Robust and adaptive construction of measure transports for Bayesian inference

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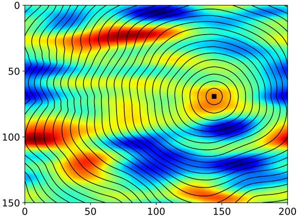
Bayesian inference – an example



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$$|\nabla \overbrace{G(\mathbf{x})}^{\text{travel time}}| = \underbrace{v(\mathbf{x})}_{\text{velocity field}}{}^{-1}$$

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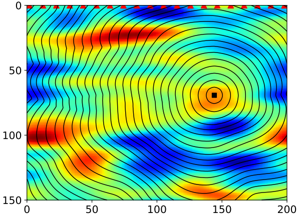

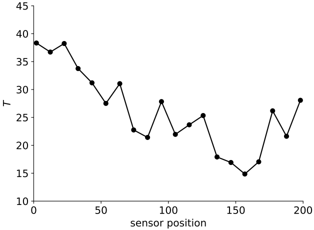

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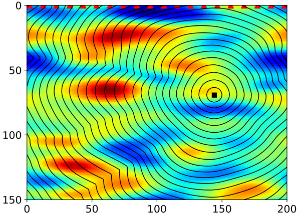

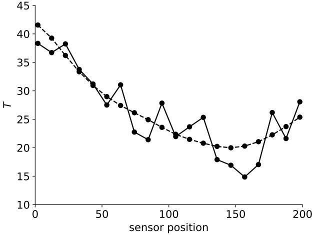

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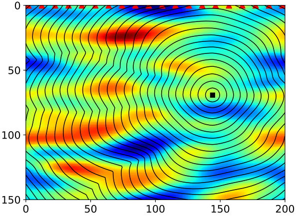

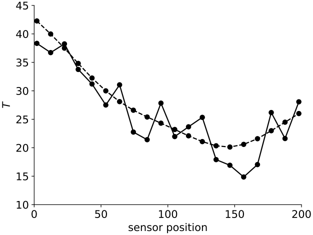

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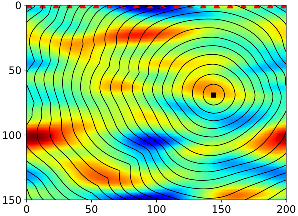

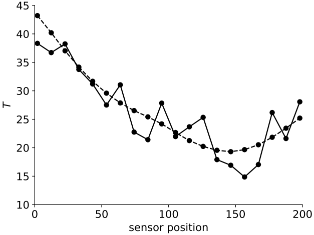

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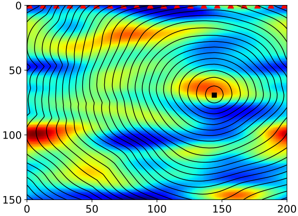

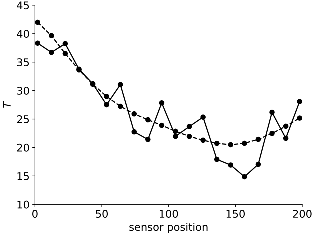

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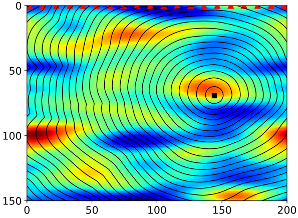

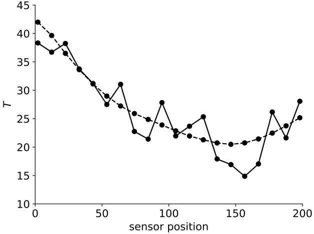

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Inference model

$$\underbrace{\pi_{\text{pos}}(\mathbf{v}|\mathbf{d})}_{\text{posterior}} \propto \overbrace{\mathcal{L}_{\mathbf{d}}(\mathbf{v})}^{\text{likelihood}} \underbrace{\pi_{\text{pr}}(\mathbf{v})}_{\text{prior}} = \pi_{\boldsymbol{\varepsilon}}(\mathbf{d} - \mathbf{G}(\mathbf{v}))\pi_{\text{pr}}(\mathbf{v})$$

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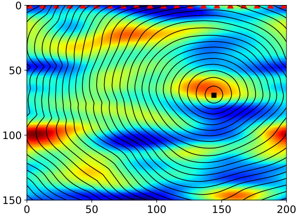

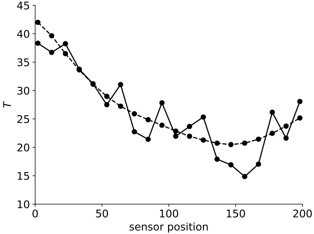

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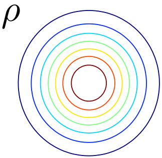
Decisions under uncertainty

$$\min_{\delta} \int L(\mathbf{v}, \delta)\pi_{\mathrm{pos}}(\mathbf{v}|\mathbf{d})d\mathbf{v}$$

Measure transport – Pullbacks [PB] and Pushforwards [PF]

