Contraction and Reaction in Generalized Schrödinger Bridges

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What is a Schrödinger Bridge Problem (SBP)



Most likely evolution between 2 distributional snapshots

This talk: Generalized SBP



Most likely evolution between 2 distributional snapshots

Motivating Application: Generalized SBP



Stochastic guidance and control of a spacecraft

Background

Optimal Mass Transport (OMT)

Static (Monge) formulation [1781]

$$egin{argsinf} rginf \ ext{measurable} \ m{ au}: \mathbb{R}^n \mapsto \mathbb{R}^n \ m{ au} \ \mathbf{x}_0 \sim
ho_0 \ \mathbf{x}_0 \sim
ho_0, \quad m{ au}(m{x}_0) \sim
ho_1 \ \mathbf{x}_0 \sim
ho_1 \end{array}$$



Optimal Mass Transport (OMT)



$$egin{argsinf} rginf times \mathbb{E}_{
ho_0}rac{1}{2}ig|oldsymbol{x}_0-oldsymbol{ au}(oldsymbol{x}_0)ig|^2 \ ext{subject to} \quad oldsymbol{x}_0\sim
ho_0, \quad oldsymbol{ au}(oldsymbol{x}_0)\sim
ho_1 \end{array}$$



Static (Kantorovich-Rubinstein) reformulation [1941]

$$egin{args}{l} rginf_{\pi\in\Pi(
ho_0,
ho_1)}\mathbb{E}_{\pi}rac{1}{2}ig|oldsymbol{x}_0-oldsymbol{x}_1ig|^2 & ext{Infinite dimensional linear program} \ ext{subject to} \quad oldsymbol{x}_0\sim
ho_0, \quad oldsymbol{x}_1\sim
ho_1 & ext{} \end{array}$$

Optimal Mass Transport (OMT)



subject to $\boldsymbol{x}_0 \sim \rho_0, \quad \boldsymbol{x}_1 \sim \rho_1$

Dynamic (Benamou-Brenier) formulation [1999] $\begin{aligned} \arg \inf_{(\rho, \boldsymbol{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\boldsymbol{v}|^2 \rho(\boldsymbol{x}, t) d\boldsymbol{x} dt \\ \frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{v}) = 0, \\ \rho(\boldsymbol{x}, t = t_0) = \rho_0, \quad \rho(\boldsymbol{x}, t = t_1) = \rho_1 \end{aligned}$ Stochastic optimal control problem

Classical SBP as Stochastic Optimal Control

$$\begin{aligned} & \underset{(\rho, \boldsymbol{v}) \in \mathcal{P}_{01} \times \mathcal{V}}{\operatorname{arginf}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\boldsymbol{v}|^2 \rho(\boldsymbol{x}, t) \mathrm{d}\boldsymbol{x} \mathrm{d}t \\ & \frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{v}) = \varepsilon \Delta_{\boldsymbol{x}} \rho, \quad \varepsilon > 0, \\ & \rho(\boldsymbol{x}, t = t_0) = \rho_0, \quad \rho(\boldsymbol{x}, t = t_1) = \rho_1, \end{aligned}$$
Fokker-Planck-Kolmogorov PDE

Classical OMT vs. Classical SBP

$$\begin{array}{|c|c|} \hline \textbf{Classical OMT} & \displaystyle \operatorname*{arg\,inf}_{(\rho, \boldsymbol{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\boldsymbol{v}|^2 \rho(\boldsymbol{x}, t) \mathrm{d} \boldsymbol{x} \mathrm{d} t \\ & \displaystyle \frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{v}) = \boldsymbol{0}, \quad \textbf{Liouville PDE} \\ & \displaystyle \rho(\boldsymbol{x}, t = t_0) = \rho_0, \quad \rho(\boldsymbol{x}, t = t_1) = \rho_1 \end{array}$$

Classical SBP

$$rginf_{(
ho,oldsymbol{v})\in\mathcal{P}_{01} imes\mathcal{V}}\int_{t_0}^{t_1}\int_{\mathbb{R}^n}rac{1}{2}|oldsymbol{v}|^2
ho(oldsymbol{x},t)\mathrm{d}oldsymbol{x}\mathrm{d}t \ rac{\partial
ho}{\partial t}+
abla_{oldsymbol{x}}\cdot\left(
hooldsymbol{v}
ight)=rac{arepsilon\Delta_{oldsymbol{x}}
ho(oldsymbol{x},t)\mathrm{d}oldsymbol{x}\mathrm{d}t \ rac{\partial
ho}{\partial t}+
abla_{oldsymbol{x}}\cdot\left(
hooldsymbol{v}
ight)=rac{arepsilon\Delta_{oldsymbol{x}}
ho,\ arepsilon\geq0, \
ho(oldsymbol{x},t=t_0)=
ho_0, \quad
ho(oldsymbol{x},t=t_1)=
ho_1, \end{cases}$$

Generalized SBP

Controlled sample path dynamics

$$d\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x},t,\boldsymbol{v}) \, dt + \sqrt{2arepsilon} \boldsymbol{g}(\boldsymbol{x},t,\boldsymbol{v}) \, d\boldsymbol{w}(t)$$

