Generalized Schrödinger Bridges

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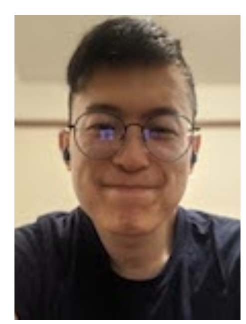
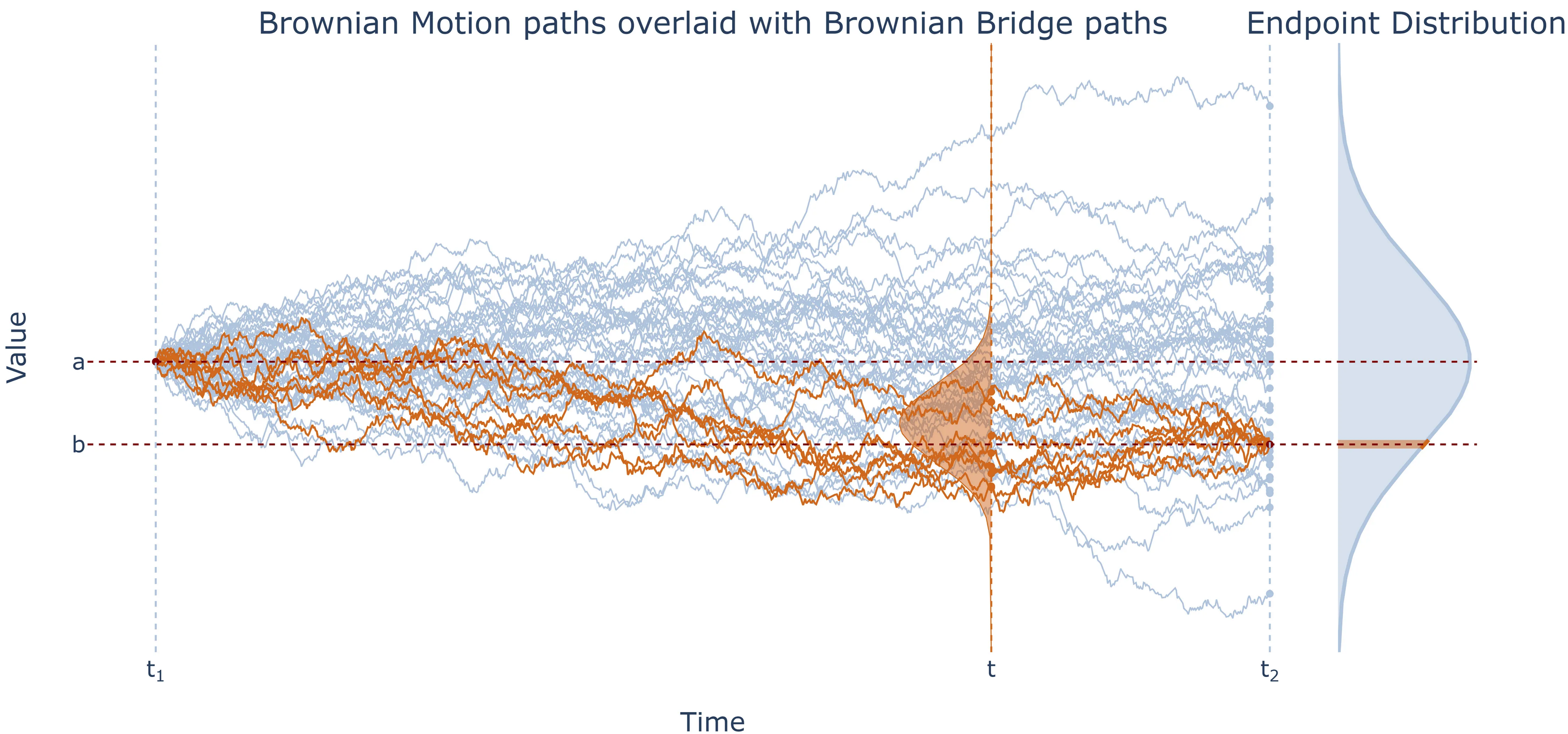
Joint work with students and collaborators

Decision Superiority Seminar, Lawrence Livermore National Lab
December 05, 2024

What is a bridge

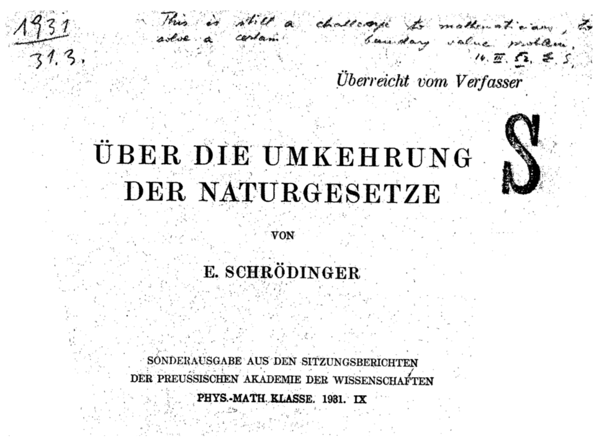
A stochastic process connecting two given states a, b in a given deadline $[t_1, t_2]$



Source: **https://medium.com/@christopher.tabori/between-certainty-and-chance-tracing-the-probability-distribution-of-paths-of-brownian-bridges-b1f97eba638d**

What is a Schrödinger bridge

Prior physics = Brownian motion


Überreicht vom Verfasser

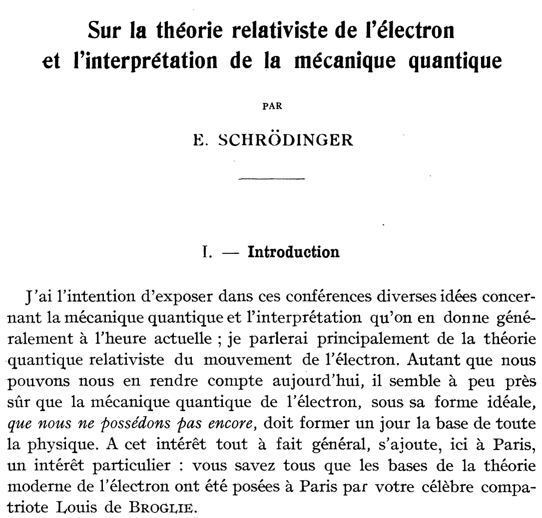
ÜBER DIE UMKEHRUNG
DER NATURGESETZE

VON

E. SCHRÖDINGER

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

[1931]


