

Schrödinger Bridge Samplers

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JB³, July 9, 2020

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(+ a note on exchangeability and optimal transport)

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Outline

- ▶ Problem setup and Monte Carlo
- ▶ The Schrödinger bridge problem
- ▶ Sequential Schrödinger bridge sampling
- ▶ Examples and numerical experiments
- ▶ Conclusion and **future directions**

Problem setup

Suppose that π_T is a Lebesgue density on $\mathbf{E} = \mathbb{R}^d$, expressed

$$\pi_T(x) = \frac{\gamma_T(x)}{Z_T}, \quad Z_T = \int_{\mathbf{E}} \gamma_T(x) dx.$$

We want to calculate

- ▶ expectations with respect to π_T ,
- ▶ the unknown normalizing constant Z_T .

Can only evaluate γ_T (and later, $\nabla \log \gamma_T$) pointwise.

A stylized Monte Carlo problem

Suppose we can **sample** x_0 from and **evaluate the density of** π_0 .

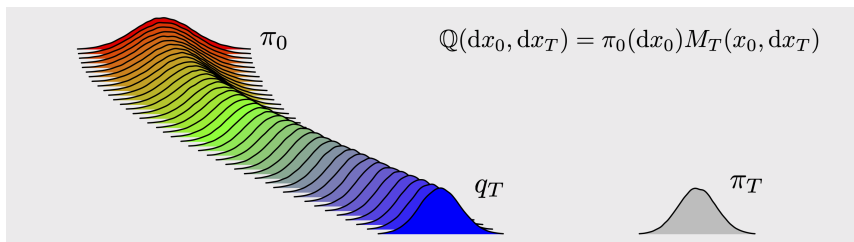
Choose and **sample a Markov kernel** $x_T \sim M_T(x_0, dx_T)$ such that $q_T = \mathcal{L}(x_T)$ is closer to π_T than π_0 .

We **want to use** q_T as the proposal in **importance sampling**.

Two challenges:

1. How do we choose M_T ?
2. The density of q_T is typically intractable.

A stylized Monte Carlo problem



Two challenges:

1. How do we choose M_T ?
2. The density of q_T is typically intractable.

Second challenge

Extend the domain of integration to \mathbb{E}^2 :

- ▶ Define $\mathbb{Q}(\mathbf{d}\mathbf{x}_0, \mathbf{d}\mathbf{x}_T) = \pi_0(\mathbf{d}\mathbf{x}_0)M_T(\mathbf{x}_0, \mathbf{d}\mathbf{x}_T)$.
- ▶ Choose an auxiliary “backward” kernel L_0 and define the auxiliary target $\mathbb{P}(\mathbf{d}\mathbf{x}_0, \mathbf{d}\mathbf{x}_T) = \pi_T(\mathbf{d}\mathbf{x}_T)L_0(\mathbf{x}_T, \mathbf{d}\mathbf{x}_0)$,

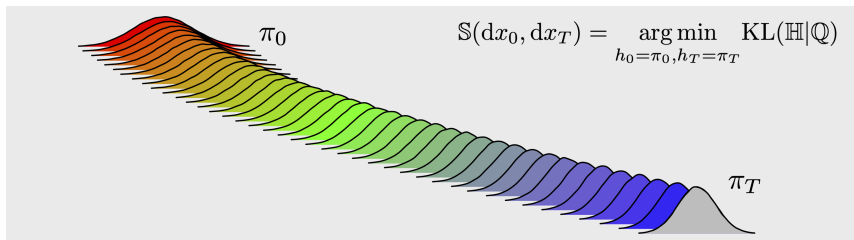
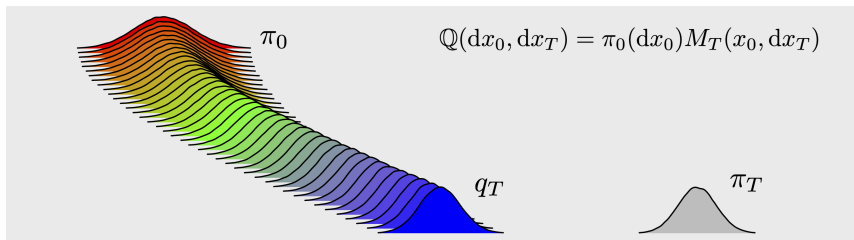
such that $\mathbb{P} \ll \mathbb{Q}$ and $w_{0,T}(x_0, x_T) = \frac{dL_0 \otimes \gamma_T}{d\pi_0 \otimes M_T}(x_0, x_T)$ can be evaluated pointwise.

