Sequential inference via low-dimensional couplings

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Sequential Bayesian inference



- State estimation (e.g., *filtering* and *smoothing*) or *joint state and* parameter estimation, in a Bayesian setting
 - Need recursive algorithms for characterizing the posterior

Deterministic couplings of distributions

Key task: sample a non-Gaussian distribution π



Idea

- Choose a reference distribution η (e.g., standard Gaussian)
- Seek a map $T : \mathbb{R}^n \to \mathbb{R}^n$ such that $T_{\sharp}\eta = \pi$
- Equivalently, find $S = T^{-1}$ such that $S_{\sharp}\pi = \eta$

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Various types of transport...

Optimal transport:

$$T_{\text{opt}} = \arg \min_{T} \int_{\mathbb{R}^{n}} c(\mathbf{x}, T(\mathbf{x})) \, \mathrm{d}\eta(\mathbf{x})$$

s.t. $T_{\sharp} \eta = \pi$

- Monge (1781) problem; many nice properties, but numerically challenging in general continuous cases
- Knothe-Rosenblatt rearrangement:

$$T(\mathbf{x}) = \begin{bmatrix} T^{1}(x_{1}) \\ T^{2}(x_{1}, x_{2}) \\ \vdots \\ T^{n}(x_{1}, x_{2}, \dots, x_{n}) \end{bmatrix}$$

- Exists and is unique (up to ordering) under mild conditions
- Inverse map $S = T^{-1}$ also lower triangular
- "Exposes" marginals, will enable conditional sampling...

Computation of triangular maps from densities

 $\min_{T} \mathcal{D}_{\mathsf{KL}}(T_{\sharp}\eta || \pi)$

► Numerical approximations can employ a monotone parameterization, guaranteeing ∂_{xk}T^k > 0 for arbitrary functions a_k, b_k

$$T^{k}(x_{1},\ldots,x_{k})=a_{k}(x_{1},\ldots,x_{k-1})+\int_{0}^{x_{k}}\exp\left(b_{k}(x_{1},\ldots,x_{k-1},w)\right)\,dw$$

Sample average approximation + (BFGS or Newton) for

$$\min_{(\boldsymbol{a}_k,\boldsymbol{b}_k)_k} \mathbb{E}_{\boldsymbol{X} \sim \boldsymbol{\eta}}[-\log \pi(\mathcal{T}(\boldsymbol{X})) - \sum_k \log \partial_{\boldsymbol{x}_k} \mathcal{T}^k(\boldsymbol{X})]$$

- Many alternatives, e.g.,
 - 1. fully nonparametric approaches (stein variational gradient) [Liu, '16]
 - 2. deep neural networks (normalizing flows) [Rezende, '15]
- Challenge: represent a high-dimensional nonlinear function

Markov properties and low-dimensional couplings

Main idea

There exists a link between the Markov properties of (η, π) and the existence of couplings that admit low-dimensional structure in terms of

- 1. Sparsity
- 2. Decomposability
- > Additional structure not discussed here: low rank



Sparse transport maps

Given a reference η and a target π, focus on the sparsity of the inverse Knothe-Rosenblatt (KR) rearrangement, i.e., S_#π = η

$$S(\mathbf{x}) = \begin{bmatrix} S^{1}(x_{1}) \\ S^{2}(x_{1}, x_{2}) \\ S^{3}(x_{1}, x_{2}, x_{3}) \\ \vdots \\ S^{n}(x_{1}, x_{2}, \dots, x_{n}) \end{bmatrix} \Longrightarrow \begin{bmatrix} S^{1}(x_{1}) \\ S^{2}(x_{1}, x_{2}) \\ S^{3}(x_{2}, x_{3}) \\ \vdots \\ S^{n}(x_{1}, x_{2}, \dots, x_{n}) \end{bmatrix}$$

Theorem:¹ The KR rearrangement (a nonlinear function) inherits the same sparsity pattern as the Cholesky factor of the incidence matrix (properly scaled) of a graphical model for π, provided that

$$\eta(\mathbf{x}) = \prod_i \eta(x_i)$$

¹Spantini et al. (2017)

Compute the inverse transport!

- Direct transports $T_{\#}\eta = \pi$, however, tend to be dense
- Sparsity in T is linked to **marginal** (not conditional) independence



Key message

Compute the inverse transport S and evaluate $T(\mathbf{x}) = S^{-1}(\mathbf{x})$ point-wise

- Trivial to invert a triangular function (sequence of 1D root findings)
- Same spirit as GMRF, but for general **non-Gaussian** densities
- The direct transport is usually dense, but low-dimensional structure might lie elsewhere...

Decomposable transport maps

▶ **Definition:** a decomposable transport is a map $T = T_1 \circ \cdots \circ T_k$ that factorizes as the composition of finitely many maps of low effective dimension and that are triangular (up to a permutation), e.g.,



► **Theorem:**² Decomposable graphical models for π lead to decomposable direct maps T, provided that $\eta(\mathbf{x}) = \prod_i \eta(x_i)$

²Spantini et al. (2017)

Applications to Bayesian filtering/smoothing

- Sparsity/decomposability apply to general Markov structures
- **Special case:** nonlinear non-Gaussian state-space models



Ideally, interested in recursively updating the full Bayesian solution:

$$\pi_{Z_{0:k}|Y_{0:k}} \to \pi_{Z_{0:k+1}|Y_{0:k+1}}$$

Let X₀, X₁,... be an independent process with marginals (η_{X_k})_k
 Coupling between X₀,..., X_N and Z₀,..., Z_N|Y₀,..., Y_N

Seek a decomposable transport for $\pi_{Z_0,...,Z_k | Y_0,...,Y_k}$ (just a chain!)

First step: compute a 2-D map



• Compute $\mathfrak{M}_0 : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ s.t.

$$\mathfrak{M}_{0}(\mathbf{x}_{0},\mathbf{x}_{1}) = \begin{bmatrix} A_{0}(\mathbf{x}_{0},\mathbf{x}_{1}) \\ B_{0}(\mathbf{x}_{1}) \end{bmatrix} \qquad T_{0}(\mathbf{x})$$

• Reference:
$$\eta_{X_0}\eta_{X_1}$$

- Target: $\pi_{Z_0} \pi_{Z_1|Z_0} \pi_{Y_0|Z_0} \pi_{Y_1|Z_1}$
- $\dim(\mathfrak{M}_0) \simeq 2 \times \dim(\mathbf{Z}_0)$

$$= \begin{bmatrix} A_0(\mathbf{x}_0, \mathbf{x}_1) \\ B_0(\mathbf{x}_1) \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \\ \mathbf{x}_5 \\ \vdots \\ \mathbf{x}_N \end{bmatrix}$$

Second step: compute a 2-D map



 $T_{1}(\mathbf{x}) = \begin{bmatrix} \mathbf{x}_{0} \\ A_{1}(\mathbf{x}_{1}, \mathbf{x}_{2}) \\ B_{1}(\mathbf{x}_{2}) \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \vdots \\ \mathbf{y} \end{bmatrix}$ • Compute $\mathfrak{M}_1 : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ s.t. $\mathfrak{M}_1(\mathbf{x}_1, \mathbf{x}_2) = \left[\begin{array}{c} A_1(\mathbf{x}_1, \mathbf{x}_2) \\ B_1(\mathbf{x}_2) \end{array} \right]$

- Reference: $\eta_{X_1}\eta_{X_2}$
- Target: $\eta_{X_1} \pi_{Y_2|Z_2} \pi_{Z_2|Z_1}(\cdot | B_0(\cdot))$
- Uses only one component of \mathfrak{M}_0

Proceed recursively forward in time



• Compute $\mathfrak{M}_2 : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ s.t.

pute
$$\mathfrak{M}_{2}: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$$
 s.t.
 $\mathfrak{M}_{2}(\mathbf{x}_{2}, \mathbf{x}_{3}) = \begin{bmatrix} A_{2}(\mathbf{x}_{2}, \mathbf{x}_{3}) \\ B_{2}(\mathbf{x}_{3}) \end{bmatrix}$
 $T_{2}(\mathbf{x}) = \begin{bmatrix} \mathbf{x}_{0} \\ \mathbf{x}_{1} \\ A_{2}(\mathbf{x}_{2}, \mathbf{x}_{3}) \\ B_{2}(\mathbf{x}_{3}) \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \vdots \\ \mathbf{x}_{N} \end{bmatrix}$
et: $\eta_{X_{2}} \pi_{Y_{3}|Z_{3}} \pi_{Z_{3}|Z_{2}}(\cdot | B_{1}(\cdot))$
only one component of \mathfrak{M}_{1}

• Reference:
$$\eta_{X_2}\eta_{X_3}$$

- Target: $\eta_{X_2} \pi_{Y_3|Z_3} \pi_{Z_3|Z_2}(\cdot | B_1(\cdot))$
- Uses only one component of \mathfrak{M}_1

XN

A decomposition theorem for chains



Theorem:^a

1.
$$(B_k)_{\sharp} \eta_{X_{k+1}} = \pi_{Z_{k+1}|Y_{0:k+1}}$$
 (filtering)
2. $(\mathfrak{M}_k)_{\sharp} \eta_{X_{k:k+1}} \simeq \pi_{Z_k, Z_{k+1}|Y_{0:k+1}}$ (lag-1 smoothing)
3. $(T_0 \circ \cdots \circ T_k)_{\sharp} \eta_{X_{0:k+1}} = \pi_{Z_{0:k+1}|Y_{0:k+1}}$ (full Bayesian solution)

^aSpantini et al. (2017)

A nested decomposable map

• $\mathfrak{T}_k = T_0 \circ T_1 \circ \cdots \circ T_k$ characterizes the full joint $\pi_{Z_{0:k+1}|Y_{0:k+1}|}$



- ▶ Trivial to go from \mathfrak{T}_k to \mathfrak{T}_{k+1} : just append a new map T_{k+1}
- No need to recompute T_0, \ldots, T_k (nested transports)
- \mathfrak{T}_k is dense and high-dimensional but **decomposable**

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A single-pass algorithm on the model

Meta-algorithm:

- 1. Compute the maps $\mathfrak{M}_0, \mathfrak{M}_1, \ldots$, each of dimension $2 \times \dim(\mathbf{Z}_0)$
- 2. Embed each \mathfrak{M}_j into an identity function to form T_j
- 3. Evaluate $T_0 \circ \cdots \circ T_k$ for the full Bayesian solution

Remarks:

- A single pass on the state-space model
- ► Non-Gaussian generalization of the Rauch-Tung-Striebel smoother
- ▶ Bias is *only* due to the numerical approximation of each map *T_i*
- Can either accept the bias or reduce it by:
 - Increasing the complexity of each map T_i, or
 - Computing weights given by the proposal density

 $(T_0 \circ T_1 \circ \cdots \circ T_k)_{\sharp} \eta_{\mathsf{X}_{0:k+1}}$

The cost of evaluating weights grows linearly with time

Joint parameter/state estimation

Can be generalized to sequential joint parameter/state estimation



 $\blacktriangleright (T_0 \circ \cdots \circ T_k)_{\sharp} \eta_{\Theta} \eta_{X_{0:k+1}} = \pi_{\Theta, Z_{0:k+1} | Y_{0:k+1}} (full Bayesian solution)$

• However, now dim $(\mathfrak{M}_j) = 2 \times \dim(\mathbf{Z}_j) + \dim(\Theta)$

Remarks:

- No artificial dynamic for the static parameters
- No a priori fixed-lag smoothing approximation

Another decomposable map



(P₀ ∘ · · · ∘ P_k)_# η_Θ = π<sub>Θ|Y_{0:k+1} (parameter estimation)
 If 𝔅_k = P₀ ∘ · · · ∘ P_k, then 𝔅_k can be computed recursively as
</sub>

$$\mathfrak{P}_k = \mathfrak{P}_{k-1} \circ P_k$$

via **regression** \implies cost of evaluating \mathfrak{P}_k does not grow with k

Numerical example: stochastic volatility model

Latent log-volatilities taking the form of an AR(1) process for t = 0, ..., N. We take N = 944.

$$\mathbf{Z}_{t+1} = \mu + \phi \left(\mathbf{Z}_t - \mu
ight) + \eta_t, \quad \eta_t \sim \mathcal{N}(0, 1), \quad \mathbf{Z}_0 \sim \mathcal{N}(0, 1/1 - \phi^2)$$

Observe the mean return for holding the asset at time t

$$\mathbf{Y}_t = arepsilon_t \, \exp(\, 0.5 \, \mathbf{Z}_t \,), \quad arepsilon_t \sim \mathcal{N}(0, 1), \quad t = 0, \dots, N$$

► The Markov structure for $\pi \sim \mu$, ϕ , $\mathbf{Z}_{0:N} | \mathbf{Y}_{0:N}$ is given by:



Joint state/parameter estimation problem

Filtering distributions

- Computed online via 4-d maps
- Can use Gauss quadratures for each map!



Smoothing marginals

- Just re-evaluate the 4-d maps backwards in time
- ► Comparison with a "reference" MCMC solution with 10⁵ ESS (in red)



Static parameter ϕ

- Sequential parameter inference
- ► Comparison with a "reference" MCMC solution (**batch** algorithm)



Static parameter μ

- Slow accumulation of error over time (sequential algorithm)
- ► Acceptance rate 75% for MCMC with transport-map proposal



Long-time smoothing (25 years)



Python code available at http://transportmaps.mit.edu

Filtering high-dimensional systems

- ▶ Now we consider the filtering of state-space models with:
 - 1. High-dimensional states
 - 2. Intractable transition kernel, i.e., can only obtain forecast samples
 - 3. Limited model evaluations, e.g., small ensemble size
 - 4. Sparse and local observations in space/time
- State-of-the-art results (in terms of tracking) are *currently* obtained with localized versions of the EnKF
- The EnKF is not consistent, but robust

Some open questions:

- ► For a given ensemble size *N*, are we doing the best we can?
- EnKF is not guaranteed to perform better as N increases, and in some situations performs worse! Can this be mitigated?
- Can we get closer to the Bayesian solution, while preserving robustness of EnKF approaches?

Main idea

- 1. Propagation: apply the dynamics to obtain the next forecast ensemble
- 2. Assimilation: transform the forecast ensemble into approx. samples from the filtering distribution via local, nonlinear couplings

Key steps of the assimilation algorithm:

- 1 Approximate the *forecast distribution* on a manifold of sparse non-Gaussian Markov random fields
- 2a Local assimilation of the observations
- 2b Propagation of information across the state

Abstraction of the assimilation problem:

▶ We have *samples* from the prior & can evaluate the likelihood

Projection onto a manifold of sparse MRFs



• **Approach:** learn an inverse map $S : \mathbb{R}^n \to \mathbb{R}^n$ from samples

$$\min_{S \in \mathcal{S}_{\Delta}} \mathcal{D}_{\mathcal{K}L}(\pi \mid\mid S_{\sharp}^{-1} \eta) = \max_{S \in \mathcal{S}_{\Delta}} \mathbb{E}_{\pi}[\log \eta(S(\boldsymbol{Z})) + \log |\nabla S(\boldsymbol{Z})|]$$

- ► Choose the approximation space S_△ (finite space of sparse lower triangular maps) to enforce a desired Markov structure
- Compute each component $S^k : \Omega \to \mathbb{R}$ via **convex** optimization
 - Choose any parameterization of S^k that departs (if desired) from linearity by adding local nonlinear terms (e.g., polynomials, RBFs)

Assimilation and propagation



► For simplicity, consider assimilating one observation at a time

$$\pi(z|y) = \pi(z_1|y) \, \pi(z_{\sim 1}|z_1)$$

• Local assimilation: simulate from $\pi(z_1|y)$

- First map component S¹ pushes forward the prior π_{Z1} to η₁; yields an approximation (S¹)⁻¹_μη₁ of the forecast marginal
- Seek a direct map \mathring{T}^1 with target density

$$\pi(z_1|y) \propto \pi(y|z_1)\eta_1\left(S^1(z_1)\right)\partial_{z_1}S^1(z_1)$$

► Then T¹ ∘ S¹ transforms forecast samples of z₁ to analysis/posterior samples of z₁

Assimilation and propagation



- ▶ Propagation: sample from the conditional π(z_{~1}|z₁) given samples from the marginal π(z₁|y)
- Given the inverse map S, notice that $S_{\xi} : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$,

$$\mathbf{z}_{2},\ldots,\mathbf{z}_{n}\mapsto\left[\begin{array}{c}S^{2}(\boldsymbol{\xi},\mathbf{z}_{2})\\\vdots\\S^{n}(\boldsymbol{\xi},\mathbf{z}_{2},\ldots,\mathbf{z}_{n})\end{array}
ight],$$

pushes forward $\pi_{Z_{2:n}|z_1=\pmb{\xi}}$ to $\eta_{2:n} \implies$ just invert $S_{\pmb{\xi}}$

- ► Sparse Markov structure yields further simplifications in *S*, e.g.,
 - 1. Sparse S
 - 2. Parallel inversion of S_{ξ}

Assimilation and propagation



Local assimilation + propagation:

▶ Then the **combined** map (for a *single* observation),

$$\mathcal{T}(\mathbf{z}) = \begin{bmatrix} T^1(\mathbf{z}_1) \\ S^{-1}_{T^1(\mathbf{z}_1)}(\mathbf{z}_2, \ldots, \mathbf{z}_n) \end{bmatrix} \circ S(\mathbf{z}),$$

transforms the forecast ensemble to the analysis ensemble!

 Can *iterate* this construction to assimilate each additional observation, or generalize to multiple/batch observations

Lorenz 96 (40-dimensional state)

► A hard test-case configuration:³

$$\frac{d\mathbf{Z}_{j}}{dt} = (\mathbf{Z}_{j+1} - \mathbf{Z}_{j-2}) \mathbf{Z}_{j-1} - \mathbf{Z}_{j} + F, \qquad j = 1, \dots, 40 \mathbf{Y}_{j} = \mathbf{Z}_{j} + \varepsilon_{j}, \qquad j = 1, 3, 5 \dots, 39$$

- F = 8 (chaotic regime) and $\varepsilon_j \sim \mathcal{N}(0, 0.5)$
- Time between observations: $\Delta_{obs} = 0.4$ (large!)
- Results averaged over 2000 assimilation cycles

	#particles: 400		#particles: 200	
	EnKF ⁶	LocNLF	≈EnKF	LocNLF
med RMSE	0.88	0.64	0.91	0.66
avg RMSE	0.97	0.74	1.02	0.79
var RMSE	0.12	0.06	0.1	0.09

• The nonlinear filter is $\sim 25\%$ more accurate in RMSE than EnKF

³Bengtsson et al. (2003)

Lorenz 96: details on the filtering approximation



- Observations were assimilated one at a time
- Approximate Markov structure: 5-way interactions
- Each conditional $\pi(x_k | x_{j_1}, \dots, x_{j_p})$ was learnt via a **separable** map

$$S^{k}(x_{j_{1}},...,x_{j_{p}},x_{k}) = \psi(x_{j_{1}}) + ... + \psi(x_{j_{p}}) + \psi(x_{k}),$$

where $\psi(x) = a_0 + a_1 \cdot x + \sum_{i>1} a_i \exp(-(x - c_i)^2 / \sigma)$.

Much more general parameterizations are of course possible!

Lorenz 96: tracking performance of the filter



Introducing simple, localized nonlinearities can make a difference!

Conclusions

Summary

► Role of **continuous** transport in problems of sequential inference

- 1. Filtering and smoothing (generalization of the RTS smoother)
- 2. Sequential parameter-state estimation
- 3. High dimensional filtering (using local couplings)

Ongoing and future work

- Approximately sparse Markov structures (e.g., graph sparsification)
- Learn Markov structure from samples

Thank You

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