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

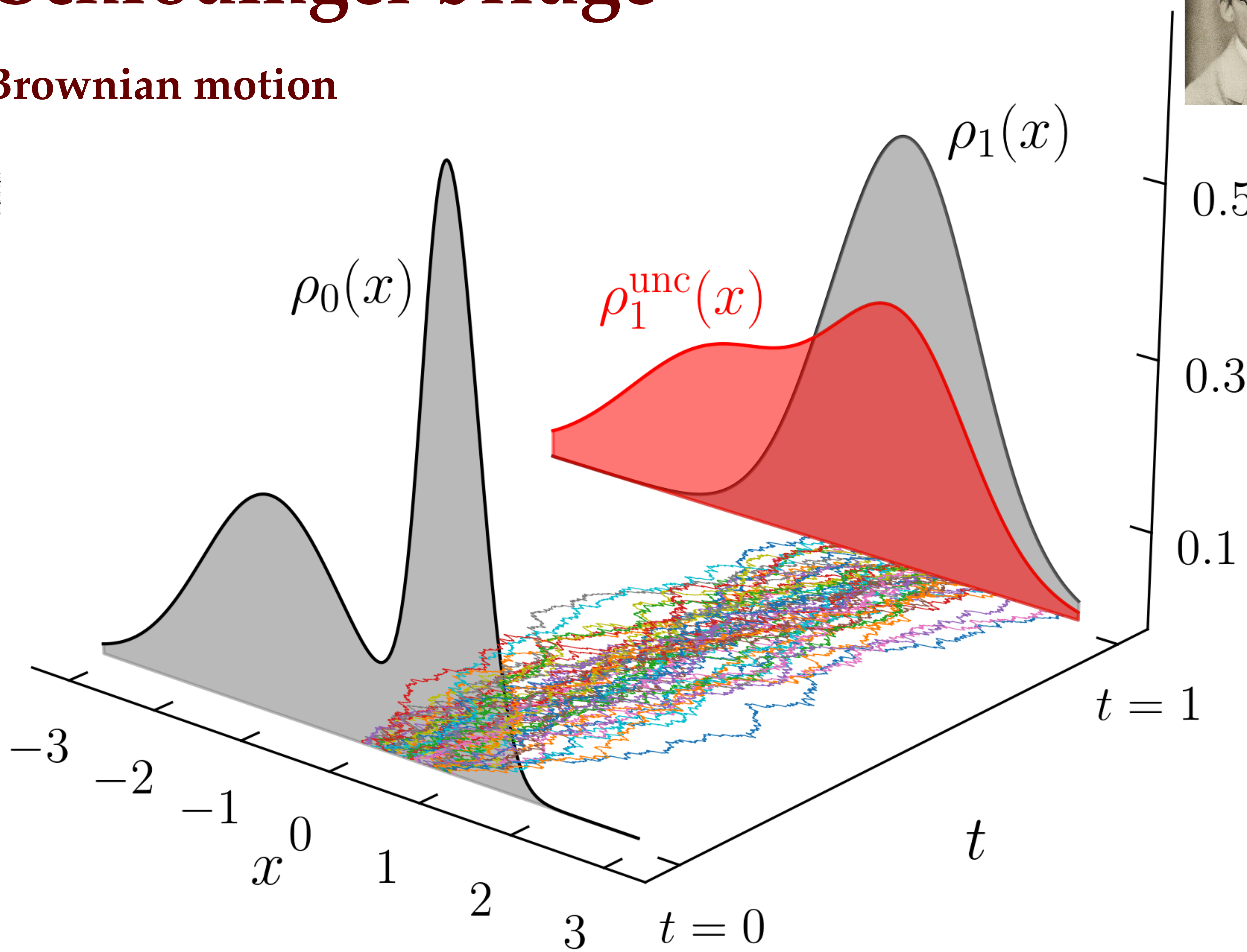
PAR

E. SCHRÖDINGER

I. — Introduction

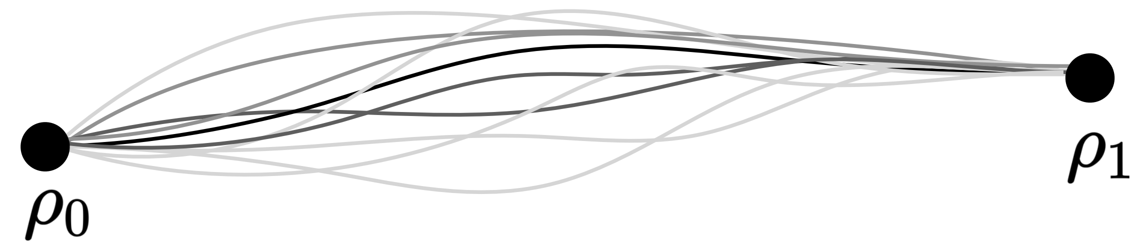
J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'on en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte 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.

[1932]



Find the most likely explanation of observation vs prior physics mismatch

What is a Schrödinger bridge



Path space $\Omega := C([t_0, t_1]; \mathbb{R}^n)$

Denote the collection of all probability measures on Ω as $\mathcal{M}(\Omega)$

$$\Pi_{01} := \{\mathbb{M} \in \mathcal{M}(\Omega) \mid \mathbb{M} \text{ has marginal } \rho_i \, \mathrm{d}\boldsymbol{x} \text{ at time } t_i \forall i \in \{0,1\}, \rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^n)\}$$

$$\text{Schrödinger bridge} = \underset{\mathbb{P} \in \Pi_{01}}{\arg\inf} \quad D_{\mathrm{KL}}(\mathbb{P} \| \mathbb{W})$$

Generated by Itô diffusion

Wiener measure

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{u}(t, \boldsymbol{x})\mathrm{d}t + \mathrm{d}\boldsymbol{w}(t)$$

Most parsimonious correction of prior physics

Constrained maximum likelihood problem on measure-valued paths

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: Sanov's theorem [1957]

$$\lim_{N\uparrow\infty} \log(\text{empiricial prob}_N \text{ under } \mathbb{W} \in \Pi_{01}) \asymp - \inf_{\mathbb{P}\in\Pi_{01}} \underbrace{D_{\mathrm{KL}}}_{\text{KL div as rate function}}(\mathbb{P} \parallel \mathbb{W})$$

Schrödinger bridge as stochastic optimal control: [1990s]

$$\begin{aligned}
&\underset{\boldsymbol{u}\in\mathcal{U}}{\text{minimize}}\, \mathbb{E}\left[\int_{t_0}^{t_1} \frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 \mathrm{d}t\right]\\
&\text{subject to}\\
&\mathrm{d}\boldsymbol{x}_t^u = \boldsymbol{u}(t,\boldsymbol{x}_t^u)\mathrm{d}t + \mathrm{d}\boldsymbol{w}_t\\
&\boldsymbol{x}_t^u(t=t_0) \sim \rho_0, \quad \boldsymbol{x}_t^u(t=t_1) \sim \rho_1
\end{aligned}$$

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: Sanov's theorem [1957]

$$\lim_{N\uparrow\infty} \log(\text{empiricial prob}_N \text{ under } \mathbb{W} \in \Pi_{01}) \asymp -\inf_{\mathbb{P}\in\Pi_{01}} D_{\mathrm{KL}}(\mathbb{P} \parallel \mathbb{W})$$

KL div as rate function

Schrödinger bridge as stochastic optimal control: [1990s]

$$\underset{\boldsymbol{u}\in\mathcal{U}}{\text{minimize}}\, \mathbb{E}\left[\int_{t_0}^{t_1} \frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 \mathrm{d}t\right]$$

subject to

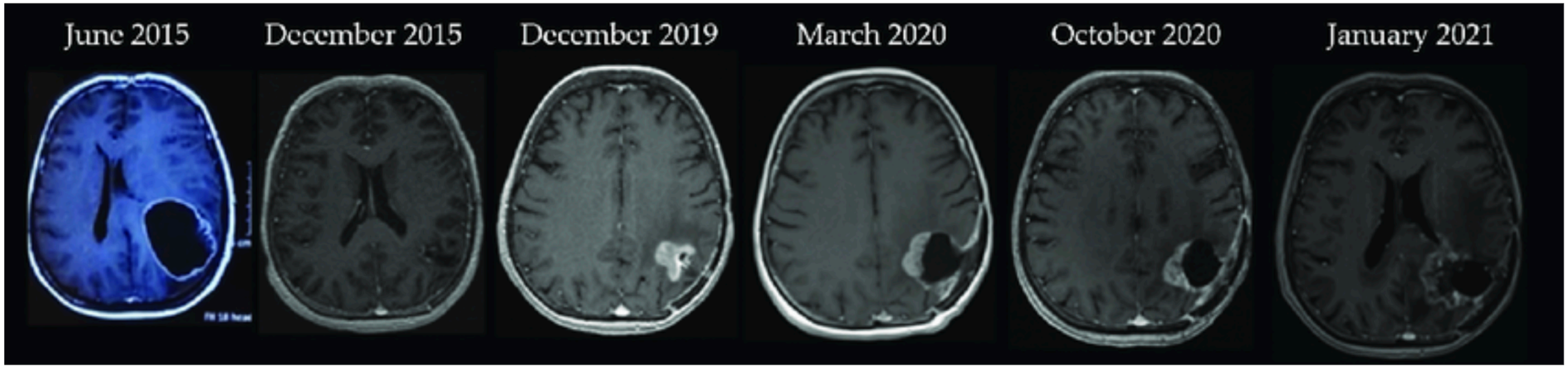
$$\mathrm{d}\boldsymbol{x}_t^u = \boldsymbol{u}(t,\boldsymbol{x}_t^u)\mathrm{d}t + \cancelto{\mathbf{0}}{\mathrm{d}\boldsymbol{w}_t}$$

Benamou-Brenier OMT [1999]

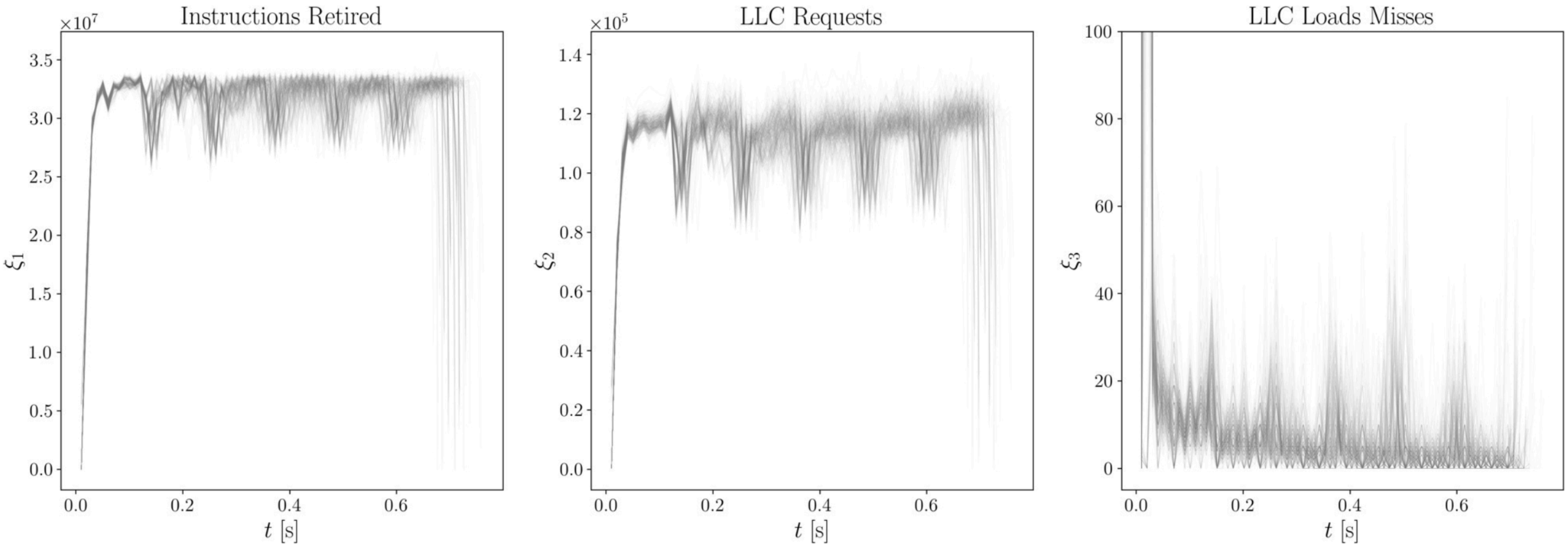
$$\boldsymbol{x}_t^u(t=t_0) \sim \rho_0, \quad \boldsymbol{x}_t^u(t=t_1) \sim \rho_1$$