- Distribution $\boldsymbol{\nu}_\rho$ with density $\rho : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$



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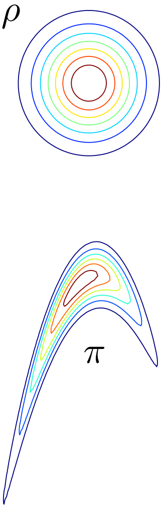

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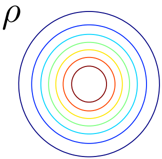

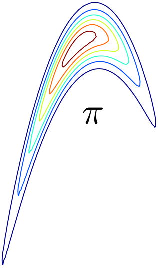

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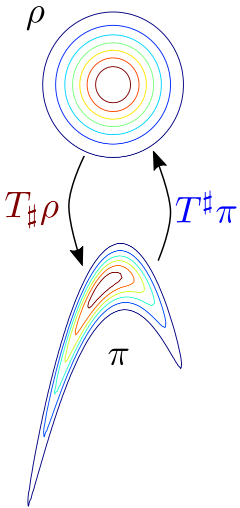

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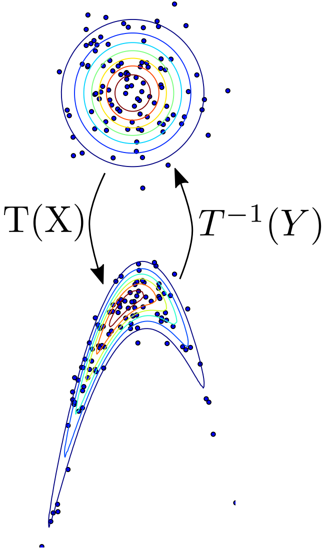

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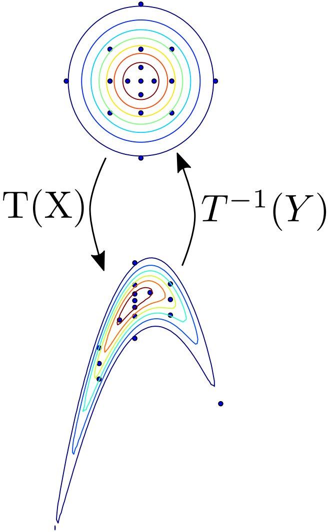

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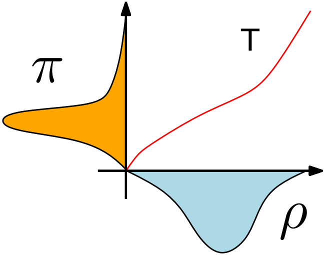

Knothe-Rosenblatt rearrangement

$\forall \boldsymbol{\nu}_\rho, \boldsymbol{\nu}_\pi$ absolutely continuous there exists a **triangular monotone** map s.t. $T(d\boldsymbol{\nu}_\rho) = d\boldsymbol{\nu}_\pi$

$$T(\mathbf{x}) = \begin{bmatrix} T^{(1)}(x_1) \\ T^{(2)}(x_1, x_2) \\ \vdots \\ T^{(d)}(x_1, \ldots, x_d) \end{bmatrix}$$

Triangular monotone maps

$$\mathcal{T}_\triangle = \left\{ T : \mathbb{R}^d \to \mathbb{R}^d : \overbrace{[T(\mathbf{x})]_k = T^{(k)}(x_1, \dots, x_k)}^{\text{triangular}} \text{ and } \overbrace{\partial_{x_k} T^{(k)} > 0}^{\text{monotone}} \right\}$$

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Integrated squared representation

$$T^{(k)}(x_{1:k}) = c_k(x_{1:k-1}) + \int_0^{x_k} \Big(h_k(x_{1:k-1}, t) + \varepsilon \Big)^2 dt$$

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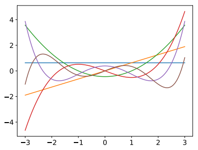
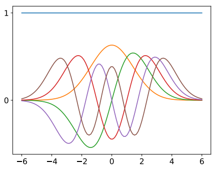
Constant part – $\mathcal{T}^0_\triangle$

$$c_k(x_{1:k-1}) = \sum_{\mathbf{i} \in \mathcal{I}_k} \mathbf{a}_\mathbf{i} \Phi_\mathbf{i}(x_{1:k-1})$$



Squared part – $\mathcal{T}^0_\triangle$

$$h_k(x_{1:k-1}, t) = \sum_{\mathbf{j} \in \mathcal{J}_k} \mathbf{b}_\mathbf{j} \Psi_\mathbf{j}(x_{1:k-1}, t)$$



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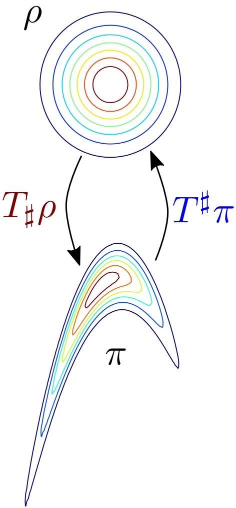

