

# Toward consistent nonlinear filtering and smoothing via measure transport

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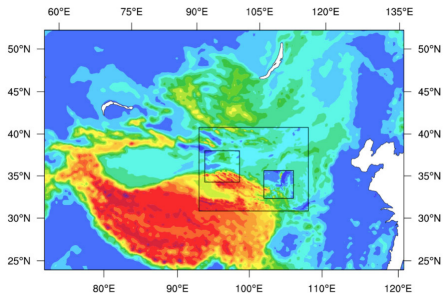
<sup>3</sup>Department of Computer Science  
Long Island University

EnKF Workshop

May 4, 2023

# Sequential inference is ubiquitous

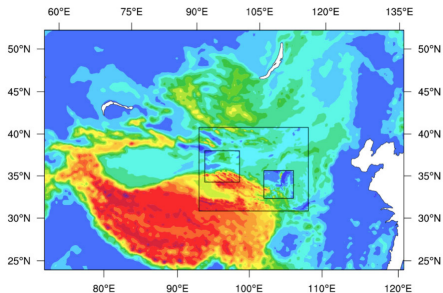
- ▶ **Goal:** Sequential state estimation in a Bayesian setting
- ▶ **Applications:** Weather prediction, oceanography, finance, population dynamics, pharmacology, robotics, aerodynamics, etc.



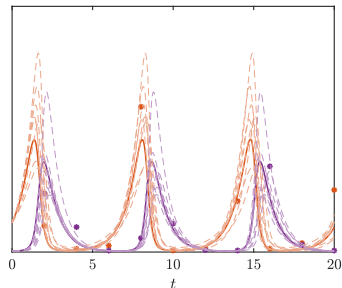
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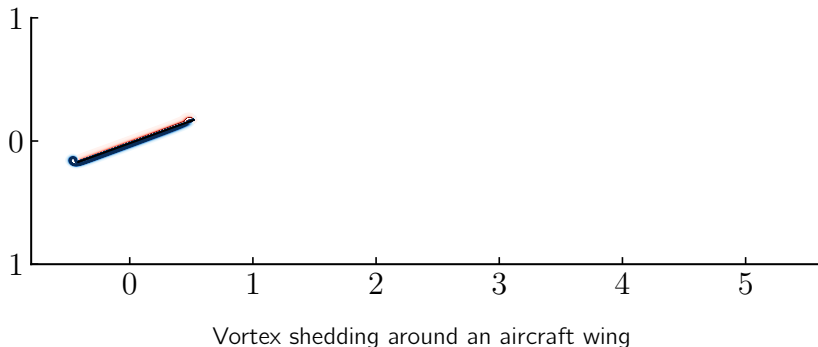
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Epidemiological forecast

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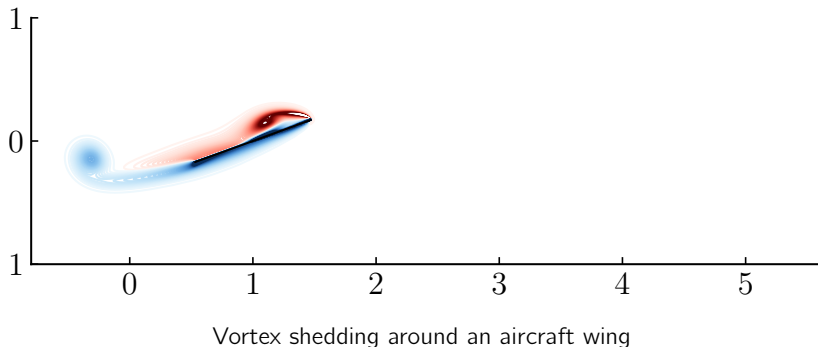
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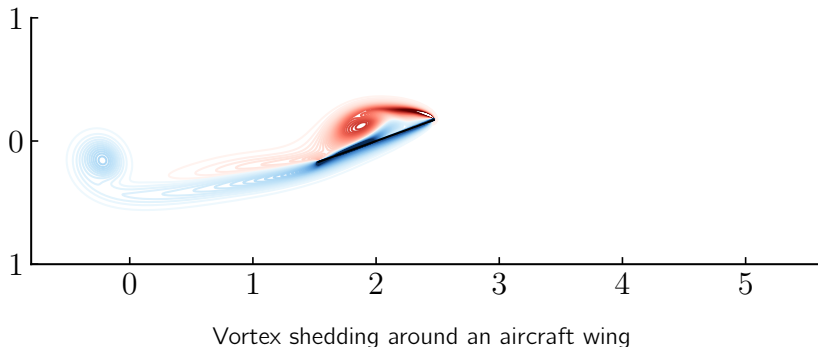
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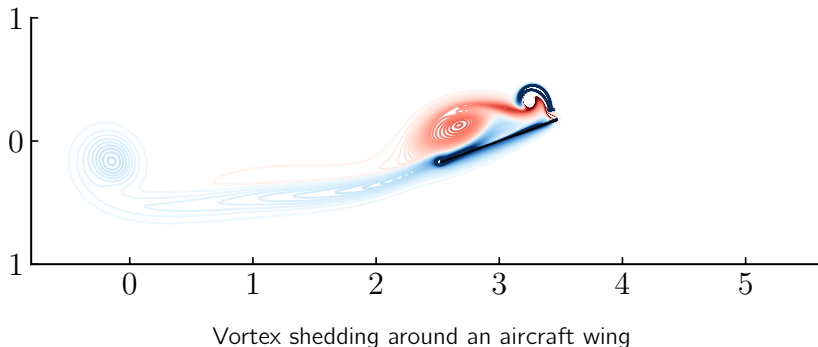
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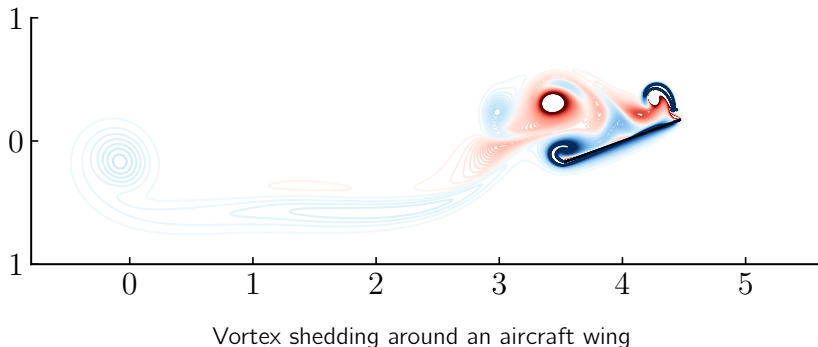
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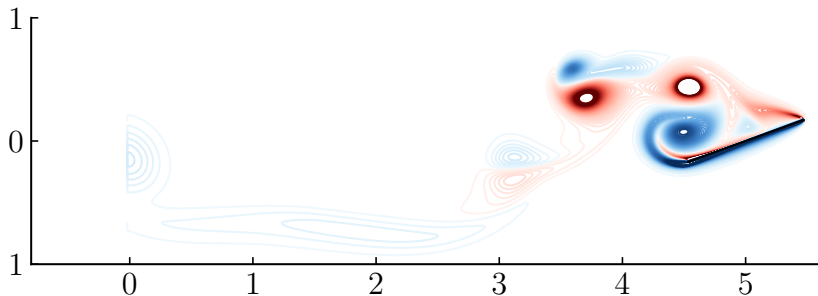
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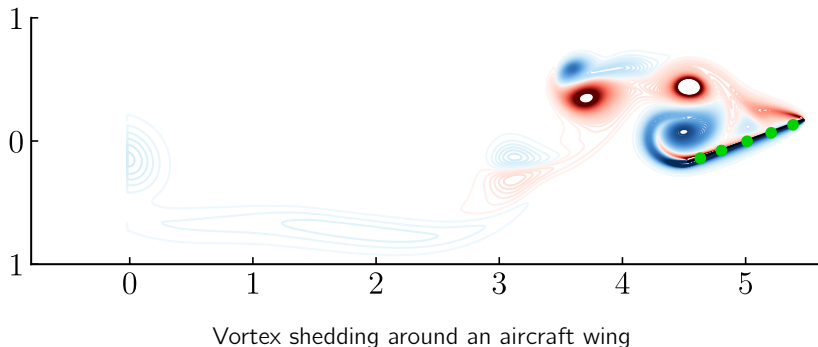
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Vortex shedding around an aircraft wing