Resurgence of Schrödinger bridge in ML/AI

Learn most likely progression of medical condition



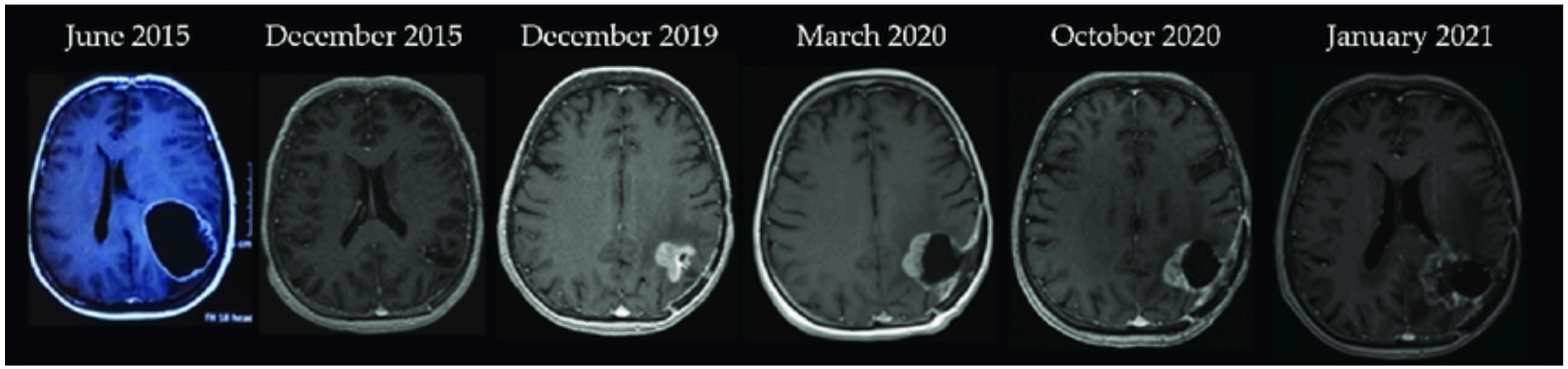
Learn joint stochastic time-varying hardware resource availability

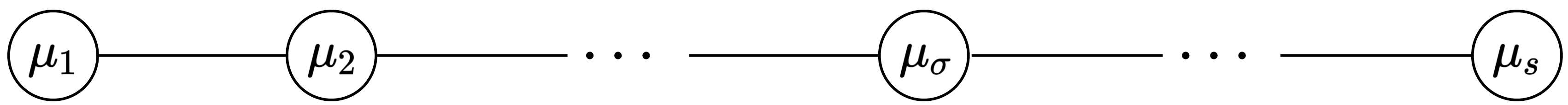


G.A. Bondar, R. Gifford, L.T.X. Phan, and A.H., ***ACC 2024,***
arXiv:2310.00604
arXiv:2405.12463

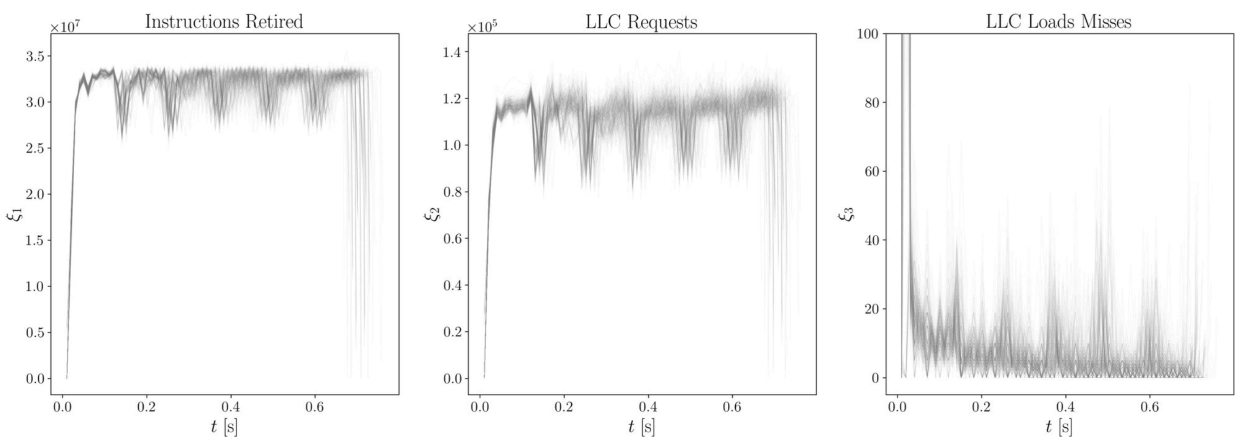
Connections with graphical models

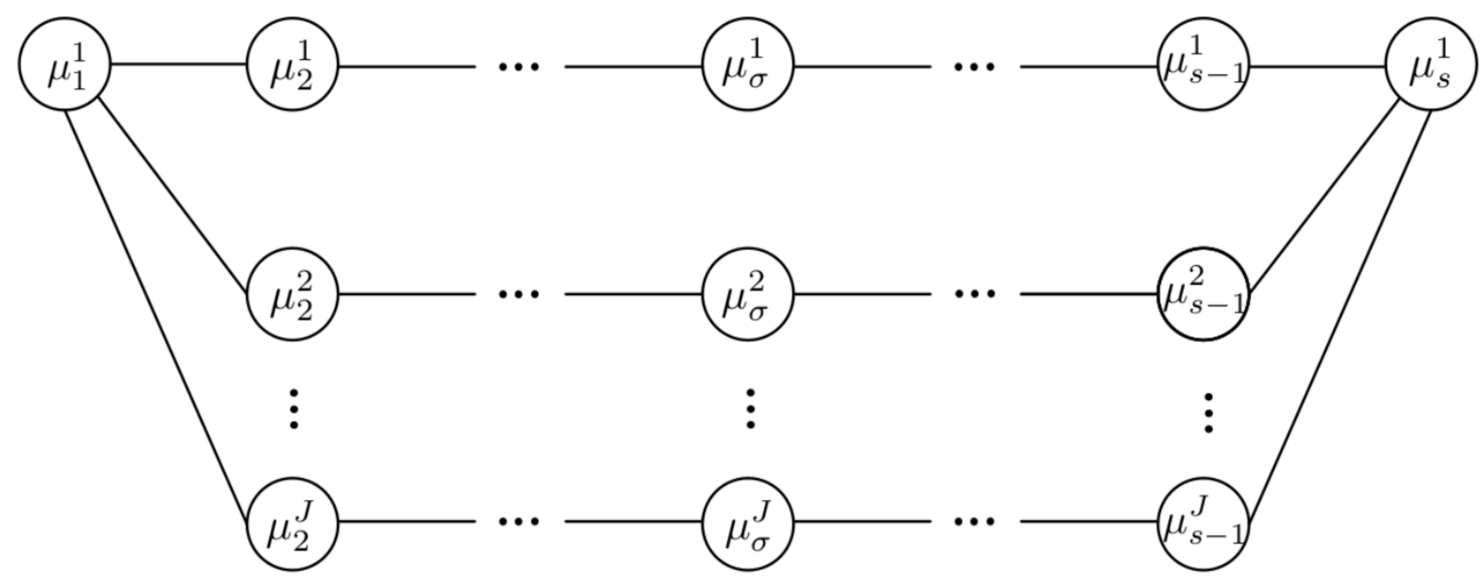
Learn most likely progression of medical condition





Learn joint stochastic time-varying hardware resource availability



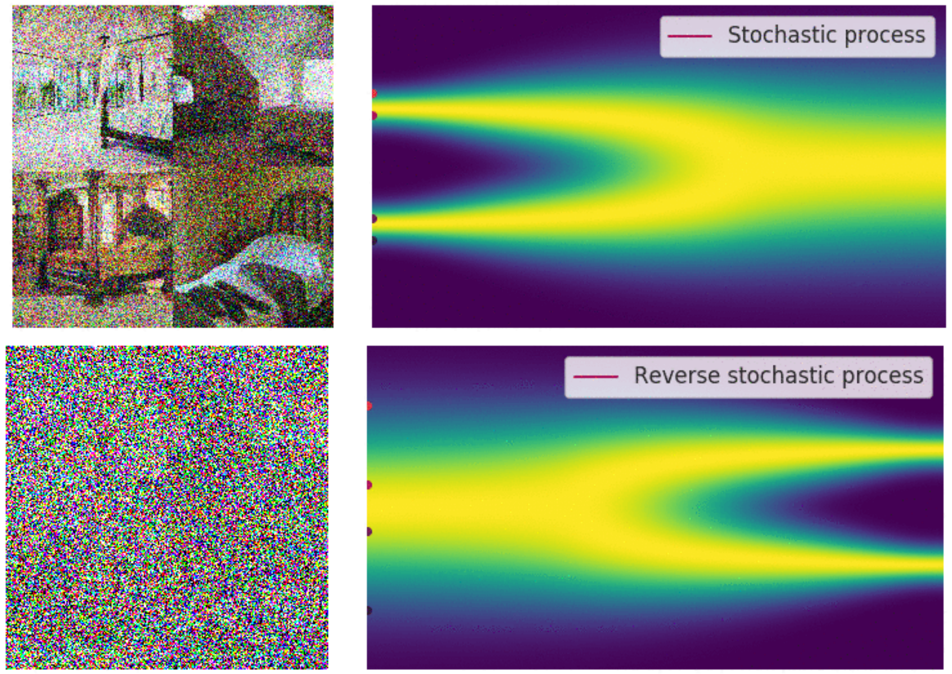


G.A. Bondar, R. Gifford, L.T.X. Phan, and A.H., ***ACC 2024,***
arXiv:2310.00604
arXiv:2405.12463

Resurgence of Schrödinger bridge in ML/AI

Diffusion models for generative AI

Source: **https://yang-song.net/blog/2021/score/**



NeurIPS 2021

Diffusion Schrödinger Bridge with Applications to Score-Based Generative Modeling

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ESSEC Business School,
Singapore

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University of Oxford, UK

UAI 2023

Aligned Diffusion Schrödinger Bridges

Vignesh Ram Somnath[*1,2] **Matteo Pariset**[*1,3] **Ya-Ping Hsieh**[1]
Maria Rodriguez Martinez[2] **Andreas Krause**[1] **Charlotte Bunne**[1]

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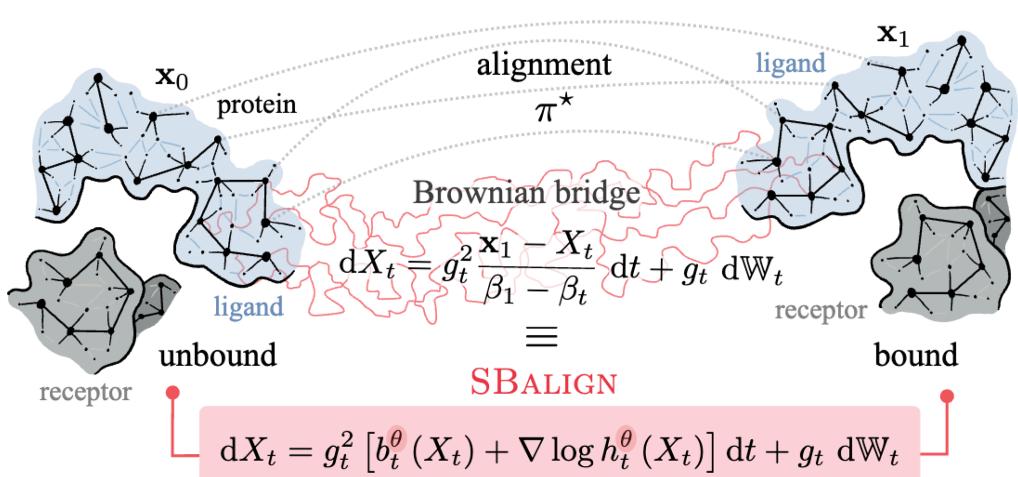
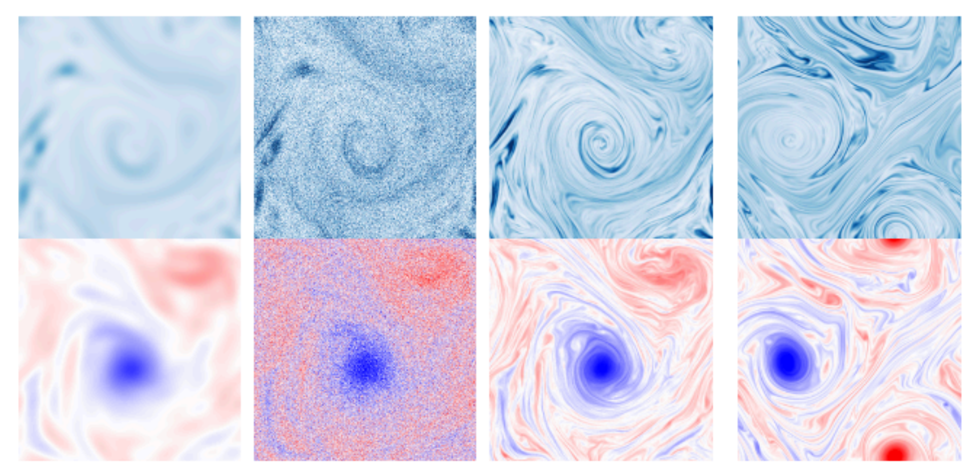
[2]IBM Research Zürich
[3]Department of Computer Science, EPFL



NeurIPS 2024

Diffusion Schrödinger Bridge Matching

Yuyang Shi* University of Oxford
Valentin De Bortoli* ENS ULM
Andrew Campbell University of Oxford
Arnaud Doucet University of Oxford



Low res **High res**

This talk: generalized Schrödinger bridges

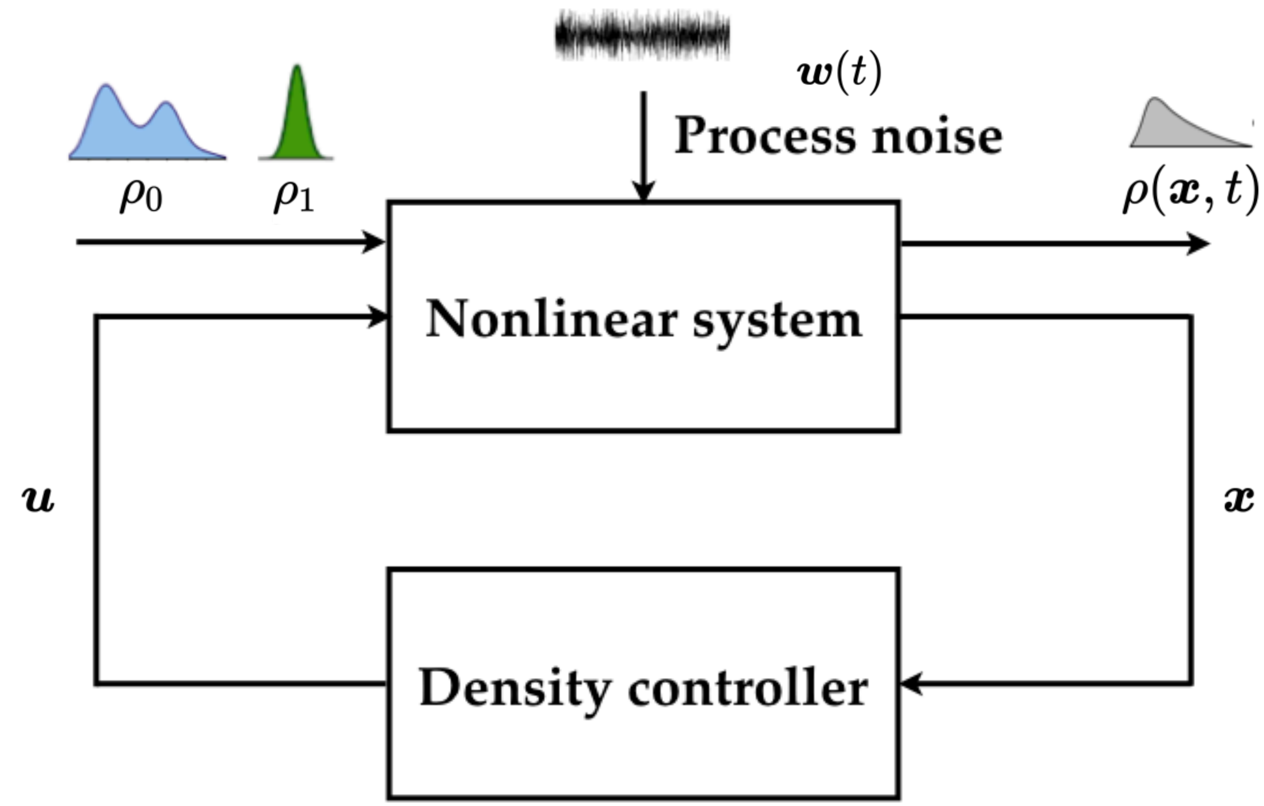
#1. general controlled dynamics

#2. extra sample path constraints

#3. additive state cost

Generalization #1: more general controlled dyn.

