Soft-constrained Schrödinger Bridge

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Schrödinger Bridge Problem

Let $X = (X_t)_{0 \leq t \leq T}$ be a diffusion process with $\mathcal{L}aw(X_0) = \mu_0$.

Given $\mu_T \neq \mathcal{L}aw(X_T)$, how to "optimally" modify the dynamics of X so that its distribution at time T coincides with μ_T?

Schrödinger Bridge Problem

Let μ_0, μ_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)

$$\begin{aligned} X_0 &= \xi, \\ \mathrm{d}X_t &= b(X_t, t)\mathrm{d}t + \sigma \mathrm{d}W_t, \end{aligned}$$

for $t \in [0, T]$,where $b \colon \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$, $\sigma \in (0, \infty)$, 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

$$\begin{aligned} X_0^u &= \xi, \\ \mathrm{d}X_t^u &= \left[b(X_t^u, t) + u_t\right] \mathrm{d}t + \sigma \mathrm{d}W_t. \end{aligned}$$

Schrödinger Bridge Problem

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

$$\mathcal{U}_0 = \{u \in \mathcal{U} \colon \mathcal{L}aw(X_T^u) = \mu_T\}.$$

Schrödinger Bridge (SB) Problem

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

$$J(u) = \mathsf{E} \int_0^T \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t,$$

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

Schrödinger Bridge Problem

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Schrödinger Bridge (SB) Problem

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

$$J(u) = \mathsf{E} \int_0^T \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t = \mathcal{D}_{\mathrm{KL}}(\mathsf{P}_X^u, \mathsf{P}_X),$$

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

$\mathcal{D}_{\mathrm{KL}}(\nu, \mu) = \int \log(\frac{\mathrm{d}\nu}{\mathrm{d}\mu})\mathrm{d}\nu$ denotes the Kullback-Leibler divergence.

Application to Denoising Diffusion Probabilistic Models

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, μ_0 is some reference distribution (e.g. normal), and μ_T is the target distribution (e.g. distribution of the images in the CelebA data set). Note μ_T is unknown but we have samples from μ_T.

Solution to the SB Problem

Let $p(x, t \,|\, y, s)$ denote the transition density of (uncontrolled process) X.
Let f_0, f_T denote the Lebesgue densities of μ_0, μ_T respectively.

Theorem 3.2 of Dai Pra [5]

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

$$f_0(y) = \rho_0(y) \int p(x, T \,|\, y, 0) \rho_T(x) \, \mathrm{d}x,$$
$$f_T(x) = \rho_T(x) \int p(x, T \,|\, y, 0) \rho_0(y) \, \mathrm{d}y.$$

If $\int \frac{f_0}{\rho_0} \mathrm{d}\mu_0 < \infty$ and $\mathcal{D}_{\mathrm{KL}}(\mu_T, \mathcal{L}aw(X_T)) < \infty$, then the optimal control for the SB problem is $u^*_t = u^*(X^{u^*}_t, t)$, where

$$u^*(x, t) = \sigma^2 \nabla_x \log \mathsf{E}[\rho_T(X_T) \,|\, X_t = x].$$

Solution to the SB Problem

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].

Example 1 for SB

Assume $b = 0$ for both examples, and let ϕ_σ be the density of $N(0, \sigma^2 I)$.

Example 1

If μ_0 is a Dirac measure at x_0,

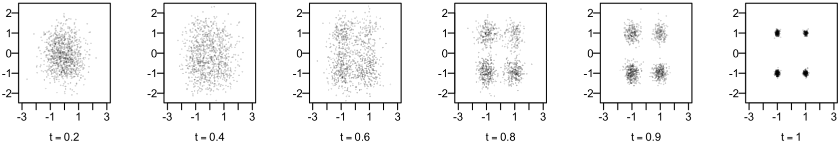
$$\rho_T(x) = \frac{f_T(x)}{\phi_{\sigma\sqrt{T}}(x - x_0)}.$$

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

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

See [17] for more sophisticated schemes.

Example 1 for SB



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

Example 2 for SB

Example 2

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

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

Example 2 for SB

Example 2

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

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

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

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

is called the *score*. If one has samples from μ_T, by adding Gaussian noise to these samples, one can train a neural network for approximating the score [19].

Example 2 for SB

Example 2 (continued)

To numerically simulate the solution to the SB problem, one still needs samples from μ_0 with density $f_0(x) = \int f_T(y)\phi_{\sigma\sqrt{T}}(x-y)\mathrm{d}y$. Some possible solutions:

- If T is sufficiently large, one can assume μ_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 μ_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 μ_0 for sufficiently many iterations.

Soft-constrained Schrödinger Bridge

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

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

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

Solution to the SSB Problem

Let $p(x, t \,|\, y, s)$ denote the transition density of (uncontrolled process) X.
Let f_0, f_T denote the Lebesgue densities of μ_0, μ_T respectively.

Theorem 4 of Garg et al. [14]

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

$$f_0(y) = \rho_0(y) \int p(x, T \,|\, y, 0) \rho_T(x) \, \mathrm{d}x,$$

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

If $\int \frac{f_0}{\rho_0} \mathrm{d}\mu_0 < \infty$, then the optimal control for the SSB problem is $u_t^* = u^*(X_t^{u^*}, t)$, where

$$u^*(x, t) = \sigma^2 \nabla_x \log \mathsf{E}[\rho_T(X_T) \,|\, X_t = x].$$

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

$$f_T(x)^{\beta/(1+\beta)} \left(\int p(x, T \,|\, y, 0) \rho_0(y) \,\mathrm{d}y \right)^{1/(1+\beta)} .$$

  So its law is a geometric mixture of μ_T and another distribution.
- For SB, the solution does not exist if $\mathcal{D}_{\mathrm{KL}}(\mu_T, \mathcal{L}aw(X_T)) = \infty$ (e.g. when μ_T is the Cauchy distribution and X is a Wiener process). For SSB, the solution always exists.
- As $\beta \to \infty$, the solution of SSB converges to that of SB. (See Garg et al. [14] for precise statements.)

Example 1 for SSB

Example 1

If μ_0 is a Dirac measure at x_0,

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

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.

$\mathcal{L}aw(X_T^{u^*})$ has density proportional to

$$f_T(x)^{\beta/(1+\beta)} p(x, T \,|\, x_0, 0)^{1/(1+\beta)}.$$

Example 2 for SSB

Example 2

Assume $b = 0$. If

$$f_0(y) = c^{-1} \int \phi_{\sigma\sqrt{T}}(x - y) f_T(x)^{\frac{\beta}{1+\beta}} \mathrm{d}x,$$

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

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

Hence,

$$u^*(x,t) = \sigma^2 \nabla_x \log \int f_T(y)^{\beta/(1+\beta)} \phi_{\sigma\sqrt{T-t}}(x - y) \mathrm{d}y.$$

Numerical Example for Normal Mixtures

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

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

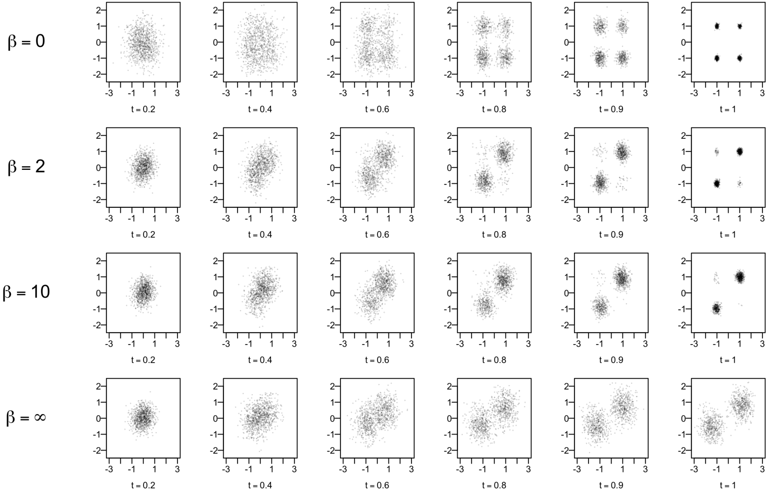
Let our target terminal distribution be

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

We solve the resulting SSB problem; that is, minimize

$$J_\beta(u) = \beta\,\mathcal{D}_{\mathrm{KL}}(\mathcal{L}aw(X_T^u), \mu_{\mathrm{obj}}) + \mathsf{E}\int_0^T \frac{\|u_t\|^2}{2\sigma^2}\mathrm{d}t.$$

Numerical Example for Normal Mixtures



SSB trajectories for normal mixture targets.

Application to Generative Modeling

Suppose we have access to two data sets.

- $\mathcal{D}_{\text{ref}}$: a large set of high-quality samples with distribution μ_{ref}
- $\mathcal{D}_{\text{obj}}$: a small set of noisy samples with distribution μ_{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 $\mathcal{L}aw(X_T^{u^*})$ has density proportional to

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

Score Matching

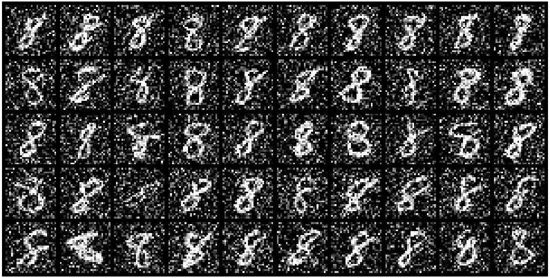
To simulate a diffusion process with terminal distribution being the geometric mixture, we need to learn the score

$$s(x,\tilde{\sigma}) = \nabla_x \log \int f_{\mathrm{ref}}(x)^{1/(1+\beta)} f_{\mathrm{obj}}(x)^{\beta/(1+\beta)} \phi_{\tilde{\sigma}}(x-y)\mathrm{d}y.$$

Given only samples from μ_{ref} and μ_{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.

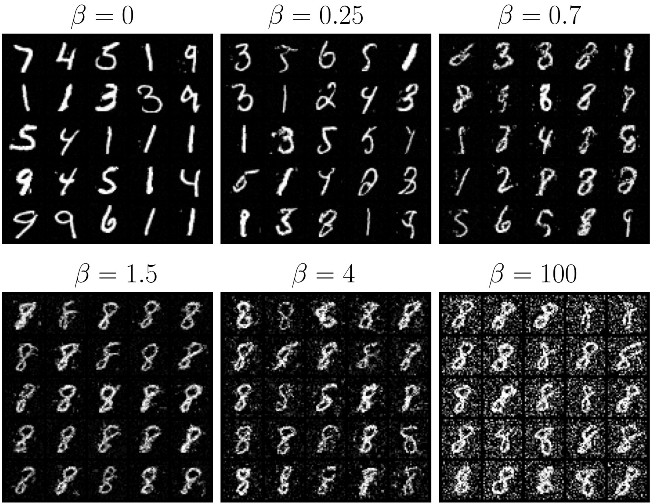
MNIST Example

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



(added entywise noise $\sim N(0, 0.4^2)$)

MNIST Example



FID scores (see our paper) indicate that $\beta = 1.5$ is the best

On the Existence of Solution to SSB

How to find the pair (ρ_0, ρ_T) that satisfies the following system?

$$(1) \qquad f_0(y) = \rho_0(y) \int p(x, T \,|\, y, 0)\rho_T(x)\,\mathrm{d}x, \tag{1}$$

$$(2) \qquad f_T(x) = \rho_T(x)^{(1+\beta)/\beta} \int p(x, T \,|\, y, 0)\rho_0(y)\,\mathrm{d}y. \tag{2}$$

Initial guess $\hat{\rho}_0 \Rightarrow$ calculate $\hat{\rho}_T$ by (2) $\Rightarrow$ update $\hat{\rho}_0$ 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].

On the Existence of Solution to SSB

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.

Time Series Extension

Time series SSB

Consider N fixed time points $0 < t_1 < \cdots < t_N = T$. Let μ_N be a probability distribution on $\mathbb{R}^{d \times N}$ such that $\mu_N \ll \lambda$. For $\beta > 0$, find $V = \inf_{u \in \mathcal{U}} J_\beta^N(u)$, where

$$J_\beta^N(u) = \beta\, \mathcal{D}_{\mathrm{KL}}(\mathcal{L}aw((X_{t_i})_{1 \le i \le N}), \mu_N) + \mathsf{E} \int_0^T \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t,$$

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

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`

Jhanvi Garg, Xianyang Zhang and Quan Zhou. "Soft-constrained Schrödinger bridge: a stochastic control approach." International Conference on Artificial Intelligence and Statistics (AISTATS 2024).

References I

[1] Peter J Bushell. Hilbert's metric and positive contraction mappings in a Banach space. *Archive for Rational Mechanics and Analysis*, 52:330–338, 1973.

[2] Yongxin Chen, Tryphon Georgiou, and Michele Pavon. Entropic and displacement interpolation: a computational approach using the Hilbert metric. *SIAM Journal on Applied Mathematics*, 76(6):2375–2396, 2016.

[3] Yongxin Chen, Tryphon T Georgiou, Michele Pavon, and Allen Tannenbaum. Relaxed Schrödinger bridges and robust network routing. *IEEE Transactions on Control of Network Systems*, 7(2):923–931, 2019.

[4] Marco Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. *Advances in neural information processing systems*, 26, 2013.

[5] Paolo Dai Pra. A stochastic control approach to reciprocal diffusion processes. *Applied Mathematics and Optimization*, 23(1):313–329, 1991.

[6] Valentin De Bortoli, James Thornton, Jeremy Heng, and Arnaud Doucet. Diffusion Schrödinger bridge with applications to score-based generative modeling. *Advances in Neural Information Processing Systems*, 34:17695–17709, 2021.

[7] George Deligiannidis, Valentin De Bortoli, and Arnaud Doucet. Quantitative uniform stability of the iterative proportional fitting procedure. *The Annals of Applied Probability*, 34(1A):501–516, 2024.

[8] W Edwards Deming and Frederick F Stephan. On a least squares adjustment of a sampled frequency table when the expected marginal totals are known. *The Annals of Mathematical Statistics*, 11(4):427–444, 1940.

[9] Montacer Essid and Michele Pavon. Traversing the Schrödinger bridge strait: Robert Fortet's marvelous proof redux. *Journal of Optimization Theory and Applications*, 181(1):23–60, 2019.

[10] Wendell H Fleming. Exit probabilities and optimal stochastic control. *Applied Mathematics and Optimization*, 4:329–346, 1977.

[11] Wendell H Fleming. Logarithmic transformations and stochastic control. In *Advances in Filtering and Optimal Stochastic Control: Proceedings of the IFIP-WG 7/1 Working Conference Cocoyoc, Mexico, February 1–6, 1982*, pages 131–141. Springer, 2005.

[12] Wendell H Fleming and Raymond W Rishel. *Deterministic and stochastic optimal control*, volume 1. Springer Science & Business Media, 2012.

[13] Robert Fortet. Résolution d'un système d'équations de m. Schrödinger. *Journal de Mathématiques Pures et Appliquées*, 19(1-4):83–105, 1940.

[14] Jhanvi Garg, Xianyang Zhang, and Quan Zhou. Soft-constrained schrödinger bridge: a stochastic control approach. In *International Conference on Artificial Intelligence and Statistics*, pages 4429–4437. PMLR, 2024.

[15] Tryphon T Georgiou and Michele Pavon. Positive contraction mappings for classical and quantum Schrödinger systems. *Journal of Mathematical Physics*, 56(3), 2015.

[16] Mohamed Hamdouche, Pierre Henry-Labordere, and Huyên Pham. Generative modeling for time series via Schrödinger bridge. *arXiv preprint arXiv:2304.05093*, 04 2023. doi: 10.13140/RG.2.2.25758.00324.

[17] Jeremy Heng, Valentin De Bortoli, and Arnaud Doucet. Diffusion Schrödinger bridges for Bayesian computation. *Statistical Science*, 39(1):90–99, 2024.

[18] Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in Neural Information Processing Systems*, 33:6840–6851, 2020.

[19] Aapo Hyvärinen. Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4):695–709, 2005.

[20] Ludger Rueschendorf. Convergence of the iterative proportional fitting procedure. *Annals of Statistics*, 23, 08 1995. doi: 10.1214/aos/1176324703.

[21] Yang Song, Jascha Sohl-Dickstein, Diederik P. Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations, 2021.

[22] Gefei Wang, Yuling Jiao, Qian Xu, Yang Wang, and Can Yang. Deep generative learning via Schrödinger bridge. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 10794–10804. PMLR, 18–24 Jul 2021.