Linear SBP: Contraction Coefficient

Related works

Y. Chen, T. Georgiou, and M. Pavon, "Entropic and displacement interpolation: a computational approach using the Hilbert metric," SIAM Journal on Applied Mathematics, vol. 76, no. 6, pp. 2375–2396, 2016

M. Kuang and E. G. Tabak, "Preconditioning of optimal transport," SIAM Journal on Scientific Computing, vol. 39, no. 4, pp. A1793–A1810, 2017

Linear SBP

$$egin{argsinf} rginf_{(
ho,oldsymbol{v})\in\mathcal{P}_{01} imes\mathcal{V}} & \int_{t_0}^{t_1}\int_{\mathbb{R}^n}rac{1}{2}|oldsymbol{v}|^2
ho(oldsymbol{x},t)\,doldsymbol{x}\,dt \ rac{\partial
ho}{\partial t}+
abla_{oldsymbol{x}}\cdot(
ho(oldsymbol{A}(t)oldsymbol{x}+oldsymbol{B}(t)oldsymbol{v}))=arepsilon\langle ext{Hess},oldsymbol{B}(t)oldsymbol{B}(t)^{ op}
ho
angle \ egin{argsinf} ext{resp. compact supports }oldsymbol{\chi}_0,oldsymbol{\chi}_1 \
ho(oldsymbol{x},t=t_0)=oldsymbol{
ho}_0, \quad
ho(oldsymbol{x},t=t_1)=oldsymbol{
ho}_1 \end{aligned}$$

Controlled sample path dynamics

$$d\boldsymbol{x}(t) = (\boldsymbol{A}(t)\boldsymbol{x}(t) + \boldsymbol{B}(t)\boldsymbol{v}(\boldsymbol{x},t))dt + \sqrt{2\varepsilon}\boldsymbol{B}(t)d\boldsymbol{w}(t)$$

State transition matrix
$$\Phi_{t\tau} := \Phi(t, \tau)$$
 $\forall t_0 \leq \tau \leq t \leq t_1$ Assume controllability: $M_{10} := \int_{t_0}^{t_1} \Phi_{t_1\tau} B(\tau) B^{\top}(\tau) \Phi_{t_1\tau}^{\top} \mathrm{d}\tau \succ \mathbf{0}$

Classical SBP is special case: $\boldsymbol{A}(t) \equiv \boldsymbol{0}, \boldsymbol{B}(t) \equiv \boldsymbol{I}$

Structure of the Solution for Linear SBP

Optimally controlled joint state PDF:
$$\rho_{\varepsilon}^{\text{opt}}(\cdot, t) = \widehat{\varphi}_{\varepsilon}(\cdot, t)\varphi_{\varepsilon}(\cdot, t)$$

Optimal control: $\boldsymbol{v}_{\varepsilon}^{\text{opt}}(\cdot, t) = 2\varepsilon \nabla_{\boldsymbol{x}} \log \varphi_{\varepsilon}(\cdot, t)$
 $\boldsymbol{\zeta} \quad \boldsymbol{\zeta} \quad \boldsymbol{\zeta}$
Schrödinger factors

Define:
$$\widehat{\varphi}_{arepsilon,0}(\cdot):=\widehat{arphi}_{arepsilon}(\cdot,t=t_0), \quad arphi_{arepsilon,1}(\cdot):=arphi_{arepsilon}(\cdot,t=t_1)$$

$$\begin{aligned} & \mathsf{Schrödinger system} \\ & \rho_0(\boldsymbol{x}) = \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{x}) \int_{\mathbb{R}^n}^{\mathbf{Markov kernel}} \underbrace{k(t_0, \boldsymbol{x}, t_1, \boldsymbol{y})}_{k(t_0, \boldsymbol{x}, t_1, \boldsymbol{y})} \varphi_{\varepsilon,1}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y} & \mathsf{Coupled nonlinear integral equations} \\ & \rho_1(\boldsymbol{x}) = \varphi_{\varepsilon,1}(\boldsymbol{x}) \int_{\mathbb{R}^n}^{\mathbf{k}} \underbrace{k(t_0, \boldsymbol{y}, t_1, \boldsymbol{x})}_{k(t_0, \boldsymbol{y}, t_1, \boldsymbol{x})} \widehat{\varphi}_{\varepsilon,0}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y} & \mathsf{Coupled nonlinear integral equations} \\ & \mathsf{Here} & \\ & k(t_0, \boldsymbol{x}_0, t_1, \boldsymbol{x}_1) := \frac{\exp\left(-\frac{(\boldsymbol{\Phi}_{t_1t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)^\top \boldsymbol{M}_{10}^{-1}(\boldsymbol{\Phi}_{t_1t_0}\boldsymbol{x}_0 - \boldsymbol{x}_1)}{4\varepsilon}\right)}{\sqrt{(4\pi\varepsilon)^n \det(\boldsymbol{M}_{10})}} \end{aligned}$$

Contractive Fixed Point Algorithm



Guaranteed linear convergence with contraction rate $\kappa \in (0, 1)$

But exact rate depends on problem data $(\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \boldsymbol{A}(t), \boldsymbol{B}(t))$

 $\begin{array}{ll} \text{Worst case contraction coefficient} \ \gamma := & \sup & \kappa \\ & \text{Linear SBPs with fixed} \left(\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \boldsymbol{A}(t), \boldsymbol{B}(t) \right) \end{array}$