If $(x_0^n, x_T^n) \sim \mathbb{Q}$ and $w_{0,T}^n = w_{0,T}(x_0^n, x_T^n)$, then $\{\mathbf{x}_T^n, \mathbf{w}_{0,T}^n\}_{n=1}^N$

- ▶ is a **weighted sample from π_T** , and
- ▶ $\hat{Z}_T = N^{-1} \sum_{n=1}^N w_{0,T}^n$ is an **unbiased estimator of Z_T** .

First challenge

Main idea: Approximate M_T^* corresponding to the **Schrödinger bridge** between π_0 and π_T for a class of kernels.



The Schrödinger bridge problem

Given a **reference distribution** $\mathbb{Q}(dx_0, dx_T)$ and **marginal constraints** π_0 and π_T , find

$$\mathbb{S}(dx_0, dx_T) = \operatorname{argmin}_{h_0=\pi_0, h_T=\pi_T} \operatorname{KL}(\mathbb{H}|\mathbb{Q}),$$

Remark:

Consider $\mathbb{Q}^\psi(dx_0, dx_T) = \pi_0(dx_0)M_T^\psi(x_0, dx_T)$, where ψ is a strictly positive function, or *policy*, and

$$M_T^\psi(x_0, dx_T) = \frac{\psi(x_T)M_T(x_0, dx_T)}{\int_{\mathbf{E}} \psi(x_T)M_T(x_0, dx_T)}.$$

Then, $\mathbb{S}(dx_0, dx_T) = \mathbb{Q}^{\psi^*}(dx_0, dx_T)$, where ψ^* is the solution to a **Schrödinger equation**.

Some notes

- ▶ Original formulation by Schrödinger in 1931: **gas with very large number of particles N** .
- ▶ The modern formulation is derived by a **large deviations principle** as $N \rightarrow \infty$, where the KL is the rate functional.
- ▶ Connection to **optimal transport**: Suppose Schrödinger's particles are Brownian with scale σ , denoted \mathbb{Q}^σ , then

$$\begin{aligned}\lim_{\sigma \rightarrow 0} \sigma^2 \text{KL}(\mathbb{S}^\sigma | \mathbb{Q}^\sigma) &= \inf_{\gamma_0 = \pi_0, \gamma_T = \pi_T} \int_{E^2} \|x_0 - x_T\|^2 \gamma(dx_0, dx_T) \\ &= \mathcal{W}_2^2(\pi_0, \pi_T).\end{aligned}$$

- ▶ Important in computation, idea behind **entropically regularized optimal transport** (Cuturi, 2013).
- ▶ We will use a formulation from **optimal control** which is amenable to computation (Heng et al., 2019).

High-level algorithm to compute $\mathbb{S}(dx_0, dx_T)$

Iterative proportional fitting (or Sinkhorn's algorithm):

Let $\mathbb{Q}^{(0)} = \mathbb{Q}$, and for $i \geq 1$, define

$$\mathbb{P}^{(i)}(dx_0, dx_T) = \operatorname{argmin}_{h_T = \pi_T} \operatorname{KL}(\mathbb{H} | \mathbb{Q}^{(i-1)}),$$

$$\mathbb{Q}^{(i)}(dx_0, dx_T) = \operatorname{argmin}_{h_0 = \pi_0} \operatorname{KL}(\mathbb{H} | \mathbb{P}^{(i)}).$$

Let $\mathbb{S}^{(2i+1)} = \mathbb{P}^{(i+1)}$ and $\mathbb{S}^{(2i)} = \mathbb{Q}^{(i)}$ for any $i \geq 0$.

Remark: Given \mathbb{Q} as the reference, $\mathbb{P}^{(1)}$ is the **optimal auxiliary target** in the sense of Del Moral et al. (2006).

