Soft-constrained Schrödinger Bridge for Diffusion Model Sampling

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Introduction: Langevin diffusion

Given a distribution π on $\mathbb{R}^d$, we can generate samples from it by simulating the Langevin diffusion (LD):

$$\mathrm{d}X_t = \sigma^2 \nabla \log \pi(X_t)\mathrm{d}t + \sqrt{2\sigma^2}\mathrm{d}W_t$$

where W_t denotes the d-dimensional standard Brownian motion.

Comments on Langevin diffusion

- Under some regularity conditions, X_t converges in distribution to π as $t \to \infty$ regardless of the initial distribution.
- If π satisfies a Poincaré inequality, then the convergence is exponentially fast.
- Convergence can be quite slow if the target is multimodal.
- To simulate the Langevin diffusion, we need access to $\nabla \log \pi(x)$.
- When simulating the unadjusted Langevin diffusion, the step size needs to be sufficiently small.

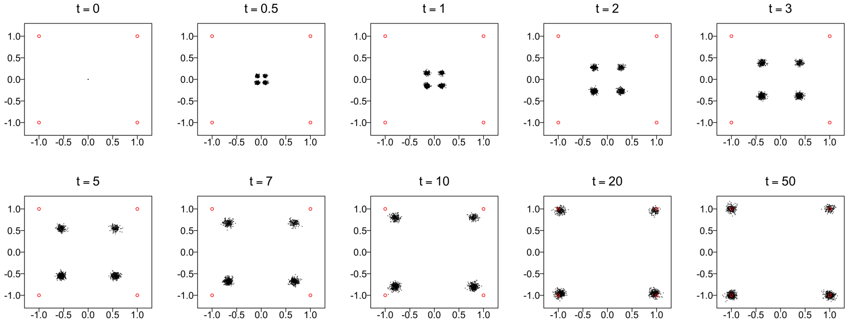
A Gaussian Mixture Example

Consider the following Gaussian mixture on $\mathbb{R}^2$:

$$\begin{aligned} &0.1\,\mathcal{N}((1,1),\,0.05^2 I) \\ +&0.2\,\mathcal{N}((-1,1),\,0.05^2 I) \\ +&0.3\,\mathcal{N}((1,-1),\,0.05^2 I) \\ +&0.4\,\mathcal{N}((-1,-1),\,0.05^2 I). \end{aligned}$$

Simulate the (unadjusted) LD with $\sigma = 0.02$ and time increment size $1/200 = 0.005$.

A Gaussian Mixture Example



1000 simulated trajectories with $X_0 = 0$.

Introduction: Schrödinger Bridge

Consider the SDE

$$\begin{aligned} \mathrm{d}X_t &= u^*(X_t, t)\mathrm{d}t + \sigma \mathrm{d}W_t, \\ X_0 &= 0, \end{aligned}$$

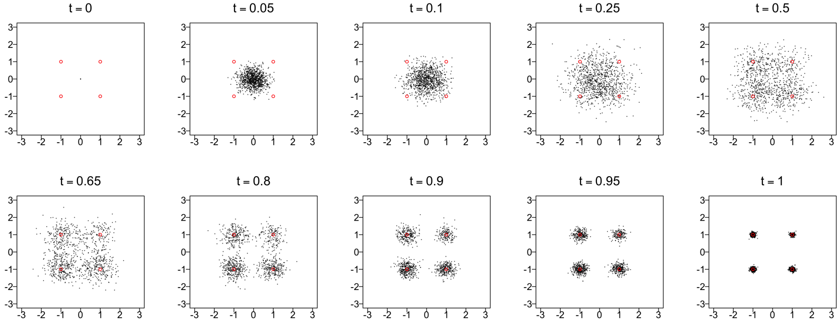
with

$$u^*(x,t) = \sigma^2 \nabla_x \log \int \frac{\pi(y)}{\phi_\sigma(y)} \phi_{\sigma\sqrt{1-t}}(y-x)\mathrm{d}y.$$

where ϕ_σ denotes the density of $\mathcal{N}(0, \sigma^2 I)$.

We have $X_1 \sim \pi$ (this is a special case of the Schrödinger bridge).