**How to find the map $T \in \mathcal{T}_\triangle$
such that $T_\sharp \rho = \pi$?**

Minimize KL-divergence to find optimal map

$$T^* = \underset{T \in \mathcal{T}_\triangle}{\arg\min}\, D_{\mathrm{KL}}(T_\sharp \rho \| \pi) = \underset{T \in \mathcal{T}_\triangle}{\arg\min}\, \mathbb{E}_\rho \left[\log \frac{\rho}{T^\sharp \pi} \right]$$

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- + **Derivative based unconstrained optimization** if gradients are available
- + We can **explore π in parallel**
- + We can **generate i.i.d. samples** from $T_\sharp^* \rho \propto \pi$ **in parallel**

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Sources of low-dimensional structure

- Smoothness
- Marginal independence
- Conditional independence
- Low-rank structure

Convergence criterion

$$T^* = \arg\min_{T \in \mathcal{T}_\triangle} D_{\mathrm{KL}}(T_\sharp \rho \| \pi) = \arg\min_{T \in \mathcal{T}_\triangle} \mathbb{E}_\rho \left[\log \frac{\rho}{T^\sharp \pi} \right]$$

Optimal $T^* \in \mathcal{T}_\triangle$ and $\int \pi = 1 \quad \Rightarrow \quad D_{\mathrm{KL}}(T^*_\sharp \rho \| \pi) = 0$

But, optimal $\tilde{T}^* \in \mathcal{T}^0_\triangle$ or $\int \pi \neq 1 \quad \Rightarrow \quad D_{\mathrm{KL}}(\tilde{T}^*_\sharp \rho \| \pi) \neq 0$

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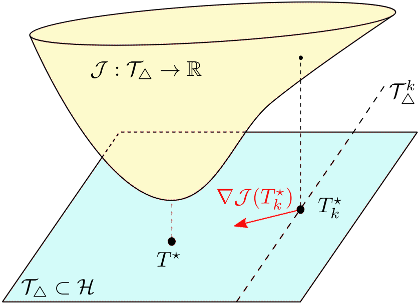
$\mathbb{V}\left[\log \frac{\rho}{T^\sharp \pi}\right] \xrightarrow{T \to T^*} 0$ as $\frac{1}{2} D_{\mathrm{KL}}(T^*_\sharp \rho \| \pi) \xrightarrow{T \to T^*} -\log \int \pi$

Refinement criterion

$$\boxed{T^* = \arg\min_{T \in \mathcal{T}_\triangle} \underbrace{D_{KL}(T_\sharp \rho \| \pi)}_{\mathcal{J}(T)}}$$



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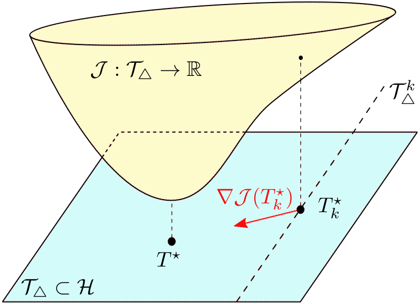

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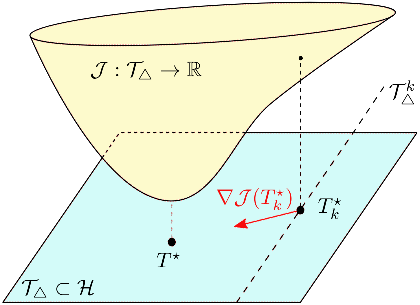

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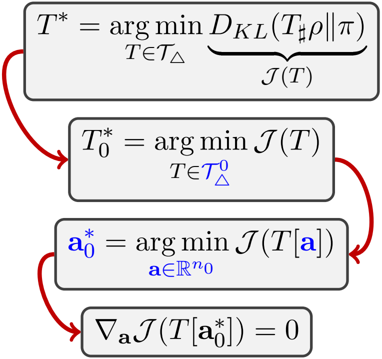

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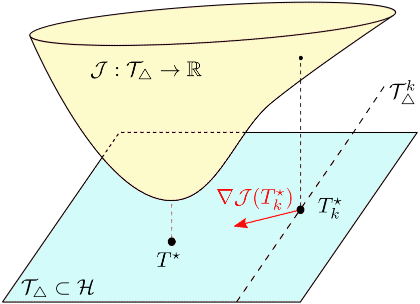
$$\nabla_{\mathbf{a}}\mathcal{J}(T[\mathbf{a}_0^*]) = 0$$



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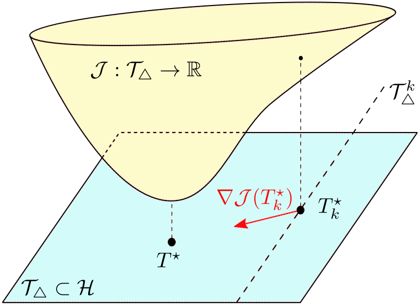
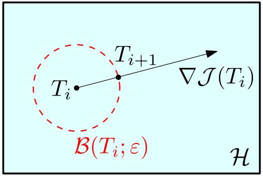


$$\mathcal{J}(T_{i+1}) < \mathcal{J}(T_i)$$



The **first variation** $\nabla\mathcal{J}\left(T[\mathbf{a}_0^*]\right) \neq 0$

There exists $\varepsilon > 0$ such that

$$\mathcal{J}\left(T[\mathbf{a}_0^*] - \varepsilon\nabla\mathcal{J}\left(T[\mathbf{a}_0^*]\right)\right) < \mathcal{J}\left(T[\mathbf{a}_0^*]\right)$$

