Soft-constrained Schrödinger Bridge

Presenter: Quan Zhou
Department of Statistics
Texas A&M University
Joint work with Jhanvi Garg and Xianyang Zhang

The research presented in this talk is supported by NSF DMS-2245591, DMS-2311307.
Let \( X = (X_t)_{0 \leq t \leq T} \) be a diffusion process with \( \mathcal{L}(X_0) = \mu_0 \).

Given \( \mu_T \neq \mathcal{L}(X_T) \), how to “optimally” modify the dynamics of \( X \) so that its distribution at time \( T \) coincides with \( \mu_T \)?
Schrödinger Bridge Problem

Let $\mu_0, \mu_T$ be two probability distributions on $\mathbb{R}^d$. Let $X = (X_t)_{0 \leq t \leq T}$ denote a weak solution to the stochastic differential equation (SDE)

$$X_0 = \xi,$$
$$dX_t = b(X_t, t)dt + \sigma dW_t,$$
for $t \in [0, T]$, where $b: \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$, $\sigma \in (0, \infty)$, and $\xi \sim \mu_0$ is independent of the Wiener process $W$.

Given a control $u = (u_t)_{0 \leq t \leq T}$, define the controlled process $X^u$ by

$$X^u_0 = \xi,$$
$$dX^u_t = [b(X^u_t, t) + u_t] dt + \sigma dW_t.$$
Schrödinger Bridge Problem

Let $\mathcal{U}$ denote the set of admissible controls, and

$$\mathcal{U}_0 = \{ u \in \mathcal{U} : \text{Law}(X^u_T) = \mu_T \}.$$

Schrödinger Bridge (SB) Problem

Find $V = \inf_{u \in \mathcal{U}_0} J(u)$, where

$$J(u) = E \int_0^T \frac{||u_t||^2}{2\sigma^2} \, dt,$$

and find the optimal control $u^*$ such that $J(u^*) = V$. 
Let $\mathcal{U}$ denote the set of admissible controls, and

$$
\mathcal{U}_0 = \{u \in \mathcal{U} : \text{Law}(X^u_T) = \mu_T\}.
$$

**Schrödinger Bridge (SB) Problem**

Find $V = \inf_{u \in \mathcal{U}_0} J(u)$, where

$$
J(u) = \mathbb{E} \int_0^T \|u_t\|^2 \frac{1}{2\sigma^2} dt = D_{KL}(P^u_X, P_X),
$$

and find the optimal control $u^*$ such that $J(u^*) = V$.

$D_{KL}(\nu, \mu) = \int \log \left( \frac{d\nu}{d\mu} \right) d\nu$ denotes the Kullback-Leibler divergence.
Many existing score-based generative modeling methods are essentially numerical approximations to the solution of SB problem.

- Denoising diffusion probabilistic models of [18, 21]
- Two-stage Schrödinger bridge algorithm of [22]
- Diffusion Schrödinger bridge algorithm of [6]
- Time-series Schrödinger bridge algorithm of [16]

In these problems, $\mu_0$ is some reference distribution (e.g. normal), and $\mu_T$ is the target distribution (e.g. distribution of the images in the CelebA data set). Note $\mu_T$ is unknown but we have samples from $\mu_T$. 
Solution to the SB Problem

Let \( p(x, t \mid y, s) \) denote the transition density of (uncontrolled process) \( X \). Let \( f_0, f_T \) denote the Lebesgue densities of \( \mu_0, \mu_T \) respectively.

**Theorem 3.2 of Dai Pra [5]**

Suppose there exist integrable functions \( \rho_0, \rho_T \geq 0 \) such that

\[
    f_0(y) = \rho_0(y) \int p(x, T \mid y, 0) \rho_T(x) \, dx,
\]

\[
    f_T(x) = \rho_T(x) \int p(x, T \mid y, 0) \rho_0(y) \, dy.
\]

If \( \int \frac{f_0}{\rho_0} \, d\mu_0 < \infty \) and \( D_{KL}(\mu_T, \text{Law}(X_T)) < \infty \), then the optimal control for the SB problem is \( u^*_t = u^*(X^*_t, t) \), where

\[
    u^*(x, t) = \sigma^2 \nabla_x \log \mathbb{E}[\rho_T(X_T) \mid X_t = x].
\]
That is, under the optimal control $u^*$, the joint distribution of $(X_0^{u^*}, X_T^{u^*})$ has density

$$\rho(y, x) = \rho_0(y)p(x, T \mid y, 0)\rho_T(x).$$

By matching the marginal distributions, one gets the Schrödinger system in the previous slide.

This is also a well studied problem in the statistical literature [8, 20].
Assume $b = 0$ for both examples, and let $\phi_\sigma$ be the density of $N(0, \sigma^2 I)$.

**Example 1**

If $\mu_0$ is a Dirac measure at $x_0$,

$$
\rho_T(x) = \frac{f_T(x)}{\phi_\sigma \sqrt{T}(x - x_0)}.
$$

If $f_T$ is known up to a normalizing constant (e.g. a posterior distribution in Bayesian statistics), one can use Monte Carlo sampling to approximate

$$
u^*(x, t) = \sigma^2 \nabla_x \log \int \rho_T(y) \phi_\sigma \sqrt{T-t}(y - x) dy.
$$

See [17] for more sophisticated schemes.
Example 1 for SB

An example on $\mathbb{R}^2$ with $T = 1$, $\mu_0 = \delta_0$ and $\mu_T$ being a mixture of four normal distributions.
Example 2 for SB

Example 2

Assume $b = 0$. If $f_0(x) = \int f_T(y) \phi_{\sigma\sqrt{T}}(x - y) dy$, then $\rho_T(x) = f_T(x)$, and

$$u^*(x, t) = \sigma^2 \nabla_x \log \int f_T(y) \phi_{\sigma\sqrt{T-t}}(x - y) dy.$$
Example 2 for SB

Example 2

Assume $b = 0$. If $f_0(x) = \int f_T(y) \phi_{\sigma \sqrt{T}}(x - y) dy$, then $\rho_T(x) = f_T(x)$,

$$u^*(x, t) = \sigma^2 \nabla_x \log \int f_T(y) \phi_{\sigma \sqrt{T-t}}(x - y) dy.$$

This integral is the density of $Y + \sigma \sqrt{T-t}Z$, where $Y \sim \mu_T$ and $Z \sim N(0, I)$. The function

$$s(x, \sigma) = \nabla_x \log \int f_T(y) \phi_{\sigma \sqrt{T-t}}(x - y) dy$$

is called the score. If one has samples from $\mu_T$, by adding Gaussian noise to these samples, one can train a neural network for approximating the score [19].
To numerically simulate the solution to the SB problem, one still needs samples from $\mu_0$ with density $f_0(x) = \int f_T(y) \phi_{\sigma \sqrt{T}}(x - y) dy$. Some possible solutions:

- If $T$ is sufficiently large, one can assume $\mu_0$ is approximately gaussian. This yields the denoising diffusion model sampling algorithm of [21].
- One can train another SB process such that the terminal distribution coincides with $\mu_0$. This is the approach taken in Wang et al. [22].
- Assuming the score $s(x, \sigma \sqrt{T})$ is available, one can run a Langevin diffusion targeting $\mu_0$ for sufficiently many iterations.
Recall $\mathcal{U}$ denotes the set of admissible controls.

**Soft-constrained Schrödinger Bridge (SSB) Problem**

For $\beta > 0$, find $V = \inf_{u \in \mathcal{U}} J_\beta(u)$, where

$$J_\beta(u) = \beta \mathcal{D}_{KL}(\mathcal{L}aw(X_u^T), \mu_T) + E \int_0^T \frac{\|u_t\|^2}{2\sigma^2} dt,$$

and find the optimal control $u^*$ such that $J_\beta(u^*) = V$. 
Solution to the SSB Problem

Let $p(x, t \mid y, s)$ denote the transition density of (uncontrolled process) $X$. Let $f_0, f_T$ denote the Lebesgue densities of $\mu_0, \mu_T$ respectively.

**Theorem 4 of Garg et al. [14]**

Suppose there exist integrable functions $\rho_0, \rho_T \geq 0$ such that

$$f_0(y) = \rho_0(y) \int p(x, T \mid y, 0) \rho_T(x) \, dx,$$

$$f_T(x) = \rho_T(x)^{(1+\beta)/\beta} \int p(x, T \mid y, 0) \rho_0(y) \, dy.$$

If $\int \frac{f_0}{\rho_0} \, d\mu_0 < \infty$, then the optimal control for the SSB problem is

$$u_t^* = u^*(X_t^u^*, t),$$

where

$$u^*(x, t) = \sigma^2 \nabla_x \log \mathbb{E}[\rho_T(X_T) \mid X_t = x].$$
Comparison between SB and SSB

- For SB, \( \mathcal{L}aw(X_T^{u^*}) = \mu_T \) (with density \( f_T \)). For SSB, the density of \( X_T^{u^*} \) is proportional to

\[
f_T(x)^{\beta/(1+\beta)} \left( \int p(x, T \mid y, 0) \rho_0(y) \, dy \right)^{1/(1+\beta)}.
\]

So its law is a geometric mixture of \( \mu_T \) and another distribution.

- For SB, the solution does not exist if \( D_{KL}(\mu_T, \mathcal{L}aw(X_T)) = \infty \) (e.g. when \( \mu_T \) is the Cauchy distribution and \( X \) is a Wiener process). For SSB, the solution always exists.

- As \( \beta \rightarrow \infty \), the solution of SSB converges to that of SB. (See Garg et al. [14] for precise statements.)
Example 1

If $\mu_0$ is a Dirac measure at $x_0$, then

$$\rho_T(x) = \left( \frac{f_T(x)}{p(x, T \mid x_0, 0)} \right)^{\beta/(1+\beta)}.$$

If $f_T$ is known up to a normalizing constant, Monte Carlo sampling can be used to simulate the resulting solution to the SSB problem. The Law of $X_T^{u*}$ has density proportional to

$$f_T(x)^{\beta/(1+\beta)} p(x, T \mid x_0, 0)^{1/(1+\beta)}.$$
Example 2 for SSB

Example 2

Assume \( b = 0 \). If

\[
f_0(y) = c^{-1} \int \phi_{\sigma \sqrt{T}}(x - y) f_T(x)^{\frac{\beta}{1 + \beta}} \, dx,
\]

where \( c = \int f_T(x)^{\beta/(1+\beta)} \, dx \) is the normalizing constant assumed to be finite. Then,

\[
\rho_0(y) = c^{-(1+\beta)}, \quad \rho_T(x) = c^{\beta} f_T(x)^{\beta/(1+\beta)}.
\]

Hence,

\[
u^*(x, t) = \sigma^2 \nabla_x \log \int f_T(y)^{\beta/(1+\beta)} \phi_{\sigma \sqrt{T-t}}(x - y) \, dy.
\]
Numerical Example for Normal Mixtures

Let the uncontrolled process $X$ be such that $\mathcal{L}aw(X_T) = \mu_{\text{ref}}$, where

$$\mu_{\text{ref}} = 0.1 \mathcal{N}((1, 1), 0.05^2 I) + 0.2 \mathcal{N}((-1, 1), 0.05^2 I) + 0.3 \mathcal{N}((1, -1), 0.05^2 I) + 0.4 \mathcal{N}((-1, -1), 0.05^2 I).$$

Let our target terminal distribution be

$$\mu_{\text{obj}} = 0.5 \mathcal{N}((1.2, 0.8), 0.5^2 I) + 0.5 \mathcal{N}((-1.5, -0.5), 0.5^2 I).$$

We solve the resulting SSB problem; that is, minimize

$$J_\beta(u) = \beta \mathcal{D}_{\text{KL}}(\mathcal{L}aw(X^u_T), \mu_{\text{obj}}) + \mathbb{E} \int_0^T \frac{\|u_t\|^2}{2\sigma^2} \, dt.$$
Numerical Example for Normal Mixtures

SSB trajectories for normal mixture targets.
Suppose we have access to two data sets.

- $\mathcal{D}_{\text{ref}}$: a large set of high-quality samples with distribution $\mu_{\text{ref}}$
- $\mathcal{D}_{\text{obj}}$: a small set of noisy samples with distribution $\mu_{\text{obj}}$

Our objective is to generate realistic samples resembling those in $\mathcal{D}_{\text{obj}}$. We can use SSB as a regularization method to mitigate overfitting to $\mathcal{D}_{\text{obj}}$.

For simplicity, we set $X_0 = 0$ (i.e., $\mu_0 = \delta_0$), and we know that $\mathcal{L}(X^u_T)$ has density proportional to

$$f_{\text{ref}}(x)^{1/(1+\beta)}f_{\text{obj}}(x)^{\beta/(1+\beta)}.$$
Score Matching

To simulate a diffusion process with terminal distribution being the geometric mixture, we need to learn the score

\[ s(x, \tilde{\sigma}) = \nabla_x \log \int f_{\text{ref}}(x)^{1/(1+\beta)} f_{\text{obj}}(x)^{\beta/(1+\beta)} \phi_{\tilde{\sigma}}(x - y) dy. \]

Given only samples from \( \mu_{\text{ref}} \) and \( \mu_{\text{obj}} \), we can combine the existing score matching algorithm with importance sampling to train a neural network for approximating \( s(x, \tilde{\sigma}) \); see Garg et al. [14] for details.
MNIST Example

- $\mathcal{D}_{\text{obj}}$: 50 noisy images labeled as “8”
- $\mathcal{D}_{\text{ref}}$: all clean images not labeled as “8”

(added entrywise noise $\sim N(0, 0.4^2)$)
FID scores (see our paper) indicate that $\beta = 1.5$ is the best
How to find the pair \((\rho_0, \rho_T)\) that satisfies the following system?

\[
(1) \quad f_0(y) = \rho_0(y) \int p(x, T \mid y, 0) \rho_T(x) \, dx,
\]

\[
(2) \quad f_T(x) = \rho_T(x)^{(1+\beta)/\beta} \int p(x, T \mid y, 0) \rho_0(y) \, dy.
\]

Initial guess \(\hat{\rho}_0 \Rightarrow \text{calculate } \hat{\rho}_T \text{ by (2)} \Rightarrow \text{update } \hat{\rho}_0 \text{ by (1)} \Rightarrow \cdots\)

- If this iteration has a fixed point, then SSB has a solution.
- When \(\beta = \infty\), this algorithm is known as iterative proportional fitting procedure (IPFP) or Sinkhorn algorithm [8, 20].
Under a compact support assumption, we show that this iteration is a strict contraction mapping with respect to the Hilbert metric [1].

The proof is similar to existing results for the SB problem [13, 15, 2, 9, 7]. However, the exponent $(1 + \beta)/\beta$ simplifies the argument significantly.
Consider $N$ fixed time points $0 < t_1 < \cdots < t_N = T$. Let $\mu_N$ be a probability distribution on $\mathbb{R}^{d \times N}$ such that $\mu_N \ll \lambda$. For $\beta > 0$, find $V = \inf_{u \in U} J_N^\beta(u)$, where

$$J_N^\beta(u) = \beta D_{KL}(\text{Law}((X_{t_i})_{1 \leq i \leq N}), \mu_N) + \mathbb{E} \int_0^T \frac{\|u_t\|^2}{2\sigma^2} \, dt,$$

and find the optimal control $u^*$ such that $J_N^\beta(u^*) = V$.

See our paper [14] for the solution.
Concluding Remarks

- Major contribution of our paper is theoretical: a rigorous solution to the SSB problem using the log transformation technique [10, 11, 12].
- Future direction: more general generative modeling algorithms based on SSB.
- Future direction: comparison between the convergence rate of IPFP for SB and that for SSB.
- There are interesting connections between SSB and the optimal transport [4]. In particular, Chen et al. [3] studied a matrix OT problem which is a discrete-time analogue to SSB on finite spaces.
Thank you!

Slides available at https://zhouquan34.github.io


References III


