

Adversarial Schrödinger bridges

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Research

The high computational inference cost of diffusion-based Schrödinger Bridge approaches is investigated.

Research objective —

suggest a method of solving Schrödinger Bridges without recovering entire Schrödinger Bridge process.

Required to suggest

1. algorithm of solving Schrödinger bridges problem that doesn't require recovering entire Schrödinger Bridge process,
2. analysis of this algorithm.

Solution

Use adversarial training instead of diffusion approaches.

Problem statement

It is given

1. $\{x_i\}_{i=0}^N = X, \{y_j\}_{j=0}^N = Y$ – two unpaired datasets, where $x_i \sim \pi_0(x)$ and $y_j \sim \pi_1(y)$,
2. \mathbb{W}^γ – path measure of reference Wiener process with drift $\sqrt{\gamma}$.

Dynamic Schrödinger Bridge Problem finds the closest path measure \mathbb{Q} with prescribed marginals of $\pi_0(x)$, $\pi_1(y)$ at times 0 and 1, to reference path measure \mathbb{W}^γ in sense of KL-divergence, i.e.:

$$\hat{\mathbb{Q}} = \arg \min_{\mathbb{Q} \in \mathcal{D}(\pi_0, \pi_1)} D_{KL}(\mathbb{Q} || \mathbb{W}^\gamma), \quad (1)$$

where $\mathcal{D}(\pi_0, \pi_1)$ is space of all path measures with prescribed marginals $\pi_0(x)$ and $\pi_1(y)$.

However, the solving of the problem requires to learn process that connects both marginals. It is computationally expensive, so, we propose a new approach that addresses this problem.

Suggested Method

Firstly, instead of solving dynamic version [1] of Schrödinger Bridge Problem we consider a Static formulation. With the same sets X and Y it is given joint distribution $p^{\mathbb{W}^\gamma}(x, y)$ of the reference Wiener process. Static Schrödinger Bridge Problem:

$$\begin{cases} q^*(x, y) = \arg \min_{q(x, y)} D_{KL}(q(x, y) || p^{\mathbb{W}^\gamma}(x, y)), \\ \pi_0(x) = \int q(x, y) dy, \\ \pi_1(y) = \int q(x, y) dx \end{cases} \quad (2)$$

To solve (2) is used Iterational Proportional Fitting (IPF), which alternates between solving two half bridges (constrained only on one distribution).

Suggested Method

To leverage adversarial approach we represent KL divergence in it's variational (dual) form (inspired by f-GAN [2]):

Backward

$$\min_{p(x,y) \in \mathcal{D}(\cdot, \pi_1)} D_{KL}(p(x,y) || q^{i-1}(x,y)) = \min_{p(x,y) \in \mathcal{D}(\cdot, \pi_1)} \max_D \mathbb{E}_{(x,y) \sim p} [D(x,y)] - \mathbb{E}_{(x,y) \sim q^{i-1}} [e^{D(x,y)-1}]$$

Forward

$$\min_{q(x,y) \in \mathcal{D}(\pi_0, \cdot)} D_{KL}(q(x,y) || p^i(x,y)) = \min_{q(x,y) \in \mathcal{D}(\pi_0, \cdot)} \max_D \mathbb{E}_{(x,y) \sim q} [D(x,y)] - \mathbb{E}_{(x,y) \sim p^i} [e^{D(x,y)-1}]$$

Suggested Method

In sense of converting one sample to another we want to learn conditional distribution:

Backward

$$\begin{aligned} & \min_{p(x,y) \in \mathcal{D}(\cdot, \pi_1)} \max_D \mathbb{E}_{(x,y) \sim p} [D(x,y)] - \mathbb{E}_{(x,y) \sim q^{i-1}} \left[e^{D(x,y)-1} \right] = \\ &= \min_{p(x|y)} \max_D \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{x \sim p(x|y)} [D(x,y)] - \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{y \sim q^{i-1}(y|x)} \left[e^{D(x,y)-1} \right] \end{aligned}$$

Forward

$$\begin{aligned} & \min_{q(x,y) \in \mathcal{D}(\pi_0, \cdot)} \max_D \mathbb{E}_{(x,y) \sim q} [D(x,y)] - \mathbb{E}_{(x,y) \sim p^i} \left[e^{D(x,y)-1} \right] = \\ &= \min_{q(y|x)} \max_D \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{y \sim q(y|x)} [D(x,y)] - \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{x \sim p^i(x|y)} \left[e^{D(x,y)-1} \right] \end{aligned}$$

Suggested Method

Using approach from Conditional GAN [3]:

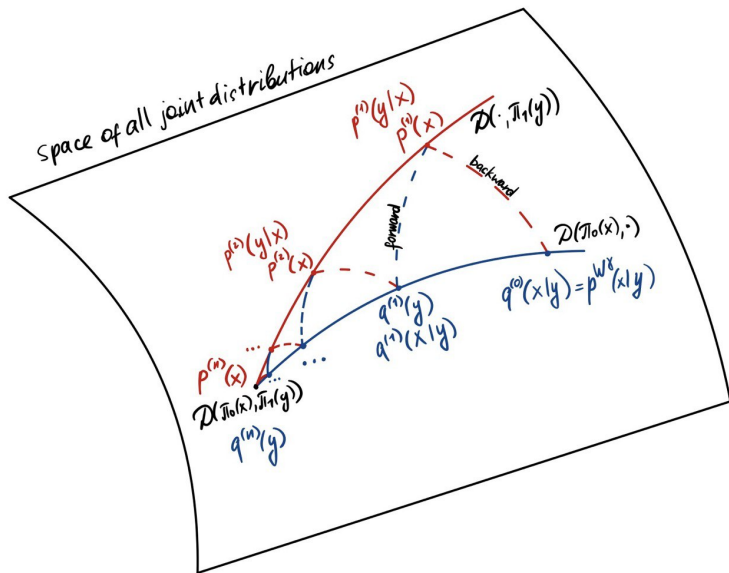
Backward

$$\begin{aligned} & \min_{p(x|y)} \max_D \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{x \sim p(x|y)} [D(x, y)] - \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{y \sim q^{i-1}(y|x)} \left[e^{D(x, y) - 1} \right] = \\ & = \min_G \max_D \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{z \sim p(z)} [D(G(z|y), y)] - \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{z \sim p(z)} \left[e^{D(x, F^{i-1}(z|x)) - 1} \right] \end{aligned}$$

Forward

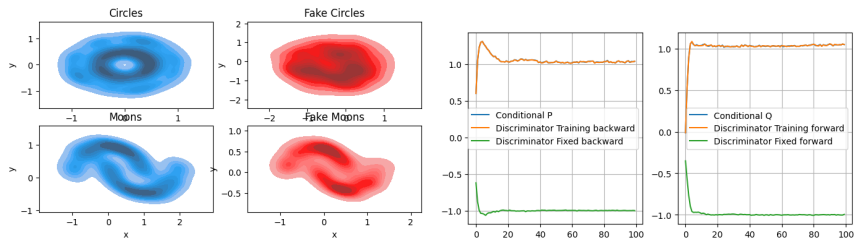
$$\begin{aligned} & \min_{q(y|x)} \max_D \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{y \sim q(y|x)} [D(x, y)] - \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{x \sim p^i(x|y)} \left[e^{D(x, y) - 1} \right] = \\ & = \min_F \max_D \mathbb{E}_{x \sim \pi_0} \mathbb{E}_{z \sim p(z)} [D(x, F(z|x))] - \mathbb{E}_{y \sim \pi_1} \mathbb{E}_{z \sim p(z)} \left[e^{D(G^i(z|y), y) - 1} \right] \end{aligned}$$

Suggested Method



Analysis of suggested method

The graphs show the adversarial loss and final generative capabilities of adversarial bridges.



It was conducted several experiments on data from multi-modal normal distributions, and no mode collapse problem was encountered.

Conclusion

1. Proposed method of solving Schrodinger Bridge Problem with adversarial training.
2. Conducted several experiments that shows great generative capability of proposed method,

Related papers

1. Machine-learning approaches for the empirical Schrodinger bridge problem¹
2. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization²
3. Conditional Generative Adversarial Nets³

¹Machine-learning approaches for the empirical Schrodinger bridge problem, F. Vargas, 2021

²f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, S. Nowozin, 2016

³Conditional Generative Adversarial Nets, Mirza M. and Osindero S., 2014

Future work plan

1. Analyse numerical error and stability of proposed algorithm;
2. Consider adversarial training without using IPF;
3. Investigate generalization of D_{KL} to other distances or metrics.