Schrödinger Bridge Problem

Wei Deng

June 2022

The classical Schrödinger Bridge problem (SBP) can be formulated into a stochastic optimal control problem as follows

$$\inf_{\boldsymbol{u} \in \mathcal{U}} \mathbb{E} \left\{ \int_0^1 \frac{1}{2} \|\boldsymbol{u}(\mathbf{x}, t)\|_2^2 dt \right\},\tag{1}$$

under the constraint

$$d\mathbf{x}_t = \mathbf{u}(\mathbf{x}, t)dt + \sqrt{2}\sigma d\mathbf{B}_t, \tag{2}$$

$$\mathbf{x}(t=0) \sim \rho_0(\mathbf{x}), \mathbf{x}(t=1) \sim \rho_1(\mathbf{x}),$$
 (3)

where $\mathcal{U} := \{ \boldsymbol{u} : \mathbb{R}^d \times [0,1] \to \mathbb{R}^n | \langle \boldsymbol{u}, \boldsymbol{u} \rangle < \infty \}$ is a set of control variables; \boldsymbol{B}_t is the standard Brownian motion in \mathbb{R}^n . The expectation is taken w.r.t the joint state PDF $\rho(\mathbf{x},t)$ given initial and terminal conditions. Rewrite SBP (1) into a fluid-dynamic formulation [CGP21], we can get that

$$\inf_{\boldsymbol{u} \in \mathcal{U}, \rho} \int_0^1 \int \frac{1}{2} \|\boldsymbol{u}(\mathbf{x}, t)\|_2^2 \rho(\mathbf{x}, t) d\mathbf{x} dt, \tag{4}$$

subject to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \sigma^2 \Delta \rho,\tag{5}$$

$$\rho(\mathbf{x},0) = \rho_0(\mathbf{x}), \quad \rho(\mathbf{x},1) = \rho_1(\mathbf{x}), \tag{6}$$

where Eq.(5) is the Fokker-Plank equation or Kolmogorov's forward PDE for the corresponding controlled diffusion process (2) based on decision variables $(\rho, \mathbf{u}) \in \mathcal{P}(\mathbb{R}^n) \times \mathcal{U}$ and $\mathcal{P}(\mathbb{R}^n)$ is the set of probability measures on \mathbb{R}^n or more generally on Polish metric spaces.

Consider the Lagrangian for Eq.(4) and introduce $\psi(\mathbf{x},t)$ as a $C^1(\mathbb{R}^n,\mathbb{R}_{>0})$ Lagrange multiplier:

$$\mathcal{L}(\rho, \boldsymbol{u}, \psi) := \int_{0}^{1} \int \frac{1}{2} \|\boldsymbol{u}(\mathbf{x}, t)\|_{2}^{2} \rho(\mathbf{x}, t) + \psi(\mathbf{x}, t) \left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) - \sigma^{2} \Delta \rho\right) d\mathbf{x} dt,$$

$$= \int_{0}^{1} \int \left(\frac{1}{2} \|\boldsymbol{u}(\mathbf{x}, t)\|_{2}^{2} - \frac{\partial \psi}{\partial t} - \langle \nabla \psi, \boldsymbol{u} \rangle - \sigma^{2} \Delta \psi \rangle\right) \rho(\mathbf{x}, t) d\mathbf{x} dt, \tag{7}$$

where the second equation is obtained through integration by parts.

Minimizing with respect to u, we get the optimal control u^* as follows

$$\boldsymbol{u}^*(\mathbf{x},t) = \nabla \psi(\mathbf{x},t). \tag{8}$$

Plugging Eq.(8) into Eq.(7), we have

$$\mathcal{L}(\rho, \boldsymbol{u}, \psi) = \int_{0}^{1} \int \left(-\frac{\partial \psi}{\partial t} - \frac{1}{2} \|\nabla \psi(\mathbf{x}, t)\|_{2}^{2} - \sigma^{2} \Delta \psi \right) \rho(\mathbf{x}, t) d\mathbf{x} dt. \tag{9}$$

To achieve the minimum control cost, we hope $\mathcal{L}(\rho, \boldsymbol{u}, \psi) = 0$, which is the dynamic programming equation. In what follows, we choose

$$\frac{\partial \psi}{\partial t} + \sigma^2 \Delta \psi = -\frac{1}{2} \|\nabla \psi(\mathbf{x}, t)\|_2^2. \tag{10}$$

Given the optimal control variable u^* , the above PDE is known as the Hamilton-Jacobi-Bellman (HJB) PDE. Since the HJB PDE is non-linear due to the presence of $\frac{1}{2}\|\nabla\psi(\mathbf{x},t)\|_2^2$, we convert it into a linear PDE through the logarithmic or Cole-Hopf transformation given by

$$\varphi(\mathbf{x},t) = \exp\left(\frac{\psi(\mathbf{x},t)}{2\sigma^2}\right)$$

$$\hat{\varphi}(\mathbf{x},t) = \rho^*(\mathbf{x},t) \exp\left(-\frac{\psi(\mathbf{x},t)}{2\sigma^2}\right).$$
(11)

We now can easily verify that the transformed variables $(\varphi, \hat{\varphi})$ solve the Schrödinger system

$$\frac{\partial \varphi}{\partial t} + \sigma^2 \Delta \psi = 0$$

$$\frac{\partial \hat{\varphi}}{\partial t} - \sigma^2 \Delta \hat{\varphi} = 0,$$
(12)

under the constraint that

$$\varphi(\mathbf{x}, t = 0)\hat{\varphi}(\mathbf{x}, t = 0) = \rho_0(\mathbf{x})$$

$$\varphi(\mathbf{x}, t = 1)\hat{\varphi}(\mathbf{x}, t = 1) = \rho_1(\mathbf{x}).$$

In what follows, the solution of Eq.(12) can be written into the Schrödinger equations

$$\varphi(\mathbf{x},t) = \int K(t,\mathbf{x},1,\mathbf{y})\hat{\varphi}(\mathbf{y},t=1)d\mathbf{y}, \quad t \le 1$$
(13)

$$\hat{\varphi}(\mathbf{x},t) = \int K(0,\mathbf{y},t,\mathbf{x})\hat{\varphi}(\mathbf{y},t=0)d\mathbf{y}, \quad t \ge 0,$$
(14)

where $K(t, \mathbf{x}, s, \mathbf{y}) := (4\pi\sigma^2(t-s))^{-n/2} \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|_2^2}{4\sigma^2(t-s)}\right)$ is the Markov kernel associated with the pure diffusion process $d\mathbf{x}_t = \sqrt{2}\sigma dB_t$.

Now, based on Eq. (11), the optimal decision variables (ρ, \mathbf{u}) can be obtained as follows

$$\begin{split} & \rho^*(\mathbf{x},t) = \varphi(\mathbf{x},t)\hat{\varphi}(\mathbf{x},t) \\ & \boldsymbol{u}^*(\mathbf{x},t) = 2\sigma^2\nabla\log\varphi(\mathbf{x},t). \end{split}$$

To compute the iterates efficiently, one may resort to the Sinkhorn algorithm with DNN approximation [CLT22] to solve it.

References

- [CGP21] Yongxin Chen, Tryphon T. Georgiou, and Michele Pavon. Stochastic Control Liaisons: Richard Sinkhorn Meets Gaspard Monge on a Schrödinger Bridge. SIAM Review, 63(2):249–313, 2021.
- [CLT22] Tianrong Chen, Guan-Horng Liu, and Evangelos A. Theodorou. Likelihood Training of Schrödinger Bridge using Forward-Backward SDEs Theory. In *Proc. of the International Conference on Learning Representation (ICLR)*, 2022.