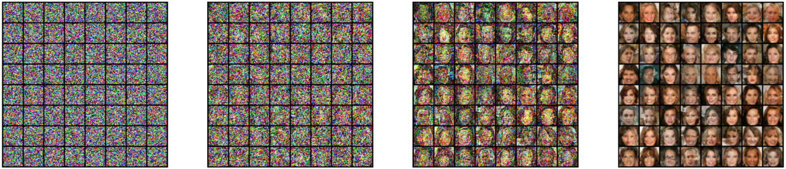
A Gaussian Mixture Example



1000 simulated trajectories with $\sigma = 1$ and time increment size $1/200 = 0.005$.

Comments on the Schrödinger Bridge

- The SB process behaves like a Brownian motion for a long time, and the "denoising" effect becomes increasingly significant as the simulation gets close to completion.
- Under some regularity conditions, it is guaranteed that $X_1 \sim \pi$, but the drift term depends on the initial distribution.
- To simulate the SB process, we need access to the score of some "perturbed" version of π instead of π itself.



$t = 0$ $t = 0.31$ $t = 0.60$ $t = 0.63$

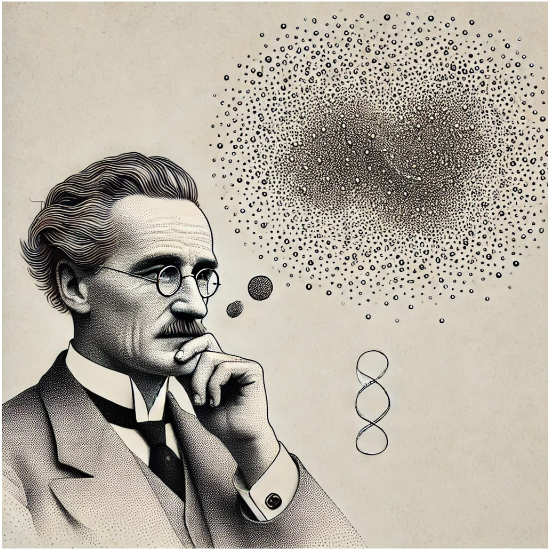
From De Bortoli et al. [6]

Schrödinger Bridge Problem

Let $X = (X_t)_{0 \le t \le 1}$ be a diffusion process with $X_0 \sim f_0$, where f_0 denotes the density w.r.t. a dominating measure ν. Denote the density of X_1 by p_1.

How to "optimally" modify the dynamics of X so that its distribution at time 1 has density $f_1 \neq p_1$ (w.r.t. the Lebesgue measure)?

Hot Gas Experiment



Schrödinger Bridge Problem

Let $X = (X_t)_{0 \leq t \leq 1}$ denote a weak solution to the SDE

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

where $b\colon \mathbb{R}^d \times [0,1] \to \mathbb{R}^d$, $\sigma \in (0, \infty)$, and $\xi \sim f_0$ is independent of W.

Given a control $u = (u_t)_{0 \leq t \leq 1}$, 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

$$\mathcal{U}_0 = \{u \in \mathcal{U} \colon \mathcal{L}aw(X_1^u) \text{ has density } f_1\}.$$

Schrödinger Bridge (SB) Problem

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

$$J(u) = \mathsf{E} \int_0^1 \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t,$$

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

Schrödinger Bridge Problem

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Schrödinger Bridge (SB) Problem

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$$J(u) = \mathsf{E} \int_0^1 \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t = \mathcal{D}_{\mathrm{KL}}(\mathsf{P}_X^u, \mathsf{P}_X),$$

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, f_0 is some reference distribution (e.g. normal), and f_1 is the target distribution (e.g. distribution of the images in CelebA). Often *f_1 is unknown* but we have *samples from f_1*.

Solution to the SB Problem

Let $p_{1|0}(x \mid y)$ denote the conditional density of $X_1 = x$ given $X_0 = y$.

Theorem 3.2 of Dai Pra [5]

Suppose there exist integrable functions $\rho_0, \rho_1 \geq 0$ such that

$$f_0(y) = \rho_0(y) \int p_{1|0}(x \mid y)\rho_1(x)\,\mathrm{d}x,$$

$$f_1(x) = \rho_1(x) \int p_{1|0}(x \mid y)\rho_0(y)\,\nu(\mathrm{d}y).$$

Under some regularity conditions, the optimal control for the SB problem is $u_t^* = u^*(X_t^{u^*}, t)$, where

$$u^*(x,t) = \sigma^2 \nabla_x \log \mathsf{E}[\rho_1(X_1) \mid X_t = x].$$

Solution to the SB Problem

That is, under the optimal control u^*, the joint distribution of $(X_0^{u^*}, X_1^{u^*})$ has density

$$\rho(y, x) = \rho_0(y) p_{1|0}(x \mid y) \rho_1(x).$$

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].

Two Examples for SB

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

$$\mathrm{d}X_t^{u^*} = u^*(X_t^{u^*}, t)\mathrm{d}t + \sigma \mathrm{d}W_t.$$

We now give two examples where $u(x, t)$ can be explicitly characterized.

Example 1 for SB

Example 1

If the initial distribution is a Dirac measure at x_0, then

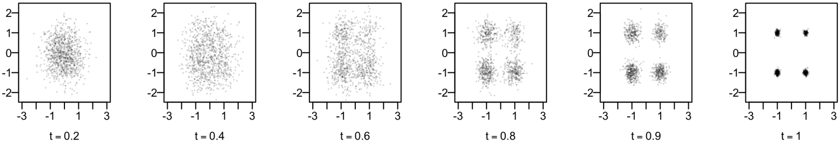
$$\rho_1(x) = \frac{f_1(x)}{\phi_\sigma(x - x_0)}.$$

If f_1 is known up to a normalizing constant (e.g. a posterior distribution in Bayesian statistics), one can use Monte Carlo sampling to approximate

$$u^*(x,t) = \sigma^2 \nabla_x \log \int \rho_1(y)\phi_{\sigma\sqrt{1-t}}(y - x)\mathrm{d}y.$$

See [17] for more sophisticated schemes.

Example 1 for SB



The Gaussian mixture example.

Example 2 for SB

Example 2

If $f_0(x) = \int f_1(y)\phi_\sigma(x-y)\mathrm{d}y$, then $\rho_1(x) = f_1(x)$,

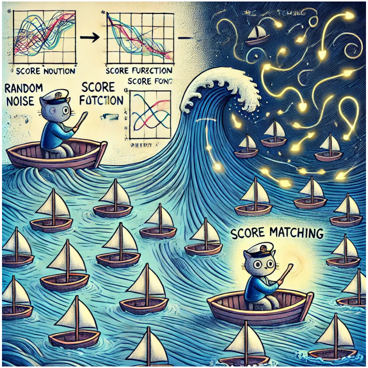
$$u^*(x,t) = \sigma^2 \nabla_x \log \int f_1(y)\phi_{\sigma\sqrt{1-t}}(x-y)\mathrm{d}y.$$

This integral is the density of $Y + \sigma\sqrt{1-t}Z$, where $Y \sim f_1$ and $Z \sim N(0,I)$. The function

$$s(x,\sigma) = \nabla_x \log \int f_1(y)\phi_{\sigma\sqrt{1-t}}(x-y)\mathrm{d}y$$

is called the *score*. How to estimate $s(x,\sigma)$ if one has samples from f_1.

Score Matching



By adding Gaussian noise to these samples, one can train a neural network for approximating the score function $s(x, \sigma)$ [19].
What happens when $\sigma = 0$?

Example 2 for SB

Example 2 (continued)

To numerically simulate the solution to the SB problem, one still needs samples from $f_0(x) = \int f_1(y)\phi_\sigma(x-y)\mathrm{d}y$. Some possible solutions:

- If σ is sufficiently large, one can assume f_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 f_0. This is the approach taken in Wang et al. [22].
- Assuming the score $s(x, \sigma)$ is available, one can run a Langevin diffusion targeting f_0 for a sufficiently long time.

Schrödinger's Cat Denoising Herself

Soft-constrained Schrödinger Bridge

Recall $\mathcal{U}$ denotes the set of admissible controls. Let μ_1 be the prob measure with density f_1.

Soft-constrained Schrödinger Bridge (SSB) Problem

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

$$J_\beta(u) = \beta \, \mathcal{D}_{\mathrm{KL}}(\mathcal{L}aw(X_1^u), \mu_1) + \mathsf{E} \int_0^1 \frac{\|u_t\|^2}{2\sigma^2} \mathrm{d}t,$$

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

Thanks to Tiziano!

Solution to the SSB Problem

Theorem 4 of Garg et al. [14]

Suppose there exist integrable functions $\rho_0, \rho_1 \geq 0$ such that

$$f_0(y) = \rho_0(y) \int p_{1|0}(x \mid y) \rho_1(x) \, \mathrm{d}x,$$

$$f_1(x) = \rho_1(x)^{(1+\beta)/\beta} \int p_{1|0}(x \mid y) \rho_0(y) \, \mathrm{d}y.$$

Under some regularity conditions, the optimal control for the SSB problem is $u_t^* = u^*(X_t^{u^*}, t)$, where

$$u^*(x, t) = \sigma^2 \nabla_x \log \mathsf{E}[\rho_1(X_1) \mid X_t = x].$$

Comparison between SB and SSB

- For SB, $\mathcal{L}aw(X_1^{u^*})$ has density f_1. For SSB, the density of $X_1^{u^*}$ is proportional to

$$f_1(x)^{\beta/(1+\beta)} \left(\int p_{1|0}(x \mid y) \rho_0(y) \, \mathrm{d}y \right)^{1/(1+\beta)} .$$

  So its law is a geometric mixture of f_1 and another distribution.
- For SB, the solution does not exist if $\mathcal{D}_{\mathrm{KL}}(\mu_1, \mathcal{L}aw(X_1)) = \infty$ (e.g. when f_1 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 the initial distribution is a Dirac measure at x_0,

$$\rho_1(x) = \left(\frac{f_1(x)}{p_{1|0}(x \mid x_0)} \right)^{\beta/(1+\beta)} .$$

If f_1 is known up to a normalizing constant, Monte Carlo sampling can be used to simulate the resulting solution to the SSB problem.

$\mathcal{L}aw(X_1^{u^*})$ has density proportional to

$$f_1(x)^{\beta/(1+\beta)} p_{1|0}(x \mid x_0)^{1/(1+\beta)}.$$

Example 2 for SSB

Example 2

Assume $b = 0$. If

$$f_0(y) = c^{-1} \int \phi_\sigma(x-y) f_1(x)^{\frac{\beta}{1+\beta}} \mathrm{d}x,$$

where $c = \int f_1(x)^{\beta/(1+\beta)} \mathrm{d}x$ is the normalizing constant assumed to be finite. Then,

$$\rho_0(y) = c^{-(1+\beta)}, \ \rho_1(x) = c^\beta f_1(x)^{\beta/(1+\beta)}.$$

Hence,

$$u^*(x,t) = \sigma^2 \nabla_x \log \int f_1(y)^{\beta/(1+\beta)} \phi_{\sigma\sqrt{1-t}}(x-y) \mathrm{d}y.$$

Numerical Example for Normal Mixtures

Let the uncontrolled process X be such that $\mathcal{L}aw(X_1)$ is

$$0.1\,N((1,1),\,0.05^2 I) + 0.2\,N((-1,1),\,0.05^2 I)+$$
$$0.3\,N((1,-1),\,0.05^2 I) + 0.4\,N((-1,-1),\,0.05^2 I).$$

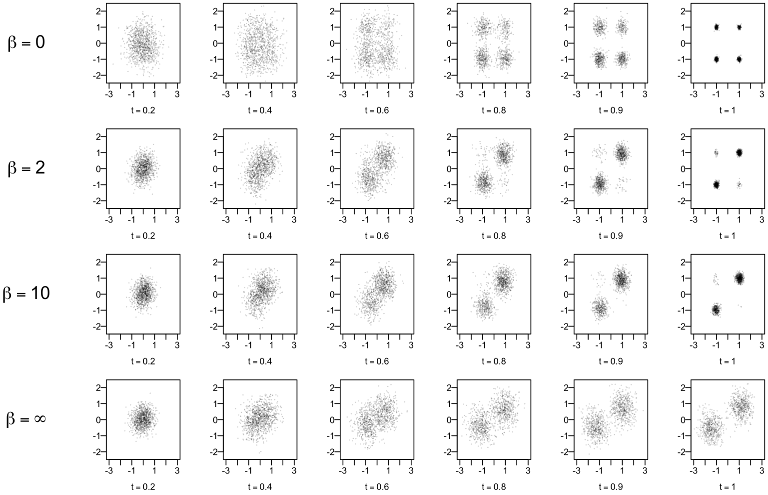
Let our target terminal distribution μ_1 be

$$0.5\,N((1.2,0.8),\,0.5^2 I) + 0.5\,N((-1.5,-0.5),\,0.5^2 I).$$

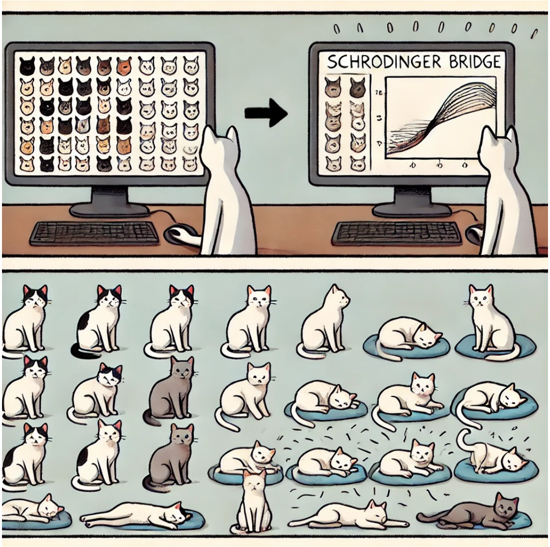
We solve the resulting SSB problem; that is, minimize

$$J_\beta(u) = \beta\,\mathcal{D}_{\mathrm{KL}}(\mathcal{L}aw(X_1^u),\mu_1) + \mathsf{E}\int_0^1 \frac{\|u_t\|^2}{2\sigma^2}\mathrm{d}t.$$

Numerical Example for Normal Mixtures



SSB trajectories for normal mixture targets.


SCHRODINGER BRIDGE

Application to Generative Modeling

Suppose we have access to two data sets.

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

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

For simplicity, we set $X_0 = 0$, and we know that $\mathcal{L}aw(X_1^{u^*})$ has density proportional to

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

Score Matching

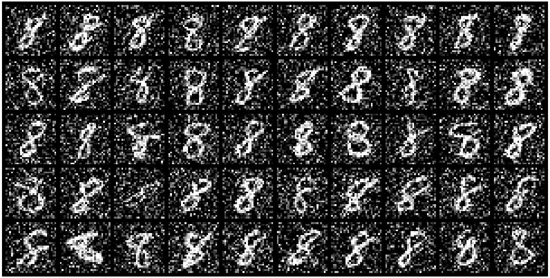
To simulate a diffusion process with terminal distribution being the geometric mixture, we need to learn the score

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

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.

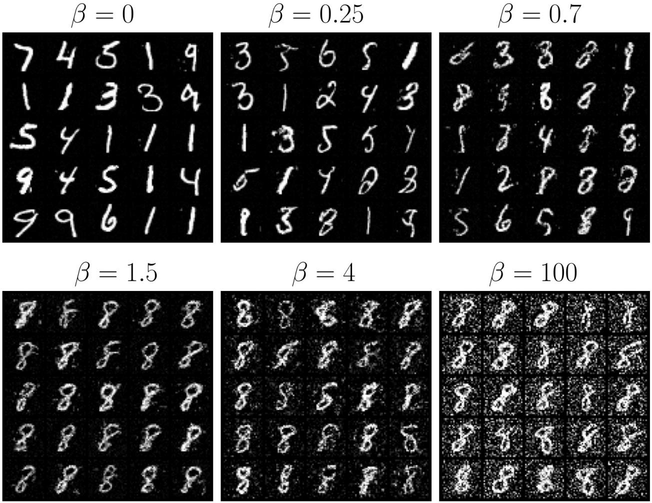
MNIST Example

- $\mathcal{D}_{\mathrm{obj}}$: 50 noisy images labeled as "8"
- $\mathcal{D}_{\mathrm{ref}}$: all 54,149 clean images not labeled as "8"



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

MNIST Example



MNIST Example

Generated 40K samples and compared them to clean digit “8” images (sample size $\approx$ 6K) using the Fréchet Inception Distance (FID) metric.

β	0	0.25	0.7	1.5	4	100
FID	67.4	66.4	61.0	*56.3*	110.9	182.4

On the Existence of Solution to SSB

How to find the pair (ρ_0, ρ_1) that satisfies the following system?

$$(1) \qquad f_0(y) = \rho_0(y) \int p_{1|0}(x \mid y)\rho_1(x)\,\mathrm{d}x, \tag{1}$$

$$(2) \qquad f_1(x) = \rho_1(x)^{(1+\beta)/\beta} \int p_{1|0}(x \mid y)\rho_0(y)\,\mathrm{d}y. \tag{2}$$

Initial guess $\hat{\rho}_0 \Rightarrow$ calculate $\hat{\rho}_1$ 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

David Hilbert (from Wiki)

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 $0 < t_1 < \cdots < t_N = 1$. 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

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

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.

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

Comics created with the help of ChatGPT & DALL·E 3.

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

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