γ in Classical SBP

$$lpha_{
m B} = rac{\exp(- ilde{lpha}_{
m B}/(4arepsilon))}{\sqrt{(4\piarepsilon)^n}}, \quad eta_{
m B} = rac{\expigg(- ilde{eta}_{
m B}/(4arepsilon)igg)}{\sqrt{(4\piarepsilon)^n}}.$$

where

Let

$$ilde{eta}_{\mathrm{B}} := \min_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1}} |oldsymbol{x}_0 - oldsymbol{x}_1|^2 \quad ext{and} \quad ilde{lpha}_{\mathrm{B}} := \max_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1}} |oldsymbol{x}_0 - oldsymbol{x}_1|^2$$

$$egin{aligned} \gamma_{ ext{B}} := ext{tanh}^2igg(rac{1}{2} ext{log}igg(rac{eta_{ ext{B}}}{lpha_{ ext{B}}}igg)igg) \in (0,1) \end{aligned}$$

Chen, Georgiou, Pavon, SIAM J. Applied Math, 2016

γ in Linear SBP



Then

$$egin{aligned} \gamma_{
m L} = anh^2 igg(rac{ ilde{lpha}_{
m L} - ilde{eta}_{
m L}}{8arepsilon} igg) \end{aligned}$$

γ in Linear SBP

Thm. (informal)

Let

$$egin{aligned} ilde{lpha}_{\mathrm{L}} &:= \max_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1)^{\!\!\!\top} oldsymbol{M}_{10}^{-1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1) \ & ilde{oldsymbol{eta}}_{\mathrm{L}} := \min_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1)^{\!\!\!\top} oldsymbol{M}_{10}^{-1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1) \ & oldsymbol{eta}_{\mathrm{L}} := \min_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1)^{\!\!\!\top} oldsymbol{M}_{10}^{-1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1) \ & oldsymbol{eta}_{\mathrm{L}} := \mathbf{D}_{\mathrm{A}} \left[oldsymbol{B}_{\mathrm{A}} oldsymbol{B}$$

Then

$$egin{aligned} \gamma_{
m L} = anh^2 igg(rac{ ilde{lpha}_{
m L} - ilde{eta}_{
m L}}{8arepsilon} igg) \end{aligned}$$

Note:

Control-theoretic Interpretation for γ_L

$$egin{aligned} \mathbf{x}_{t_0} & \mathbf$$

Minimum cost for deterministic OCP

Control-theoretic Interpretation for γ_L

$$\gamma_{\rm L} = \tanh^2 \left(\begin{array}{c} \tilde{\alpha}_{\rm L} - \tilde{\beta}_{\rm L} \\ \hline 8\varepsilon \end{array} \right)$$

Process noise

Conforms with intuition:

$$\left(ilde{lpha}_{
m L} - ilde{eta}_{
m L}^{} \uparrow \quad \Rightarrow \quad \gamma_{
m L}^{} \uparrow
ight)$$

$$egin{array}{ccc} arepsilon \uparrow & \Rightarrow & \gamma_{
m L}\downarrow \end{array}$$

Support Functions



The support function $h_{\mathcal{K}}(\cdot)$ for closed convex set \mathcal{K} is

$$h_{\mathcal{K}}(oldsymbol{y}):=\sup_{oldsymbol{x}\in\mathcal{K}}~\langleoldsymbol{y},oldsymbol{x}
angle,~~oldsymbol{y}\in\mathbb{R}^n$$

e.g., distance from the origin to a supporting hyperplane of $\,\mathcal{K}$ with normal in direction of $\,m{y}$

γ in Linear SBP

$$\gamma_{
m L} = anh^2 igg(rac{ ilde{lpha}_{
m L} - ilde{eta}_{
m L}}{8arepsilon} igg)$$

Thm. (informal)

With support functions of \mathcal{X}_0 and \mathcal{X}_1 , and Euclidean unit sphere \mathcal{S}^{n-1}

$$egin{aligned} ilde{lpha}_{
m L} &= \{ \max_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^ opm{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ ilde{eta}_{
m L} &= \{ \min_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^ opm{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ \end{pmatrix} \end{aligned}$$

γ in Linear SBP

$$\gamma_{
m L} = anh^2igg(rac{ ilde{lpha}_{
m L} - ilde{eta}_{
m L}}{8arepsilon}igg)$$

Thm. (informal)

With support functions of \mathcal{X}_0 and \mathcal{X}_1 , and Euclidean unit sphere \mathcal{S}^{n-1}

$$egin{aligned} & ilde{lpha}_{
m L} = \{ \max_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^ opm{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ & ilde{eta}_{
m L} = \{ \min_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^ opm{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ \end{aligned}$$

Note:

$$\begin{split} \mathbf{\tilde{\alpha}_{B}} &= \mathbf{I} \\ \mathbf{M}_{10} &= \frac{1}{t_{1} - t_{0}} \mathbf{I} \\ \mathbf{M}_{B} &= \frac{1}{t_{1} - t_{0}} \{ \max_{\boldsymbol{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_{0}}(\boldsymbol{y}) + h_{\mathcal{X}_{1}}(-\boldsymbol{y}) \}^{2} \\ \tilde{\alpha}_{B} &= \frac{1}{t_{1} - t_{0}} \{ \min_{\boldsymbol{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_{0}}(\boldsymbol{y}) + h_{\mathcal{X}_{1}}(-\boldsymbol{y}) \}^{2} \\ \end{split}$$

