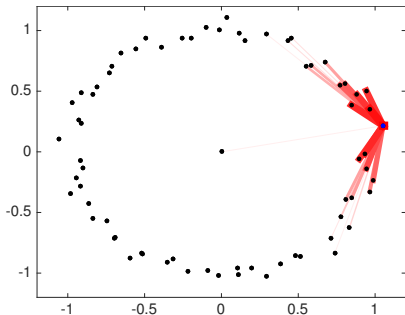
► **Problem:** Noise and outliers can lead to *bridging*



# SO HOW DO WE FIND THE LAPLACIAN FROM DATA?

► To prevent bridging we weight the edges

► Edges are given weights  $K_\delta(x, y) = e^{-\frac{\|x-y\|^2}{4\delta^2}}$



# SO HOW DO WE FIND THE LAPLACIAN FROM DATA?

- ▶ Data set  $\Rightarrow$  *weighted graph*
- ▶ Edge Weights defined by a kernel function

$$K_{\delta}(x_i, x_j) = e^{-\frac{\|x_i - x_j\|^2}{4\delta^2}}$$

- ▶ Bandwidth  $\delta$  determines localization
- ▶ ‘Adjacency’ matrix:  $\mathbf{K}_{ij} = K(x_i, x_j)$
- ▶ ‘Degree’ matrix:  $\mathbf{D}_{ii} = \sum_j \mathbf{K}_{ij}$
- ▶ Normalized graph Laplacian:  $\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{K}$

# POINTWISE CONVERGENCE

**Theorem:** (Belkin & Niyogi, 2005, Singer, 2006)

For  $\{x_i\}_{i=1}^N \subset \mathcal{M} \subset \mathbb{R}^m$  uniformly sampled on a compact manifold and for  $\vec{f}_i = f(x_i)$  where  $f \in C^3(\mathcal{M})$

$$\frac{1}{\delta^2} \left( \mathbf{L}\vec{f} \right)_i = \Delta f(x_i) + \mathcal{O} \left( \delta^2, \frac{1}{N^{1/2}\delta^{1+d/2}} \right)$$

$\delta =$  bandwidth

$N =$  number of points

# RESTRICTIONS THAT HAVE BEEN OVERCOME TO DEAL WITH **REAL DATA**:

- ▶ **Arbitrary sampling** (Coifman & Lafon, 'Diffusion maps', ACHA 2006)
- ▶ **Non-compact manifolds** (Berry & Harlim, ACHA 2015)
- ▶ **Other kernel functions** (Thesis 2013; Berry & Sauer, ACHA 2015)
- ▶ **Boundary** (Coifman & Lafon, ACHA 2006; Berry & Sauer, J. Comp. Stat. 2016)
- ▶ **Spectral convergence** (Luxburg et al., Ann. Stat. 2008, Berry & Sauer, submitted)



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# LOCAL KERNELS

- ▶ A *local kernel* has exponential decay:

$$K_\delta(x, x + \delta y) < c_1 e^{-c_2 \|y\|^2}$$

- ▶ **Theorem:** Symmetric **local kernels** converge to Laplacians
  - ▶ Every local kernel determines a geometry
  - ▶ Every geometry accessible by a local kernel
- ▶ Explain success of **'kernel methods'** in data science:
  - ▶ **KPCA:** Kernel Principal Component Analysis
  - ▶ **KSVM:** Kernel Support Vector Machines
  - ▶ **KDE:** Kernel Density Estimation
  - ▶ **RKHS:** Reproducing Kernel Hilbert Spaces
  - ▶ Spectral Clustering (**KPCA**)

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# TANGIBLE MANIFOLDS

- ▶ Compute ambient distance  $\|x - y\|_{\mathbb{R}^m}$
- ▶ Need localization in  $d_{\mathcal{I}}(x, y) = \inf_{\gamma} \left\{ \int_0^1 |\gamma'(t)| dt \right\}$
- ▶ **Assume** ratio  $R(x, y) = \frac{\|x - y\|_{\mathbb{R}^m}}{d_{\mathcal{I}}(x, y)}$  bounded away from zero
- ▶ We will use the exponential map to change variables
- ▶ **Assume** injectivity radius  $\text{inj}(x)$  bounded away from zero

**Definition:** A manifold is **uniformly tangible** if there are lower bounds on  $\text{inj}(x)$  and  $\inf_{y \in \mathcal{M}} R(x, y)$  independent of  $x$