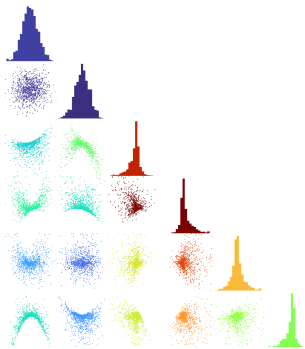
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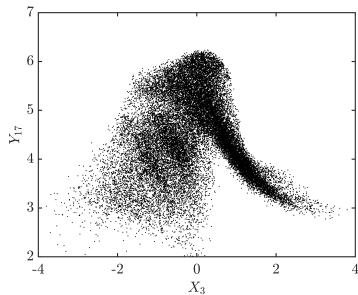


# Non-Gaussianity is ubiquitous

- ▶ Non-Gaussianity can include multi-modality and/or tail-heaviness
- ▶ Mathieu's talk (this morning) will address heavy-tailed distributions



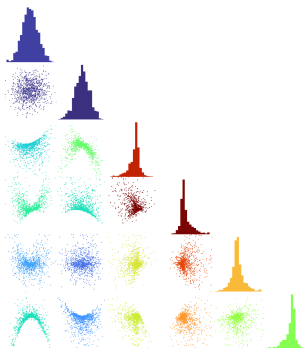
Lorenz-63 smoothing ensemble



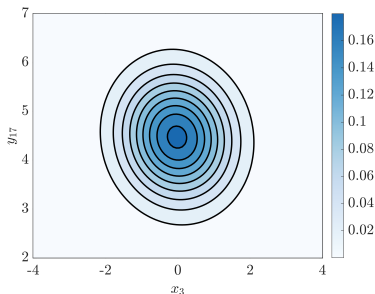
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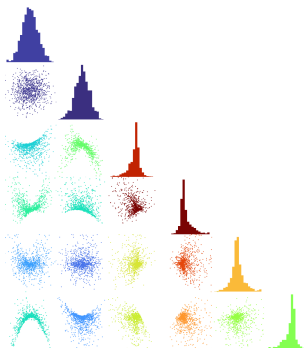


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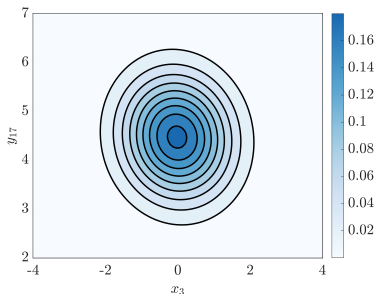


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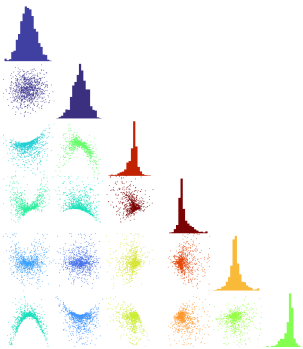


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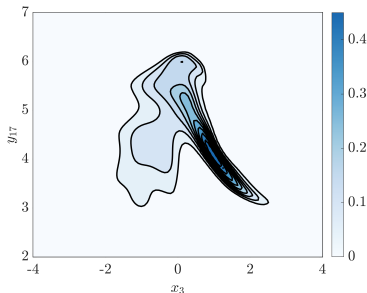
**Takeaway:** Gaussian approximations under-predict data informativeness

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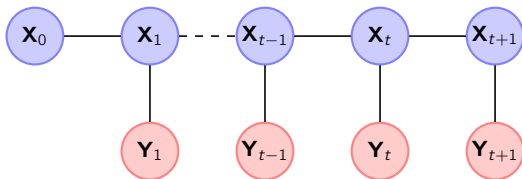
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**Takeaway:** Gaussian approximations under-predict data informativeness

**Goal:** Develop **consistent** inference methods for non-Gaussian problems

## State-space models

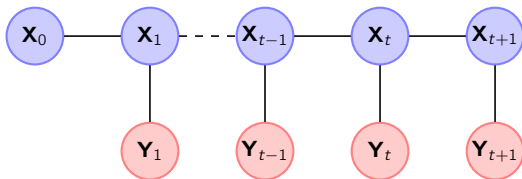
- ▶ States follow model dynamics  $\pi_{\mathbf{x}_t|\mathbf{x}_{t-1}}$
- ▶ Observations follow likelihood function  $\pi_{\mathbf{y}_t|\mathbf{x}_t}$



**Goal:** Recursively sample distributions  $\pi_{\mathbf{x}_t|y_1^*, \dots, y_t^*}$  or  $\pi_{\mathbf{x}_{1:t}|y_1^*, \dots, y_t^*}$

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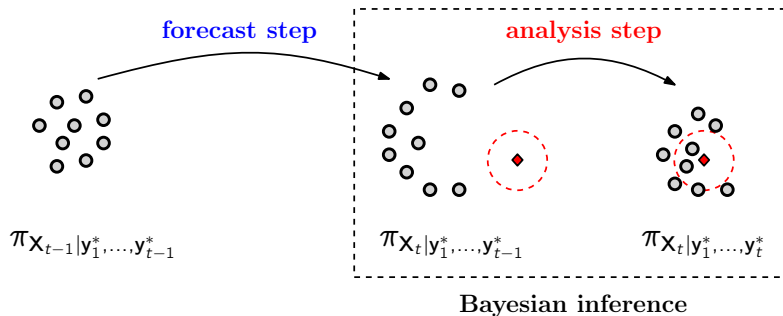
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## Common challenges leading to non-Gaussianity

- ▶ Nonlinear dynamical models or observation operators
- ▶ Sparse observations in space and time

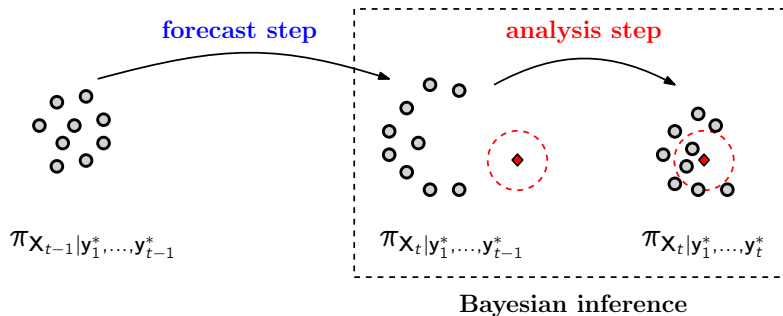
# Ensemble filtering and smoothing

**Approach:** Approximate distributions using limited samples



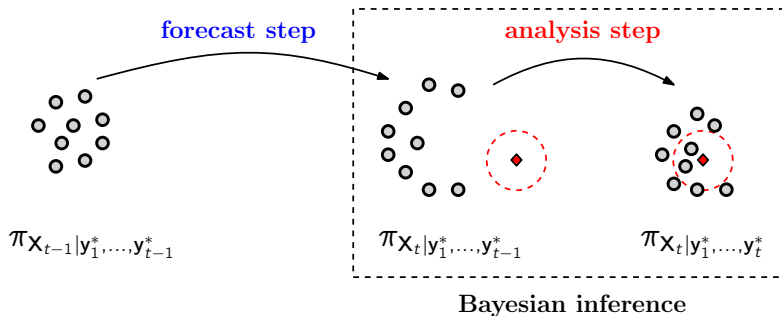
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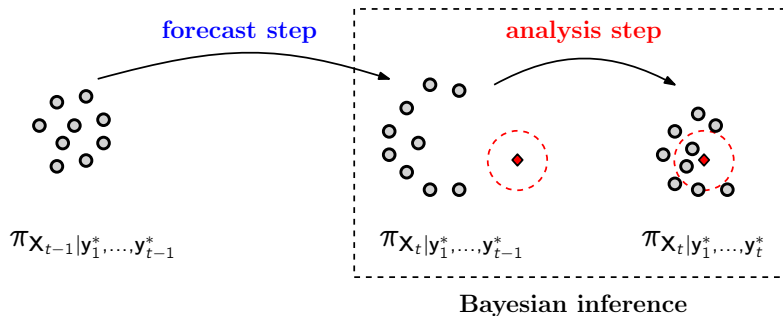