Geometric Interpretation for γ_L

$$\gamma_{
m L} = {
m tanh}^2 igg(rac{ ilde{lpha}_{
m L} - ilde{eta}_{
m L}}{8arepsilon} igg)$$

Geometric interpretation:

 $\tilde{\alpha}_{\rm L}$ and $\tilde{\beta}_{\rm L}$ can be considered the maximum and minimal separation of $\Phi_{t_1t_0}\mathcal{X}_0$ M $M_{10}^{-1/2} oldsymbol{\Phi}_{t_1 t_0} \mathcal{X}_0$ and $M_{10}^{-1/2} \mathcal{X}_1$ 1 -2

Applications to Preconditioning:

Preconditioning to improve optimal transport algorithms ~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017

Example: Linear SBP: $\varepsilon = 0.5$ $d\boldsymbol{x}(t) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \boldsymbol{x}(t) dt + \sqrt{2\varepsilon} \begin{bmatrix} 0 \\ 1 \end{bmatrix} d\boldsymbol{w}(t)$ $\boldsymbol{\Phi}_{t_1t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad \boldsymbol{M}_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$ $\frac{4}{3}$ 2 1 \mathcal{X}_1 -2 2 2 24

Applications to Preconditioning:

Preconditioning to improve optimal transport algorithms ~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017



$$egin{array}{lll} ilde{lpha}_{
m L} = 2 + 2\sqrt{3} & \longrightarrow & \gamma_{
m L} = anh^2(1) pprox 0.580 \ ilde{eta}_{
m L} = -2 + 2\sqrt{3} & & & \end{array}$$

Applications to Preconditioning:

Preconditioning to improve optimal transport algorithms ~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017



SBP with State Cost

Related works

Dawson, D., Gorostiza, L., and Wakolbinger, A., "Schrödinger processes and large deviations," Journal of mathematical physics, Vol. 31, No. 10, 1990, pp. 2385–2388. https://doi.org/10.1063/1.528840

Aebi, R., and Nagasawa, M., "Large deviations and the propagation of chaos for Schrödinger processes," Probability Theory and Related Fields, Vol. 94, No. 1, 1992, pp. 53–68. https://doi.org/10.1007/BF01222509

SBP with State Cost

$$egin{argsinf} rginf_{(
ho,oldsymbol{v})\in\mathcal{P}_{01} imes\mathcal{V}} & \int_{t_0}^{t_1}\int_{\mathbb{R}^n}igg(rac{1}{2}|oldsymbol{v}|^2+oldsymbol{q}(oldsymbol{x})igg)
ho(oldsymbol{x},t)\,doldsymbol{x}\,dt \ & rac{\partial
ho}{\partial t}+
abla_{oldsymbol{x}}\cdot(
hooldsymbol{v})=arepsilon\Delta_{oldsymbol{x}}
ho \ &oldsymbol{x}(t=t_0)\sim
ho_0\ (ext{given}), \quad oldsymbol{x}(t=t_1)\sim
ho_1\ (ext{given}) \end{array}$$

Controlled sample path dynamics

$$d\boldsymbol{x} = \boldsymbol{v}(\boldsymbol{x},t)dt + \sqrt{2\varepsilon}d\boldsymbol{w}(t)$$

Solution for the SBP with State Cost

Thm. (informal)

SBP with state cost admits a unique solution

Proof idea:

Reformulate as Kullback-Leibler minimization over path space:



Conditions for Optimality

Necessary conditions of optimality for the SBP with state cost

The pair $(\rho_{\varepsilon}^{\text{opt}}, \boldsymbol{v}_{\varepsilon}^{\text{opt}})$ solves the coupled nonlinear PDEs

$$egin{aligned} &rac{\partial \psi_arepsilon}{\partial t}+rac{1}{2}|
abla_{oldsymbol{x}}\psi_arepsilon|^2+arepsilon\Delta_{oldsymbol{x}}\psi_arepsilon=oldsymbol{q}(oldsymbol{x})\ &rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t}+
abla_{oldsymbol{x}}\cdotig(
ho_arepsilon^{ ext{opt}}
abla_{oldsymbol{x}}\psi_arepsilonig)=arepsilon\Delta_{oldsymbol{x}}
ho_arepsilon^{ ext{opt}}\ &rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t}+
abla_{oldsymbol{x}}\cdotig(
ho_arepsilon^{ ext{opt}}
abla_{oldsymbol{x}}\psi_arepsilonig)=arepsilon\Delta_{oldsymbol{x}}
ho_arepsilon^{ ext{opt}}\ &rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t}+
abla_{oldsymbol{x}}\cdotig(
ho_arepsilon^{ ext{opt}}
abla_{oldsymbol{x}}\psi_arepsilonig)=arepsilon\Delta_{oldsymbol{x}}
ho_arepsilon^{ ext{opt}}\ &rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t}+
abla_{oldsymbol{x}}\cdotig(
ho_arepsilon^{ ext{opt}}
abla_{oldsymbol{x}}\psi_arepsilonig)=arepsilon\Delta_{oldsymbol{x}}
ho_arepsilon^{ ext{opt}}\ &rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t}+
abla_{oldsymbol{x}}\cdotig(
ho_arepsilon^{ ext{opt}}
abla_{oldsymbol{x}}\psi_arepsilonig)=arepsilon\Delta_{oldsymbol{x}}
ho_arepsilon^{ ext{opt}}\ & ext{opt}\ & ext{$$

with boundary conditions

$$egin{aligned} &
ho^{ ext{opt}}_arepsilon\left(oldsymbol{x},t=t_0
ight) =
ho_0(oldsymbol{x}) \ &
ho^{ ext{opt}}_arepsilon\left(oldsymbol{x},t=t_1
ight) =
ho_1(oldsymbol{x}) \end{aligned}$$