# CONSISTENCY PART 1

- ▶ Matrix times vector converges to integral operator:

$$\left(\mathbf{K}\vec{f}\right)_i = \sum_{j=1}^N K_\delta(x_i, x_j) f(x_j) \xrightarrow{N \rightarrow \infty} \int_{\mathcal{M}} K_\delta(x_i, y) f(y) dV(y)$$

- ▶ Assume kernel has fast decay:  $K_\delta(x, y) < e^{-\|x-y\|^2/\delta^2}$
- ▶ Localize integral, requires  $R(x_i, y) = \frac{\|x_i - y\|}{d_i(x_i, y)} > 0$

$$\left(\mathbf{K}\vec{f}\right)_i \rightarrow \int_{\mathcal{M} \cap \exp_{x_i}(B_\delta(0))} K_\delta(x_i, y) f(y) dV(y) + \mathcal{O}(\delta^k)$$

- ▶ Change variables to the tangent space  $y = \exp_{x_i}(s)$ :

$$\left(\mathbf{K}\vec{f}\right)_i \rightarrow \int_{B_\delta(0)} K_\delta(x_i, \exp_{x_i}(s)) f(\exp_{x_i}(s)) ds + \mathcal{O}(\delta^k)$$

- ▶ Requires injectivity radius  $\text{inj}(x_i) > \delta > 0$

## CONSISTENCY PART 2

- ▶ Taylor expansion in normal coordinates:

$$f(\exp_x(s)) = f(x) + \nabla f(x) \cdot s + \frac{1}{2} s^\top H(f \circ \exp_x)(0) s$$

- ▶ Symmetric kernel  $\Rightarrow$  Odd terms integrate to zero

$$\begin{aligned} (\mathbf{K}\vec{f})_i &\rightarrow \int_{\|s\| < \delta} \left( K(\|s\|) + \mathcal{O}(\delta^2 s_i^4) K'(\|s\|) / \|s\| \right) \cdot \\ &\quad \left( f(x_i) + \delta \nabla f(x_i) \cdot s + \frac{\delta^2}{2} s^\top H(f \circ \exp_{x_i})(0) s \right) ds + \mathcal{O}(\delta^4) \\ &= f(x_i) + m\delta^2 (f(x_i)\omega(x) + \Delta f(x_i)) + \mathcal{O}(\delta^4) \end{aligned}$$

- ▶ Normalize:  $\mathbf{D}^{-1}\mathbf{K}\vec{f} = \frac{\mathbf{K}\vec{f}}{\mathbf{K}\mathbf{1}} \rightarrow \vec{f} + m\delta^2 \overrightarrow{\Delta f} + \mathcal{O}(\delta^4)$

- ▶ **Consistency:**  $\frac{1}{m\delta^2} (\mathbf{D}^{-1}\mathbf{K} - \mathbf{I})\vec{f} \rightarrow \overrightarrow{\Delta f} + \mathcal{O}(\delta^2)$

# CONSISTENCY IS NOT ENOUGH!

- ▶ Extend to arbitrary sampling  $x_i \sim q$  (Coifman & Lafon)
- ▶ **Variance:**  $\mathbb{E}[(\vec{L}f)_i - \Delta f(x_i)]^2 = \mathcal{O}\left(\frac{q(x_i)^{3-4d}}{N\delta^{2+d}}\right)$
- ▶ Negative exponent:  $3 - 4d < 0$
- ▶ As density  $q$  approaches zero the variance blows up!
- ▶ **Solution:** Variable bandwidth

Berry and Harlim (ACHA, 2015)

# VARIABLE BANDWIDTH KERNELS

We introduced the **variable bandwidth** kernel:

$$K_{\delta,\beta}(x, y) = K \left( \frac{\|x - y\|}{\delta \sqrt{q(x)^\beta q(y)^\beta}} \right)$$

**Theorem** (Berry and Harlim, ACHA, 2015):

$$\mathbf{L}_{\delta,\alpha,\beta} \vec{f} = \Delta f + c_1 \nabla f \cdot \nabla \log q + \mathcal{O} \left( \delta^2, \frac{q^{-c_2}}{\sqrt{N} h^{1+d/2}} \right)$$

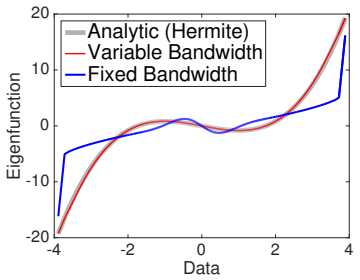
- ▶ Operator defined by:  $c_1 = 2 - 2\alpha + d\beta + 2\beta$
- ▶ Variance determined by:  $c_2 = 1/2 - 2\alpha + 2d\alpha + d\beta/2 + \beta$