Use the first variation to enrich the approximation space

$$\boxed{\nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) = \left(\nabla_{\mathbf{x}} T\right)^{-1}\left(\nabla_{\mathbf{x}} \log \frac{\rho}{T[\mathbf{a}_0^*]^\sharp \pi}\right)}$$

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- $\nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) : \mathbb{R}^d \to \mathbb{R}^d$ **is a map** in $\mathcal{H} \supset \mathcal{T}_\triangle$

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Projection on $\mathcal{T}_\triangle^1 \supset \mathcal{T}_\triangle^0$

$$\mathbf{b}_1^* = \arg\min_{\mathbf{b} \in \mathbb{R}^{n_1}} \left\| U[\mathbf{b}] - \nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) \right\|_{L^2_\rho}$$

Use the first variation to enrich the approximation space

$$\boxed{\nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) = \left(\nabla_{\mathbf{x}} T\right)^{-1}\left(\nabla_{\mathbf{x}} \log \frac{\rho}{T[\mathbf{a}_0^*]^\sharp \pi}\right)}$$

- $\nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) : \mathbb{R}^d \to \mathbb{R}^d$ **is a map** in $\mathcal{H} \supset \mathcal{T}_\triangle$

Projection on $\mathcal{T}_\triangle^1 \supset \mathcal{T}_\triangle^0$

$$\mathbf{b}_1^* = \underset{\mathbf{b} \in \mathbb{R}^{n_1}}{\arg\min} \left\| U[\mathbf{b}] - \nabla \mathcal{J}\left(T[\mathbf{a}_0^*]\right) \right\|_{L^2_\rho}$$

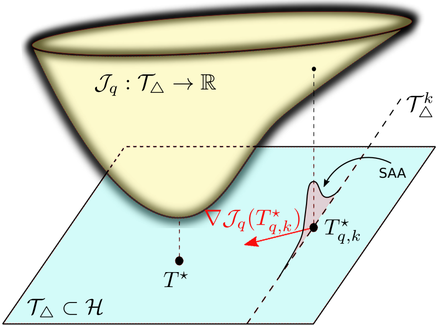
- **No new evaluation** of $\nabla_{\mathbf{x}} \log \pi$ is required
- $U[\mathbf{b}_1^*]$ informs about **active variables** to be included
- $U[\mathbf{b}_1^*]$ informs about **active coefficients** to be included

Controlling the sample average accuracy

$$T_k^* = \underset{T \in \mathcal{T}_\triangle^k}{\arg\min} -\mathbb{E}_\rho \left[\log T^\sharp \pi \right] \approx \underset{T \in \mathcal{T}_\triangle^k}{\arg\min} \overbrace{- \sum_{1 \leq i \leq q} \log T^\sharp \pi(\mathbf{x}_i)}^{\mathcal{J}_q(T)} =: T_{q,k}^*$$

Controlling the sample average accuracy

$$T_k^* = \arg\min_{T\in\mathcal{T}_\triangle^k} -\mathbb{E}_\rho\left[\log T^\sharp\pi\right] \approx \arg\min_{T\in\mathcal{T}_\triangle^k} \overbrace{-\sum_{1\le i\le q}\log T^\sharp\pi(\mathbf{x}_i)}^{\mathcal{J}_q(T)} =: T^*_{q,k}$$

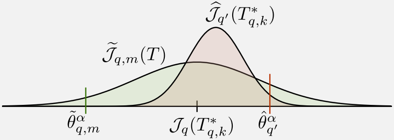


Controlling the sample average accuracy

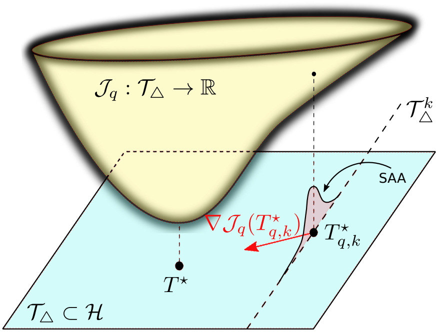
$$T^*_k = \underset{T\in\mathcal{T}^k_\triangle}{\arg\min} -\mathbb{E}_\rho\left[\log T^\sharp\pi\right] \approx \underset{T\in\mathcal{T}^k_\triangle}{\arg\min} - \overbrace{\sum_{1\leq i\leq q} \log T^\sharp\pi(\mathbf{x}_i)}^{\mathcal{J}_q(T)} =: T^*_{q,k}$$

Sample average approximation

$$\tilde{\theta}_{q,m} \leq \mathcal{J}(T^*_k) \leq \hat{\theta}_{q'}$$

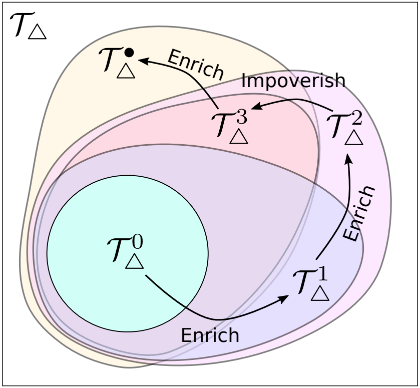


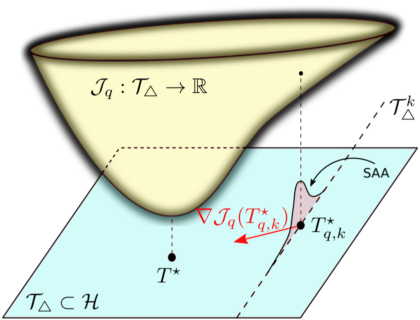
$$\widetilde{J}_{q,m}(T) = \frac{1}{m}\sum_{i=1}^{m} \min_{T\in\mathcal{T}^k_\triangle} \mathcal{J}_q(T)$$



Adaptivity ingredients

- **Convergence criterion – Variance diagnostic** : $\mathbb{V}\left[\log \frac{\rho}{T^\sharp \pi}\right]$
- **Refinement criterion – First variation** : $\nabla \mathcal{J}\left(T[\mathbf{a}^*]\right)$
- **Stability criterion – Sample average approximation** : $\tilde{\theta}_{q,m} \leq \mathcal{J}(T_k^*) \leq \hat{\theta}_{q'}$





The banana distribution – $d = 2$

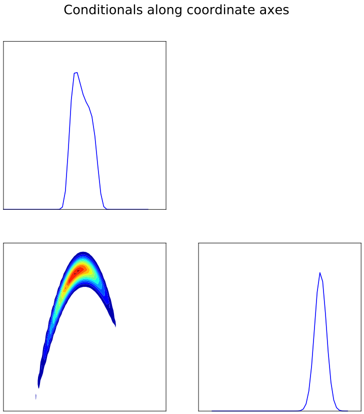
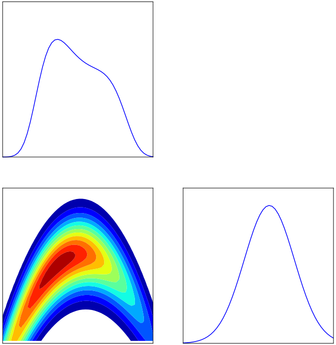


Figure: Target π

The banana distribution – $d = 2$

Iteration 1 – Pullback $T^\sharp \pi$


Conditionals along coordinate axes

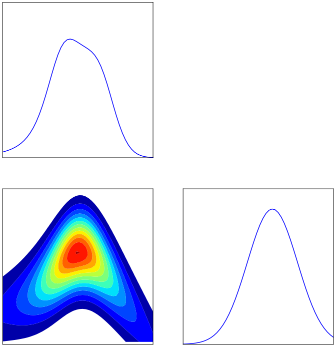

Intensity coefficients map

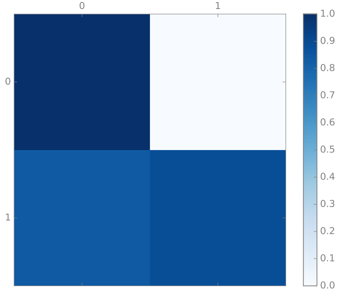
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

The banana distribution – $d = 2$

Iteration 2 – Pullback $T^\sharp \pi$


Conditionals along coordinate axes

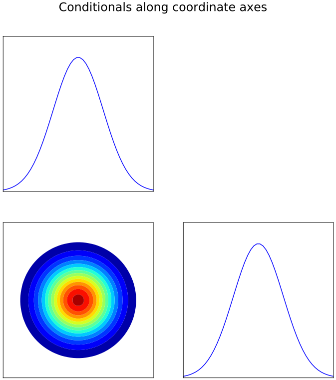

Intensity coefficients map

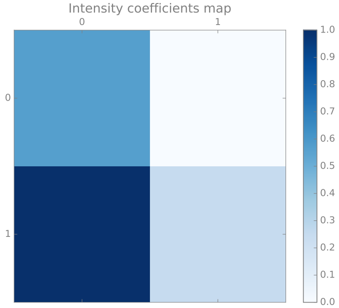
$$\nabla_{\mathbf{x}} T$$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