Structure of the solution for SBP with State Cost

Boundary-coupled system of linear PDEs for the Schrödinger factors

$$\begin{cases} \text{Reaction-diffusion PDEs} & \frac{\partial \widehat{\varphi}_{\varepsilon}}{\partial t} = \left(\varepsilon \Delta_{\boldsymbol{x}} - \frac{1}{2\varepsilon}q(\boldsymbol{x})\right)\widehat{\varphi}_{\varepsilon} \leftarrow \mathcal{L}_{\text{forward}}\widehat{\varphi} \\ & \frac{\partial \varphi_{\varepsilon}}{\partial t} = \left(-\varepsilon \Delta_{\boldsymbol{x}} + \frac{1}{2\varepsilon}q(\boldsymbol{x})\right)\varphi_{\varepsilon} \leftarrow \mathcal{L}_{\text{backward}}\varphi \\ & \widehat{\varphi}_{\varepsilon}(\cdot, t = t_{0})\varphi_{\varepsilon}(\cdot, t = t_{0}) = \rho_{0} \\ & \widehat{\varphi}_{\varepsilon}(\cdot, t = t_{1})\varphi_{\varepsilon}(\cdot, t = t_{1}) = \rho_{1}. \end{cases}$$

Optimally controlled joint state PDF

$$ho^{opt}_arepsilon(\cdot,t)=\hatarphi_arepsilon(\cdot,t)arphi_arepsilon(\cdot,t)$$

Optimal control

$$oldsymbol{v}^{ ext{opt}}_arepsilon(\cdot,t) = 2arepsilon
abla_oldsymbol{x} \log arphi_arepsilon(\cdot,t)$$

Algorithm

Fixed point recursion over pair $(\varphi_{\varepsilon,1}, \widehat{\varphi}_{\varepsilon,0})$

$$\widehat{\varphi}_{\varepsilon,0}(\cdot) \xrightarrow{\int \mathcal{L}_{\text{forward}} \widehat{\varphi}} \widehat{\varphi}_{\varepsilon}(\cdot, t = t_{1})$$

$$\rho_{0}(\cdot)/\varphi_{\varepsilon}(\cdot, t = t_{0}) \xrightarrow{\qquad} \rho_{1}(\cdot)/\widehat{\varphi}_{\varepsilon}(\cdot, t = t_{1})$$

$$\varphi_{\varepsilon}(\cdot, t = t_{0}) \xrightarrow{\qquad} \varphi_{\varepsilon,1}(\cdot)$$

$$\int \mathcal{L}_{\text{backward}} \widehat{\varphi}$$

Schrödinger system:

$$egin{aligned} &
ho_0(oldsymbol{x}) = \widehat{arphi}_{arepsilon,0}(oldsymbol{x}) \int_{\mathbb{R}^n} oldsymbol{k}(t_0,oldsymbol{x},t_1,oldsymbol{y}) arphi_{arepsilon,1}(oldsymbol{y}) \mathrm{d}oldsymbol{y} \ &
ho_1(oldsymbol{x}) = arphi_{arepsilon,1}(oldsymbol{x}) \int_{\mathbb{R}^n} oldsymbol{k}(t_0,oldsymbol{y},t_1,oldsymbol{x}) \widehat{arphi}_{arepsilon,0}(oldsymbol{y}) \mathrm{d}oldsymbol{y} \end{aligned}$$

Fredholm Integral Equation of 2nd Kind

Thm. (informal)

Solution of linear reaction-diffusion PDE IVP with state-dependent reaction rate:

$$rac{\partial u}{\partial t} = a \Delta_{oldsymbol{x}} u + q(oldsymbol{x}) u, \quad oldsymbol{x} \in \mathbb{R}^n, \quad u(oldsymbol{x},t=t_0) = u_0(oldsymbol{x}) ext{ given }$$

admits space-time Fredholm integral representation

$$egin{aligned} u(oldsymbol{x},t) &= \underbrace{rac{1}{\sqrt{\left(4\pi at
ight)^n}} \int_{\mathbb{R}^n} \expigg(-rac{|oldsymbol{x}-oldsymbol{y}|^2}{4at}igg) u_0(oldsymbol{y})doldsymbol{y}}_{ ext{term 1}} \ &+ \underbrace{\int_{t_0}^t rac{1}{\sqrt{\left(4\pi a(t- au)
ight)^n}} \int_{\mathbb{R}^n} \expigg(-rac{|oldsymbol{x}-oldsymbol{y}|^2}{4a(t- au)}igg) q(oldsymbol{y}) u(oldsymbol{y}, au)\,doldsymbol{y}\,d au}_{ ext{term 2}} \end{aligned}$$