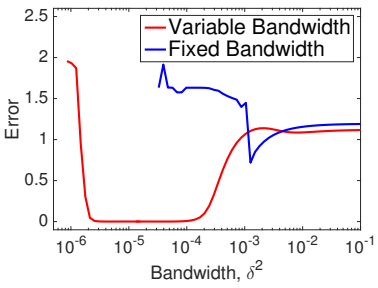
# EXAMPLE: VARIABLE BANDWIDTH KERNEL

**Gaussian data:** Brownian motion in quadratic potential

### Eigenfunctions (Hermite)



### Error vs. Bandwidth



# SUMMARY OF MANIFOLD LEARNING

- ▶ Manifold learning  $\Leftrightarrow$  Estimating Laplace-Beltrami
- ▶ Can estimate Laplace-Beltrami with a graph Laplacian
- ▶ For a non-compact manifold:
  - ▶ Manifold must be tangible
  - ▶ Requires a variable bandwidth kernel
- ▶ My other contributions:
  - ▶ Access any desired geometry (local kernels)
  - ▶ Manifolds with boundary
  - ▶ Spectral convergence

# CONTINUOUS K-NEAREST NEIGHBORS (CKNN)

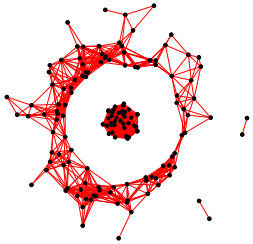
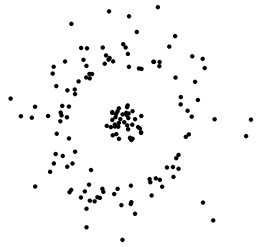
## Building unweighted graphs from data (TDA)

**CkNN Graph:** Edge  $\{x, y\}$  added if  $\frac{\|x-y\|}{\sqrt{\|x-x_k\| \|y-y_k\|}} < \delta$

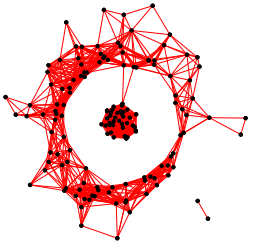
- ▶  $x_k = k$ -th nearest neighbor of  $x$
- ▶ Unnormalized graph Laplacian:  $\mathbf{L}_{\text{un}} = \mathbf{D} - \mathbf{K}$
- ▶ **Corollary:**  $\mathbf{L}_{\text{un}} \vec{f} \rightarrow \overrightarrow{\Delta_{\tilde{g}}} \vec{f}$  where  $(\tilde{g} = q^{2/d} g, d\tilde{V} = q dV)$
- ▶ **New result:** Spectral convergence  $\mathbf{L}_{\text{un}} \rightarrow \Delta_{\tilde{g}}$
- ▶ Consistency of CkNN clustering:
  - ▶ Conn. comp. of graph  $\Leftrightarrow$  Kernel of  $L_{\text{un}}$
  - ▶ Conn. comp. of  $\mathcal{M} \Leftrightarrow$  Kernel of  $\Delta_{\tilde{g}}$  (Hodge theorem)

# CKNN YIELDS IMPROVED GRAPH CONSTRUCTION

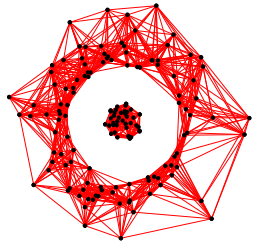
2D Gaussian with annulus removed:  
 Persistent vs. consistent homology



Small bandwidth

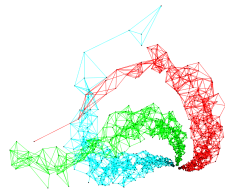
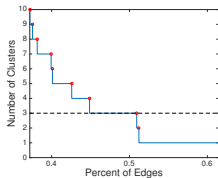
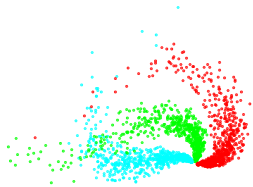
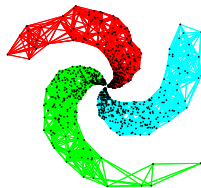
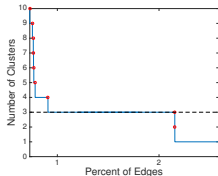
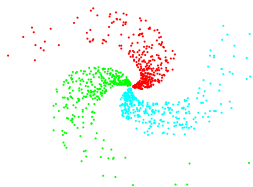


Large bandwidth

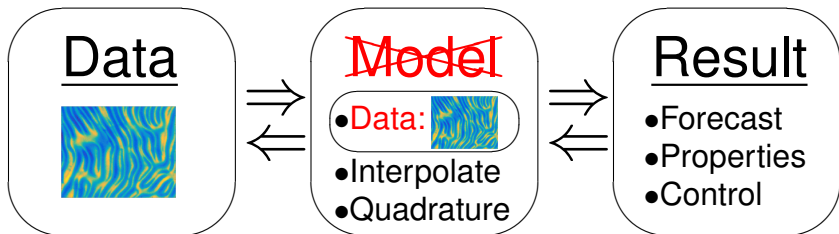


CkNN

# IMPROVED CLUSTERING USING CKNN



# NONPARAMETRIC MODELING



► **Tools:** Geometry and Harmonic/Functional Analysis

► Interpolate:  $f(x) = \sum_j \langle f, \varphi_j \rangle \varphi_j(x)$

► Quadrature:  $\langle f, \varphi_i \rangle \approx \sum_j f(x_j) \varphi_i(x_j)$

► Operator Representation:  $\mathbf{A}_{jk} = \langle \varphi_j, \mathcal{A} \varphi_k \rangle$

► All require a **basis**  $\{\varphi_j\}$ !

# DIFFUSION FORECAST

- ▶ **Autonomous** SDE:  $dx = a(x) dt + b(x) dW_t$
- ▶ Density solves **Fokker-Planck PDE**:  $\frac{\partial}{\partial t} p = \mathcal{L}^* p$
- ▶ **Shift map**:  $S(f)(x_i) = f(x_{i+1})$  estimates  $\mathbb{E}[S(f)] = e^{\tau \mathcal{L}} f$
- ▶  $\vec{c}(t)$  are the custom Fourier coefficients of  $p$

$$p(x, t) \xrightarrow{\text{Diffusion Forecast}} p(x, t + \tau) = e^{\tau \mathcal{L}^*} p(x, t)$$

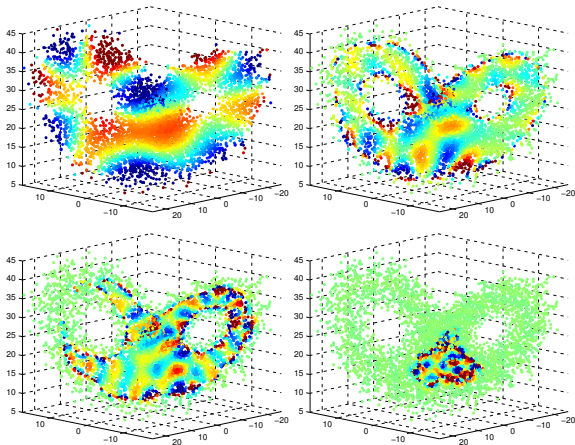
$$\downarrow \langle p, \varphi_j \rangle$$

$$\uparrow \sum_j c_j \varphi_j$$

$$\vec{c}(t) \xrightarrow{A_{ij} \equiv \mathbb{E}[\langle \varphi_j, S \varphi_i \rangle_q]} \vec{c}(t + \tau) = A \vec{c}(t).$$

# MANIFOLD LEARNING $\Rightarrow$ CUSTOM 'FOURIER' BASIS

- ▶ **Optimal basis:** Minimum variance  $A_{lj} \equiv \mathbb{E}[\langle \varphi_j, S\varphi_l \rangle_q]$





# DIFFUSION FORECAST EXAMPLE

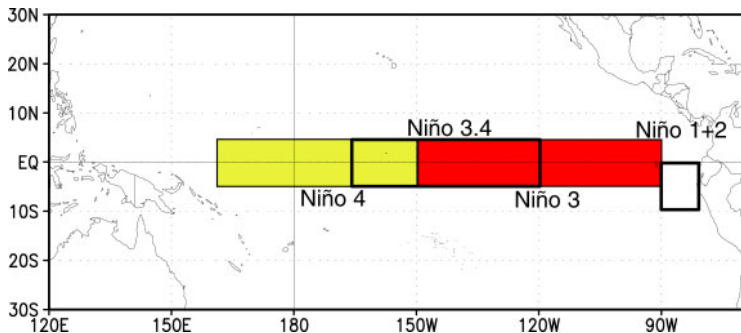
No Model

Perfect Model

Berry, Harlim, and Giannakis (PRE, 2015)

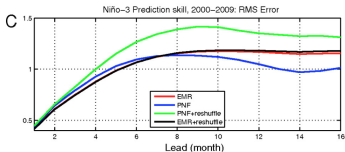
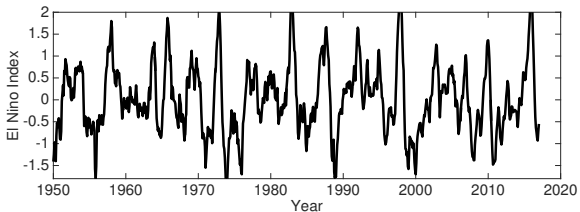
# FORECASTING THE EL NIÑO INDEX

Sea surface temperatures (SST) in the Niño indices:

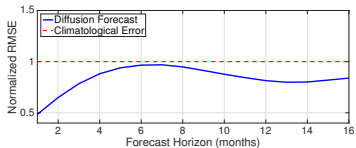


Index: 3-month running average SST anomaly

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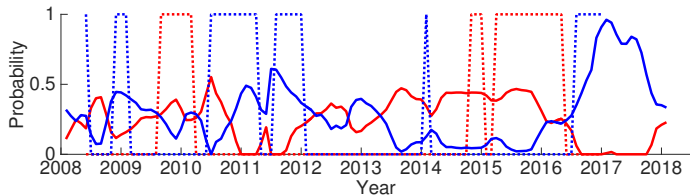
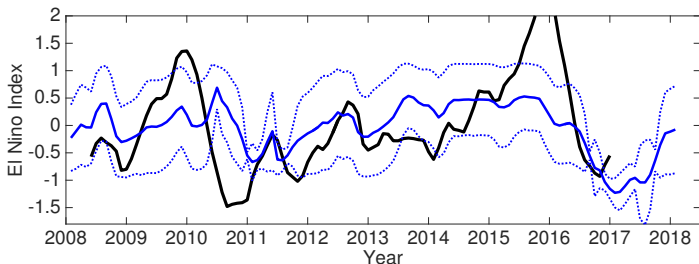
Chekrouna, Kondrashov, and Ghil, PNAS 2011,108,no.29



## Diffusion Forecast

Berry, Harlim, and Giannakis (PRE, 2015)

# YOUR 13-MONTH FORECAST

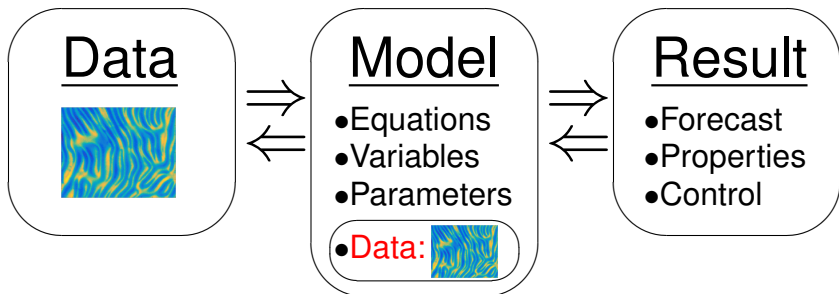


— Probability of El Niño — Actual El Niño — Probability of La Niña — Actual La Niña

El Niño = Index > 0.5

La Niña = Index < -0.5

# SEMIPARAMETRIC MODELING

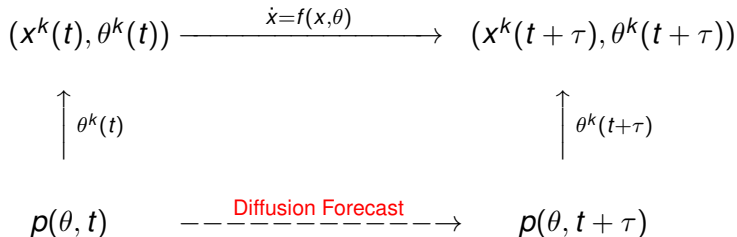


► **Data becomes part of the model:**

- Start with **imperfect** parametric model
- Assimilate data (adaptive), collect **residual errors**
- Build **nonparametric** model for the residuals

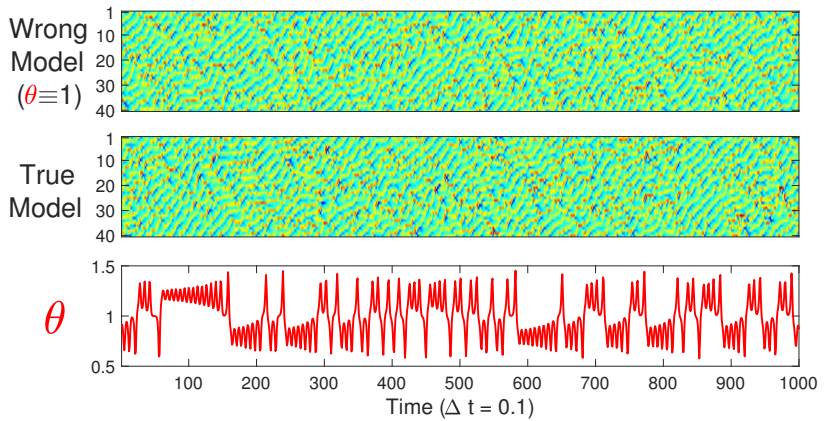
# SEMIPARAMETRIC FORECAST MODEL

- ▶ Partially known model  $\dot{x} = f(x, \theta)$
- ▶ No equations for  $\theta$ !
- ▶ Apply the **Diffusion Forecast** to  $p(\theta, t)$
- ▶ **Sample**  $\theta^k(t) \sim p(\theta, t)$  and pair with **ensemble**  $x^k(t)$



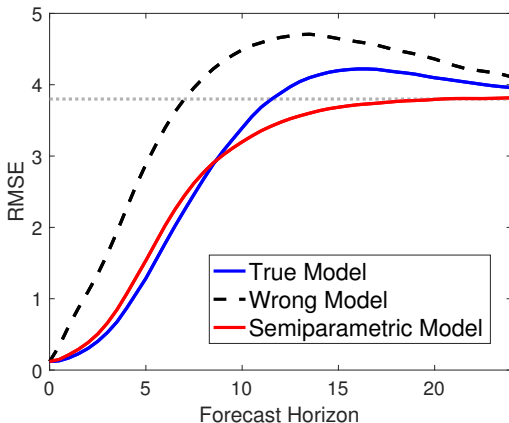
# EXAMPLE: 40-DIMENSIONAL LORENZ-96 SYSTEM DRIVEN BY LORENZ-63

$$\dot{x}_i = \theta x_{i-1} x_{i+1} - x_{i-1} x_{i-2} - x_i + 8$$



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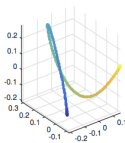
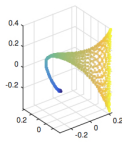
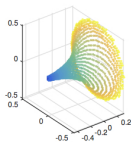
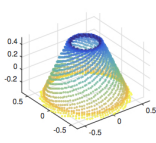
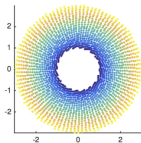


# FUTURE DIRECTION #1: FEATURE MAPS

- ▶ Want to represent map  $\mathcal{H} : \mathcal{M} \rightarrow \mathcal{N}$
- ▶ For  $\mathcal{H}$  a diffeomorphism: pull-back metric
- ▶ Otherwise: Apply the Iterated Diffusion Map (IDM)

$$\frac{dg}{dt} = \frac{1}{2} \left( (D\mathcal{H}^\top D\mathcal{H} - I)g + g(D\mathcal{H}^\top D\mathcal{H} - I) \right)$$

- ▶ Example:  $\mathcal{H}(x, y) = \sqrt{x^2 + y^2}$



Berry & Sauer, (ACHA, 2015)

Berry & Harlim (ACHA, 2016)

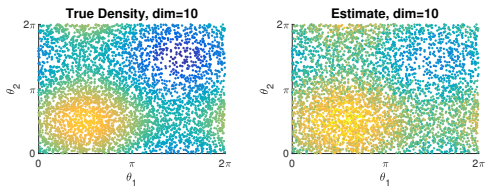
## FUTURE DIRECTION #2: CONSISTENCY OF TOPOLOGICAL DATA ANALYSIS (TDA)

- ▶ **Topological Consistency:** VR homology  $\rightarrow H_k(\mathcal{M})$
- ▶ Spectral convergence proves consistency of  $H_0(\mathcal{M})$
- ▶ Discrete Exterior Calculus (DEC):
  - ▶ TDA uses simplicial complexes to compute homology
  - ▶ Weighted simplices correspond to differential forms
  - ▶ Kernel on simplices can define Laplacians on forms
  - ▶ Which kernels recover the Laplace de-Rham operator?
- ▶ Smooth Exterior Calculus (SEC):
  - ▶ Start with the smooth eigenfunctions  $\Delta\varphi_i = \lambda_i\varphi_i$
  - ▶ Define a frame for 1-forms:  $b^{ij} = \varphi_i d\varphi_j - \varphi_j d\varphi_i$
  - ▶ Define Laplace-de Rham operators on  $b^{ij}$
  - ▶  $\langle b^{kl}, \Delta^1(b^{ij}) \rangle = \sum_r (c_{kir}c_{ijr} - c_{kjr}c_{ilir})(\lambda_r^2 - \lambda_r(\lambda_k + \lambda_i + \lambda_l + \lambda_j)) + c_{ijr}c_{klr}(\lambda_j - \lambda_i)(\lambda_l - \lambda_k)$

# FUTURE DIRECTION #3: SMOOTHNESS PRIORS

- ▶ Manifold learning suffers from the curse-of-dimensionality
  - ▶ Bias-squared:  $\mathcal{O}(\delta^4)$
  - ▶ Variance:  $\mathcal{O}(N^{-1}\delta^{-2-d})$
  - ▶ Optimal bandwidth:  $\delta = \mathcal{O}(N^{-1/(6+d)})$
  - ▶ Minimal Error:  $\mathcal{O}(N^{-2/(6+d)})$
- ▶ Richardson Extrapolation: Combine multiple  $\delta$ 's
  - ▶ Reduces bias to  $\mathcal{O}(\delta^{2k})$
  - ▶ Increases variance by a constant
  - ▶ Requires  $\mathcal{M}$  to be  $C^k$
- ▶ 'Solves' curse-of-dimensionality by assuming smoothness

- ▶ 5000 points
- ▶ 10-dim torus
- ▶ In  $\mathbb{R}^{20}$



# SUMMARY

- ▶ Manifold learning  $\Leftrightarrow$  Estimating Laplace-Beltrami
- ▶ Can estimate Laplace-Beltrami with a graph Laplacian
- ▶ Need an appropriate kernel (variable bandwidth)
- ▶ Results imply better method for graph construction (CkNN)
- ▶ Spectral convergence gives us a custom Fourier basis
- ▶ Allows model-free forecasting and correcting model error

# A BIT OF GEOMETRY

- ▶ Let  $\iota : \mathcal{M} \rightarrow \mathbb{R}^m$  be the embedding into data space
- ▶ Tangent space  $T_x\mathcal{M}$  inherits an inner product

$$g_x(v, w) = \langle D\iota(x)v, D\iota(x)w \rangle_{\mathbb{R}^m}$$

- ▶  $g$  is called the **Riemannian metric**
- ▶ If  $e_1, \dots, e_d \in T_x\mathcal{M}$  is a basis, define  $g_{ij}(x) = g_x(e_i, e_j)$
- ▶ Define the **volume form**  $dV(x) = \sqrt{\det(g(x))}$
- ▶  $\text{vol}(\mathcal{M}) = \int_{x \in \mathcal{M}} 1 dV(x)$

# A BIT MORE GEOMETRY: THE EXPONENTIAL MAP

- ▶ The **exponential map** takes tangent vectors to the manifold

$$\exp_x : T_x \mathcal{M} \rightarrow U \subset \mathcal{M}$$

- ▶ Let  $\gamma : [0, 1] \rightarrow \mathcal{M}$  be **geodesic curve** with  $\gamma'(t) = 1$
- ▶ If  $\gamma'(0) = s/\|s\|$  then  $\exp_x(s) = \gamma(1)$  and  $\exp_x(0) = x$  so

$$y = x + s + \frac{1}{2} \mathbb{I}(s, s) + \mathcal{O}(s_i^3)$$

- ▶ **Fact 1:**  $\|y - x\|^2 = \|s\|^2 + \mathcal{O}(s_i^4)$
- ▶ **Fact 2:** Natural volume element,  $dV(y) = ds$
- ▶ **Fact 3:** **Gradient**,  $D_s(f \circ \exp_x) = \nabla f$
- ▶ **Fact 4:** **Laplace-Beltrami operator**,  $\sum_{i=1}^d \frac{d^2(f \circ \exp_x)}{ds_i^2} = \Delta f$

# DIFFUSION MAPS: ALLOWING ARBITRARY SAMPLING

- ▶ For  $X_i \sim q$

$$\mathbb{E}[Kf(x)] = f(x)q(x) + mh^2(f(x)q(x)\omega(x) + \Delta(fq)(x)) + \mathcal{O}(h^4)$$

$$D(x) = K1(x) = q(x) + mh^2(q(x)\omega(x) + \Delta q(x)) + \mathcal{O}(h^4)$$

- ▶ Right normalize:

$$\hat{K}f \equiv K\left(\frac{f}{D}\right) = f(x) + mh^2\left(\Delta f(x) - f(x)\frac{\Delta q(x)}{q(x)}\right)$$

- ▶ Left normalize:  $\hat{D} \equiv \hat{K}1 = 1 - mh^2\frac{\Delta q(x)}{q(x)}$

$$\frac{\hat{K}f}{\hat{D}} = f(x) + mh^2\Delta f(x)$$

# CONTINUOUS K-NEAREST NEIGHBORS (CKNN)

- ▶ Let  $x_k$  denote the  $k$ th nearest neighbor of  $x$

**CkNN:** Edge between the points  $x, y$  if  $\frac{\|x-y\|}{\sqrt{\|x-x_k\| \|y-y_k\|}} < \delta$

- ▶ Corresponds to variable bandwidth kernel with  $\beta = -1/d$
- ▶ **Corollary:**  $L_{\text{un}} \vec{f} \rightarrow \overrightarrow{\Delta_{\vec{g}} f}$
- ▶ For fixed  $k$ ,  $\|x - x_k\| \propto q(x)^{-1/d}$  so  $\beta = -1/d$
- ▶ This is a variable bandwidth kernel with  $K(t) = 1_{\{t < 1\}}$  so

$$K\left(\frac{\|x-y\|}{\delta \sqrt{q(x)^{-1/d} q(y)^{-1/d}}}\right) = 1_{\left\{\frac{\|x-y\|}{\sqrt{\|x-x_k\| \|y-y_k\|}} < \delta\right\}}$$



# CKNN CONVERGENCE RESULT

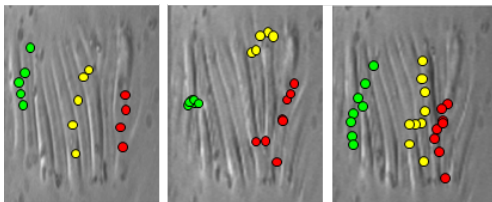
- ▶ Define the unnormalized graph Laplacian  $L_{\text{un}} = D - K$
- ▶ **Corollary:**  $L_{\text{un}} \vec{f} \rightarrow \overrightarrow{\Delta_{\tilde{g}} f}$
- ▶ Only  $\beta = -1/d$  yields a Laplace-Beltrami operator
- ▶  $\tilde{g} \equiv q^{2/d} g$  is a conformal change of metric on  $\mathcal{M}$
- ▶ Natural volume form:

$$d\tilde{V} = \sqrt{|\tilde{g}|} = \sqrt{|q^{2/d} g|} = q \sqrt{|g|} = q dV$$

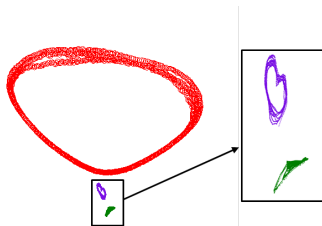
- ▶  $\text{vol}_{\tilde{g}}(\mathcal{M}) = \int_{\mathcal{M}} d\tilde{V} = \int_{\mathcal{M}} q dV = 1$

# ATTRACTOR CLUSTERING

Multi-stability in Nematic Liquid Crystals:

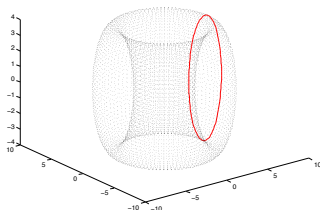
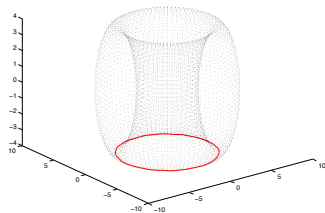


Finding good metrics/coordinates:



# THE DISCRETE EXTERIOR CALCULUS (DEC)

- ▶ Estimate Laplace-de Rham:  $\Delta^k = \delta^{k+1} d^k + d^{k-1} \delta^k$
- ▶ Compute Betti numbers:  $H^k(\mathcal{M}) \cong \text{Kernel}(\Delta^k)$
- ▶ Eigenforms in the kernel of  $\Delta^1$  on  $T^2$ :



► Representatives of  $H^1(\mathcal{M})$  on a genus two surface:

