école normale supérieure paris—saclay

Project presentation

Likelihood training of Schrödinger bridge using Forward-backward SDEs theory

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MVA

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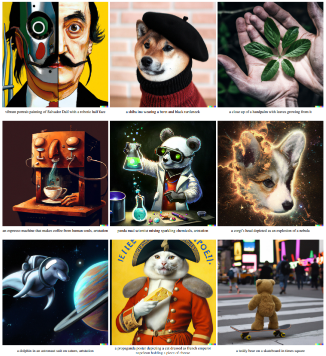
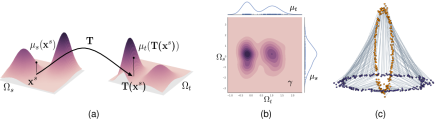
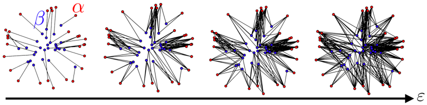
Likelihood training of Schrödinger bridge using Forward-backward SDEs theory



Generative Modelling

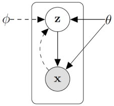




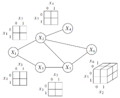
Optimal Transport

Generative Models

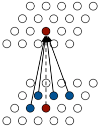
Likelihood-based models:



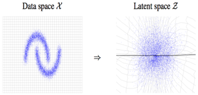
Bayesian networks (e.g., VAEs)



MRF

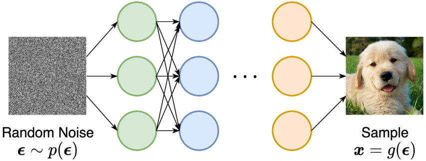


Autoregressive models



Flow models

Implicit models:



Yang Song, Generative Modeling by Estimating Gradients of the Data Distribution

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Diffusion models and Score-based generative models

SGM: $\begin{cases} \mathrm{d}\mathbf{X}_t = f(t, \mathbf{X}_t)\mathrm{d}t + g(t)\mathrm{d}W_t & \mathbf{X}_0 \sim p_{\mathrm{data}} \\ \mathrm{d}\mathbf{X}_t = [f(t, \mathbf{X}_t) - g(t)^2 \nabla_x \log p_t(\mathbf{X}_t)]\,\mathrm{d}t + g(t)\mathrm{d}\mathbf{W}_t & \mathbf{X}_T \sim p_T \end{cases}$

- Score-Based models (SGMs) learn a mapping between an easy-to-sample distribution (typically Gaussian) and the data distribution (more complex).
- We can model the diffusion process only with a linear or degenerate drift, in the stochastic differential equations (SDEs). That problem can be dealt with thanks to other formulations.

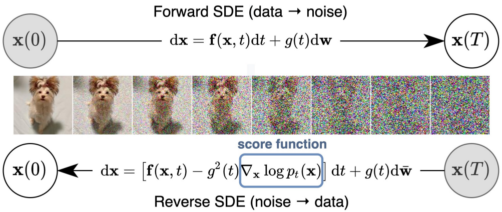

Figure: Solving a reversing-time SDE. Illustration taken from Song et al. (2019)

$$\log p_0^{\mathrm{SGM}}(\mathbf{x}_0) \geq \mathbb{E}\left[\log p_T(\mathbf{X}_t)\right] - \int_0^T \mathbb{E}\left[\tfrac{1}{2} g^2 ||\mathbf{s}_t||^2 - \nabla_x \cdot (g^2 s_t - f)\right] \mathrm{d}t$$

Entropy-regularized OT and Schrödinger-Bridge problem

- The Schrödinger-Bridge problem (SB) is an Optimal Transport entropy-regularized problem. The main difference with the previous model is that this one is based on partial differential equations (PDEs) whereas the former relies on SDEs.

SB: $\Pi^\star = \operatorname{argmin}\{\mathrm{KL}(\Pi|\mathbb{P}) \,|\, \Pi \in \mathcal{P}(\mathcal{C}),\ \Pi_0 = p_{\mathrm{data}},\ \Pi_T = p_{\mathrm{prior}}\}$

$\mathrm{L}_c^\varepsilon(\alpha, \beta) = \min_{\pi \in \mathcal{U}(\alpha,\beta)} \int_{X\times Y} c(x, y)\mathrm{d}\pi(x, y) + \varepsilon \mathrm{KL}(\pi|\alpha \otimes \beta)$

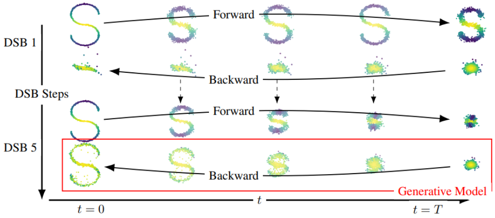

Figure: DSB steps until convergence. Illustration taken from De Bortoli et al. (2021)

Some reminders about score-based model and SB

- The Benamou-Brenier reformulation of the entropy-regularized optimal transport problem gives the following partial differential equations (PDEs).
- First, let's remind the Benamou-Brenier formulation of the Optimal Transport problem:

$$\begin{cases} \mathcal{W}_2^2(\nu_0, \nu_1) = \inf\limits_{(\mu, v)} \int_0^1 \int_{\mathbb{R}^n} ||v(t,x)||^2 \mu_t(\mathrm{d}x)\mathrm{d}t, \\ \dfrac{\partial \mu}{\partial t} + \nabla.(v\mu) = 0, \\ \mu_0 = \nu_0, \quad \mu_1 = \nu_1 \end{cases} \tag{1}$$

Some reminders about score-based model and SB

- With the entropy-regularized optimal transport problem of Schrödinger-Briges, it gives the following PDEs:

$$\begin{cases} \frac{\partial \Psi}{\partial t} = -\nabla_x \Psi^\top f - \frac{1}{2}\mathrm{Tr}(g^2 \nabla_x^2 \Psi) \\ \frac{\partial \widehat{\Psi}}{\partial t} = -\nabla_x \cdot (\widehat{\Psi} f) + \frac{1}{2}\mathrm{Tr}(g^2 \nabla_x^2 \widehat{\Psi}) \end{cases} \quad \text{s.t.} \quad \begin{aligned} \Psi(0,\cdot)\widehat{\Psi}(0,\cdot) &= p_{\mathrm{data}} \\ \Psi(T,\cdot)\widehat{\Psi}(T,\cdot) &= p_{\mathrm{prior}} \end{aligned} \tag{2}$$

- Ψ and $\widehat{\Psi}$ can also be seen as solutions to the Schrödinger system of equations (we recall that the trace of the Hessian is the Laplace operator)

Seeing Schrödinger Bridge as SDEs

- If Ψ and $\widehat{\Psi}$ are solutions of these PDEs, then the solution of the SB problem is the path measure that is in $\mathcal{P}(p_{\mathrm{data}}, p_{\mathrm{prior}})$, of the following SDEs:

$$
\begin{cases}
\mathrm{d}\mathbf{X}_t = [f + \overbrace{g^2 \nabla_x \log \Psi(t, \mathbf{X}_t)}^{\text{Non linear forward drift}}]\mathrm{d}t + g\mathrm{d}\mathbf{W}_t, \quad \mathbf{X}_0 \sim p_{\mathrm{data}} \\
\mathrm{d}\mathbf{X}_t = [f - \underbrace{g^2 \nabla_x \log \widehat{\Psi}(t, \mathbf{X}_t)}_{\text{"score function"}}]\mathrm{d}t + g\mathrm{d}\mathbf{W}_t, \quad \mathbf{X}_T \sim p_{\mathrm{prior}}
\end{cases}
\tag{3}
$$

- This establishes a first link between PDEs founding the SB problem and SDEs characterizing the SGM model. In this situation, we have to learn both the score function and the drift function, while SGM only learns the score.

Overview

In this section, we will explain how to solve the PDEs associated with Schrödinger Bridge

1. The Schrödinger Bridge entropy-regularized problem can be expressed as coupled PDEs (2)
2. The solutions to those PDEs equivalently solve control-affine SDEs (3) similar to SGM with non-linear drift
3. The Forward-Backward SDE theory propose a way to solve such SDEs
4. We can then make a link between this solution and the training of SGM, bridging the gap between SBs and SGMs

Second Order PDE

$$\begin{cases} \dfrac{\partial}{\partial t}\Psi = -\nabla\Psi^\top f - \dfrac{1}{2}\sigma_t^2\Delta\Psi \\ \dfrac{\partial}{\partial t}\widehat{\Psi} = -\nabla\cdot(\widehat{\Psi} f) + \dfrac{1}{2}\sigma_t^2\Delta\widehat{\Psi} \end{cases} \text{s.t.} \begin{aligned} \Psi(0,\cdot)\widehat{\Psi}(0,\cdot) &= p_{\mathcal{A}} \\ \Psi(T,\cdot)\widehat{\Psi}(T,\cdot) &= p_{\mathcal{B}} \end{aligned}$$

Itô's Formula and Exarchos and Theodorou (2018)

$$\frac{\partial v}{\partial t} + \nabla v^\top f + \frac{1}{2}\sigma^2\Delta v + h(t, x, v, \sigma\nabla v) = 0, \quad v(x,1) = \phi(x)$$

Forward Backward SDE theory

- Second order PDE

$$\frac{\partial v}{\partial t} + \nabla v^\top f + \frac{1}{2}\sigma^2 \Delta v + h\big(t, x, v, \sigma \nabla v\big) = 0, \quad v(x, 1) = \phi(x) \tag{4}$$

- Forward-Backward SDEs

$$\begin{cases} \mathrm{d}X_t = f\big(X_t, t\big)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t, & X_0 = x_0 \\ \mathrm{d}Y_t = -h\big(t, X_t, Y_t, Z_t\big)\,\mathrm{d}t + Z_t^\top\,\mathrm{d}W_t, & Y_1 = \phi\big(X_1\big) \end{cases} \tag{5}$$

- Link between v, X_t and Y_t via conditional expectations

$$v\big(x, t\big) = \mathbb{E}\big[Y_t \big| X_t = x\big], \quad \sigma \nabla v\big(x, t\big) = \mathbb{E}\big[Z_t \big| X_t = x\big] \tag{6}$$

Exarchos and Theodorou (2018), "Stochastic optimal control via forward and backward stochastic differential equations and importance sampling"

In the case of Schrödinger Bridges

- Applying this method in the context of Schrödinger Bridges:

$$\begin{cases} \mathrm{d}\mathbf{X}_t = (f + g\mathbf{Z}_t)\mathrm{d}t + g\mathrm{d}\mathbf{W}_t \\ \mathrm{d}\mathbf{Y}_t = \frac{1}{2}\mathbf{Z}_t^\top \mathbf{Z}_t \mathrm{d}t + \mathbf{Z}_t^\top \mathrm{d}\mathbf{W}_t \\ \mathrm{d}\widehat{\mathbf{Y}}_t = \left(\frac{1}{2}\widehat{\mathbf{Z}}_t^\top \widehat{\mathbf{Z}}_t + \nabla_{\mathbf{x}}.(g\widehat{\mathbf{Z}}_t - f) + \widehat{\mathbf{Z}}_t^\top \mathbf{Z}_t\right)\mathrm{d}t + \widehat{\mathbf{Z}}_t^\top \mathrm{d}\mathbf{W}_t \end{cases} \tag{7}$$

- The constraints are $X_0 = x_0$ and $\mathbf{Y}_T + \widehat{\mathbf{Y}}_T = \log p_{\mathcal{B}}(\mathbf{X}_T)$.
- The link between Ψ, $\widehat{\Psi}$, X_t and Y_t is:

$$\log \Psi(x, t) = \mathbb{E}[Y_t | X_t = x], \log \widehat{\Psi}(x, t) = \mathbb{E}[\widehat{Y}_t | X_t = x] \tag{8}$$

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Path Integral Formulation of the log-likelihood

- From there, we can use the path integral formulation of the log-likelihood introduced in Song et al. (2021):

$$\log p_{\mathcal{A}}(x_0) = \mathbb{E}[\log p_{\mathcal{B}}] - \int_0^T \mathbb{E}\left[\frac{1}{2}\|\mathbf{z}_t\|^2 + \frac{1}{2}\|\widehat{\mathbf{z}}_t\|^2 + \nabla_x \cdot (g\widehat{\mathbf{z}}_t - f) + \widehat{\mathbf{z}}_t^\top \mathbf{z}_t\right] \mathrm{d}t \quad (9)$$

- This is a generalisation of SGM, indeed, for $\left(\mathbf{z}_t^\theta, \widehat{\mathbf{z}}_t^\phi\right) = \left(0, gs_t\right)$, the SB log-likelihood objective is the same as (5). SBs allow for a wider array of drifts:

$$\log p_{\mathrm{data}}(x_0) \geq \mathbb{E}\left[\log p_{\mathrm{prior}}(X_1)\right] - \int_0^T \mathbb{E}\left[\frac{1}{2}\sigma_t^2 \|s_t\|^2 - \nabla \cdot (\sigma_t^2 s_t - f)\right] \mathrm{d}t$$

From SB-FBSDE to Mean Field Game

1. FBSDE links SDEs and PDEs
2. SB is composed by two PDEs
3. we can show that those two PDEs are equivalent SB
4. SB-FBSDE can solves this set of PDEs too

Generalisation of Benamou Brenier Formulation

- Ideas introduced by Caluya and Halder (2021)

$$
\begin{cases}
\inf\limits_{(\rho,u)} \int_0^1 \int_{\mathbb{R}^n} \frac{1}{2} \left\| u(x,t) \right\|^2 \rho(x,t) \, \mathrm{d}x \, \mathrm{d}t \\
\frac{\partial \rho}{\partial t} + \nabla.(\rho(f + g(t)u)) = 0 \\
\text{subject to } \rho(x,0) = \rho_0(x), \quad \rho(x,1) = \rho_1(x)
\end{cases}
\tag{10}
$$

Hamilton-Jacobi-Bellman (HJB) equation

- When we take this formulation of the SBD
- We compute the Lagrangian associated
- At the optimum, we have the following PDEs

$$\boxed{-\frac{\partial u}{\partial t} + H(t, x, \nabla u, \rho) - \frac{1}{2}\nabla^2 u = 0} \tag{SOC-HJB}$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nabla_\rho H(x, \nabla u, \rho)) - \frac{1}{2}\nabla^2 \rho = 0} \tag{FK}$$

Mean Field Games

$$\boxed{-\frac{\partial u}{\partial t} + H(t, x, \nabla u, \rho) - \frac{1}{2}\nabla^2 u = F(x, \rho)}, \tag{11}$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nabla_\rho H(x, \nabla u, \rho)) - \frac{1}{2}\nabla^2 \rho = 0} \tag{12}$$

- model the behavior of a large number of interacting agents in a dynamic setting
- ρ the density of population
- u the strategy at the equilibrium (optimal)

$$\begin{cases} \psi(x,t) := \exp(-u(x,t)) \\ \widehat{\psi}(x,t) := \rho(x,t)\exp(u(x,t)) \end{cases} \tag{13}$$

Some examples of mean field games

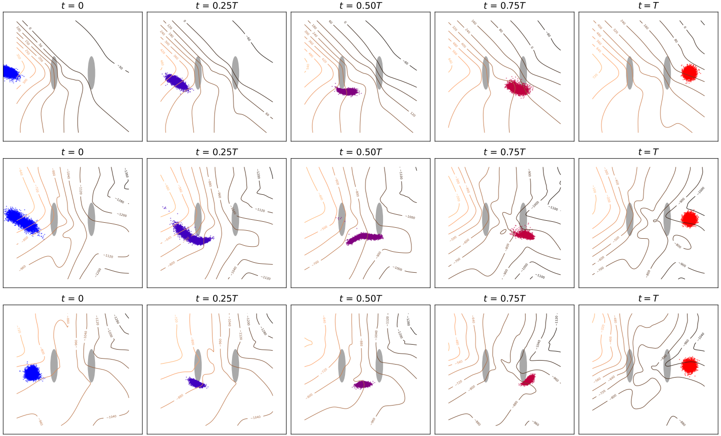

Figure: Forward process. From top to bottom, Step n° 10, 20, 40 of forward-backward pass.

The Silo Clogging Reduction

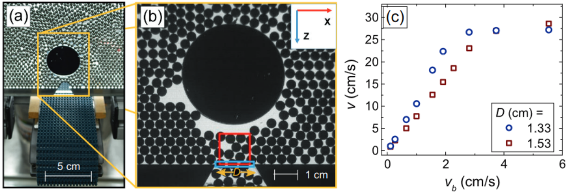

Fig. 1 Outline of the experimental setup. a Photograph of the bottom part of the silo where the obstacle, the orifice, and the conveyor belt can be distinguished. **b** Frame taken from a film recorded with the high-speed camera where the orifice size is defined. The blue box is the region located at the outlet where the velocity of particles is averaged to compute v. The red box is the representative area above the orifice and below the obstacle where the magnitudes are averaged to obtain v_x, v_z, and the solid fraction ϕ. The coordinate system (where for convenience, positive values are considered in the downwards direction) is also shown in this figure. **c** Experimental data of the mean velocity of the particles when exiting the silo v, versus the belt velocity v_b, in the silo with the obstacle, for the two orifice sizes indicated in the legend. Uncertainties are smaller than the point size as the velocities come from averages over a large amount of data.

Figure: Extract from https://doi.org/10.1038/s42005-021-00756-4

The Silo Clogging Reduction

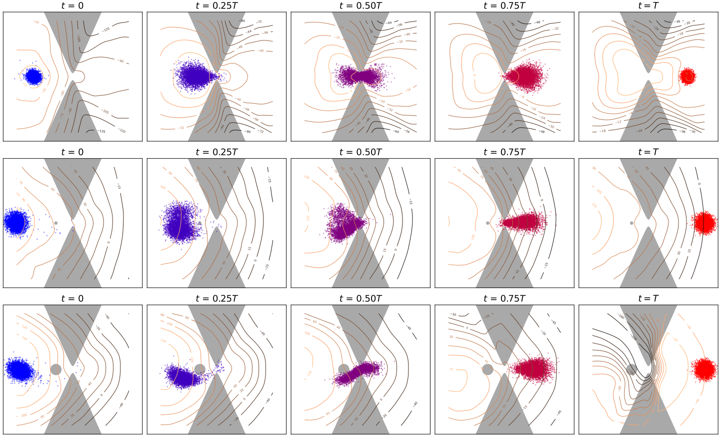

Figure: Forward process. From top to bottom, no obstacle, little obstacle, bigger obstacle école normale supérieure paris-saclay

Conclusion

- Chen et al. (2023) have proposed a new method leveraging the power of Schrödinger Bridges in the context of generative modelling.
- Allow interpolation, more freedom in the framework (starting distribution, steps ...)
- SB-FBSDE cannot be leverage to solves any PDEs
- but can solve MFG (problems in economic, financial, neuronal field)

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