## Ensemble Kalman filters and smoothers

- ▶ Analysis step updates particles by estimating a **linear transformation**
- ▶ **Inconsistent** for capturing Bayesian solution

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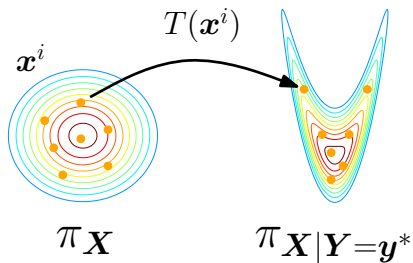
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**Goal:** Perform analysis **consistently and robustly** in non-Gaussian settings



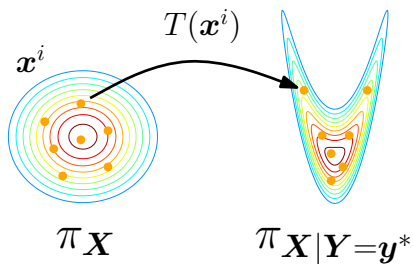
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**Idea:** Find map  $T$  that take samples from prior  $\pi_X$  to posterior  $\pi_{X|Y}$



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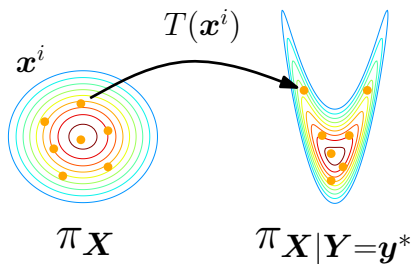


**Plan for this talk:**

- 1 Maps for filtering  $\mathbf{X} = \mathbf{X}_t$

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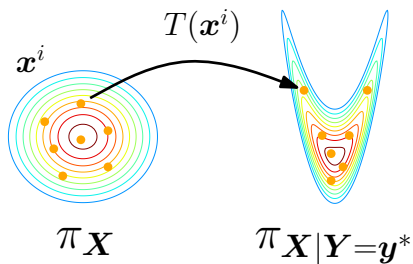


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- 2 Maps for smoothing  $\mathbf{X} = \mathbf{X}_{1:t}$ ?

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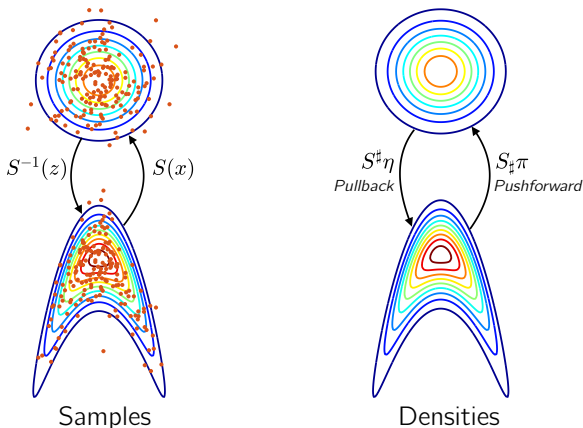


**Plan for this talk:**

- 1 Maps for filtering  $\mathbf{X} = \mathbf{X}_t$ ?
- 2 Maps for smoothing  $\mathbf{X} = \mathbf{X}_{1:t}$ ?
- 3 Leveraging structure in  $T$  to tackle high-dimensional problems

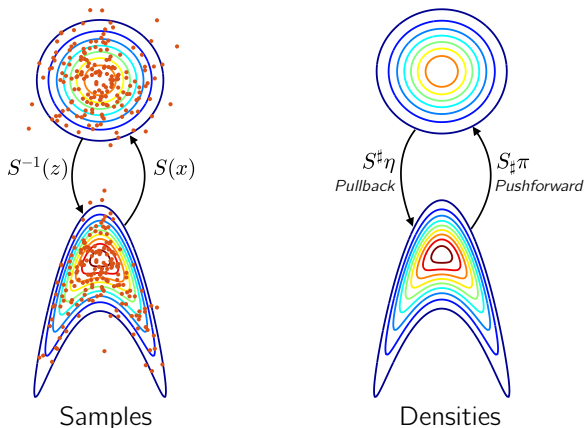
# Transport maps characterize distributions

- ▶ **Transport map**  $S$  induces a deterministic coupling between a target density  $\pi$  and a reference density  $\eta$  (e.g., standard normal)
  - ▶ Generate cheap and independent samples:  $\mathbf{x} \sim \pi \Leftrightarrow S(\mathbf{x}) \sim \eta$
  - ▶ Evaluate the target density:  $\pi(\mathbf{x}) = S^\# \eta(\mathbf{x}) := \eta \circ S(\mathbf{x}) |\det \nabla S(\mathbf{x})|$



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As a building block, consider the **Knothe-Rosenblatt rearrangement**

$$S(\mathbf{x}) = \begin{bmatrix} S_1(x_1) \\ S_2(x_1, x_2) \\ \vdots \\ S_d(x_1, x_2, \dots, x_d) \end{bmatrix}$$

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- ① Unique under mild assumptions on  $\pi$  and  $\eta$
- ② Invertibility is guaranteed by one-dimensional monotonicity  $\partial_k S_k > 0$
- ③  $S^{-1}(\mathbf{z})$  and  $\det \nabla S(\mathbf{x})$  are simple to evaluate
- ④ Each component  $S_k$  characterizes one marginal conditional

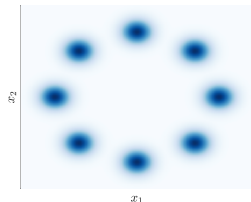
$$\pi_{\mathbf{X}} = \pi_{X_1} \pi_{X_2|X_1} \cdots \pi_{X_d|X_1, \dots, X_{d-1}}$$



# Learning expressive triangular maps from samples

Given target density  $\pi$  and standard Gaussian  $\eta$ ,

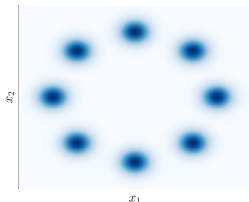
$$\begin{aligned} & \min_S D_{\text{KL}}(\pi || S^\# \eta) \\ \Leftrightarrow & \min_{\{s: \partial_k s > 0\}} \mathbb{E}_\pi \left[ \frac{1}{2} s(\mathbf{x}_{1:k})^2 - \log |\partial_k s(\mathbf{x}_{1:k})| \right] \forall k \end{aligned}$$



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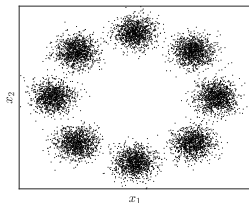
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Given samples  $\{\mathbf{x}^i\}_{i=1}^n \sim \pi$ , find  $\hat{S}_k$  via

$$\arg \min_{\{s: \partial_k s > 0\}} \frac{1}{n} \sum_{i=1}^n \left[ \frac{1}{2} s(\mathbf{x}_{1:k}^i)^2 - \log |\partial_k s(\mathbf{x}_{1:k}^i)| \right]$$



**Target density approximation:**  $\hat{\pi}(\mathbf{x}) := \hat{S}^\# \eta(\mathbf{x})$

## Triangular maps enable conditional sampling

Consider the triangular map pushing forward  $\pi_{\mathbf{Y}, \mathbf{X}}$  to  $\eta_{\mathbf{Z}_1, \mathbf{Z}_2}$ :

$$S(\mathbf{y}, \mathbf{x}) = \begin{bmatrix} S^{\mathcal{Y}}(\mathbf{y}) \\ S^{\mathcal{X}}(\mathbf{y}, \mathbf{x}) \end{bmatrix}$$

- ▶  $S^{\mathcal{Y}}$  pushes forward  $\pi_{\mathbf{Y}}$  to  $\eta_{\mathbf{Z}_1}$
- ▶  $S^{\mathcal{X}}(\mathbf{y}, \cdot)$  pushes forward  $\pi_{\mathbf{X}|\mathbf{y}}$  to  $\eta_{\mathbf{Z}_2}$  for any  $\mathbf{y}$

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## Recipe for amortized inference:

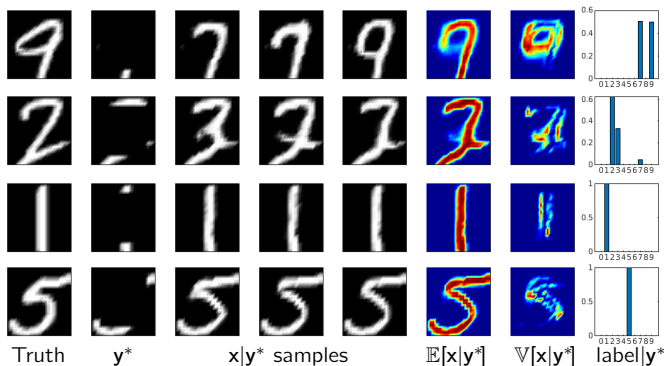
To characterize posterior  $\pi_{\mathbf{X}|\mathbf{y}^*} \propto \pi_{\mathbf{y}^*|\mathbf{X}}\pi_{\mathbf{X}}$  given an observation  $\mathbf{y}^*$ :

- ▶ Simulate from the model:  $\mathbf{x}^i \sim \pi_{\mathbf{X}}, \mathbf{y}^i \sim \pi_{\mathbf{Y}|\mathbf{X}^i}$
- ▶ Estimate  $S^{\mathcal{X}}$  from joint samples  $(\mathbf{x}^i, \mathbf{y}^i) \sim \pi_{\mathbf{X}, \mathbf{Y}}$
- ▶ Simulate  $\hat{S}^{\mathcal{X}}(\mathbf{y}^*, \cdot)^{-1} \Big|_{\mathbf{z}^i} \sim \pi_{\mathbf{X}|\mathbf{y}^*}$  for  $\mathbf{z}^i \sim \eta_{\mathbf{Z}_2}$

**Related Work:** Simulation-based or likelihood-free inference [Papamakarios & Murray, 2016; Lueckmann et al., 2017; Greenberg et al., 2019]

# Numerical example: image in-painting [Kovachki, B, et al., 2021]

- ▶ **Goal:** Reconstruct image after removing its center section
- ▶ Use map to sample from the conditional distribution for the  $14 \times 14$  center pixels of a  $28 \times 28$  MNIST handwritten digit
- ▶ Estimate conditional mean and variance and classify digit probability

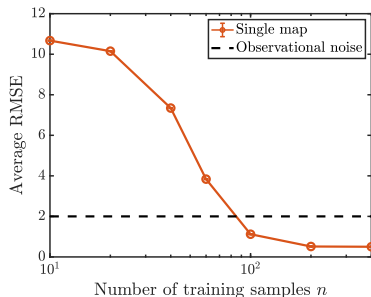
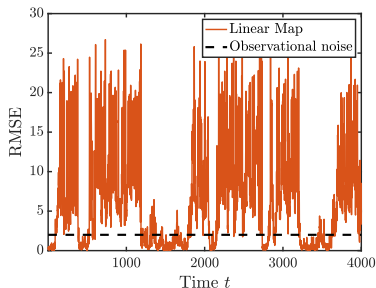


**Note:** Prior distributions in imaging problems have no analytic form

# Will this always work well?

## Lorenz-63 model

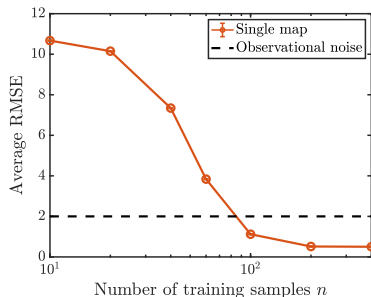
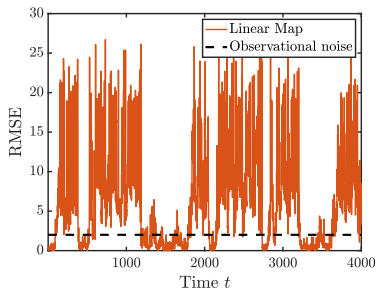
- ▶ Infer the hidden state given noisy point-wise observations
- ▶ With  $N = 50$  samples, we can *at best* estimate linear maps
- ▶ Measure root-mean-squared error (RMSE) of ensemble mean



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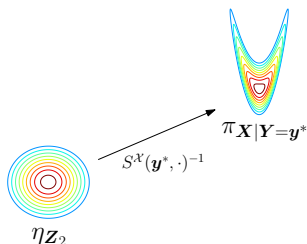
**Takeaway:** This approach yields large errors with limited samples

## Another approach: compose maps for sampling

For  $\pi_{\mathbf{Y}, \mathbf{X}}$  and  $\eta_{\mathbf{Z}_1, \mathbf{Z}_2}$ , consider the triangular map

$$S(\mathbf{y}, \mathbf{x}) = \begin{bmatrix} S^{\mathbf{y}}(\mathbf{y}) \\ S^{\mathbf{x}}(\mathbf{y}, \mathbf{x}) \end{bmatrix}$$

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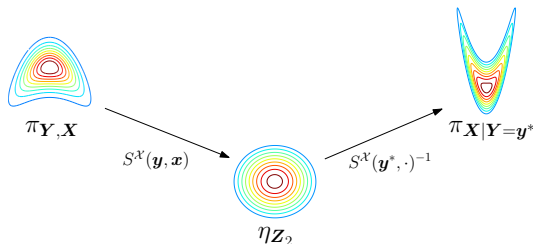


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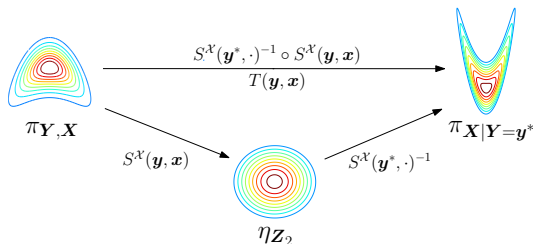


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## Another approach: compose maps for sampling

The **prior-to-posterior map** that pushes  $\pi_{\mathbf{Y}, \mathbf{X}}$  to  $\pi_{\mathbf{X}|\mathbf{y}^*}$  is

$$\boxed{T_{\mathbf{y}^*}(\mathbf{y}, \mathbf{x}) = S^{\mathcal{X}}(\mathbf{y}^*, \cdot)^{-1} \circ S^{\mathcal{X}}(\mathbf{y}, \mathbf{x})}$$

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**Stochastic map algorithm:**

- 1 Estimate  $S^{\mathcal{X}}$  using  $(\mathbf{y}^i, \mathbf{x}^i) \sim \pi_{\mathbf{Y}, \mathbf{X}}$
- 2 Evaluate composed map  $T_{\mathbf{y}^*}(\mathbf{y}, \mathbf{x})$  to approximately sample posterior

## Forecast step

- 1 Apply dynamics to generate forecast ensemble  $(\mathbf{x}_t^f)^i \sim \pi_{\mathbf{x}_t | \mathbf{x}_{t-1}^i}$

## Analysis step

- 1 Sample observations  $\mathbf{y}_t^i \sim \pi_{\mathbf{Y}_t | (\mathbf{x}_t^f)^i}$  using forecast samples
- 2 Estimate lower-triangular map  $S$  that couples  $\pi_{\mathbf{Y}_t, \mathbf{x}_t}$  and  $\mathcal{N}(\mathbf{0}, \mathbf{I})$

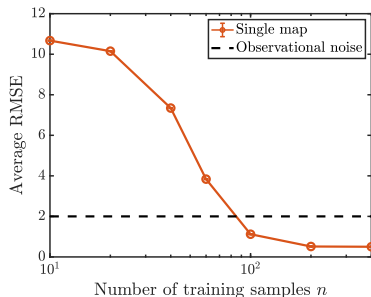
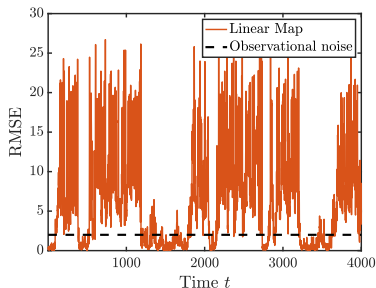
$$S(\mathbf{y}_t, \mathbf{x}_t) = \begin{bmatrix} S^{\mathbf{y}}(\mathbf{y}_t) \\ S^{\mathbf{x}}(\mathbf{y}_t, \mathbf{x}_t) \end{bmatrix}$$

- 3 Compose maps  $T_{\mathbf{y}_t^*}(\mathbf{y}_t, \mathbf{x}_t) = S^{\mathbf{x}}(\mathbf{y}_t^*, \cdot)^{-1} \circ S^{\mathbf{x}}(\mathbf{y}_t, \mathbf{x}_t)$
- 4 Generate analysis ensemble  $\mathbf{x}_t^i = T_{\mathbf{y}_t^*}(\mathbf{y}_t^i, \mathbf{x}_t^i)$  for  $i = 1, \dots, N$

# Composed maps are stable for tracking

## Lorenz-63 model

- ▶ Infer the hidden state given noisy point-wise observations
- ▶ With  $N = 50$  samples, we can *at best* estimate linear maps
- ▶ Measure root-mean-squared error (RMSE) of ensemble mean

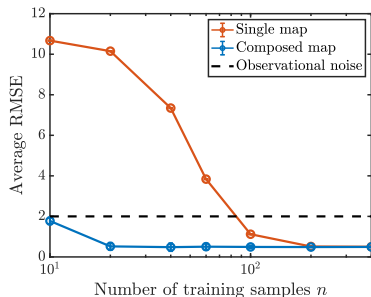
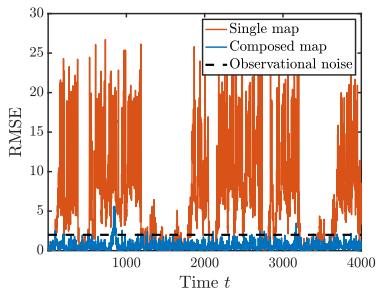


**Takeaway:** Composed maps have **stable RMSE with limited samples**

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**Takeaway:** Composed maps have **stable RMSE with limited samples**

## Generalization of the EnKF

- ▶ Restricting  $S^{\mathcal{X}}$  to be affine in  $\mathbf{x}_t, \mathbf{y}_t$ , we recover the transformation

$$T_{\mathbf{y}_t^*}(\mathbf{y}_t, \mathbf{x}_t) = \mathbf{x}_t - \Sigma_{\mathbf{x}_t, \mathbf{y}_t} \Sigma_{\mathbf{y}_t}^{-1} (\mathbf{y}_t - \mathbf{y}_t^*),$$

- ▶ Transport maps allow for the gradual introduction of nonlinear terms
- ▶ Nonlinear maps  $T_{\mathbf{y}_t^*}$  capture non-Gaussian structure of  $\pi_{\mathbf{Y}_t, \mathbf{X}_t}$



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## Example map parameterization

- ▶ Each component is the sum of nonlinear univariate functions

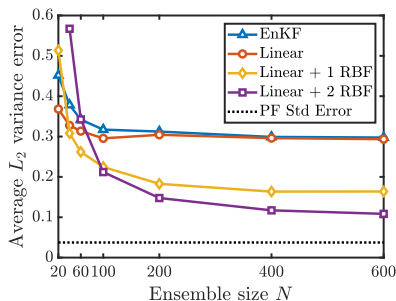
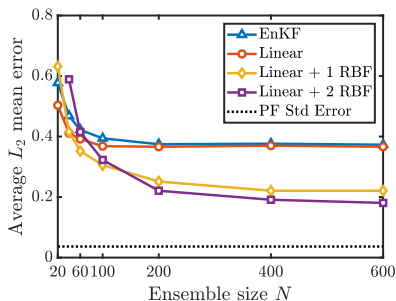
$$S_k(z_1, \dots, z_k) = \mathbf{u}_1(z_1) + \dots + \mathbf{u}_k(z_k),$$

where  $\mathbf{u}_i(z) = u_{i,0}z + \sum_{j=1}^p u_{ij} \mathcal{N}(z; \xi_j, \sigma_j^2)$  and  $\mathbf{u}_k(z_k)$  is monotone

# Nonlinear maps capture filtering distribution

## Lorenz-63 model

- ▶  $d = 3$  with  $\Delta t_{obs} = 0.1$  and fully-observed state
- ▶ Observations follow  $\mathbf{y}_t = \mathbf{x}_t + \boldsymbol{\eta}_t$  with  $\boldsymbol{\eta}_t \sim \mathcal{N}(\mathbf{0}, 4\mathbf{I})$
- ▶ Measure root-mean-squared-error  $\text{RMSE}(t) = \|\mathbf{x}_t^* - \mathbb{E}[\mathbf{x}_t | \mathbf{y}_{1:t}^*]\|_2 / \sqrt{d}$
- ▶ Compare statistics to a particle filter (PF) with 1M samples

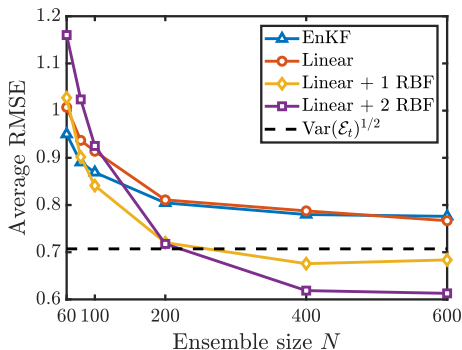


Improved posterior estimates is also **stable with increasing  $\Delta t_{obs}$**

# Nonlinear maps improve tracking

## Lorenz-96 model: chaotic dynamics

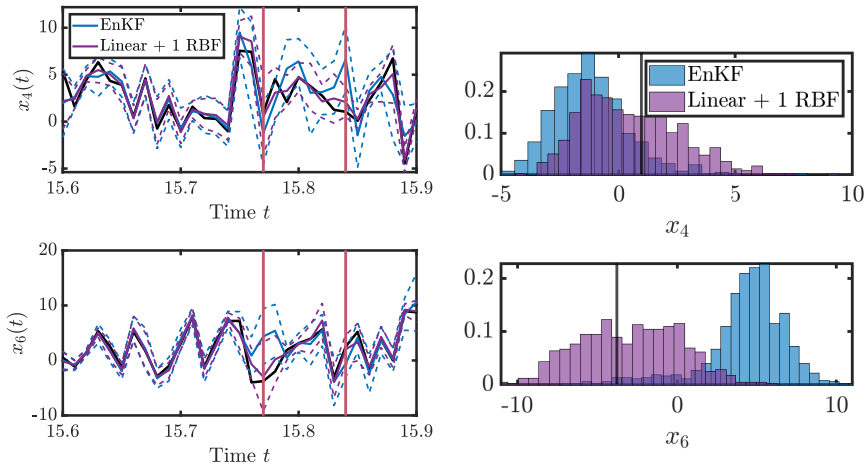
- ▶ 40 states, 20 observations, and  $\Delta t_{obs} = 0.4$  (**large!**)
- ▶ Measure average RMSE (*left*) over 2000 assimilation cycles
- ▶ Parametrize maps with increasing nonlinearity using RBFs



Nonlinear maps also **improve estimates of posterior moments**

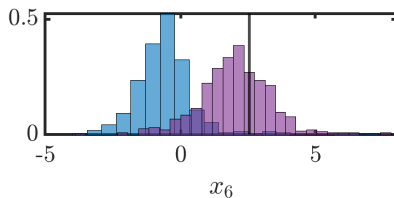
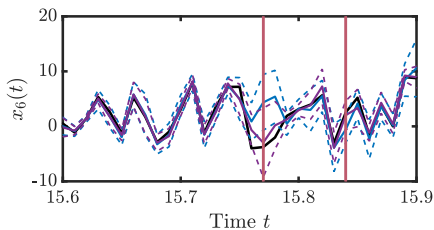
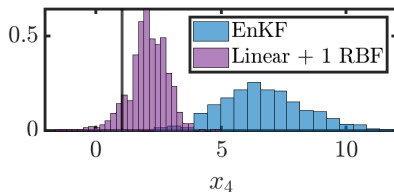
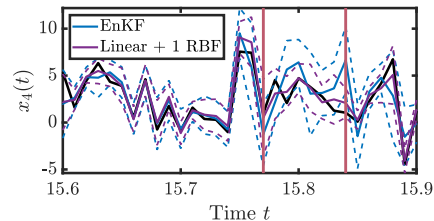
# Nonlinear maps better capture uncertainty in true state

- ▶ Tracking two marginals of Lorenz-96 system at two assimilation times
- ▶ Compare ensemble distribution from EnKF and nonlinear maps



# Nonlinear maps better capture uncertainty in true state

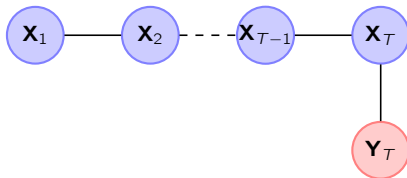
- ▶ Tracking two marginals of Lorenz-96 system at two assimilation times
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## Extension to smoothing

**Goal:** Characterize full smoothing distribution  $\pi_{\mathbf{x}_{1:T}|\mathbf{y}_{1:T}}$  or a marginal

- Consider update for all states given a single observation at time  $T$



**Ensemble Transport Smoother:** Apply stochastic map algorithm on joint states over time:

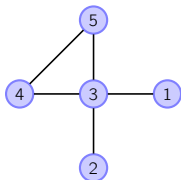
$$T_{\mathbf{y}_T^*}(\mathbf{y}_T, \mathbf{x}_{1:T}) = S^{\mathcal{X}}(\mathbf{y}_T^*, \cdot)^{-1} \circ S^{\mathcal{X}}(\mathbf{y}_T, \mathbf{x}_{1:T})$$

- Ordering of states in  $S^{\mathcal{X}}$  defines different smoothing algorithms
- Exploiting the Markov structure of the states yields sparse maps

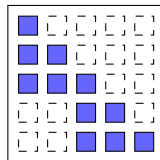
# Transport maps exploit conditional independence

Theorem: Sparsity of triangular maps [Spantini et al., 2018]

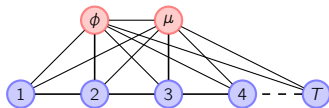
Conditional independence of target distribution  $\pi$  (encoded by graph) defines functional dependence of  $S$  such that  $S^\# \eta = \pi$



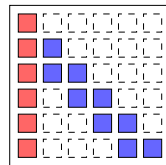
Markov structure of 5-dimensional distribution



Sparsity of  $\partial_j S_k$



Markov structure of hidden Markov model



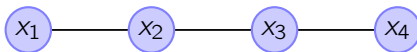
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Conditional independence of target distribution  $\pi$  (encoded by graph) defines functional dependence of  $S$  such that  $S^\# \eta = \pi$


$$\begin{bmatrix} S_1(x_1) \\ S_2(x_1, x_2) \\ S_3(x_1, x_2, x_3) \\ S_4(x_1, x_2, x_3, x_4) \end{bmatrix} \rightarrow \begin{array}{l} \pi(x_1) \\ \pi(x_2|x_1) \\ \pi(x_3|x_1, x_2) \\ \pi(x_4|x_1, x_2, x_3) \end{array} \quad \begin{array}{l} \\ \\ = \pi(x_3|x_2) \\ = \pi(x_4|x_3) \end{array} \quad \begin{array}{l} \\ \\ X_3 \perp\!\!\!\perp X_1|X_2 \\ X_4 \perp\!\!\!\perp (X_1, X_2)|X_3 \end{array}$$





## Two new classes of smoothers [Ramgraber, B et al., 2022]


**Backwards-in-time:** uses the ordering  $\mathbf{x}_T, \dots, \mathbf{x}_1$

$$S^{\mathcal{X}}(\mathbf{y}_T, \mathbf{x}_{1:T}) \stackrel{CI}{=} \begin{bmatrix} S_T(\mathbf{y}_T, \mathbf{x}_T) \\ S_{T-1}(\mathbf{x}_T, \mathbf{x}_{T-1}) \\ \vdots \\ S_1(\mathbf{x}_2, \mathbf{x}_1) \end{bmatrix} \cdot$$


(CI) exploits chain structure:  $\mathbf{x}_{1:T-1} \perp\!\!\!\perp \mathbf{y}_T | \mathbf{x}_T$  and  $\mathbf{x}_{1:s-1} \perp\!\!\!\perp \mathbf{x}_{s+1:T} | \mathbf{x}_s$

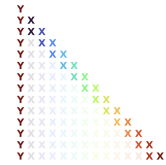
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**Forwards-in-time:** uses the ordering  $\mathbf{x}_1, \dots, \mathbf{x}_T$

$$S^x(\mathbf{y}_T, \mathbf{x}_{1:T}) \stackrel{CI}{=} \begin{bmatrix} S_1(\mathbf{y}_T, \mathbf{x}_1) \\ S_2(\mathbf{y}_T, \mathbf{x}_1, \mathbf{x}_2) \\ \vdots \\ S_T(\mathbf{y}_T, \mathbf{x}_{T-1}, \mathbf{x}_T) \end{bmatrix}$$

(CI) exploits chain structure:  $\mathbf{x}_s \perp\!\!\!\perp \mathbf{x}_{1:s-2} | \mathbf{x}_{s-1}$  for  $s \geq 2$

- ▶ Empirical results suggest backward-in-time accumulates less errors
- ▶ Forwards smoother constrains state trajectories by dynamics

**Sequential context:** The joint decomposition simplifies

$$\begin{aligned}\pi(\mathbf{x}_{1:T}|\mathbf{y}_{1:T}^*) &= \pi(\mathbf{x}_T|\mathbf{y}_{1:T}^*) \prod_{s=1}^{T-1} \pi(\mathbf{x}_s|\mathbf{x}_{s+1}, \mathbf{y}_{1:T}^*) \\ &= \pi(\mathbf{x}_T|\mathbf{y}_{1:T}^*) \prod_{s=1}^{T-1} \pi(\mathbf{x}_s|\mathbf{x}_{s+1}, \mathbf{y}_{1:s}^*)\end{aligned}$$

- ▶ Component  $S_s$  samples  $\pi(\mathbf{x}_s|\mathbf{x}_{s+1}, \mathbf{y}_{1:s}^*)$
- ▶ We estimate  $S_s$  using filtering ensemble  $(\mathbf{x}_s^i, \mathbf{x}_{s+1}^i) \sim \pi(\mathbf{x}_s, \mathbf{x}_{s+1}|\mathbf{y}_{1:s}^*)$

## Generalization of the Ensemble RTS smoother

- ▶ Restricting  $S^{\mathcal{X}}$  to be affine in  $\mathbf{y}_t, \mathbf{x}_{1:t}$ , we recover the transformation

$$\begin{aligned}T_{\mathbf{y}_T^*}(\mathbf{y}_T, \mathbf{x}_T) &= \mathbf{x}_T - \Sigma_{\mathbf{x}_T, \mathbf{y}_T} \Sigma_{\mathbf{y}_T}^{-1} (\mathbf{y}_T - \mathbf{y}_T^*) \\ T_{\mathbf{x}_{s+1}^*}(\mathbf{x}_s, \mathbf{x}_{s+1}) &= \mathbf{x}_s - \Sigma_{\mathbf{x}_s, \mathbf{x}_{s+1}} \Sigma_{\mathbf{x}_{s+1}}^{-1} (\mathbf{x}_{s+1} - \mathbf{x}_{s+1}^*), \quad s < t\end{aligned}$$

## Special case: fixed-point smoothing

**Idea:** Apply backwards-in-time smoother to  $\pi(\mathbf{x}_s, \mathbf{x}_T | \mathbf{y}_{1:T^*})$  for  $s < T$

$$S^{\mathcal{X}}(\mathbf{y}_T, \mathbf{x}_s, \mathbf{x}_T) \stackrel{CI}{=} \begin{bmatrix} S_T(\mathbf{y}_T, \mathbf{x}_T) \\ S_s(\mathbf{x}_T, \mathbf{x}_s) \end{bmatrix}.$$

- ▶ Estimate map using augmented filtering ensemble  $\pi(\mathbf{x}_s, \mathbf{x}_t | \mathbf{y}_{1:t-1}^*)$
- ▶ Pushing forward through composed maps samples  $\pi(\mathbf{x}_s, \mathbf{x}_t | \mathbf{y}_{1:t}^*)$

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- ▶ Pushing forward through composed maps samples  $\pi(\mathbf{x}_s, \mathbf{x}_t | \mathbf{y}_{1:t}^*)$

### Generalization of the ensemble Kalman smoother (EnKS)

For affine  $S^x$ , the combined composed map recovers the transformation

$$\mathbf{x}_s^* = \mathbf{x}_s - \Sigma_{\mathbf{x}_s, \mathbf{y}_t} \Sigma_{\mathbf{y}_t}^{-1} (\mathbf{y}_t - \mathbf{y}_t^*)$$

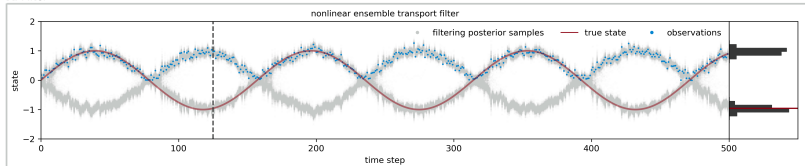
Key feature for affine maps: Update each state variable in parallel

**Takeaway:** Non-linear transport maps generalize linear smoothers

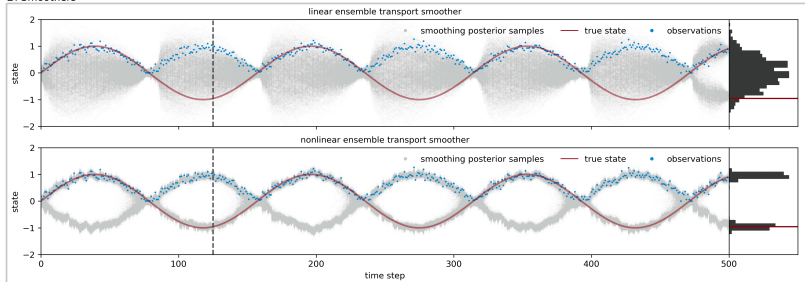
# Nonlinear smoothers capture bimodal distributions

- ▶ Sinusoidal state  $x_t$  with observation  $y_t = |x_t + \gamma|$  for  $\gamma \sim \mathcal{N}(0, 0.1)$
- ▶ Infer state using random walk model without knowing true dynamics
- ▶ Backward smoother is initialized from nonlinear transport filter

A: Filter



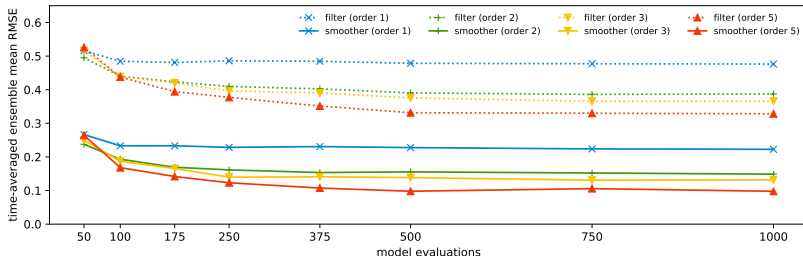
B: Smoothers



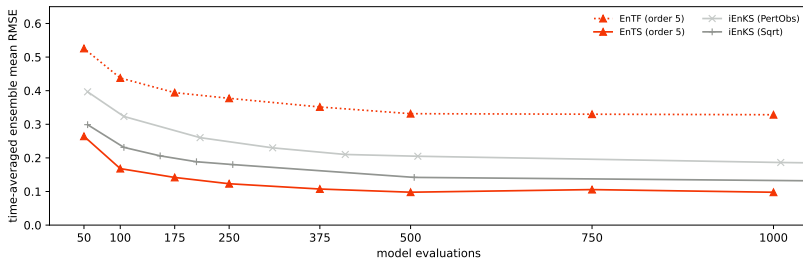
# Nonlinear smoothers improve state estimation

## Lorenz-63 model

A: Lorenz-63 EnTF and EnTS results



B: Lorenz-63 iEnKS results





**So far:** Transport maps are **consistent for sampling non-Gaussian filtering and smoothing distributions** without requiring importance weights

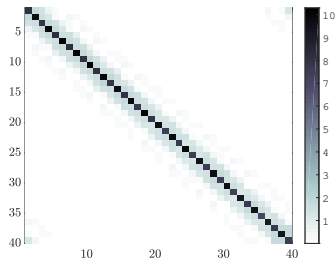
**So far:** Transport maps are [consistent for sampling non-Gaussian filtering and smoothing distributions](#) without requiring importance weights

How do we compute transport maps given small ensemble sizes?

- 1 Localize estimators with approximate Markov structure
- 2 Targeted non-linearity using hybrid nonlinear+linear maps
- 3 Restrict inference to relevant low-dimensional subspaces

# 1. Transport maps are easy to “localize” in high dimensions

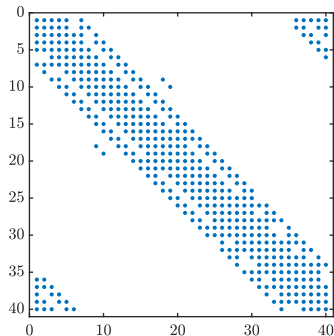
Many spatial fields satisfy approximate Markov properties



Inverse covariance matrix for  
Lorenz-96 model forecast is **sparse**

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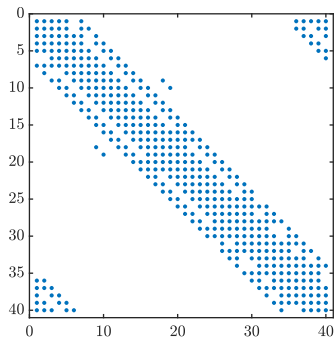
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# 1. Transport maps are easy to “localize” in high dimensions

## Many spatial fields satisfy approximate Markov properties



Inverse covariance matrix for  
Lorenz-96 model forecast is **sparse**

- **Idea:** Regularize the estimation of  $S$  by *imposing sparsity*:

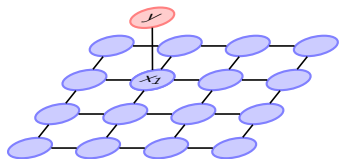
$$\hat{S}(\mathbf{x}) = \begin{bmatrix} \hat{S}^1(x_1) \\ \hat{S}^2(x_1, x_2) \\ \hat{S}^3(\quad, x_2, x_3) \\ \hat{S}^4(\quad, x_3, x_4) \end{bmatrix}$$

- **Heuristic:** Let  $\hat{S}^k$  depend on neighboring variables  $(x_j)_{j < k}$  that are physically close to  $x_k$ :

$$\hat{S}^k(x_1, \dots, x_k) \approx \hat{S}^k(x_{N(k)}, x_k)$$

## 2. Structured hybrid linear and nonlinear maps

**Local-likelihood models:** Scalar observation  $y \sim \pi_{Y|X_1}$

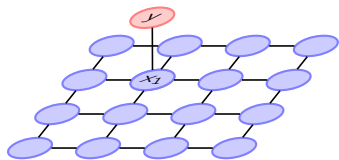


$$T(y, \mathbf{x}) = \left[ \begin{array}{c} T_1(y, x_1) \\ \vdots \\ T_l(x_1, \dots, x_l) \\ L_{l+1}(x_1, \dots, x_{l+1}) \\ \vdots \\ L_d(x_1, \dots, x_d) \end{array} \right] \left\{ \begin{array}{l} \text{Nonlinear maps} \\ \text{Affine maps: EnKF update} \end{array} \right.$$

**Idea:** For conditionally Gaussian models, use nonlinear updates  $T_k$  for state variables  $\mathbf{x}_{1:l}$  and use linear updates  $L_k$  for  $\mathbf{x}_{l+1:d}$

## 2. Structured hybrid linear and nonlinear maps

**Local-likelihood models:** Scalar observation  $y \sim \pi_{Y|X_1}$



$$T(y, \mathbf{x}) = \left[ \begin{array}{c} T_1(y, x_1) \\ \vdots \\ T_I(x_1, \dots, x_I) \\ L_{I+1}(x_1, \dots, x_{I+1}) \\ \vdots \\ L_d(x_1, \dots, x_d) \end{array} \right] \left\{ \begin{array}{l} \text{Nonlinear maps} \\ \text{Affine maps: EnKF update} \end{array} \right.$$

**Idea:** For conditionally Gaussian models, use nonlinear updates  $T_k$  for state variables  $\mathbf{x}_{1:I}$  and use linear updates  $L_k$  for  $\mathbf{x}_{I+1:d}$

**Special cases:**

- ▶  $I = 1$ : Nonlinear  $T_1$  and keeping all other components affine **recovers the rank histogram filter** [Andersen 2010]
- ▶ With decay in correlation,  $L_{I+1}, \dots, L_d$  reverts to an identity map

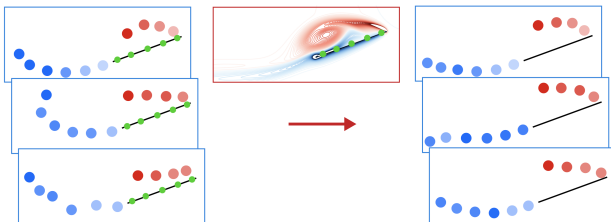
See Max's talk (today) on adapting map complexity to ensemble size!