Case Study Probabilistic Lambert's Problem

Lambert's Problem



3D position coordinate $\boldsymbol{x} := \left(\begin{array}{c} y \end{array} \right)$

$$igg(egin{array}{c} x \ y \ z \ \end{pmatrix} \in \mathbb{R}^3$$

Find velocity control policy $\dot{\boldsymbol{x}} := \boldsymbol{v}(\boldsymbol{r}, t)$ such that

 $oldsymbol{\ddot{x}} = abla_{oldsymbol{x}}V(oldsymbol{x}), \quad oldsymbol{x}(t=t_0) = oldsymbol{x}_0 ext{ (given)}, \quad oldsymbol{x}(t=t_1) = oldsymbol{x}_1 ext{ (given)}$

Probabilistic Lambert's Problem



Probabilistic Lambert's Problem



3D position coordinate $\boldsymbol{x} := \left(\begin{array}{c} y \end{array} \right)$

$$egin{pmatrix} x \ y \ z \end{pmatrix} \in \mathbb{R}^3$$

(m)

Find velocity control policy $\dot{\boldsymbol{x}} := \boldsymbol{v}(\boldsymbol{r}, t)$ such that

 $m{\ddot{x}} = abla_{m{x}} V(m{x}), \ egin{pmatrix} m{x}(t=t_0) \sim
ho_0 \ (ext{given}), \quad m{x}(t=t_1) \sim
ho_1 \ (ext{given}) \end{pmatrix}$

Connection with OMT

Lambert Problem \Leftrightarrow Deterministic OCP

Reformulate Lambert's problem as deterministic OCP [Bando and Yamakawa, *JGCD*, 2010]

 $oldsymbol{\ddot{x}} = abla_{oldsymbol{x}}V(oldsymbol{x}), \quad oldsymbol{x}(t=t_0) = oldsymbol{x}_0 ext{ (given)}, \quad oldsymbol{x}(t=t_1) = oldsymbol{x}_1 ext{ (given)}$ $rgin_{oldsymbol{v}} \operatorname{arg\,inf}_{oldsymbol{v}} \int_{t_0}^{t_1} \left(rac{1}{2} |oldsymbol{v}|^2 - V(oldsymbol{x})
ight) dt$ Potential as state cost $\dot{\boldsymbol{x}} = \boldsymbol{v}$ $\boldsymbol{x}(t=t_0) = \boldsymbol{x}_0 ext{ (given)}, \quad \boldsymbol{x}(t=t_1) = \boldsymbol{x}_1 ext{ (given)}$

Lambertian OMT (L-OMT)

Probabilistic Lambert's Problem ⇔ Generalized OMT

$$\ddot{oldsymbol{x}} = -
abla_{oldsymbol{x}} V(oldsymbol{x}), \quad oldsymbol{x}(t=t_0) \sim
ho_0 ext{ (given)}, \quad oldsymbol{x}(t=t_1) \sim
ho_1 ext{ (given)}$$

\mathbf{r}

$$egin{aligned} &rginf\ (
ho,oldsymbol{v})\in\mathcal{P}_{01} imes\mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} igg(rac{1}{2}|oldsymbol{v}|^2 - V(oldsymbol{x})igg)
ho(oldsymbol{x},t) \, doldsymbol{x} dt \ ec{oldsymbol{x}} & ec{oldsymbol{v}} = oldsymbol{v} \ oldsymbol{v} = 0 \ oldsymbol{is} \ oldsymbol{OMT} \ oldsymbol{x}(t=t_0) = oldsymbol{x}_0 \ (ext{given}), \quad oldsymbol{x}(t=t_1) = oldsymbol{x}_1 \ (ext{given}) \end{aligned}$$

Existence and Uniqueness of Solution for L-OMT

Thm. (informal)

L-OMT with negative potential admits a unique solution

Proof Idea:

Consider Lagrangian for L-OMT problem

Show that the Lagrangian is strictly convex and superlinear in \boldsymbol{v}

Use Figalli's theory for Tonelli Lagrangians induced by action integrals

Connection to SBP with state cost

$$rginf_{(
ho,oldsymbol{v})\in\mathcal{P}_{01} imes\mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left(rac{1}{2} |oldsymbol{v}|^2 - V(oldsymbol{x})
ight) \,
ho(oldsymbol{x},t) \, doldsymbol{x} dt$$

$$egin{aligned} &rac{\partial
ho}{\partial t}+
abla_{m{r}}\cdot(
hom{v})=0,\ &
ho(t=t_0,\cdot)=
ho_0, &
ho(t=t_1,\cdot)=
ho_1. \end{aligned}$$

Lambertian SBP (L-SBP)

$$\begin{split} & \underset{(\rho, \boldsymbol{v}) \in \mathcal{P}_{01} \times \mathcal{V}}{\operatorname{arg inf}} \int_{\mathbb{R}^{n}}^{t_{1}} \int_{\mathbb{R}^{n}} \left(\frac{1}{2} |\boldsymbol{v}|^{2} - \boldsymbol{V}(\boldsymbol{x}) \right) \rho(\boldsymbol{x}, t) \, d\boldsymbol{x} dt \\ & \underset{\mathbf{Regularization} > \mathbf{0}}{\operatorname{Regularization} > \mathbf{0}} \\ & \frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}) = \varepsilon \Delta_{\boldsymbol{r}} \rho, \\ & \rho(t = t_{0}, \cdot) = \rho_{0}, \quad \rho(t = t_{1}, \cdot) = \rho_{1} \end{split}$$

