Data-driven Correction of Model and Representation Error in Data Assimilation

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Roadmap: Correcting model error

- What is manifold learning? $\Rightarrow$ Custom Fourier Basis
- Nonparametric methods (no model)
  - Diffusion Forecast
- Semiparametric methods (model error)
- Correcting observation model error

Manifold Learning

- Geometric prior: Data lie on smooth manifold $\mathcal{M} \subset \mathbb{R}^m$
- **Manifold learning $\Leftrightarrow$ Estimating Laplace-Beltrami**
- Eigenfunctions $\Delta \varphi_i = \lambda_i \varphi_i$ orthonormal basis for $L^2(\mathcal{M})$
- Smoothest functions: φ_i minimizes the functional

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

- Eigenfunctions of Δ are custom Fourier basis
  - Smoothest orthonormal basis for $L^2(\mathcal{M})$
  - Can be used to define wavelets
  - Define the Hilbert/Sobolev spaces on $\mathcal{M}$

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 δ 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 $f \in C^3(\mathcal{M})$

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

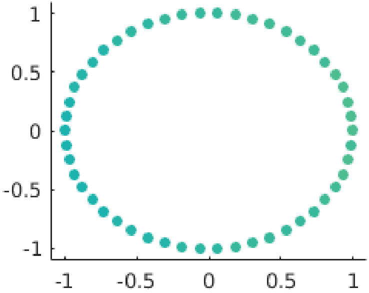
$\delta =$ bandwidth
$N =$ number of points

RESTRICTIONS THAT HAVE BEEN OVERCOME TO DEAL WITH REAL DATA:

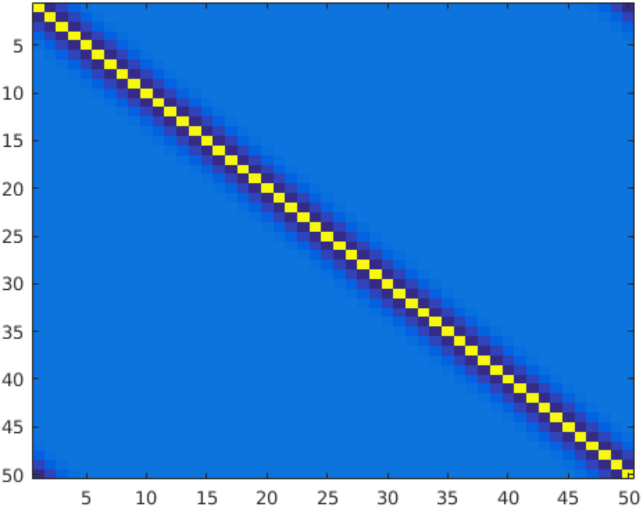
- Arbitrary sampling (Coifman & Lafon, 'Diffusion maps', ACHA 2006)
- Non-compact manifolds (Berry & Harlim, ACHA 2015)
- Other kernel functions (Thesis 2013; Berry & Sauer, ACHA 2015)
- Boundary (Coifman & Lafon, ACHA 2006; Berry & Sauer, J. Comp. Stat. 2016)
- Spectral convergence (Luxburg et al.,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

EXAMPLE: 50 DATA POINTS ON S^1

- True Laplacian: $\Delta = \frac{d^2}{d\theta^2}$
- True Eigenfunctions: $\{\sin(k\theta), \cos(k\theta)\}$

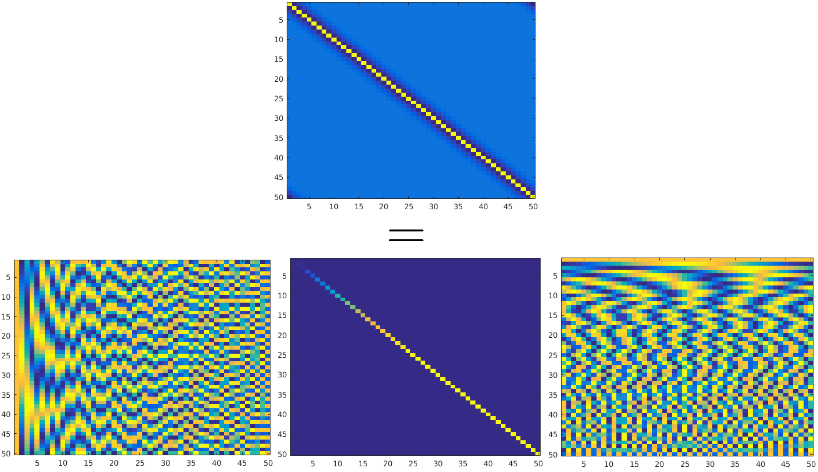


Example: L matrix for S^1



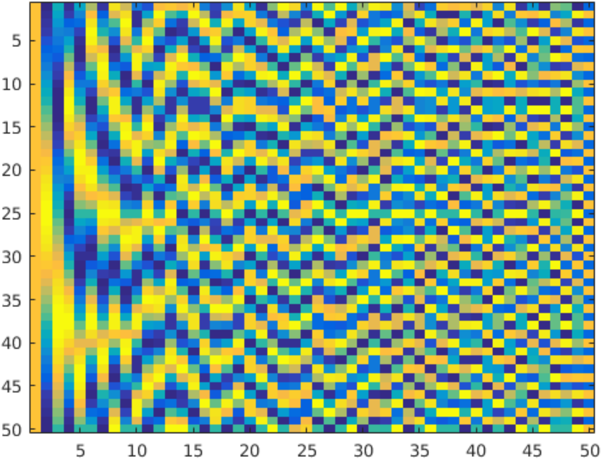
Example S^1: Eigenvector Decomposition

$$L = U \Lambda U^\top$$

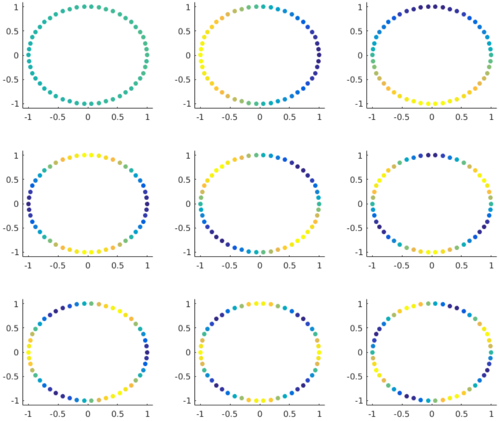


U Λ $U^\top$

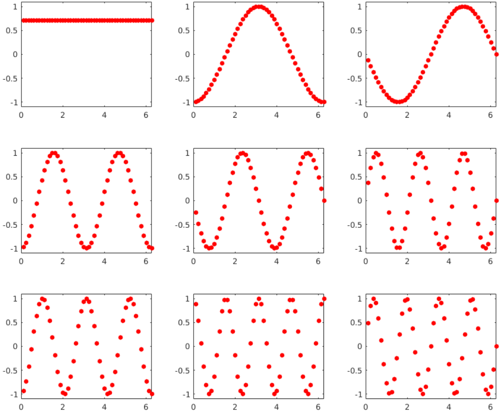
Example S^1: Matrix of Eigenvectors, U



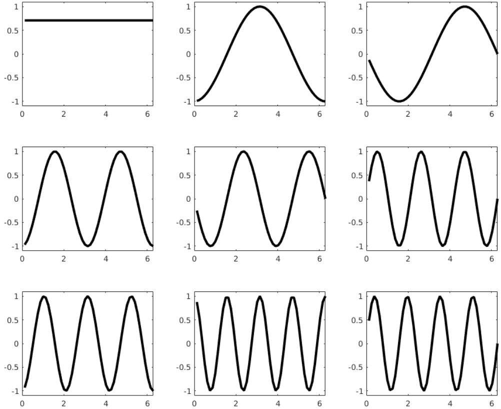
EXAMPLE S^1: EIGENVECTORS ON DATA



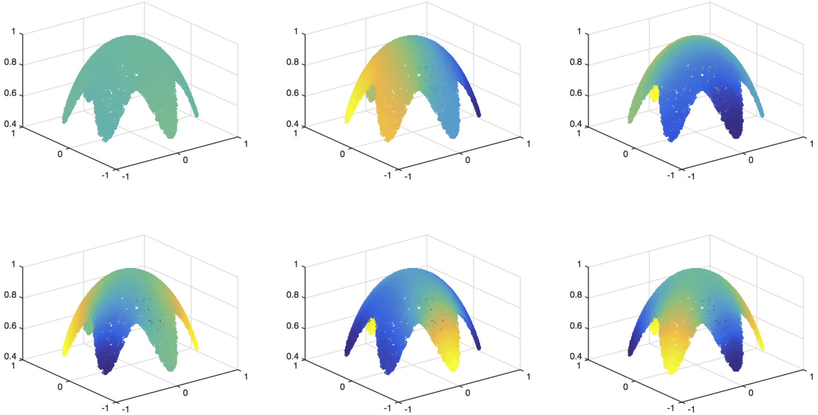
Example S^1: Eigenvectors vs. θ



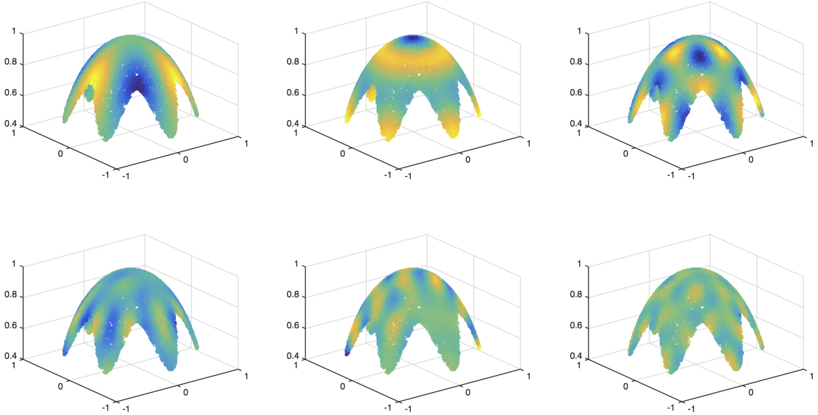
EXAMPLE S^1: CONNECTING THE DOTS



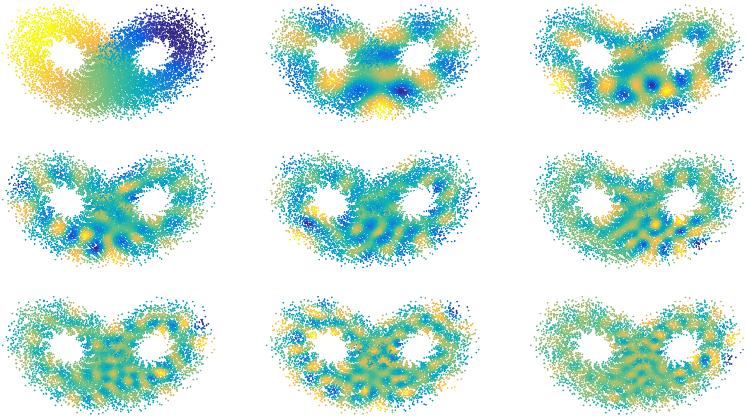
Harmonic Analysis on Manifolds/Data Sets



Harmonic Analysis on Manifolds/Data Sets



HARMONIC ANALYSIS ON MANIFOLDS/DATA SETS



DIFFUSION FORECAST

- Autonomous SDE: $dx = a(x)\,dt + b(x)\,dW_t$
- Density solves Fokker-Planck PDE: $\frac{\partial}{\partial t}p = \mathcal{L}^* p$
- Project onto the custom Fourier basis $\{\varphi_j\}$
- Forecast operator is linear $\Rightarrow$ Matrix $A_{lj} = \langle \varphi_j, e^{t\mathcal{L}} \varphi_l \rangle$

$$\begin{tikzcd}
p(x,t) \arrow[r, dashed, "\text{Diffusion Forecast}"] \arrow[d, "\langle p, \varphi_j \rangle"] & p(x,t+\tau) = e^{\tau\mathcal{L}^*} p(x,t) \\
\vec{c}(t) \arrow[r, "A_{lj} \equiv \mathbb{E}[\langle \varphi_j, S\varphi_l \rangle_{p_{\mathrm{eq}}}]"] & \vec{c}(t+\tau) = A\vec{c}(t). \arrow[u, "\sum_j c_j \varphi_j q"']
\end{tikzcd}$$

Diffusion Forecast Lorenz-63 Example

(Loading Video...)

NONPARAMETRIC FORECAST ON A TORUS

- Stochastic dynamics on a torus $(\theta, \phi) \in [0, 2\pi)^2$

$$d(\theta,\phi)^\top = a(\theta,\phi)\,dt + b(\theta,\phi)\,dW_t$$

- Drift and diffusion coefficients,

$$a(\theta,\phi) = \begin{pmatrix} \frac{1}{2} + \frac{1}{8}\cos(\theta)\cos(2\phi) + \frac{1}{2}\cos(\theta+\pi/2) \\ 10 + \frac{1}{2}\cos(\theta+\phi/2) + \cos(\theta+\pi/2)) \end{pmatrix},$$

$$b(\theta,\phi) = \begin{pmatrix} \frac{1}{4} + \frac{1}{4}\sin(\theta) & \frac{1}{4}\cos(\theta+\phi) \\ \frac{1}{4}\cos(\theta+\phi) & \frac{1}{40} + \frac{1}{40}\sin(\phi)\cos(\theta) \end{pmatrix}.$$

DIFFUSION FORECAST TORUS EXAMPLE

(Loading Video...)

Problem: Curse of dimensionality

- Learning the basis → Data exponential in manifold dim
- Monte-Carlo type estimates $\mathcal{O}(N^{-1/2})$:
  - Coefficients:

$$c_l(t) = \langle p(x,t), \varphi_l \rangle \approx \frac{1}{N}\sum_{i=1}^{N} \varphi_l(x_i) p(x_i,t)/p_{\mathrm{eq}}(x_i)$$

  - Markov Matrix:

$$A_{lj} = \left\langle \varphi_j, e^{\tau\mathcal{L}}\varphi_l \right\rangle_{p_{\mathrm{eq}}} \approx \frac{1}{N}\sum_{i=1}^{N} \varphi_j(x_i)\varphi_l(x_{i+1})$$

- Maybe we shouldn't throw out the model...
- Use diffusion forecast to fix model error!

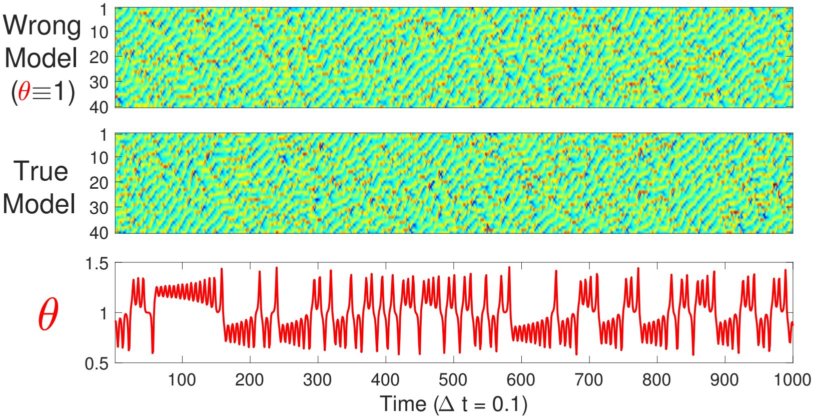
Semiparametric Forecast Model

- Partially known model $\dot{x} = f(x, \theta)$
- Unknown: $d\theta = a(\theta)\, dt + b(\theta)\, dW_t$
- Apply the Diffusion Forecast to $p(\theta, t)$
- Sample $\theta^k(t) \sim p(\theta, t)$ and pair with ensemble $x^k(t)$

$$\begin{tikzcd}
(x^k(t), \theta^k(t)) \arrow[r, "\dot{x}=f(x,\theta)"] & (x^k(t+\tau), \theta^k(t+\tau)) \\
p(\theta, t) \arrow[u, "\theta^k(t)"'] \arrow[r, dashed, "\text{Diffusion Forecast}"] & p(\theta, t+\tau) \arrow[u, "\theta^k(t+\tau)"']
\end{tikzcd}$$

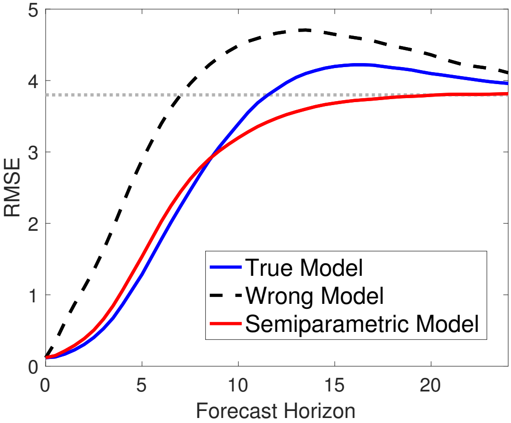
Example: 40-dimensional Lorenz-96 system

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



Example: 40-dimensional Lorenz-96 system

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



SEMIPARAMETRIC FILTER: PUT IT ALL TOGETHER...

$$\begin{tikzcd}
\begin{pmatrix} x^{k,a}(t-\tau) \\ \theta^{k,a}(t-\tau) \end{pmatrix} \arrow[r, "\dot{x}=f(x,\theta)"] \arrow[d, "\theta^a"] & \begin{pmatrix} x^{k,f}(t) \\ \theta^{k,f}(t) \end{pmatrix} \arrow[r, "\text{EnKF } y^o(t)"] & \begin{pmatrix} x^{k,a}(t) \\ \theta^{k,a}(t) \end{pmatrix} \arrow[d, "p(\theta^a(t)\,|\,\theta(t))"'] \\
p^a(\theta,t-\tau) \arrow[r, dashed, "\text{Diffusion Forecast}"] \arrow[d, "\langle p^a,\varphi_j\rangle"] & p^f(\theta,t) \arrow[u, "\theta^{k,f}(t)"'] \arrow[r, "p^f(\theta)p(y\,|\,\theta)"] & p^a(\theta,t) \arrow[d, "\langle p^a,\varphi_j\rangle"'] \\
\vec{c}^{\,a}(t-\tau) \arrow[r, "A_{lj}c^{\,a}(t-\tau)"] & \vec{c}^{\,f}(t) \arrow[u, "\sum_j c_j^f\varphi_j p_{\mathrm{eq}}"'] \arrow[r, dashed, "\text{Bayesian Update}"] & \vec{c}^{\,a}(t)
\end{tikzcd}$$

MODEL ERROR OVERVIEW

- Consider the standard filtering problem,

$$\begin{aligned} x_i &= f(x_{i-1}, \theta) + \omega_{i-1} \\ y_i &= h(x_i) + \eta_i \end{aligned}$$

- So far we have focused on the dynamics, *f*
  - Diffusion Forecast ⇒ Learn *f* from data
  - Diffusion Forecast for θ to correct model error
- We have assumed that *h* is fully known...

BIAS IN OBSERVATION MODELS

- Consider the standard filtering problem,

$$x_i = f(x_{i-1}) + \omega_{i-1}$$
$$y_i = h(x_i) + \eta_i$$

- We assume the true observation function $h(x)$ is unknown
- An approximate model is available $\tilde{h}(x)$ so that

$$y_i = h(x_i) + \eta_i = \tilde{h}(x_i) + b_i + \eta_i$$

- Where $b_i \equiv h(x_i) - \tilde{h}(x_i)$ is called the bias

EXAMPLE 1: LORENZ-96

- Consider the standard 40-dimensional Lorenz-96,

$$\dot{x}_j = x_{j-1}(x_{j+1} - x_{j-2}) - x_j + 8$$

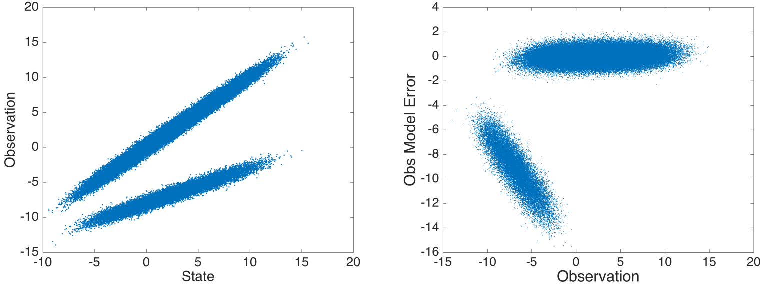
- We observe 20 of the 40 variables
- We draw $\xi_i \sim \mathcal{U}(0,1)$ and let the observations be,

$$h(x_k) = \begin{cases} x_k & \xi_i > 0.8 \\ \beta_k x_k - 8 & \text{else} \end{cases}$$
$$\beta_k \sim \mathcal{N}(0.5, 1/50).$$

- *h* is applied to 7 randomly chosen variables
- Remaining 13 are directly observed

Example 1: Lorenz-96

- The result is a bimodal distribution, “cloudy/clear”
- Obs Model Error = True Obs - $\tilde{h}$(True State)



CORRECTING THE BIAS

- Our goal is to find $p(b_i \,|\, y_i)$
- We can then correct our observation function

$$\hat{h}(x_i^f) \equiv \tilde{h}(x_i^f) + \hat{b}_i$$

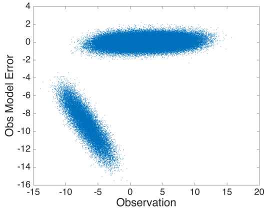
- Where $\hat{b}_i = \mathbb{E}_{p(b_i \,|\, y_i)}[b_i]$
- Since $\hat{b}_i$ random:
  - Inflate the obs noise covariance
  - Use $\hat{R}_{b_i} = \mathbb{E}_{p(b_i \,|\, y_i)}[(b_i - \hat{b}_i)(b_i - \hat{b}_i)^\top]$

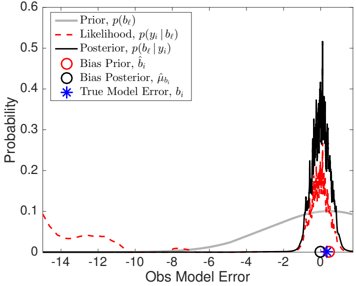
Correcting the bias

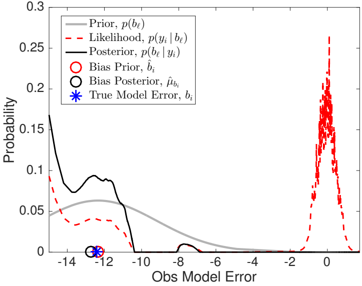
- If we can estimate $p(b_i \mid y_i)$ we can fix the obs
- From the forecast step we have a prior $p(b_i)$
- Can use Bayes' $p(b_i \mid y_i) = p(b_i)p(y_i \mid b_i)$
- Need the likelihood $p(y_i \mid b_i)$
- Use kernel estimation of conditional distributions

Correcting the bias

- Below plots have $y_i \approx -4$
- Left is clear, right is cloudy
- Notice bimodal likelihood







Learning the conditional distribution

- Given training data (y_i, b_i) our goal is to learn $p(y_i \mid b_i)$
- For a kernel $K(\alpha, \beta) = e^{-\frac{||\alpha-\beta||^2}{\delta^2}}$ we define Hilbert spaces

$$\mathcal{H}_y = \left\{ \sum_{i=1}^{N} a_i K(y_i, \cdot) \,:\, \vec{a} \in \mathbb{R}^N \right\}, \mathcal{H}_b = \left\{ \sum_{i=1}^{N} a_i K(b_i, \cdot) \,:\, \vec{a} \in \mathbb{R}^N \right\}$$

- For example the kernel density estimate (KDE) $\hat{q}$ is in $\mathcal{H}_y$

$$\hat{q}(y) = \frac{1}{m_0 N} \sum_{i=1}^{N} K(y_i, y)$$

- Eigenvectors ϕ_ℓ of $K_{ij} = K(y_i, y_j)$ form an orthonormal basis for $\mathcal{H}_y$. Similarly φ_k are a basis for $\mathcal{H}_b$.

Learning the conditional distribution

- We assume that $p(y \mid b)$ can be approximated in $\mathcal{H}_y \otimes \mathcal{H}_b$
- Let $C^{yb}_{ij} = \langle \phi_i, \varphi_j \rangle$ and $C^{bb}_{ij} = \langle \varphi_i, \varphi_j \rangle$ then define

$$C^{y|b} = C^{yb} \left(C^{bb} + \lambda I \right)^{-1}$$

- We can then define a consistent estimator of $p(y \mid b)$ by

$$\hat{p}(y \mid b) = \sum_{i,j=1}^{N} C^{y|b}_{i,j} \phi_i(y) \varphi_j(b) \hat{q}(y)$$

- We define eigenfunctions with Nystöm extension

$$\varphi_j(b) = \lambda_j^{-1} \sum_{i=1}^{N} \varphi_j(b_i) K(b_i, b)$$

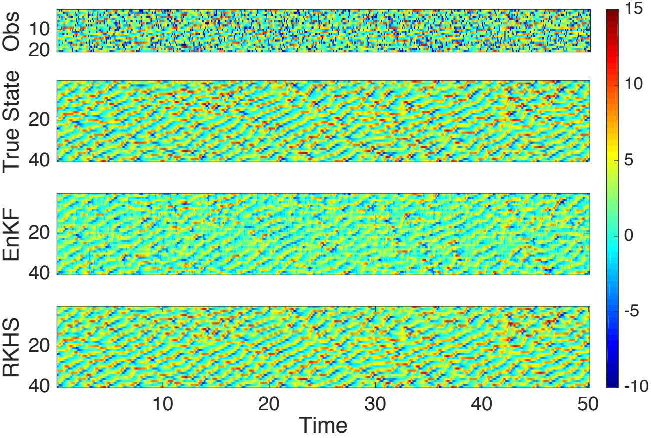
OVERVIEW

- **Learning Phase:** Given training data set (x_i, y_i)
  - Compute the biases $b_i = y_i - \tilde{h}(x_i)$
  - Learn the conditional distribution $p(y \,|\, b)$
- **Filtering:** Forecast $x_i^f \Rightarrow$ innovation $\epsilon_i = y_i - \tilde{h}(x_i^f)$
- Use prior $p(b) = \mathcal{N}(\epsilon_i, P_i^y)$
- Combine with conditional to find $p(b \,|\, y_i) = p(b)p(y_i \,|\, b)$
- Estimate conditional mean $\hat{b}_i$ and covariance $\hat{R}_{b_i}$
- Adjust innovation $\hat{\epsilon}_i = \epsilon_i + \hat{b}_i$ and $R_i = R^o + \hat{R}_{b_i}$
- Apply Kalman update, continue to the next filter step

OVERVIEW

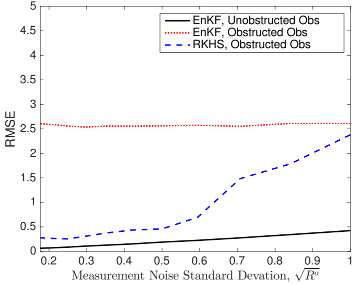
$$\begin{tikzcd}
\begin{array}{c}\text{Prior}\\ p(x_i)\end{array} \arrow[r, "\text{Primary Filter}"] \arrow[d] & \begin{array}{c}\text{Posterior}\\ p(x_i \mid y_i)\end{array} \\
\begin{array}{c}\text{Error Prior}\\ p(b)\end{array} \arrow[r, "\text{Secondary Filter}"] & \begin{array}{c}\text{Error Posterior}\\ p(b \mid y_i)\end{array} \arrow[u] \\
\begin{array}{c}\text{Observation}\\ y_i\end{array} \arrow[u] \arrow[r, "\text{RKHS+Training Data}"] & \begin{array}{c}\text{Likelihood}\\ p(y_i \mid b)\end{array} \arrow[u]
\end{tikzcd}$$

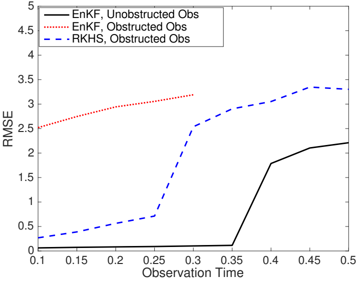
LORENZ-96 RESULTS



Lorenz-96 Results

- Works well with small measurement noise
- Observations need to be precise, but not accurate


EnKF, Unobstructed Obs
EnKF, Obstructed Obs
RKHS, Obstructed Obs
RMSE
Measurement Noise Standard Devation, $\sqrt{R^o}$


EnKF, Unobstructed Obs
EnKF, Obstructed Obs
RKHS, Obstructed Obs
RMSE
Observation Time