### 3. Low-rank updates via an example in turbulent flows

#### Inference problem:

- ▶ States  $\mathbf{x}_t$ : Positions and strengths of point vortices
- ▶ Observations  $\mathbf{y}_t$ : Pressure observations along airfoil

Truth from CFD/ experiment



#### Challenges:

- ▶ High-dimensional states and observations  $d = 180$  and  $m = 50$
- ▶ Observations are non-local:  $\mathbf{y}_t$  is related to all  $\mathbf{x}_t$  by Poisson equation
- ▶ Limited ensemble of size  $N = \mathcal{O}(100)$



## Main ideas

- ▶ Only part of the state  $\mathbf{x}_r = U_r^T \mathbf{x}$  is informed by the observations
- ▶ Only part of the observation  $\mathbf{y}_s = V_s^T \mathbf{y}$  is relevant to the states

## Main ideas

- ▶ Only part of the state  $\mathbf{x}_r = U_r^T \mathbf{x}$  is informed by the observations
- ▶ Only part of the observation  $\mathbf{y}_s = V_s^T \mathbf{y}$  is relevant to the states
- ▶ Consider the posterior approximation at each assimilation step

$$\hat{\pi}_{\mathbf{X}|\mathbf{Y}}(\mathbf{x}|\mathbf{y}) = \hat{\pi}_{\mathbf{X}_r|\mathbf{Y}_s}(\mathbf{x}_r|\mathbf{y}_s)\pi_{\mathbf{X}_\perp|\mathbf{X}_r}(\mathbf{x}_\perp|\mathbf{x}_r)$$

- ▶ **Approach:** Find  $U_r, V_s$  with small  $r$  and  $s$  from prior ensemble and observation operator such that  $\pi_{\mathbf{X}|\mathbf{Y}} \approx \hat{\pi}_{\mathbf{X}|\mathbf{Y}}$  [B, Marzouk et al., 2022]

## Main ideas

- ▶ Only part of the state  $\mathbf{x}_r = U_r^T \mathbf{x}$  is informed by the observations
- ▶ Only part of the observation  $\mathbf{y}_s = V_s^T \mathbf{y}$  is relevant to the states
- ▶ Consider the posterior approximation at each assimilation step

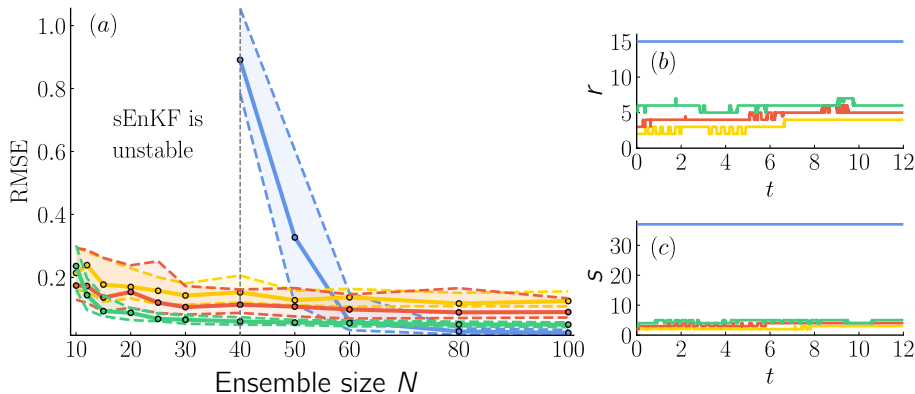
$$\hat{\pi}_{\mathbf{X}|\mathbf{Y}}(\mathbf{x}|\mathbf{y}) = \hat{\pi}_{\mathbf{X}_r|\mathbf{Y}_s}(\mathbf{x}_r|\mathbf{y}_s)\pi_{\mathbf{X}_\perp|\mathbf{X}_r}(\mathbf{x}_\perp|\mathbf{x}_r)$$

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- ▶ **Result:** Prior-to-posterior **map only acts on low-dimensional variables**

$$T_{\mathbf{y}^*}(\mathbf{y}, \mathbf{x}) = U_r T_{\mathbf{y}_s^*}^r(V_s^T \mathbf{y}, U_r^T \mathbf{x}) + U_\perp U_\perp^T \mathbf{x}$$

- ▶  $T_r$  can be linear [Le Provost, B et al., 2022] or non-linear

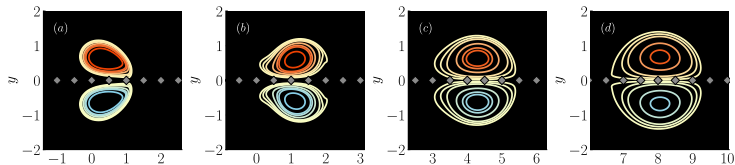
# Low-rank filter is stable for small ensemble sizes



## Observations:

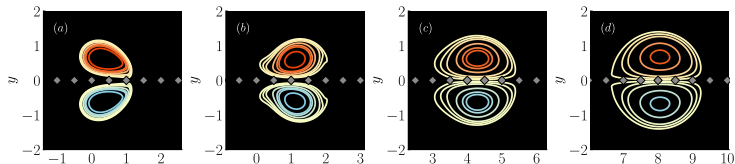
- ▶ RMSE is stable for small  $N$  for different energy ratios
- ▶ Adaptive reduced dimensions  $r, s$  do not increase over time

## High-fidelity numerical simulation at Reynolds number 1000

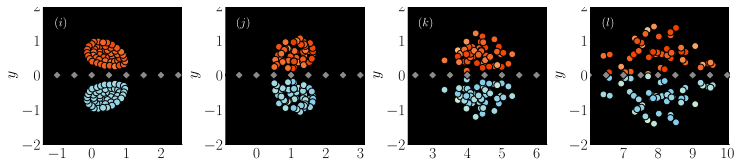


# Low-rank EnKF is stable with model error

## High-fidelity numerical simulation at Reynolds number 1000

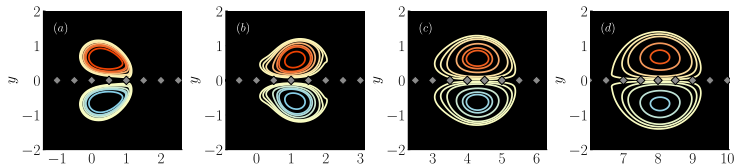


## Inviscid vortex model with EnKF

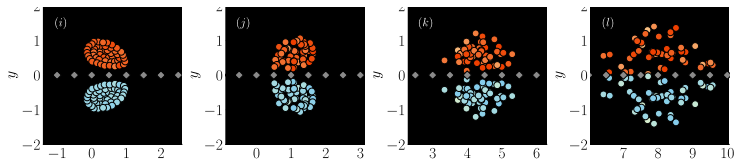


# Low-rank EnKF is stable with model error

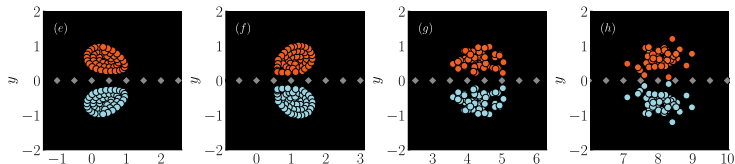
## High-fidelity numerical simulation at Reynolds number 1000



## Inviscid vortex model with EnKF



## Inviscid vortex model with LR-EnKF



# Conclusions and outlook



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Central idea: consistent data assimilation using measure transport

- ▶ **Composed transport maps** generalize ensemble filters and smoothers
- ▶ Nonlinear maps **improve state estimation** for chaotic systems
- ▶ **Exploit (approximate) conditional independence structure** for scaling to high-dimensional inference problems

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## Ongoing work

- ▶ Square-root versions of nonlinear filters and smoothers
- ▶ Conditional sampling with other generative models, e.g., score-based diffusion models [Song et al., 2020]

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Main references: [arXiv:1907.00389](https://arxiv.org/abs/1907.00389), [arXiv:2203.05120](https://arxiv.org/abs/2203.05120), [arXiv:2210.17000](https://arxiv.org/abs/2210.17000)

## Thank You

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