Convergence of iterative proportional fitting

Rüschendorf (1995) shows that if there exists $c > 0$ such that

$$M_T(x_0, dx_T) \geq c\pi_T(dx_T), \quad \text{for } \pi_0\text{-a.e. } x_0 \in \mathbf{E},$$

then $\mathbf{S}^{(i)}$ converges to \mathbf{S} in KL and TV as $i \rightarrow \infty$.

Proposition: For any $\varepsilon > 0$, IPF returns an $\mathbf{S}^{(i)}$ that satisfies

$$\text{KL}(\pi_0 | s_0^{(i)}) + \text{KL}(\pi_T | s_T^{(i)}) < \varepsilon$$

in fewer than $\lceil \text{KL}(\mathbf{S} | \mathbf{Q}) / \varepsilon \rceil$ iterations.

IPF as policy refinement

Using the ψ -parameterization, it turns out that we can express

$$\mathbb{Q}^{(i)} = \mathbb{Q}^{\psi^{(i)}},$$

for two sequences $\psi^{(i)}$ and $\phi^{(i)}$, satisfying

$$\phi^{(i)}(\mathbf{x}_T) = \frac{\mathbf{d}\pi_T}{\mathbf{d}q_T^{\psi^{(i-1)}}}(\mathbf{x}_T), \quad \psi^{(i)} = \psi^{(i-1)} \cdot \phi^{(i)}.$$

The sequence $\psi^{(i)} \rightarrow \psi^*$ as $i \rightarrow \infty$.

IPF as policy refinement

For any $\mathbb{H} \ll \mathbb{Q}^\psi$ such that $h_T = \pi_T$, we have that

$$\frac{d\pi_T}{dq_T^\psi}(x_T) = \int_{\mathbb{E}} \frac{d\mathbb{H}}{d\mathbb{Q}^\psi}(x_0, x_T) \mathbb{Q}^\psi(dx_0|x_T).$$

If $(x_0, x_T) \sim \mathbb{Q}^\psi$, then, conditional on x_T , we have $x_0 \sim \mathbb{Q}^\psi(dx_0|x_T)$.

Thus, if $\mathbb{H}(dx_0, dx_T) = \pi_T(dx_T)L_0^\psi(x_T, dx_0)$, then $\mathbf{w}_{0,T}^\psi(\mathbf{x}_0, \mathbf{x}_T)$ is an **unbiased estimator of $\frac{d\pi_T}{dq_T^\psi}(x_T)$** .

- Can borrow ideas from **conditional SMC** to reduce variance.

Approximate IPF

Given $\{(\mathbf{x}_0^n, \mathbf{x}_T^n)\}_{n=1}^N \sim \mathbf{Q}^{\hat{\psi}^{(i-1)}}$, approximate $\phi^{(i)}$ with

$$\hat{\phi}^{(i)} = \operatorname{argmin}_{f \in \mathbf{F}} \sum_{n=1}^N \left| \log f(\mathbf{x}_T^n) - \log R^{\hat{\psi}^{(i-1)}}(\mathbf{x}_T^n) \right|^2,$$

- ▶ \mathbf{F} is a **function class**,
- ▶ $R^{\hat{\psi}^{(i-1)}}(\mathbf{x}_T)$ is an **estimator** of $\frac{d\pi_T}{dq_T^{\hat{\psi}^{(i-1)}}}(\mathbf{x}_T)$.

Choice of kernels and function classes

Restrictions: Must be able to

- ▶ sample from $\mathbb{Q}^{\hat{\psi}^{(i-1)}}$, i.e. **sample from** $M_T^{\hat{\psi}^{(i-1)}}$,
- ▶ **evaluate** $w_{0,T}^{\hat{\psi}^{(i-1)}}$ at the points $\{(x_0^n, x_T^n)\}_{n=1}^N \sim \mathbb{Q}^{\hat{\psi}^{(i-1)}}$.

Important example:

- ▶ the kernel $M_T(x_0, dx_T)$ is **Gaussian**,
- ▶ the function class $\log F$ is the **quadratic forms**,
- ▶ approximate the optimal backward kernel $L_0^{(i)}$, in the sense of Del Moral et al. (2006), with similar regressions.