L-SBP Solution

Thm. (informal) Existence and uniqueness of L-SBP is guaranteed

$$V(oldsymbol{x}) = -rac{\mu}{|oldsymbol{x}|} \left(1 + rac{J_2 R_{ ext{Earth}}^2}{2|oldsymbol{x}|^2} \left(1 - rac{3z^2}{|oldsymbol{x}|^2}
ight)
ight) \longrightarrow egin{array}{c} ext{Bounded and} & \ ext{negative for} & \ ext{negative for} & \ ext{|oldsymbol{x}|}^2 \ge ext{R}_{ ext{Earth}}^2 \end{array}$$

Thm. (Necessary conditions of optimality for L-SBP)

$$egin{aligned} &rac{\partial \psi_arepsilon}{\partial t}+rac{1}{2}|
abla_{m{x}}\psi_arepsilon|^2+arepsilon\Delta_{m{x}}\psi_arepsilon=-V(m{x})\ &rac{\partial
ho^{ ext{opt}}_arepsilon}{\partial t}+
abla_{m{x}}\cdotig(
ho^{ ext{opt}}_arepsilon
abla_{m{x}}\psi_arepsilonig)=arepsilon\Delta_{m{x}}
ho^{ ext{opt}}_arepsilon\ &
ho^{ ext{opt}}_arepsilon(t=t_0,\cdot)=
ho_0, \quad
ho^{ ext{opt}}_arepsilon(t=t_1,\cdot)=
ho_1 \end{aligned}$$

L-SBP Computation via Schrödinger Factors

Recursion over pair $(\varphi_1, \hat{\varphi}_0)$

L-SBP Computation via Schrödinger Factors

Recursion over pair $(\varphi_1, \hat{\varphi}_0)$



Thm. (Fredholm Integral Representation)

$$egin{aligned} \widehat{arphi}_arepsilon(oldsymbol{x},t) &= rac{1}{\sqrt{(4\piarepsilon t)^3}} \int_{\mathbb{R}^3} \expigg(-rac{|oldsymbol{x}-oldsymbol{ ilde{x}}|^2}{4arepsilon t}igg) \widehat{arphi}_{arepsilon,0}(oldsymbol{ ilde{x}}) \,doldsymbol{ ilde{x}} \ &- \int_{t_0}^t rac{1}{2arepsilon\sqrt{(4\piarepsilon(t- au))^3}} \int_{\mathbb{R}^3} \expigg(-rac{|oldsymbol{x}-oldsymbol{ ilde{x}}|^2}{4arepsilon(t- au)}igg) V(oldsymbol{ ilde{x}}) \widehat{arphi}_arepsilon(oldsymbol{ ilde{x}}) \,doldsymbol{ ilde{x}} \,d au \end{aligned}$$

Numerical Case Study

Prescribed time horizon $[t_0, t_1] \equiv [0, 1]$ hours

Endpoint joint PDFs

$$oldsymbol{x}_0 \sim \mathcal{N}(\mu_0, \Sigma_0) \ oldsymbol{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$$

where

$$\mu_0 = egin{pmatrix} 5000\ 10000\ 2100 \end{pmatrix}, \quad \mu_1 = egin{pmatrix} -14600\ 2500\ 7000 \end{pmatrix}$$

$$\Sigma_0 = rac{1}{100} \mathrm{diag}ig(\mu_0^2ig), \quad \Sigma_1 = rac{1}{100} \mathrm{diag}ig(\mu_1^2ig),$$

Solution: Computation

IDEA: Fixed point recursion over pair $(\varphi_1, \hat{\varphi}_0)$

Idea: Left Riemann Approximation of Second Term

$$egin{aligned} &\int_{t_0}^{t_1} \int_{\mathbb{R}^n} f(\widetilde{oldsymbol{x}},oldsymbol{x}, au,t) d\widetilde{oldsymbol{x}}d au \ &pprox \sum_{q=0}^{k-1} \sum_{m=0}^{N_x} \sum_{n=0}^{N_y} \sum_{j=0}^{N_z} f(\widetilde{oldsymbol{x}}_{(m,n,j)},oldsymbol{x},t_0+k\Delta t,t)\Delta z\Delta y\Delta x\Delta t \ & ext{where} \ \ &\widetilde{oldsymbol{x}}_{(m,n,j)} = (x_0+\Delta x,y_0+\Delta y,z_0+\Delta z) \end{aligned}$$

Numerical Case Study (cont.)

Optimally controlled closed loop state sample paths



Numerical Case Study (cont.)



Numerical Case Study (cont.)

Univariate marginals for optimally controlled joint PDFs



Tentative Timeline for Research

Winter-Spring 2024: Further investigation of convergence guarantees for reactiondiffusion PDEs associated with SBPs with additive state costs.

Summer-Fall 2024: Deriving conditions for optimality of generalized SBPs.