The banana distribution – $d = 2$

Iteration 3 – Pullback $T^\sharp \pi$

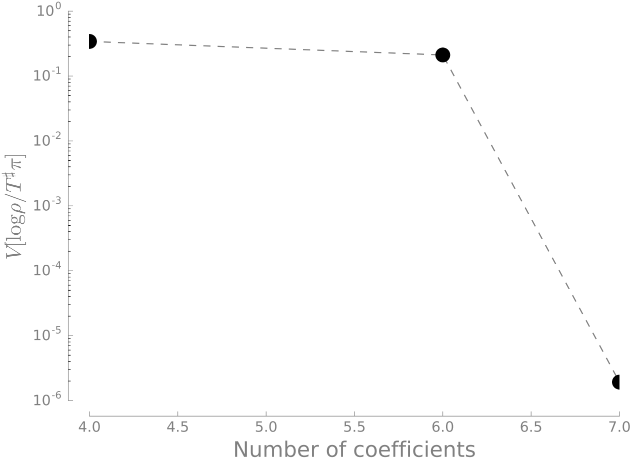




$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

The banana distribution – $d = 2$



Variance diagnostic

Stochastic volatility of financial assets – $d = 32$

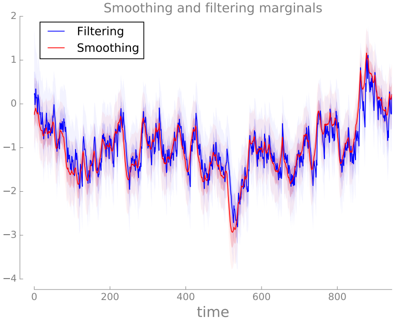
- Latent log-volatilities modeled with an AR(1) process for $t = 1, \ldots, N$ $(N = 30)$

$$X_{t+1} = \mu + \phi(X_t - \mu) + \eta_t \ , \quad \eta_t \sim \mathcal{N}(0,1) \ , \quad X_1 \sim \mathcal{N}\left(0, 1/\left(1-\phi^2\right)\right)$$

- Observe the mean return for holding the asset at time t

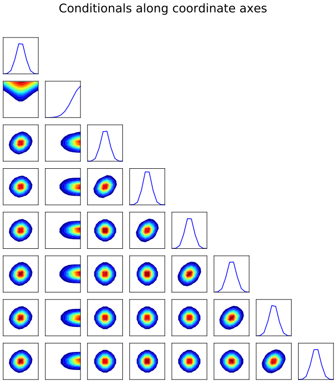
$$Y_t = \varepsilon_t \exp(X_t/2) \ , \quad \varepsilon_t \sim \mathcal{N}(0,1)$$

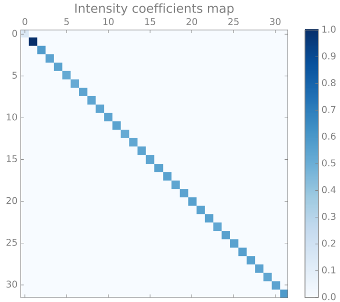
- We want to characterize $\pi \sim \mu, \phi, \mathbf{X}_{1:N} | \mathbf{Y}_{1:N}$



Stochastic volatility of financial assets – $d = 32$

Iteration 1 – Pullback $T^\sharp \pi$



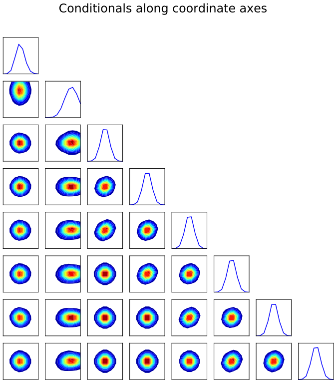


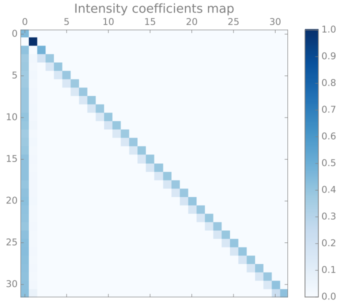
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 2 – Pullback $T^{\sharp}\pi$



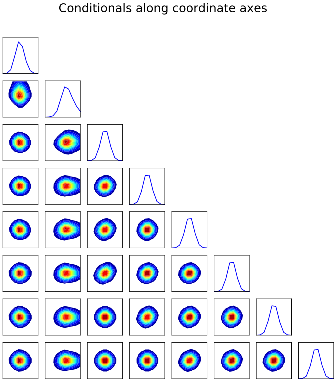


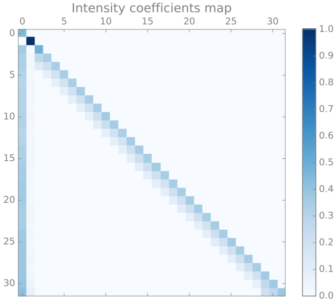
$\nabla_{\mathbf{x}} T$

Reminder: $T^{\sharp}\pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 3 – Pullback $T^{\sharp}\pi$



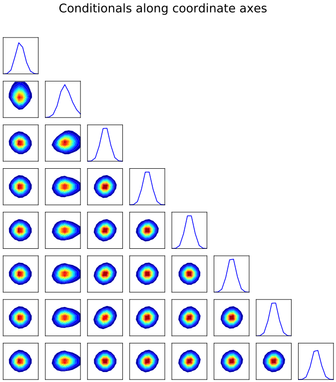


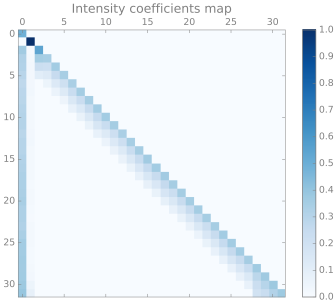
$\nabla_{\mathbf{x}} T$

Reminder: $T^{\sharp}\pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 4 – Pullback $T^\sharp \pi$



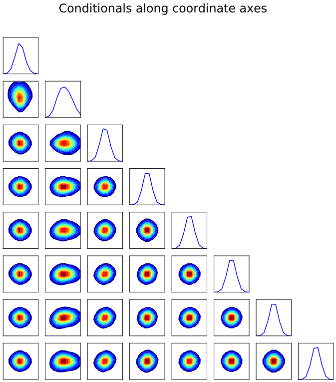


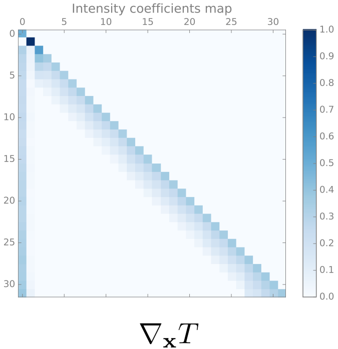
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 5 – Pullback $T^\sharp \pi$

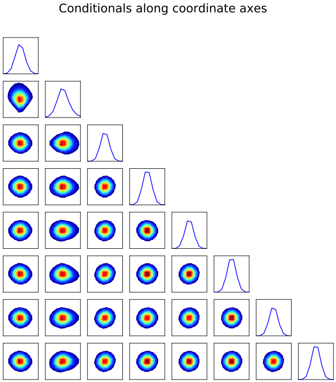


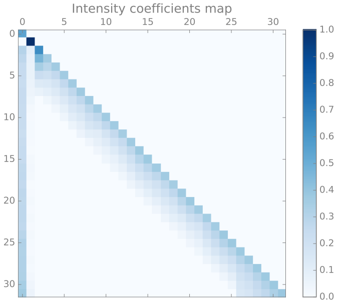


Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 6 – Pullback $T^\sharp\pi$



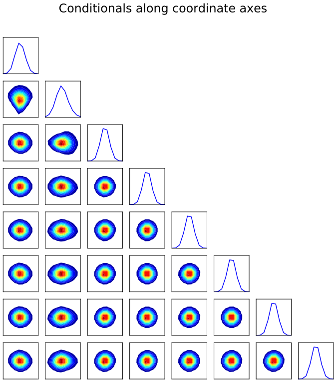


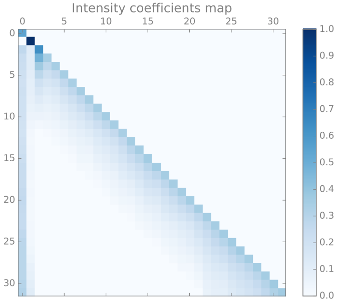
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp\pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 7 – Pullback $T^\sharp\pi$



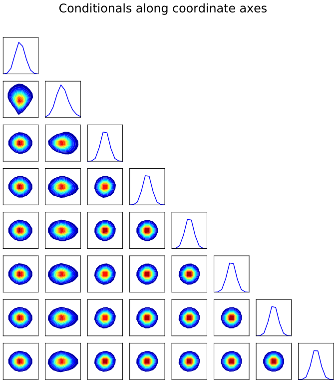


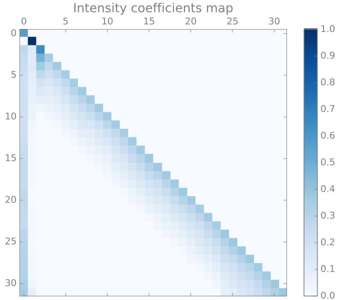
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp\pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 7 – Pullback $T^\sharp \pi$



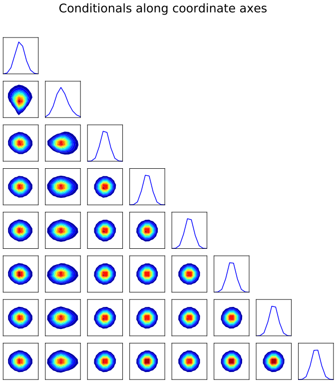


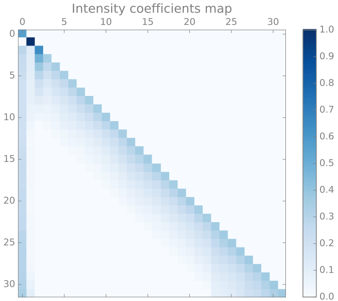
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 9 – Pullback $T^\sharp \pi$



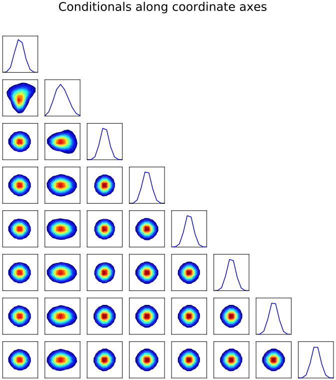


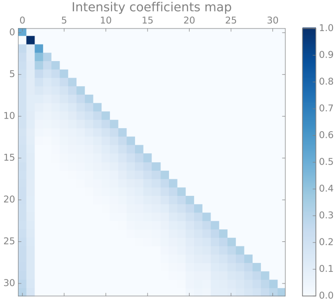
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 10 – Pullback $T^\sharp \pi$



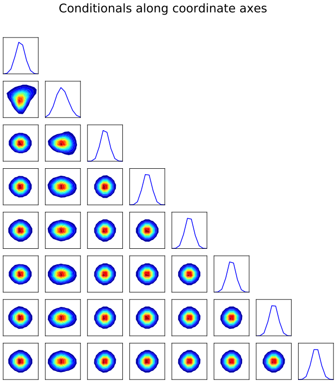


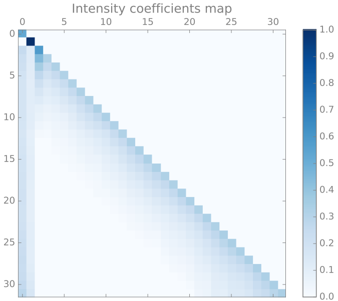
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 11 – Pullback $T^\sharp \pi$



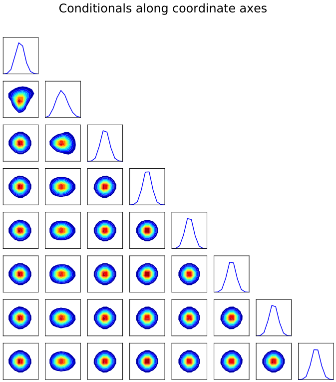


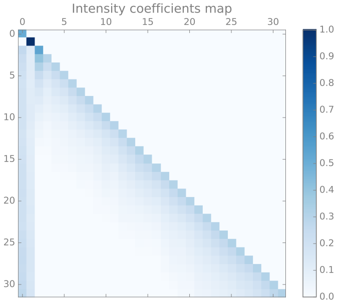
$$\nabla_{\mathbf{x}} T$$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 12 – Pullback $T^\sharp \pi$



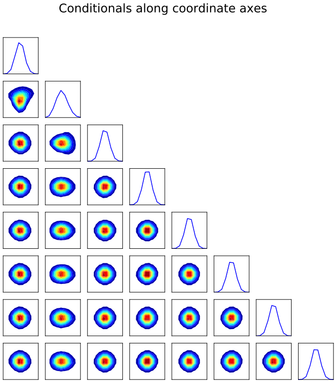


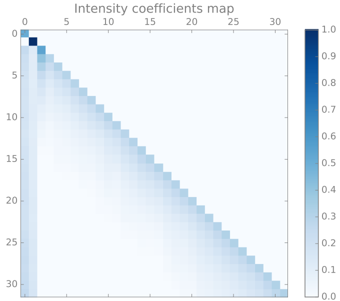
$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$

Iteration 13 – Pullback $T^\sharp \pi$

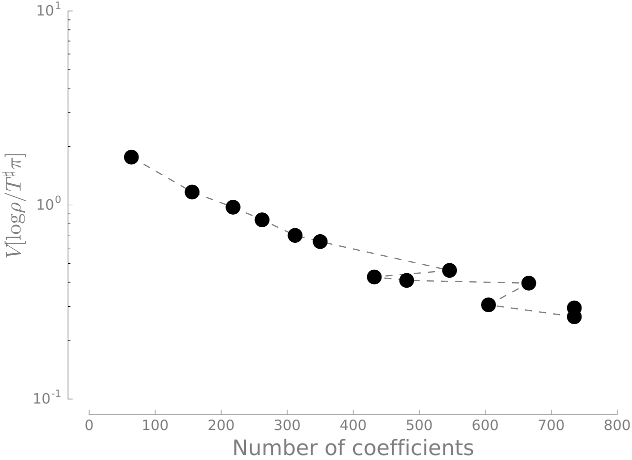




$\nabla_{\mathbf{x}} T$

Reminder: $T^\sharp \pi \approx \rho$, where ρ is the density of $\mathcal{N}(0, \mathbf{I})$

Stochastic volatility of financial assets – $d = 32$



Variance diagnostic

Key contributions

Robust adaptive algorithm for characterizing probability measures via **deterministic couplings** and **optimization**, exploiting **smoothness** and **marginal independence**

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Youssef Marzouk – **ymarz@mit.edu**

Thanks to: U.S. DEPARTMENT OF ENERGY

References:

El Moselhy et al. “Bayesian inference with optimal maps”
Parno et al. “Transport map accelerated Markov chain Monte Carlo”
Marzouk et al. “An introduction to sampling via measure transport”
Spantini et al. “Inference via low-dimensional couplings”