Toy example

Suppose $\pi_0 = \mathcal{N}(\mathbf{0}, \mathcal{I})$, $\pi_T = \mathcal{N}(\mu_T, \Sigma_T)$, where

$$\mu_T = (17.9, 17.9), \quad \Sigma_T = \begin{pmatrix} 0.40 & 0.24 \\ 0.24 & 0.40 \end{pmatrix}$$

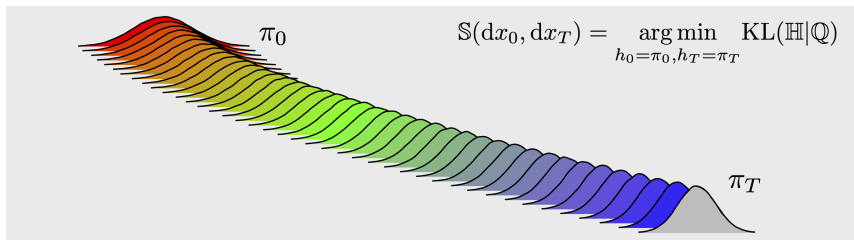
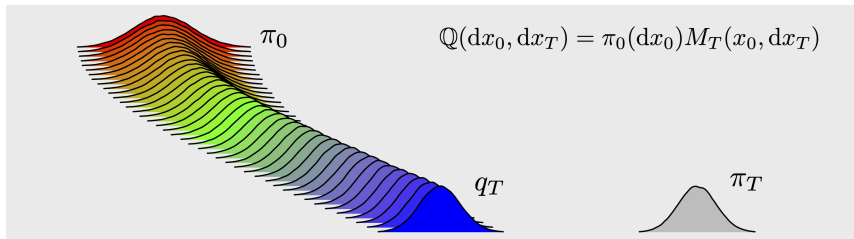
Let M_T be the kernel arising from an **Euler-Maruyama discretization** of the Langevin diffusion

$$dX_s = \frac{1}{2} \nabla \log \pi_s(X_s) ds + dW_s, \quad \text{for } s \in [0, \tau], \quad X_0 \sim \pi_0,$$

where $(\pi_s)_{s \in [0, \tau]}$ is the geometric interpolation of π_0 and π_T .

Suppose we take $\tau = 2$ and **40 steps** of Euler-Maruyama, and $i = 5$ iterations of IPF.

Toy example: Illustration of first marginal



Sequential Schrödinger bridge sampling

Instead of targeting π_T directly, we introduce an **interpolation** $\{\pi_t\}_{t=0}^T$, for example

$$\gamma_t(x_t) = \pi_0(x_t)^{1-\lambda_t} \gamma_T(x_t)^{\lambda_t}, \quad \pi_t(x_t) = \gamma_t(x_t) / Z_t,$$

where $\{\lambda_t\}_{t=0}^T \subset [0, 1]$ is increasing, $\lambda_0 = 0$ and $\lambda_T = 1$.

Introduce a **sequence of Markov kernels** $\{M_t\}_{t=1}^T$, and let

$$\mathbb{Q}(\mathrm{d}x_{0:T}) = \pi_0(\mathrm{d}x_0) \prod_{t=1}^T M_t(x_{t-1}, \mathrm{d}x_t).$$

Sequential Schrödinger bridge sampling

Consider the **multi-marginal** Schrödinger bridge problem:

$$\mathbb{S}(dx_{0:T}) = \operatorname{argmin}_{h_t = \pi_t, \forall t \in \{0, \dots, T\}} \text{KL}(\mathbb{H} | \mathbb{Q}).$$

Proposition: Can be solved **sequentially**. Consider the sequence of intermediate problems

$$\begin{aligned} \mathbb{S}_{t-1,t}(dx_{t-1}, dx_t) &= \operatorname{argmin}_{h_{t-1} = \pi_{t-1}, h_t = \pi_t} \text{KL}(\mathbb{H}_{t-1,t} | \mathbb{Q}_{t-1,t}), \\ &= \pi_{t-1}(dx_{t-1}) M_t^{\psi_t^*}(\mathbf{x}_{t-1}, \mathbf{d}\mathbf{x}_t). \end{aligned}$$

Then, $\mathbb{S}(d\mathbf{x}_{0:T}) = \pi_0(d\mathbf{x}_0) \prod_{t=1}^T M_t^{\psi_t^*}(\mathbf{x}_{t-1}, \mathbf{d}\mathbf{x}_t)$, where $\{\psi_t^*\}_{t=1}^T$ similarly solve a set of Schrödinger equations.

Algorithm

Initialize $\{x_0^n\}_{n=1}^N \sim \pi_0$. For each $t = 1, \dots, T$,

- ▶ Perform i iterations of approximate IPF to obtain $x_t^n \sim M_t^{(i)}(x_{t-1}^n, dx_t^n)$ and

$$w_{t-1,t}^{(i)}(x_{t-1}^n, x_t^n) = \frac{dL_{t-1}^{(i)} \otimes \gamma_t}{d\gamma_{t-1} \otimes M_t^{(i)}}(x_{t-1}^n, x_t^n),$$

for $n = 1, \dots, N$.

Return $\{(x_T^n, w_{0:T}^n)\}_{n=1}^N$, where $w_{0:T}^n = \prod_{t=1}^T w_{t-1,t}^{(i)}(x_{t-1}^n, x_t^n)$.

Optional: Add resampling steps.

Generic choice of kernels

For $t = 1, \dots, T$, let M_t denote the t -th step of the Euler-Maruyama **discretization of Langevin diffusion**:

$$dX_s = \frac{1}{2} \nabla \log \pi_s(X_s) ds + dW_s, \quad \text{for } s \in [0, \tau], \quad X_0 \sim \pi_0.$$

Let $\log F_t$ be the **quadratic forms**, then M_t^ψ is **Gaussian** for every t and ψ .

Can similarly approximate the optimal backward kernels using quadratic forms.

Small step-size regime

For sufficiently large τ and small step size $h > 0$, q_t should provide a **reasonable approximation** of π_t .

For small h , we can also leverage **flexible function classes** by approximating the underlying continuous-time SBP:

$$M_t^\psi(x_{t-1}, dx_t) \approx \mathcal{N}(dx_t; x_{t-1} + \frac{h}{2} \nabla \log \pi_t(x_{t-1}) + h \nabla \log \psi_t(x_{t-1}), h \mathcal{I}_d).$$

Continuous-time Schrödinger bridge problem:

Find $(\psi_s^*)_{s \in [0, \tau]}$ such that $\mathbf{X}_0 \sim \pi_0, \mathbf{X}_\tau \sim \pi_\tau$,

$$d\mathbf{X}_s = \frac{1}{2} \nabla \log \pi_s(\mathbf{X}_s) ds + \nabla \log \psi_s(\mathbf{X}_s) ds + dW_s, \quad \text{for } s \in [0, \tau],$$

and $(\psi_s^*)_{s \in [0, \tau]}$ **minimizes** $\int_0^\tau \mathbb{E} \|\nabla \log \psi_s(\mathbf{X}_s)\|^2 ds$.

Example: Linear Quadratic Gaussian

Prior: $\pi_0(dx_0) = \mathcal{N}(dx_0; 0, \mathcal{I})$.

Log-likelihood: $\ell(x) = -(y - x)^\top R^{-1}(y - x)/2$, observation $y \in \mathbb{R}^d$, symmetric positive definite $R \in \mathbb{R}^{2 \times 2}$.

Posterior: $\pi_T(dx_T) = \mathcal{N}(dx_T; \mu_T, \Sigma_T)$ with $\Sigma_T = (\Sigma_0^{-1} + R^{-1})^{-1}$, $\mu_T = \Sigma_T (\Sigma_0^{-1} \mu_0 + R^{-1} y)$.

Parameters: $y = (8, 8)^\top$, $R_{11} = R_{22} = 1$, $R_{12} = R_{21} = 0.8$.

Example: Linear Quadratic Gaussian

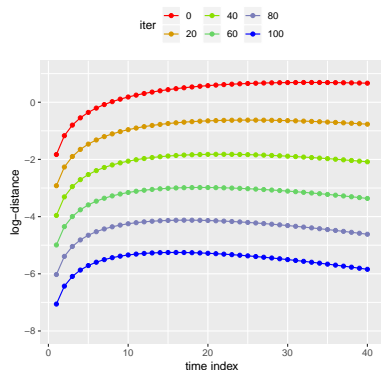
Kernels: Discretized Langevin diffusion with $h = 1/20$.

Interpolation: $\tau = 2$, $T = 40$, $\lambda_t = t/T$.

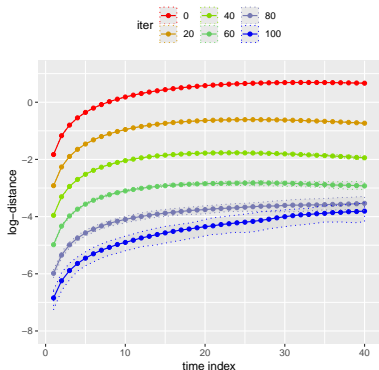
Function classes: If $f \in \mathbb{F}_t$, then $\log f$ is quadratic.

Example: Linear Quadratic Gaussian

Plot: $\log \mathcal{W}_2(\pi_t, q_t^{(i)})$ as a function of t , for different $i \geq 0$.



Left: Exact IPF.



Right: SSB with $N = 1,000$.

Example: Linear Quadratic Gaussian

Comparing the reference sampler with the SSB sampler for $N = 1,000$,

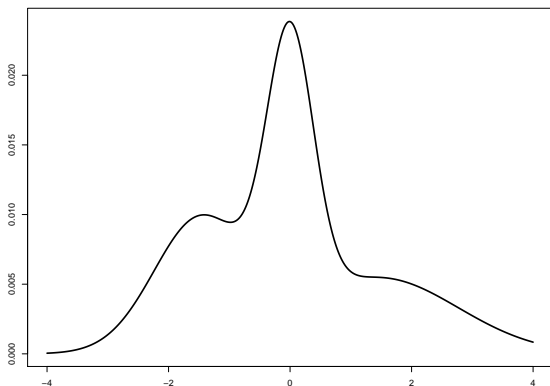
- ▶ The MSE of $\log \hat{Z}_T$ obtained with reference sampler was **7396 times higher** than the SSB estimator.
- ▶ The wall-clock time consumed by the SSB sampler was **7.4 times higher** than the reference sampler.

SSB about **1,000 times more efficient** in terms of MSE per unit of computation time.

Example: 1D mixture

Target distribution: $\pi_T(dx_T) = \sum_{i=1}^p w_i \mathcal{N}(dx_T; \mu_i, \sigma_i^2)$.

Parameters: $p = 3$, $\mu = (-1.5, 0, 1.5)$, $\sigma = (0.6, 0.15, 1.8)$,
 $w = (1/3, 1/3, 1/3)$.



Example: 1D mixture

Kernels: Discretized Langevin diffusion with $h = 1/50$.

Interpolation: $\pi_0(dx_0) = \mathcal{N}(dx_0; 0, 50)$, $\tau = 2$, $T = 100$, $\lambda_t = t^2/T^2$.

Function classes: If $f \in \mathbb{F}_t$, then $\log f$ is a cubic smoothing spline with 25 knots, estimated with `smooth.spline` in R.

Example: 1D mixture

For the SSB sampler and reference sampler with $N = 500$,

- ▶ The MSE of $\log \hat{Z}_T$ obtained with the reference sampler was **53.4 times higher** than the SSB estimator.
- ▶ The wall-clock time consumed by the SSB sampler was **17.8 times higher** than the reference sampler.

SSB about **3 times more efficient** in terms of MSE per unit of computation time.

Example: Logistic regression

Data: Cleveland heart disease database, $M = 297$ individuals, each with $d = 20$ binary and continuous covariates X_m .

Prior: Weakly informative prior from Gelman et al. (2008).

Log-likelihood: $\ell(x) = y^\top Xx - \sum_{m=1}^M \log(1 + \exp(x^\top X_m))$,
response variable $y \in \{0, 1\}^M$, covariate matrix $X \in \mathbb{R}^{M \times d}$.

Example: Logistic regression

Interpolation: $\tau = 2$, $T = 40$, $\lambda_t = t^2/T^2$.

Kernels: Discretized Langevin diffusion with $h = 1/20$.

Function classes: If $f \in F_t$, then $\log f(x) = x^\top Ax + b^\top x + c$, where $A \in \mathbb{R}^{d \times d}$ is diagonal.

Example: Logistic regression

Over 100 repeated simulations with $N = 4,000$, the average estimates of $\log Z_T$ were

- ▶ SSB: **-126.7** (sd = **0.09**),
- ▶ Reference: **-130.5** (sd = **2.7**),

Summary

Using the SMC framework, we leverage approximations of **Schrödinger bridges to do Monte Carlo sampling**.

Important features of the algorithm include

- ▶ iterative proportional fitting,
- ▶ function approximation,
- ▶ estimation of normalizing constants and Radon-Nikodym derivatives.

Compared to a well-tuned reference processes, the SSB sampler showed **computational gains** in a few simple examples.

Future directions

Extend the method to **other kinds of kernels**, e.g.

- ▶ Gibbs sampling,
- ▶ Kernels that utilize model structure in high dimensions.

Many **theoretical aspects** left to consider, e.g.

- ▶ Asymptotic properties in N , i and T ,
- ▶ Behavior of IPF with **misspecified** function classes.

Optimal transport and statistics

Ideas from optimal transport and related literatures has inspired many recent methods and results in statistics.

Relatively small community using **statistical ideas to learn about optimal transport**.

Example: Optimal transport from exchangeability.

Optimal transport from exchangeability

Optimal transport problem:

Given

- ▶ marginals μ on X and ν on Y ,
- ▶ a cost function $c : X \times Y \rightarrow [0, \infty]$,

solve

$$\min_{\gamma_x=\mu, \gamma_y=\nu} \int_{X \times Y} c(x, y) \gamma(dx, dy),$$

and find the argmin.

Notably studied by **Monge** (1781) and **Kantorovich** (1942).

Optimal transport from exchangeability

Consider the following scheme:

- ▶ sample $z_k = [(x_i, y_i)]_{i=1}^k \sim (\mu \otimes \nu)^k$,
- ▶ find $M(z_k) = \operatorname{argmin}_{\sigma \in \mathcal{S}(k)} \sum_{i=1}^k c(x_i, y_{\sigma(i)})$,
- ▶ sample $\bar{\sigma} \sim \operatorname{Unif}\{M(z_k)\}$,
- ▶ return $\bar{z}_k = [(x_i, y_{\sigma(i)})]_{i=1}^k = [(\bar{x}_i, \bar{y}_i)]_{i=1}^k$.

Define $\Gamma_{\mathbf{k}} = \mathcal{L}(\bar{z}_{\mathbf{k}})$, which takes values on $\mathcal{C}_{\mathbf{k}} = \{\bar{z}_{\mathbf{k}} : \sigma_{\text{id}} \in M(\bar{z}_{\mathbf{k}})\}$.

Note that $\hat{\gamma}_{\bar{z}_{\mathbf{k}}} = \frac{1}{k} \sum_{i=1}^k \delta_{(\bar{x}_i, \bar{y}_i)} \in \mathbf{OT}(\hat{\mu}_{\mathbf{k}}, \hat{\nu}_{\mathbf{k}})$.

Optimal transport from exchangeability

For every $k \geq 1$, the rows of $\bar{z}_k \sim \Gamma_k$ are **exchangeable**.

By the Diaconis-Freedman theorem, one can derive a limit of Γ_k on $(X \times Y)^\infty$:

$$\Gamma(A) = \int \gamma^\infty(A) d\mathcal{L}(\gamma),$$

where $\mathcal{L}(\gamma)$ is the weak limit of $\mathcal{L}(\hat{\gamma}_{\bar{z}_k})$.

By **stability results** on optimal transport, we know that the limit points of $\hat{\gamma}_{\bar{z}_k}$ almost surely belong to $\text{OT}(\mu, \nu)$.

Optimal transport from exchangeability

Hence, $\mathcal{L}(\gamma)$ takes values in $\text{OT}(\mu, \nu)$, and

$$\gamma^*(B) = \int_{\text{OT}(\mu, \nu)} \gamma(B) d\mathcal{L}(\gamma)$$

is an optimal transport measure.

Thanks!