Reflected Schrödinger Bridge: Density Control with Path Constraints

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Schrödinger Bridge Problem (SBP)

Finite horizon minimum effort density steering

$$\underset{\boldsymbol{u}\in\mathcal{U}}{\text{minimize}} \quad \mathbb{E}\left[\int_0^1 \frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^{\boldsymbol{u}})\|_2^2 \,\mathrm{d}t\right]$$

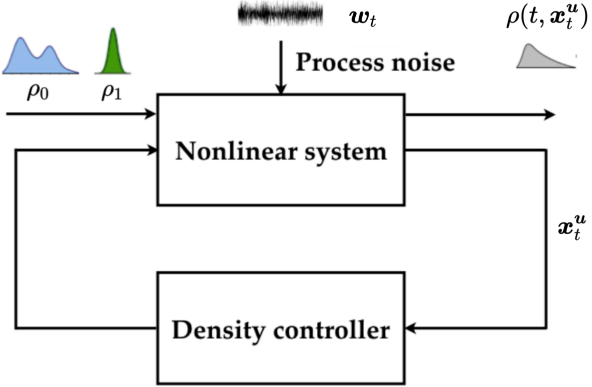
subject to

$$\mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}} = \{\boldsymbol{f}(t,\boldsymbol{x}_t^{\boldsymbol{u}}) + \boldsymbol{B}(t)\boldsymbol{u}(t,\boldsymbol{x}_t^{\boldsymbol{u}})\}\mathrm{d}t + \sqrt{2\theta}\boldsymbol{G}(t)\mathrm{d}\boldsymbol{w}_t$$

$$\boldsymbol{x}_0^{\boldsymbol{u}} := \boldsymbol{x}_t^{\boldsymbol{u}}(t=0) \sim \rho_0, \quad \boldsymbol{x}_1^{\boldsymbol{u}} := \boldsymbol{x}_t^{\boldsymbol{u}}(t=1) \sim \rho_1$$

- $\boldsymbol{x}_t^{\boldsymbol{u}}$ is the controlled state vector
- $\boldsymbol{w}_t$ is the standard Wiener process
- endpoint densities ρ_0, ρ_1 given

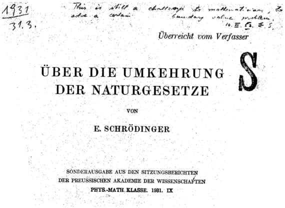
Motivation



- **Population density:** reshape robotic swarm for dynamic coverage, control cell population, sync. and desync. neuronal population, control TCL ensemble

- **Probability density:** belief space motion planning

Prior Works in SBP


1931
31.3.
This is still a challenge to mathematicians, to solve a certain boundary value problem.

Überreicht vom Verfasser

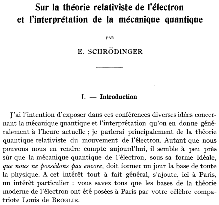
S

ÜBER DIE UMKEHRUNG
DER NATURGESETZE

VON

E. SCHRÖDINGER

SONDERAUSGABE AUS DEN SITZUNGSBERICHTEN
DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN
PHYS.-MATH. KLASSE. 1931. IX


Sur la théorie relativiste de l'électron
et l'interprétation de la mécanique quantique

PAR

E. SCHRÖDINGER

I. — **Introduction**

J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'on en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte aujourd'hui, il semble à peu près sûr que la mécanique quantique de l'électron, sous sa forme idéale, *que nous ne possédons pas encore*, doit former un jour la base de toute la physique. A cet intérêt tout à fait général, s'ajoute, ici à Paris, un intérêt particulier : vous savez tous que les bases de la théorie moderne de l'électron ont été posées à Paris par votre célèbre compatriote Louis de Broglie.

- Schrödinger [1931-32]: $\boldsymbol{f} \equiv \mathbf{0}$, $\boldsymbol{B} = \boldsymbol{G} \equiv \boldsymbol{I}$

- **Connections with stochastic optimal control and optimal transport:** Fortet [1940], Beurling [1960], Jamison [1975], Mikami [1990], Dai Pra and Pavon [1990-1991], Chen-Georgiou-Pavon [2016]

- **Surveys:** Wakolbinger [1990], Léonard [2014]

Many Works in Systems-control

- **Early literature in covariance control:** Skelton et. al. [late 80's and early '90s]

- **Linear quadratic theory for the SBP:** Chen-Georgiou-Pavon [2014-18]

- **Input constrained covariance steering:** Bakolas [2018], Okamoto-Tsiotras [2019]

- **SBP with nonlinear drift:** Chen-Georgiou-Pavon [2015], Bakshi-Fan-Theodorou [2020], Caluya-Halder [2020-21]

- **Probabilistic state constraints:** Tsiotras et. al. [2018-20]

The Present Paper

SBP with deterministic state constraints $\rightsquigarrow$ safety

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SBP with deterministic state constraints $\rightsquigarrow$ safety

Main idea: path constraints $\sim$ reflected Itô SDEs
modify the controlled sample path dynamics to

$$\boxed{\mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}} = \{\boldsymbol{f}(t,\boldsymbol{x}_t^{\boldsymbol{u}}) + \boldsymbol{B}(t)\boldsymbol{u}(t,\boldsymbol{x}_t^{\boldsymbol{u}})\}\mathrm{d}t + \sqrt{2\theta}\boldsymbol{G}(t)\mathrm{d}\boldsymbol{w}_t + \boldsymbol{n}(\boldsymbol{x}_t^{\boldsymbol{u}})\mathrm{d}\gamma_t}$$

$\boldsymbol{x}_t^{\boldsymbol{u}} \in \overline{\mathcal{X}} := \mathcal{X} \cup \partial\mathcal{X}$, closure of connected smooth $\mathcal{X}$

$\boldsymbol{n}$ is inward unit normal to the boundary $\partial\mathcal{X}$

γ_t is minimal local time stochastic process

Reflected SBP for $B = G \equiv I$

Boundary value problem on joint state density

$$\inf_{(\rho,\boldsymbol{u})\in\mathcal{P}_2(\overline{\mathcal{X}})\times\mathcal{U}} \quad \int_0^1 \int_{\overline{\mathcal{X}}}^1 \frac{1}{2} \left\|\boldsymbol{u}\left(t,\boldsymbol{x}_t^u\right)\right\|_2^2 \, \rho\left(t,\boldsymbol{x}_t^u\right) \mathrm{d}\boldsymbol{x}_t^u \, \mathrm{d}t$$

subject to

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\left(\rho(\boldsymbol{u}+\boldsymbol{f})\right) = \theta\Delta\rho,$$

$$\langle -(\boldsymbol{u}+\boldsymbol{f})\rho + \theta\nabla\rho, \boldsymbol{n}\rangle\big|_{\partial\mathcal{X}} = 0$$

$$\rho\left(0,\boldsymbol{x}_t^u\right) = \rho_0, \quad \rho\left(1,\boldsymbol{x}_t^u\right) = \rho_1$$

Condition for Optimality

Theorem: The pair $(\rho^{\text{opt}}, \boldsymbol{u}^{\text{opt}})$ solves

$$\frac{\partial \rho^{\text{opt}}}{\partial t} + \nabla \cdot \left(\rho^{\text{opt}}(\nabla \psi + \boldsymbol{f})\right) = \theta \Delta \rho^{\text{opt}}$$

$$\frac{\partial \psi}{\partial t} + \tfrac{1}{2}\|\nabla \psi\|_2^2 + \langle \nabla \psi, \boldsymbol{f} \rangle = -\theta \Delta \psi$$

where $\boldsymbol{u}^{\text{opt}}(t, \cdot) = \nabla \psi(t, \cdot)$, subject to

$$\langle \nabla \psi, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = 0, \quad \text{for all } \; t \in [0, 1]$$

$$\rho^{\text{opt}}(0, \cdot) = \rho_0, \quad \rho^{\text{opt}}(1, \cdot) = \rho_1,$$

$$\langle \rho^{\text{opt}}(\nabla \psi + \boldsymbol{f}) - \theta \nabla \rho^{\text{opt}}, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = 0, \quad \text{for all } \; t \in [0, 1]$$

Schrödinger System

Theorem: Consider $(\rho^{\text{opt}}, \boldsymbol{u}^{\text{opt}}) \mapsto (\varphi, \hat{\varphi})$ as

$$\varphi := \exp\left(\frac{\psi(t,\cdot)}{2\theta}\right), \quad \hat{\varphi} := \rho^{\text{opt}}(t,\cdot)\exp\left(-\frac{\psi(t,\cdot)}{2\theta}\right).$$

The pair $(\varphi, \hat{\varphi})$ solves

$$\frac{\partial \varphi}{\partial t} = -\langle \nabla \varphi, \boldsymbol{f} \rangle - \theta \Delta \varphi, \qquad \frac{\partial \hat{\varphi}}{\partial t} = -\nabla \cdot (\boldsymbol{f} \hat{\varphi}) + \theta \Delta \hat{\varphi},$$

subject to b.c.

$$\varphi_0 \hat{\varphi}_0 = \rho_0, \quad \varphi_1 \hat{\varphi}_1 = \rho_1,$$

$$\underbrace{\langle \nabla \varphi, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = 0}_{\text{Neumann b.c.}}, \quad \underbrace{\langle \boldsymbol{f} \hat{\varphi} - \theta \nabla \hat{\varphi}, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = 0}_{\text{Robin b.c.}}.$$

Fixed Point Recursion for the pair $(\varphi_1, \hat{\varphi}_0)$

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\hat{\varphi}_0(\boldsymbol{x}) \arrow[r, "\displaystyle\int \text{with b.c. } \langle \boldsymbol{f}\hat{\varphi} - \theta\nabla\hat{\varphi}, \boldsymbol{n}\rangle\big|_{\partial\mathcal{X}} = 0"] & \hat{\varphi}_1(\boldsymbol{x}) \arrow[d, "\rho_1(\boldsymbol{x}) \oslash \hat{\varphi}_1(\boldsymbol{x})"] \\
\varphi_0(\boldsymbol{x}) \arrow[u, "\rho_0(\boldsymbol{x}) \oslash \varphi_0(\boldsymbol{x})"] & \varphi_1(\boldsymbol{x}) \arrow[l, "\displaystyle\int \text{with b.c. } \langle \nabla\varphi, \boldsymbol{n}\rangle\big|_{\partial\mathcal{X}} = 0"]
\end{tikzcd}
$$

Numerical Results: 1D RSBP, no drift

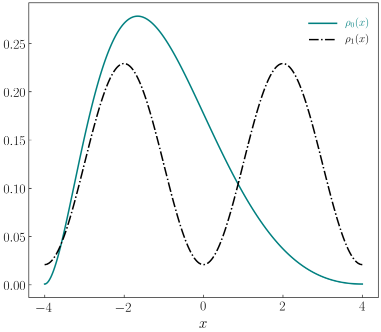
$f \equiv 0$ **and** $\overline{\mathcal{X}} = [a, b] \subset \mathbb{R}$

$$\begin{aligned} \varphi(x,t) &= \int_{[a,b]} K_\theta(x,y,1-t)\,\varphi_1(y)\mathrm{d}y, \quad && t \leq 1 \\ \hat{\varphi}(x,t) &= \int_{[a,b]} K_\theta(y,x,t)\,\hat{\varphi}_0(y)\mathrm{d}y, && t \geq 0 \end{aligned}$$

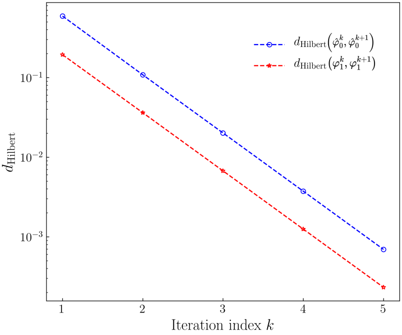
where

$$\begin{aligned} K_\theta(x,y,t) := \frac{1}{b-a} + \frac{2}{b-a} \sum_{m=1}^{\infty} \exp\left(-\frac{\theta\pi^2 m^2}{(b-a)^2} t\right) \\ \times \cos\left(\frac{m\pi(x-a)}{b-a}\right) \cos\left(\frac{m\pi(y-a)}{b-a}\right) \end{aligned}$$

Numerical Results: 1D RSBP, no drift

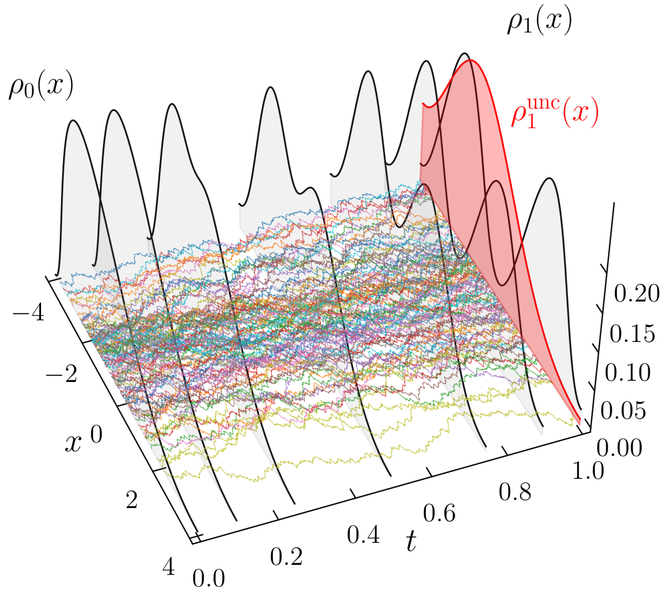


(a) Endpoint PDFs ρ_0, ρ_1



(b) Convergence of the fixed point recursion w.r.t. the Hilbert metric

Numerical Results: 1D RSBP, no drift



RSBP with Gradient Drift

$\boldsymbol{f} \equiv -\nabla V \in C^2\left(\overline{\mathcal{X}}\right)$ and $\overline{\mathcal{X}} \subset \mathbb{R}^n$

Theorem: Let $s := 1-t$, and let $\varphi \mapsto p\left(s, \boldsymbol{x}_s\right) := \varphi(1-s, \boldsymbol{x}_{1-s}) \exp\left(-V(\boldsymbol{x}_s)/\theta\right)$. Then

$$\frac{\partial p}{\partial s} = \nabla \cdot (p \nabla V) + \theta \Delta p, \quad \frac{\partial \hat{\varphi}}{\partial t} = \nabla \cdot (\hat{\varphi} \nabla V) + \theta \Delta \hat{\varphi},$$

subject to

$$p(s=1, \boldsymbol{x}) \exp(V(\boldsymbol{x})/\theta) \hat{\varphi}_0(\boldsymbol{x}) = \rho_0,$$

$$p(s=0, \boldsymbol{x}) \exp(V(\boldsymbol{x})/\theta) \hat{\varphi}_1(\boldsymbol{x}) = \rho_1,$$

$$\langle \nabla V p + \theta \nabla p, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = \langle \nabla V \hat{\varphi} + \theta \nabla \hat{\varphi}, \boldsymbol{n} \rangle|_{\partial \mathcal{X}} = 0,$$

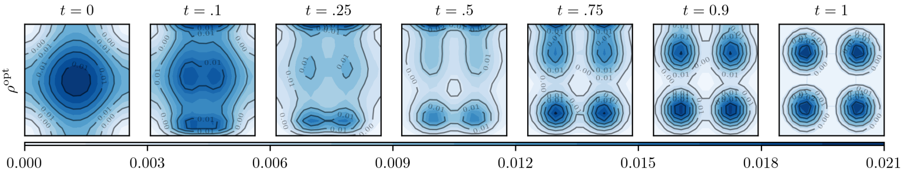
and

$$\varphi\left(t, \boldsymbol{x}_t\right) = \varphi\left(1-s, \boldsymbol{x}_{1-s}\right) = p\left(s, \boldsymbol{x}_s\right) \exp\left(-V\left(\boldsymbol{x}_s\right)/\theta\right).$$

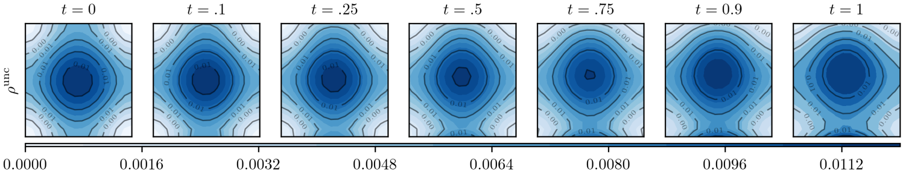
Numerical Results: 2D RSBP, gradient drift

$$V(x_1, x_2) = (x_1^2 + x_2^3)/5, \quad \overline{\mathcal{X}} = [-4, 4]^2$$

Optimal controlled state PDFs:



Uncontrolled state PDFs:



Summary

- Finite horizon minimum effort PDF steering with hard state constraints

- Controlled reflected state SDEs

- Computation: Skorokhod map + proximal updates + contractive fixed point recursion

Thank You

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