Winter-Spring 2025: Publishing results, writing my dissertation.

Summer 2025: Ph.D. defense.

Publications

Alexis M.H. Teter, Yongxin Chen, Abhishek Halder "On the contraction coefficient of the Schrödinger bridge for stochastic linear systems" *IEEE Control Systems Letters*, Vol. 7, pp. 3325–3330, 2023 doi: 10.1109/LCSYS.2023.3326836 (also accepted for presentation at the 2024 American Control Conference)

Alexis M.H. Teter, Iman Nodozi, Abhishek Halder "Probabilistic Lambert Problem: Connections with Optimal Transport, Schrödinger Bridge and Reaction-Diffusion PDEs" under review arXiv:2401.07961, 2024

Alexis M.H. Teter, Iman Nodozi, Abhishek Halder "Proximal mean field learning in shallow neural networks" *Transactions on Machine Learning Research*, 2024 URL: https://openreview.net/forum?id=vyRBsqj5iG

Thank You

Backup Slides

γ in Linear SBP

Thm. (informal)

$$egin{aligned} ilde{lpha}_{\mathrm{L}} &= \{ \max_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^{ op}m{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ ilde{eta}_{\mathrm{L}} &= \{ \min_{m{y}\in\mathcal{S}^{n-1}}(h_{\mathcal{X}_0}(m{\Phi}_{t_1t_0}^{ op}m{M}_{10}^{-1/2}m{y}) + h_{\mathcal{X}_1}(-m{M}_{10}^{-1/2}m{y})) \}^2 \ \end{aligned}$$

Proof idea:

$$ilde{lpha}_{\mathrm{L}} = \max_{oldsymbol{x}_0 \in \mathcal{X}_0, oldsymbol{x}_1 \in \mathcal{X}_1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1)^{\!\!\!\top} \!\! oldsymbol{M}_{10}^{-1} (oldsymbol{\Phi}_{t_1 t_0} oldsymbol{x}_0 - oldsymbol{x}_1)^{\!\!\!}$$

$$ilde{lpha}_{
m L} = \max_{m{x}\inm{M}_{10}^{-1/2}m{\Phi}_{10}\mathcal{X}_0 - m{M}_{10}^{-1/2}\mathcal{X}_1} ig|^{m{x}} = \{\max_{m{x}\inm{M}_{10}^{-1/2}m{\Phi}_{10}\mathcal{X}_0 - m{M}_{10}^{-1/2}\mathcal{X}_1} ig\langle rac{m{x}}{ig|m{x}ig|},m{x} ig
angle \}^2$$

$$ilde{lpha}_{
m L} = \{ \max_{m{y} \in \mathbb{S}^{n-1}} h_{m{M}_{10}^{-1/2} m{\Phi}_{10} \mathcal{X}_0 - m{M}_{10}^{-1/2} \mathcal{X}_1}(m{y}) \}^2$$

Solution to the Classical SBP

Thm. (Necessary conditions of optimality for the classical SBP):

The pair $(\rho_{\varepsilon}^{\text{opt}}, \boldsymbol{v}_{\varepsilon}^{\text{opt}})$ solves the coupled PDEs

 $egin{aligned} & \operatorname{Value \ function} \ & \displaystyle rac{\partial \psi_arepsilon}{\partial t} + \displaystyle rac{1}{2} |
abla_x \psi_arepsilon|^2 + arepsilon \Delta_x \psi_arepsilon &= 0, \ & \displaystyle rac{\partial
ho_arepsilon^{ ext{opt}}}{\partial t} +
abla_x \cdot \left(
ho_arepsilon^{ ext{opt}}
abla_x \psi_arepsilon
ight) &= arepsilon \Delta_x
ho_arepsilon^{ ext{opt}}
onumber \ \end{aligned}$

with boundary conditions

$$egin{aligned} &
ho^{ ext{opt}}_arepsilon \left(oldsymbol{x},t=t_0
ight) =
ho_0(oldsymbol{x}) \ &
ho^{ ext{opt}}_arepsilon \left(oldsymbol{x},t=t_1
ight) =
ho_1(oldsymbol{x}) \end{aligned}$$

Solution to the Classical SBP

Hopf-Cole transform

Schrödinger factors

results in

$$egin{aligned} rac{\partial \hat{arphi}_arepsilon}{\partial t} &= arepsilon \Delta_x \hat{arphi}_arepsilon \ rac{\partial arphi_arepsilon}{\partial t} &= arepsilon \Delta_x arphi_arepsilon \ rac{\partial arphi_arepsilon}{\partial t} &= -arepsilon \Delta_x arphi_arepsilon \ \hat{arphi}_arepsilon(oldsymbol{x},t=t_0) arphi_arepsilon(oldsymbol{x},t=t_0) &=
ho_0(oldsymbol{x}), \ \hat{arphi}_arepsilon(oldsymbol{x},t=t_1) arphi_arepsilon(oldsymbol{x},t=t_1) &=
ho_1(oldsymbol{x}) \end{aligned}$$

Contraction Coefficient for Linear SBP

Thm. (informal)

$$\gamma_{
m L} = {
m tanh}^2 igg({ ar lpha_{
m L} - {ar eta_{
m L}} \over 8 arepsilon} igg)$$

Proof Idea: