Machine Learning for Inverse Problems and Data Assimilation: A Practical Session

Ricardo Baptista

Statistical Sciences
University of Toronto

Collaborators: Eviatar Bach, Edo Calvello, Bohan Chen, Daniel Sanz-Alonso, Andrew Stuart

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Some background first on me

Trajectory from aviation to probabilistic modeling

- BASc in aerospace engineering
- PhD in computational science from MIT
- Instructor in applied mathematics at Caltech
- Postdoc at Amazon Stores AI
- Current: faculty at UToronto

Current research interests

- Computational Bayesian inference
- Data assimilation
- Measure transport
- Mathematics of probabilistic machine learning

Overview of Tutorial

1. **Transport for Inverse Problems**
   - Variational Inference
   - Data Amortization

2. **Learning Filters for Data Assimilation**
   - Learning The Gain

Code: www.github.com/baptistar/MLforIPDA

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Variational Inference

Goal: Approximate the posterior distribution for parameters u given data y

$$\pi^y(u) = \frac{1}{Z} \underbrace{l(y|u)}_{\textit{Likelihood}} \underbrace{\rho(u)}_{\textit{Prior}}$$

Approximate $\pi^y(u) \approx q(u)$ by minimizing the KL divergence over a family of distributions $\mathcal{Q}$:

$$\min_{q \in \mathcal{Q}} D_{KL}(q||\pi^y)$$

Minimizing the *reverse* KL is equivalent to

$$\arg\min_q D_{KL}(q||\pi^y) = \arg\min_q \mathbb{E}_{u\sim q}[\log q(u) - \log \rho(u) - \log \mathrm{l}(y|u)]$$

Takeaway:

- Minimization is tractable without knowing Z
- Requires evaluating $\mathrm{l}(y|\cdot)$; alternative is to use D_E with ρ samples

Gaussian Variational Inference

Gaussian Posterior Approximations:

$$\mathcal{Q} = \left\{ q = \mathcal{N}(m, \Sigma), m \in \mathbb{R}^d, \Sigma \in \mathbb{R}^{d \times d}, \Sigma \succ 0 \right\}$$

Two Gaussian Families:

- Mean-field:

$$q(u) = \prod_{i=1}^{d} q_i(u_i), \qquad q_i = \mathcal{N}(m_i, \sigma_i^2)$$

- General multivariate distribution:

$$\Sigma = LL^T, \qquad L \in \mathbb{R}^{d \times d}$$

Optimization Problem:

$$\begin{aligned} &\arg\min_q \mathbb{E}_{u \sim q}[\log q(u) - \log \rho(u) - \log \mathrm{l}(y|u)] \\ =&\arg\min_{m,\Sigma} -\frac{1}{2} \log |\Sigma| - \mathbb{E}_{u \sim q}[\log \rho(u) - \log \mathrm{l}(y|u)] \end{aligned}$$

Application: Bio-chemical oxygen demand model

Parameters:

$$A \sim U(0.4, 1.2), \text{ and } B \sim U(0.01, 0.31) \quad A \perp\!\!\!\perp B,$$

Transform independent standard Gaussian variables u to uniform (A, B) using CDF: $\Phi : \mathbb{R} \to [0, 1]$

$$A = 0.4 + 0.4\Phi(u_1)$$
$$B = 0.01 + 0.15\Phi(u_2)$$

Prior:

$$u \sim \mathcal{N}(0, I_2)$$

Forward Model:

$$\mathfrak{B}(t; u) = A(1 - \exp(-Bt))$$
$$G(u) = [\mathfrak{B}(1; u), \mathfrak{B}(2; u), \mathfrak{B}(3; u), \mathfrak{B}(4; u), \mathfrak{B}(5; u)]$$
$$y = G(u) + \eta, \quad \eta \sim \mathcal{N}(0, \Gamma), \quad \Gamma = 10^{-3} I_5$$

Goal: Sample $u \in \mathbb{R}^2$ conditioned on a data measurement $y \in \mathbb{R}^5$

Transport Variational Inference

Transport Approximation: Choose reference distribution $\varrho \in \mathcal{P}(\mathbb{R}^d)$

$$\mathcal{Q} = \left\{ q = T(\cdot;\theta)_{\#}\varrho, \theta \in \mathbb{R}^p \right\}$$

Sample posterior using: $T(z;\theta) \sim q, \quad z \sim \varrho$

Optimization Problem

$$\arg\min_{\theta} -\mathbb{E}_{z\sim\varrho}[\log \rho \circ T(z,\theta) + \log \mathsf{l}(y|\,T(z;\theta)) + \log\det \nabla_z T(z;\theta)]$$

Given i.i.d. samples $z^{(1)}, \ldots, z^{(N)}$ from the reference distribution ϱ:

$$\arg\min_{\theta} -\frac{1}{N}\sum_{i=1}^{N} \log \rho \circ T(z^{(i)};\theta) + \log \mathsf{l}(y|\,T(z^{(i)};\theta)) + \log\det \nabla_z T(z^{(i)};\theta)$$

Requirement: T must be smooth and monotone: $\nabla_z T \succ 0$

Normalizing Flows Define Invertible Transports

Idea: Compose K invertible maps L_j to create a *flow*

$$T(z;\theta) = L_K \circ L_{K-1} \circ \cdots \circ L_1(z)$$

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Benefit: The inverse (needed later) and log-determinant are computable layer-wise

$$T^{-1}(u;\theta) = L_1^{-1} \circ L_2^{-1} \circ \ldots L_K^{-1}(u)$$
$$\log\det \nabla T(z;\theta) = \sum_{j=1}^{K} \log\det \nabla L_j(y^j),$$

where $y^j = L_j \circ \cdots \circ L_1(z)$ are hidden features

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Practical remarks:

- Each layer is chosen to be a simple transformation
- There is a trade-off in the expressiveness of each layer and the number of layers K

How do we parameterize each flow layer?

Real non-volume preserving flow

Split input $y \in \mathbb{R}^d$ into two blocks y_1 and y_2 of equal size and apply:

$$L(y) = \begin{bmatrix} y_1 \\ a(y_1) + \exp(b(y_1))y_2 \end{bmatrix}$$

where a and b are neural network modeling translation and scale

Inverse by construction:

$$L^{-1}(w) = \begin{bmatrix} w_1 \\ (w_2 - a(w_1))/\exp(b(w_1)) \end{bmatrix}, \qquad \log\det \nabla_y L(y) = b(y_1)$$

Key Properties:

- Variable permutations are used between the layers
- Each layer can only represent conditional Gaussian distributions

Alternative approaches: Residual flows, masked autoregressive flows, diffusion models

Learning Data Dependence of Transports

Target: Posterior distribution for any observation y

$$\pi(u|y) \propto \rho(u)\mathsf{l}(y|u)$$

Goal: Approximate $\pi(u|y) \approx T(\cdot; y, \theta)_{\#}\varrho(u)$ by minimizing forward KL (flipped order):

$$\arg\min_{\theta} \mathbb{E}_y[D_{KL}(\pi^y || T(\cdot; y, \theta)_{\#}\varrho)]$$

Minimizing the forward KL is equivalent to

$$\arg\min_{\theta} \mathbb{E}_y[D_{KL}(\pi^y || T(\cdot; y, \theta)_{\#}\varrho)] = \arg\min_{\theta} \mathbb{E}_{(u,y)}[-\log T(\cdot; y, \theta)_{\#}\varrho(u)]$$

Note: Objective is likelihood and prior-free!

Output: After learning the map, sample any posterior $\pi(u|y^*)$:

$$u^{(i)} = \widehat{T}(z^{(i)}; y^*\theta), \quad z^{(i)} \sim \varrho$$

Maximum Likelihood Training

Given target density $\gamma(u, y) = \rho(u)\mathsf{l}(y|u)$:

$$\arg\min_{\theta} \mathbb{E}_{(u,y)\sim\gamma}[-\log T(\cdot; y, \theta)_{\#}\varrho(u)]$$

For standard Gaussian ϱ:

$$\arg\min_{\theta} \mathbb{E}_{(u,y)\sim\gamma}\left[\|T(\cdot; y, \theta)\|^2 - \log\det \nabla_u T^{-1}(u; y, \theta)\right]$$

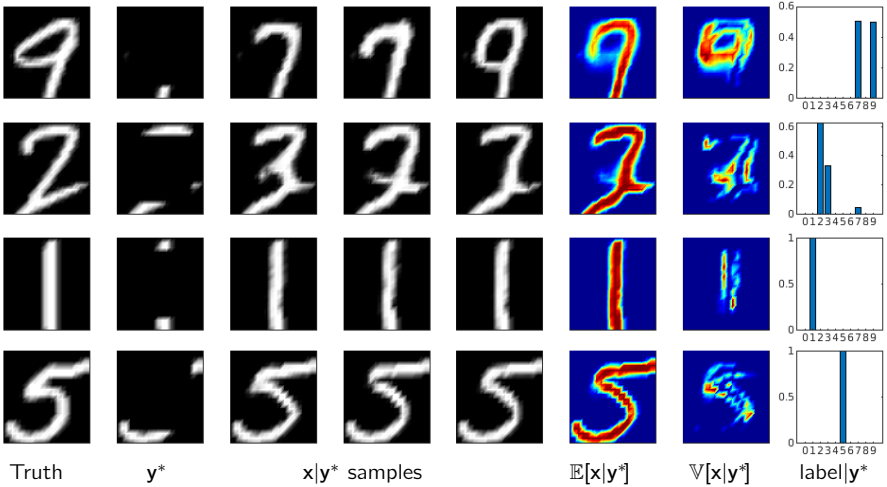
Given i.i.d. samples $(u^{(1)}, y^{(1)}), \ldots, (u^{(N)}, y^{(N)})$ from γ:

$$\arg\min_{\theta} \frac{1}{N}\sum_{i=1}^{N} -\log \varrho \circ T^{-1}(u^{(i)}; y^{(i)}, \theta) - \log\det \nabla_u T^{-1}(u^{(i)}; y^{(i)}, \theta),$$

Remark: Training requires T^{-1}, but generating samples only needs to evaluate T

Another Numerical Example: Image In-Painting [B et al., 2024]

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



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Data Assimilation Recap

Setup: Markov model for states and observations

$$v_{j+1}^\dagger = \Psi(v_j^\dagger) + \xi_{j+1}^\dagger, \qquad \xi_{j+1}^\dagger \sim \mathcal{N}(0, \Sigma)$$
$$y_{j+1}^\dagger = h(v_{j+1}^\dagger) + \eta_{j+1}^\dagger, \qquad \eta_{j+1}^\dagger \sim \mathcal{N}(0, \Gamma)$$

Goal: Approximate the filtering distribution for state at times $j = 1, \ldots, J$:

$$\pi_j := \mathbb{P}(v_j | y_1^\dagger, \ldots, y_j^\dagger)$$

Filtering evolves according to the recursion:

- Prediction step: $\widehat{\pi}_{j+1} = \mathsf{P}\pi_j$, where $\widehat{\pi}_{j+1} = \mathbb{P}(v_{j+1} | y_1^\dagger, \ldots, y_j^\dagger)$
- Analysis step: $\pi_{j+1} = \mathsf{A}(\widehat{\pi}_{j+1}; y_{j+1}^\dagger)$

Note: $\mathsf{A}(\cdot; y) = \mathsf{B}(\cdot; y) \circ \mathsf{Q}$ in the earlier lectures

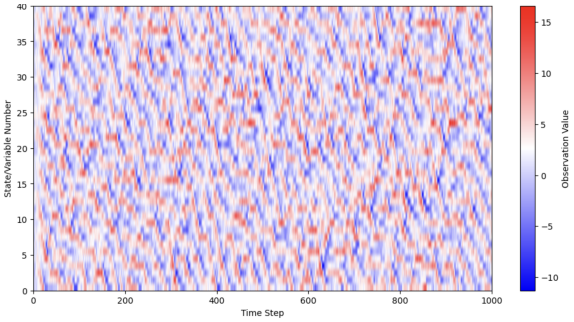
Model Problem: Lorenz-96 System

Continuous-Time System: Coupled ODE with $n = 40$ states:

$$\frac{dv_i}{dt} = (v_{i+1} - v_{i-2})v_{i-1} - v_i + F, \qquad i = 1, \ldots, n$$

starting from initial condition $v(0) \sim \mathcal{N}(0, I_n)$

Discretized System: Discretize ODE using RK4 and evolve state v_j at discrete time-steps
Direct Observations: $y_j = v_j + \eta_j, \qquad \eta_j \sim \mathcal{N}(0, \Gamma)$



Goal: Approximate $\pi_{j+1} \approx q_{j+1}(\theta)$ using variational inference

Recall:

$$\begin{aligned} &\arg\min_{\theta} D_{KL}(q_{j+1}(\theta)||\pi_{j+1}) \\ =&\arg\min_{\theta} D_{KL}(q_{j+1}(\theta)||\widehat{\pi}_{j+1}) - \mathbb{E}_{u\sim q_{j+1}(\theta)}[\log l(y_{j+1}^{\dagger}; u)] \end{aligned}$$

Approximate π_{j+1} for all steps by minimizing the sum of KL divergences:

$$\min_{\theta} \frac{1}{J}\sum_{j=0}^{J-1} D_{KL}(q_{j+1}(\theta)||\widehat{\pi}_{j+1}) - \mathbb{E}_{u\sim q_{j+1}(\theta)}[\log l(y_{j+1}^{\dagger}; u)]$$

Approximate Distributions

Consider Gaussian distributions $q_j(\theta)$ defined recursively given $K = \theta$:

- Prediction step

$$\widehat{m}_{j+1} = \Psi(m_j)$$
$$\widehat{C}_{j+1} = J_j C_j J_j^T + \Sigma, \qquad J_j = \text{ Jacobian of } \Psi$$

- Analysis step

$$m_{j+1} = \widehat{m}_{j+1} + K(y_{j+1}^\dagger - H m_{j+1})$$
$$C_{j+1} = (I - KH)\widehat{C}_{j+1}(I - KH)^T + K\Gamma K^T$$

Define: $\widehat{\pi}_{j+1} = \mathcal{N}(\widehat{m}_{j+1}, \widehat{C}_{j+1})$ and $q_{j+1}(K) = \mathcal{N}(m_{j+1}(K), C_{j+1}(K))$

Goal: Learn K that yields close filters for all time j

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Thank You to attendees and organizers

astuart@caltech.edu, r.baptista@utoronto.ca