Steer joint state PDF via feedback control over finite time horizon



Common scenario: $G \equiv B$

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

subject to

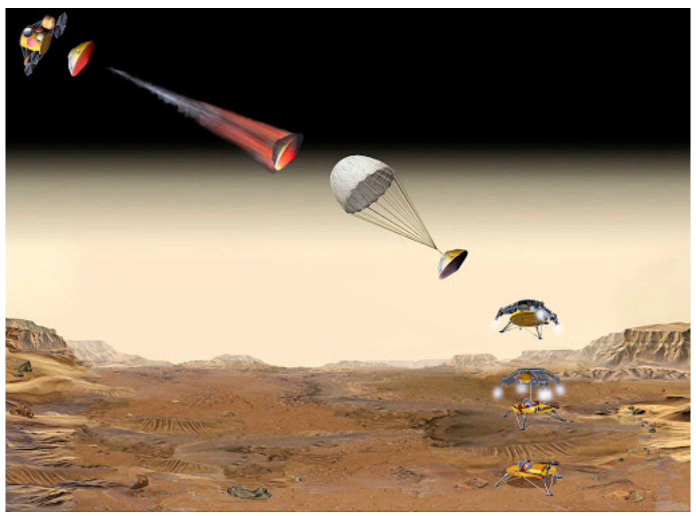
$$\mathrm{d}\boldsymbol{x}_t^u = \{\boldsymbol{f}(t,\boldsymbol{x}_t^u) + \boldsymbol{B}(t,\boldsymbol{x}_t^u)\boldsymbol{u}\}\mathrm{d}t + \sqrt{2}\boldsymbol{G}(t,\boldsymbol{x}_t^u)\mathrm{d}\boldsymbol{w}_t$$

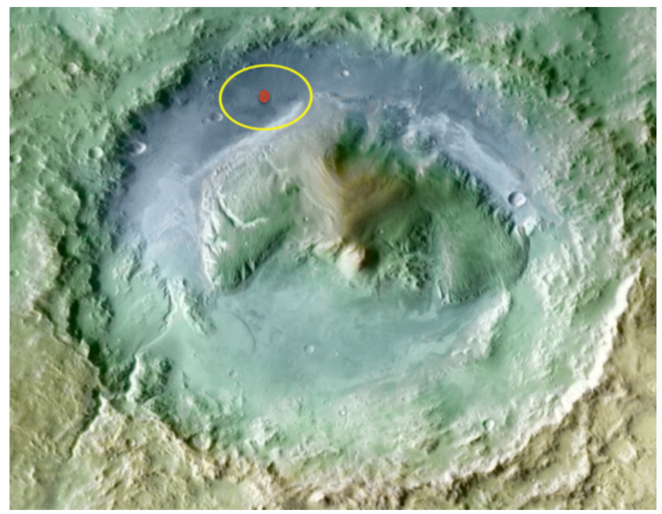
$$\boldsymbol{x}_0^u := \boldsymbol{x}_t^u(t=0) \sim \rho_0, \quad \boldsymbol{x}_1^u := \boldsymbol{x}_t^u(t=1) \sim \rho_1$$

Motivating applications

Distribution ~ Probability

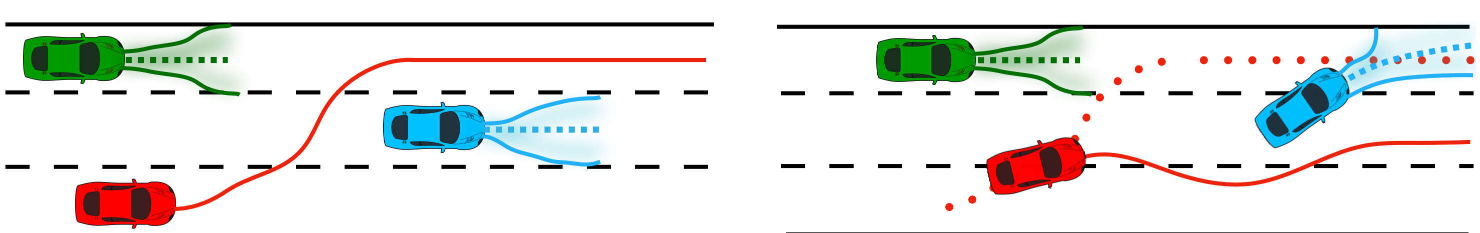
Spacecraft landing with desired statistical accuracy





Gale Crater (4.49S, 137.42E)

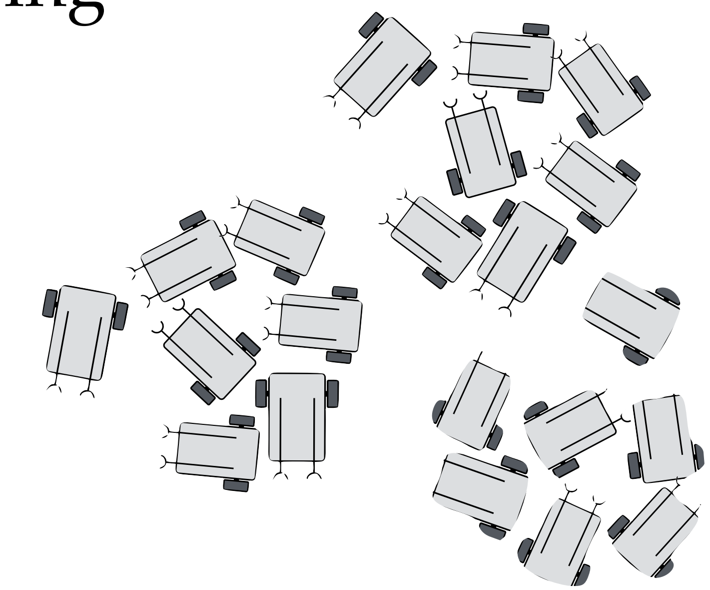
Risk management for automated driving in multi-lane highways



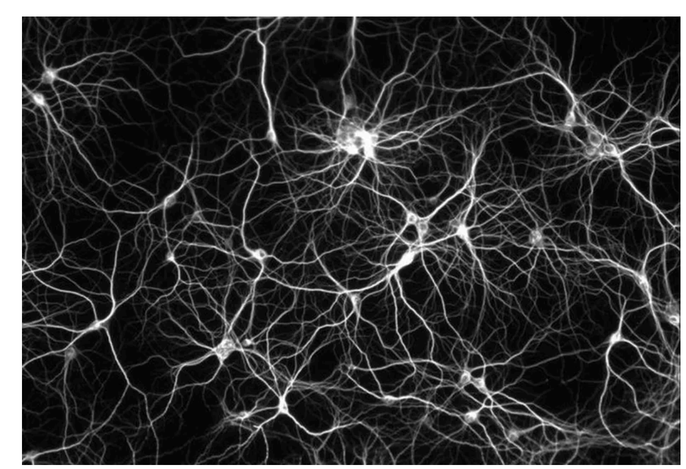
Control of uncertainties

Distribution ~ Population

Dynamic shaping of swarms



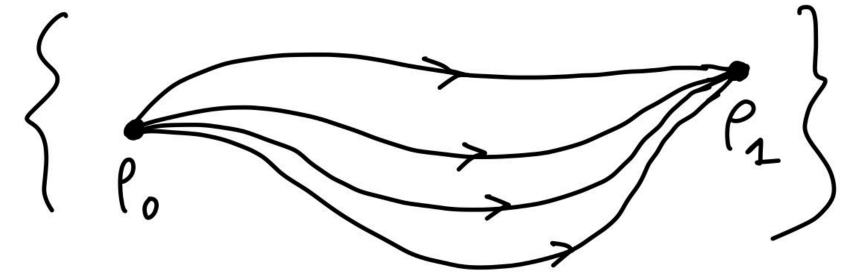
Feedback sync. and desync. of neuronal population



Control of ensemble

Generalized Schrödinger bridge

$\mathcal{P}_{01} :=$



Diffusion tensor: $\boldsymbol{D} := \boldsymbol{G}\boldsymbol{G}^{\top}$

Hessian operator w.r.t. state: Hess

$$\inf_{(\rho,\boldsymbol{u})\in\mathcal{P}_{01}\times\mathcal{U}} \int_{\mathbb{R}^n}\int_0^1 \left(\frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 + q(t,\boldsymbol{x}_t^u)\right)\rho(t,\boldsymbol{x}_t^u)\mathrm{d}t\,\mathrm{d}\boldsymbol{x}_t^u$$

subject to

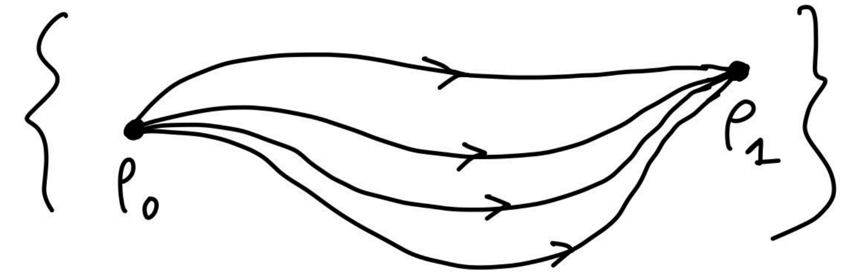
$$\frac{\partial\rho}{\partial t} + \nabla\cdot((\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u})\rho) = \Delta_{\boldsymbol{D}}\rho$$

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

Controlled Fokker-Planck or Kolmogorov's forward PDE

Zero process noise ⇝ Generalized OMT

Diffusion tensor: $\boldsymbol{D} := \boldsymbol{G}\boldsymbol{G}^{\top}$

$\mathcal{P}_{01} :=$ 

Hessian operator w.r.t. state: Hess

$$\inf_{(\rho,\boldsymbol{u})\in\mathcal{P}_{01}\times\mathcal{U}} \int_{\mathbb{R}^n}\int_0^1 \left(\frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 + q(t,\boldsymbol{x}_t^u)\right)\rho(t,\boldsymbol{x}_t^u)\mathrm{d}t\,\mathrm{d}\boldsymbol{x}_t^u$$

subject to

$$\frac{\partial\rho}{\partial t} + \nabla\cdot((\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u})\rho) = \cancel{\Delta_{\boldsymbol{D}}\rho}$$

0

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

Controlled Liouville PDE

Necessary Conditions of Optimality (Assuming $G \equiv B$)

Coupled nonlinear PDEs + linear boundary conditions

Controlled Fokker-Planck or Kolmogorov's forward PDE

$$\frac{\partial \rho^{\mathrm{opt}}}{\partial t} + \nabla \cdot \left(\left(\boldsymbol{f} + \boldsymbol{D} \nabla \psi \right) \rho^{\mathrm{opt}} \right) = \Delta_{\boldsymbol{D}} \rho^{\mathrm{opt}}$$

Hamilton-Jacobi-Bellman-like PDE

$$\frac{\partial \psi}{\partial t} + \langle \nabla \psi, \boldsymbol{f} \rangle + \langle \boldsymbol{D}, \mathrm{Hess}(\psi) \rangle + \frac{1}{2} \langle \nabla \psi, \boldsymbol{D} \nabla \psi \rangle = q$$

Boundary conditions:

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

Optimal control: $\boldsymbol{u}^{\mathrm{opt}} = \boldsymbol{B}^{\top} \nabla \psi$

Feedback synthesis via the Schrödinger factors

Hopf-Cole a.k.a. Fleming's logarithmic transform:

$$\left(\rho^{\mathrm{opt}}, \psi\right) \mapsto \boxed{\left(\widehat{\varphi}, \varphi\right)}$$ — **Schrödinger factors**

$$\widehat{\varphi}(\boldsymbol{x},t) = \rho^{\mathrm{opt}}(\boldsymbol{x},t)\exp\left(-\psi\left(\boldsymbol{x},t\right)\right)$$

$$\varphi(\boldsymbol{x},t) = \exp\left(\psi\left(\boldsymbol{x},t\right)\right)$$

2 coupled nonlinear PDEs $\longrightarrow$ boundary-coupled linear PDEs!!

Uncontrolled forward-backward advection-reaction-diffusion PDEs:

$$\frac{\partial\widehat{\varphi}}{\partial t} = \overbrace{\boxed{-\nabla\cdot\left(\widehat{\varphi}\boldsymbol{f}\right) + \Delta_{\boldsymbol{D}}\widehat{\varphi} - q\widehat{\varphi},}}^{\mathcal{L}_{\text{forward}}\widehat{\varphi}} \qquad \widehat{\varphi}_0\varphi_0 = \rho_0$$

$$\frac{\partial\varphi}{\partial t} = \overbrace{\boxed{-\langle\nabla\varphi, \boldsymbol{f}\rangle - \Delta_{\boldsymbol{D}}\widehat{\varphi} + q\widehat{\varphi},}}^{\mathcal{L}_{\text{backward}}\varphi} \qquad \widehat{\varphi}_1\varphi_1 = \rho_1$$

Optimal controlled joint state PDF: $\rho^{\mathrm{opt}}(\boldsymbol{x},t) = \widehat{\varphi}(\boldsymbol{x},t)\varphi(\boldsymbol{x},t)$

Optimal control: $\boldsymbol{u}^{\mathrm{opt}}(\boldsymbol{x},t) = 2\boldsymbol{B}^{\top}\nabla_{\boldsymbol{x}}\log\varphi(\boldsymbol{x},t)$

What exactly are Schrödinger factors?

Consider Schrödinger's original case: $\boldsymbol{f} = \mathbf{0}, \boldsymbol{B} = \boldsymbol{D} = \boldsymbol{I}$

Classical: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \varphi(\boldsymbol{x}, t)\widehat{\varphi}(\boldsymbol{x}, t)$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q\right)\varphi = 0$$ [Backward reaction-diffusion PDE]

$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\varphi} = 0$$ [Forward reaction-diffusion PDE]

Quantum: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \Psi(\boldsymbol{x}, t)\widehat{\Psi}(\boldsymbol{x}, t)$ [Born's relation]

wave function

$$\left(\sqrt{-1}\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q\right)\Psi = 0$$ [Schrödinger PDE]

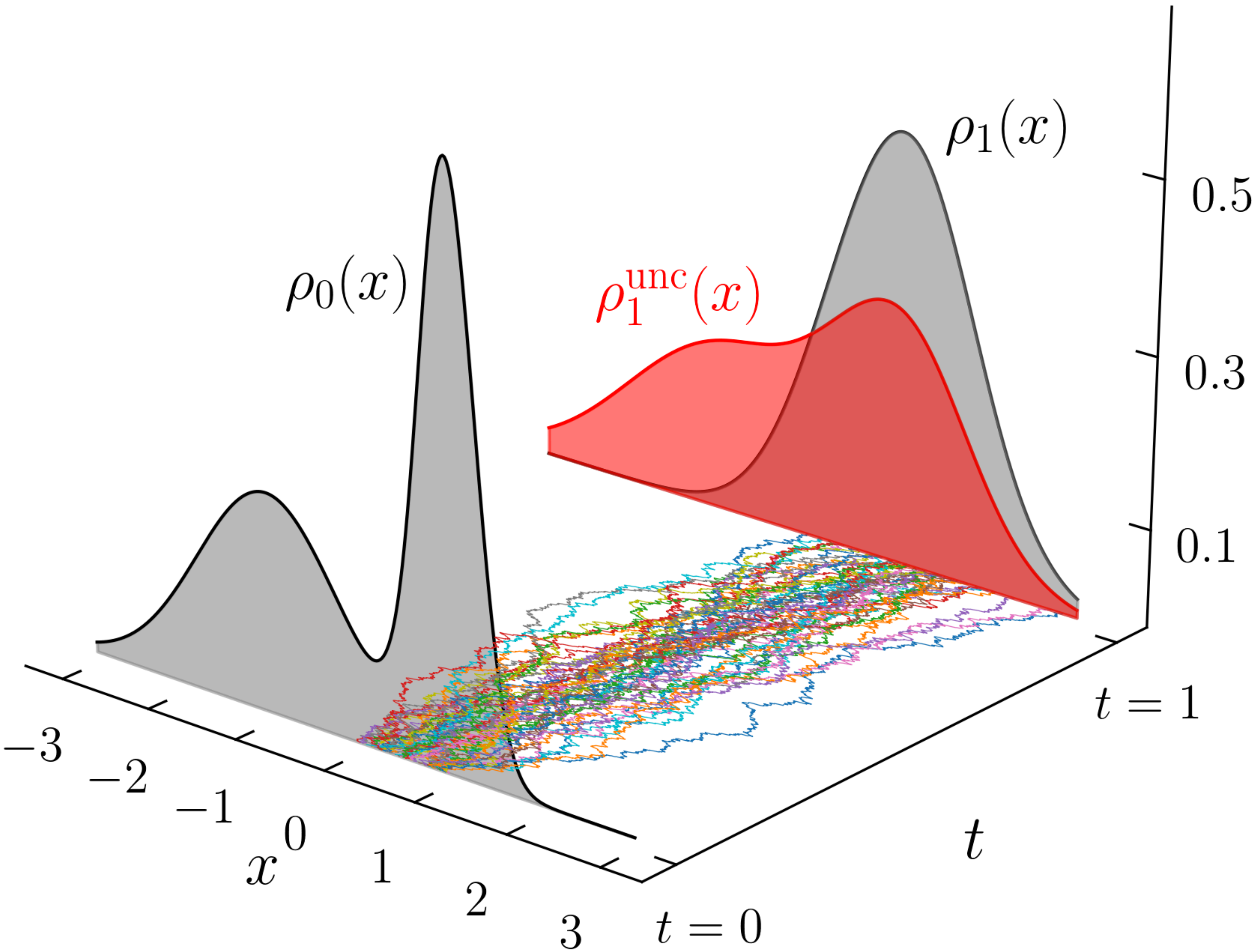
$$\left(-\sqrt{-1}\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\Psi} = 0$$ [Adjoint Schrödinger PDE]

Fixed Point Recursion Over Pair $\left(\varphi_1, \hat{\varphi}_0\right)$

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\hat{\varphi}_0(\boldsymbol{x}) \arrow[r, "\int \mathcal{L}_{\text{forward}}"] & \hat{\varphi}_1(\boldsymbol{x}) \arrow[d, "\rho_1(\boldsymbol{x}) \oslash \hat{\varphi}_1(\boldsymbol{x})"] \\
\varphi_0(\boldsymbol{x}) \arrow[u, "\rho_0(\boldsymbol{x}) \oslash \varphi_0(\boldsymbol{x})"] & \varphi_1(\boldsymbol{x}) \arrow[l, "\int \mathcal{L}_{\text{backward}}"]
\end{tikzcd}
$$

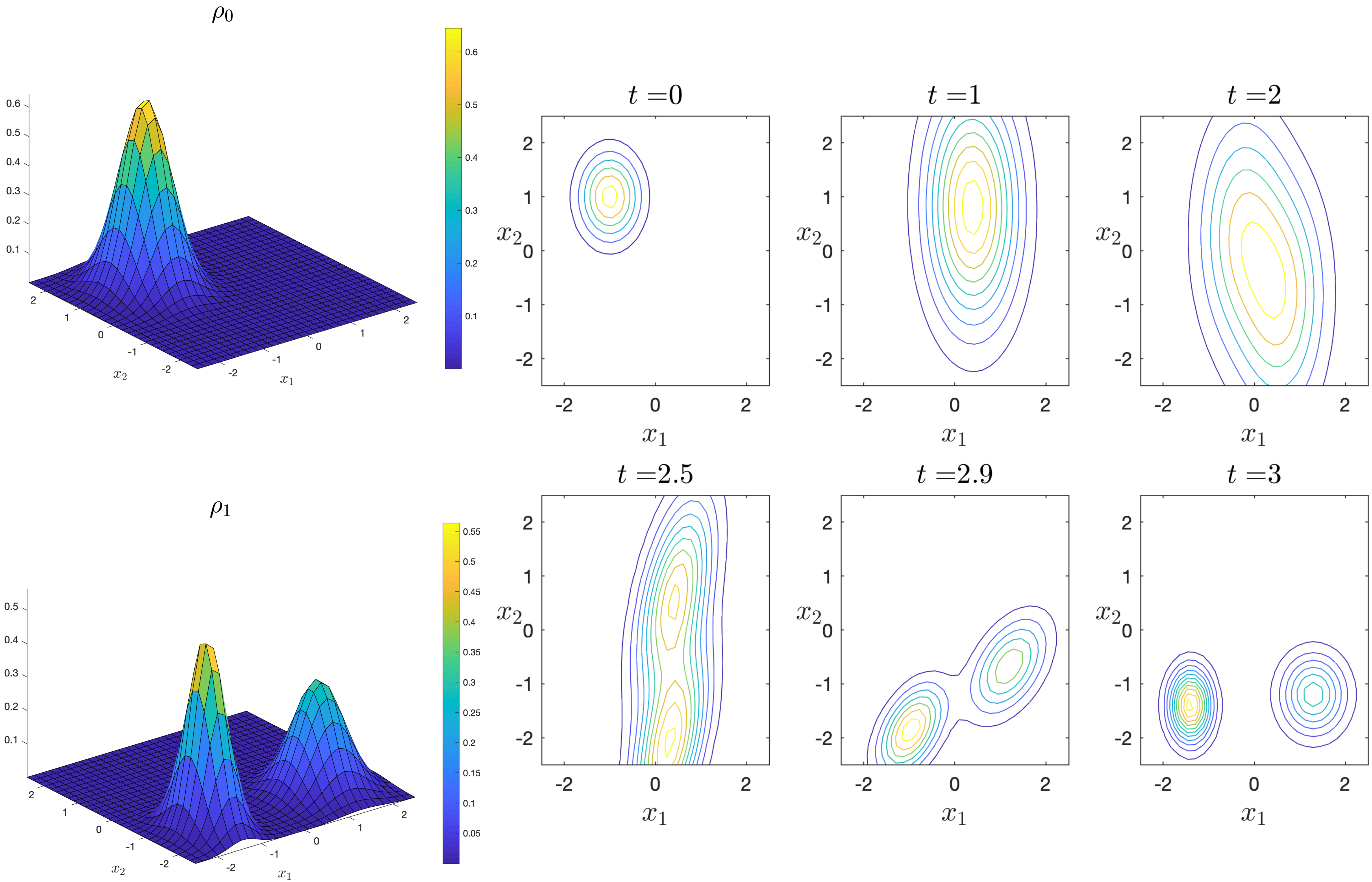
This recursion is contractive in the Hilbert's projective metric!!

Feedback Density Control: $\boldsymbol{f} \equiv \mathbf{0}, \boldsymbol{B} = \boldsymbol{G} \equiv \boldsymbol{I}, q \equiv 0$



Zero prior dynamics

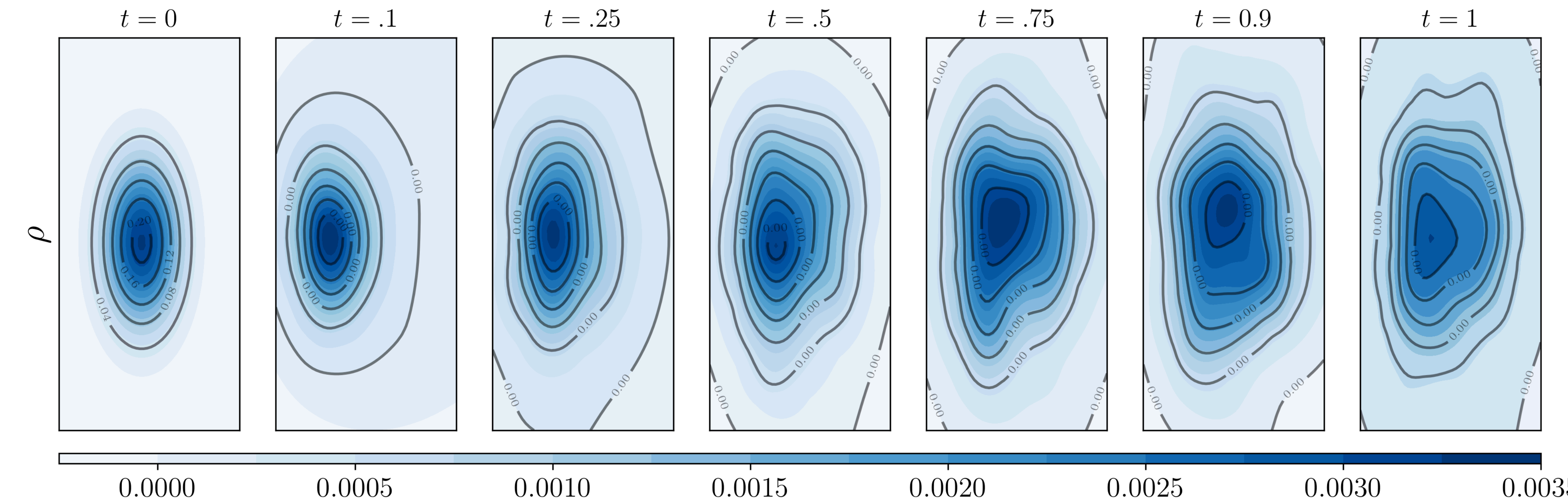
Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$



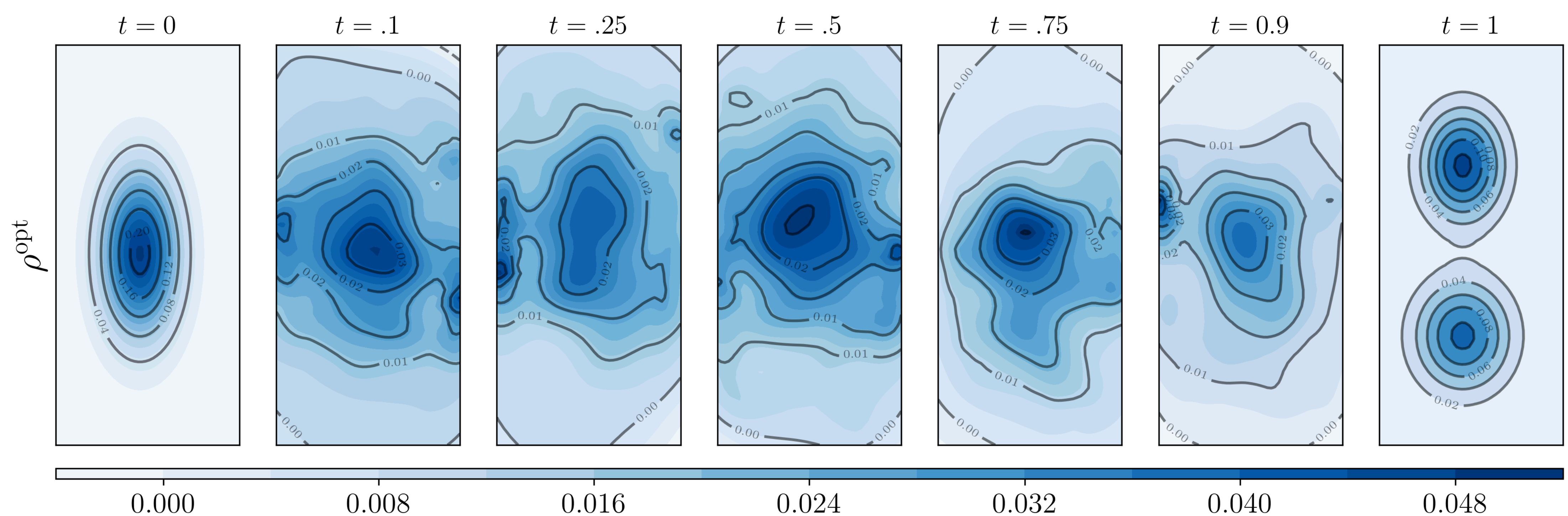
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

Uncontrolled joint PDF evolution:



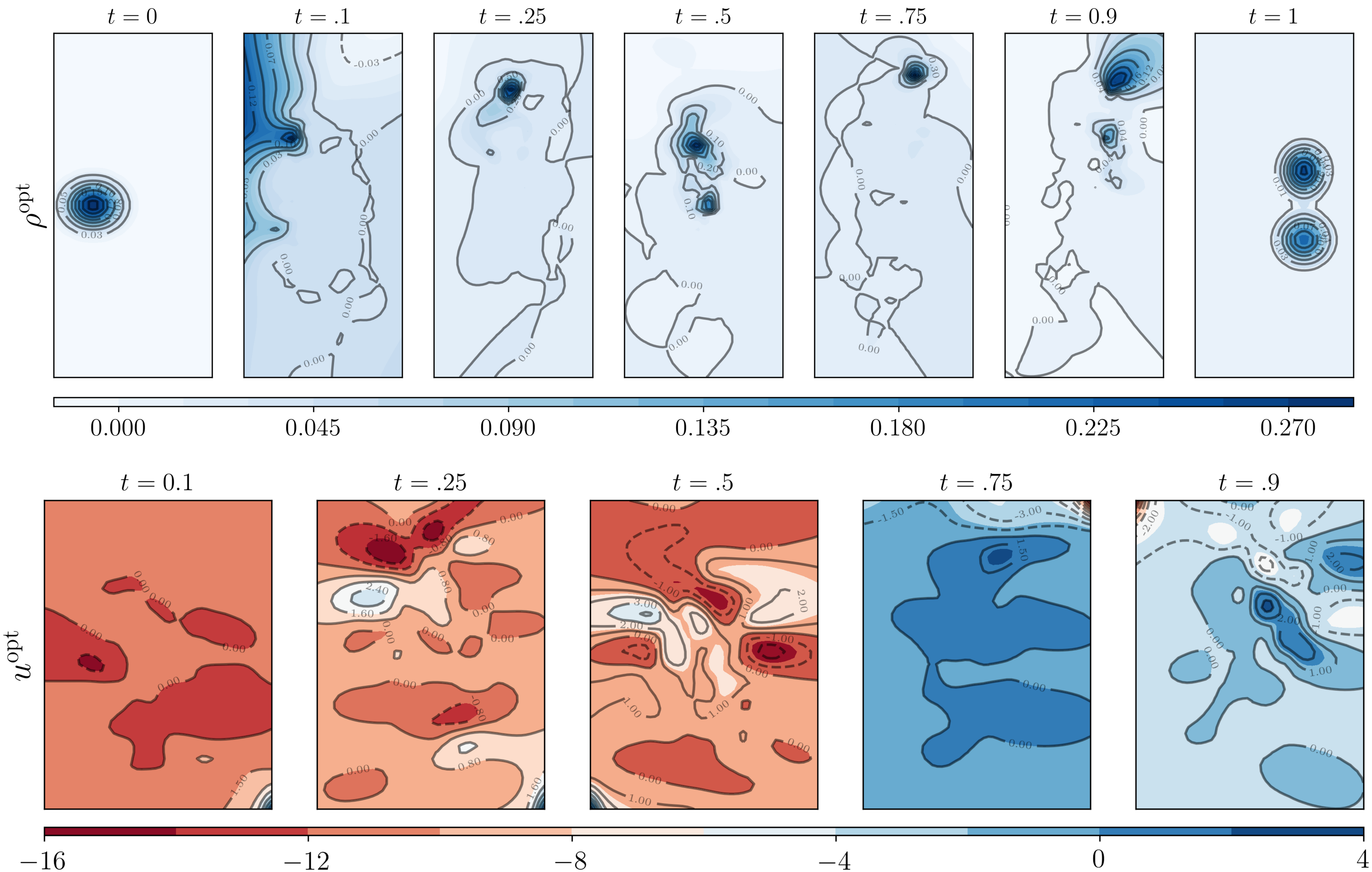
Optimal controlled joint PDF evolution:



K.F. Caluya, and A.H., *TAC 2022*

K.F. Caluya, and A.H., *TAC 2019*

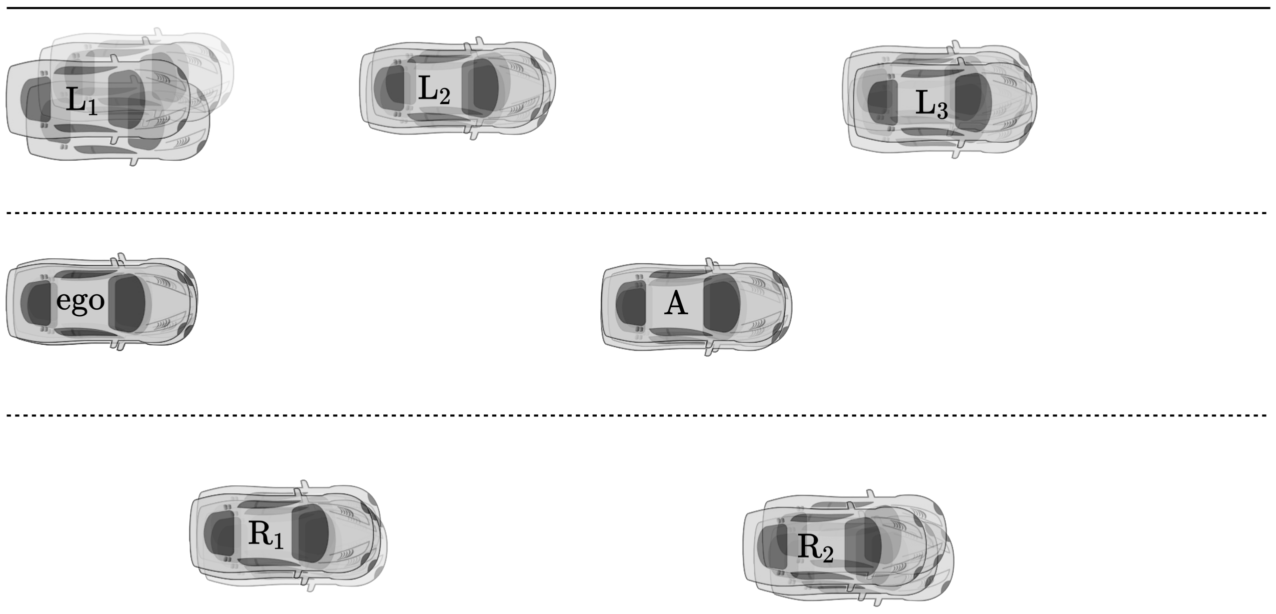
Feedback Density Control: Mixed Conservative-Dissipative Drift

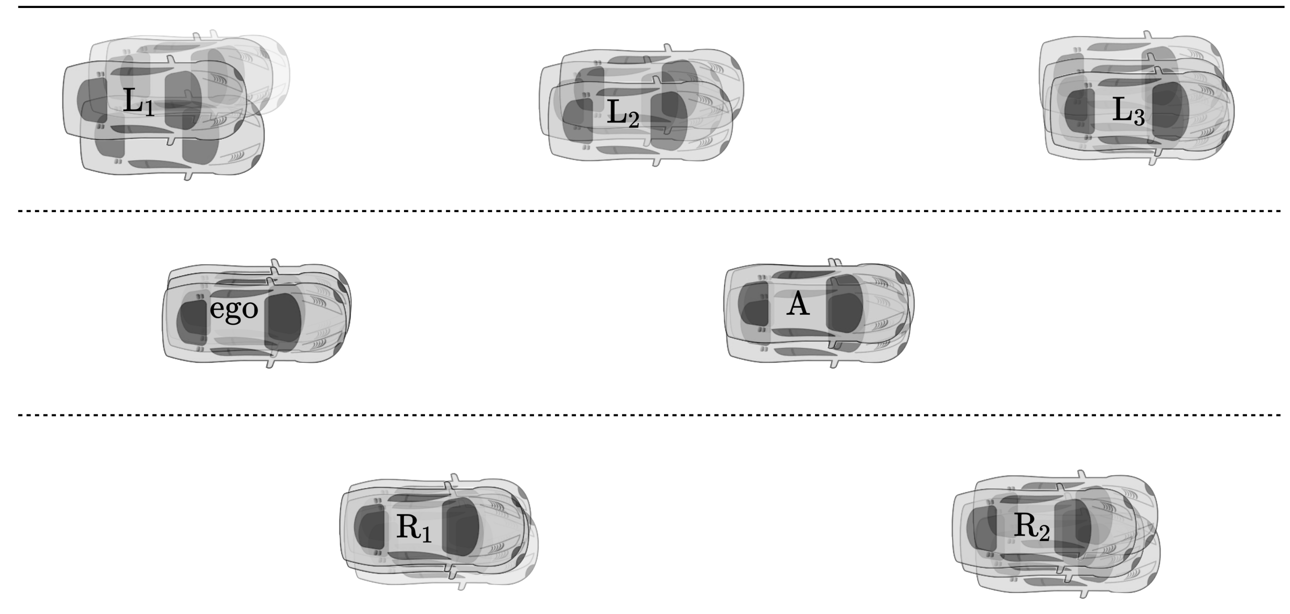


K.F. Caluya, and A.H., *TAC 2022*

K.F. Caluya, and A.H., *TAC 2019*

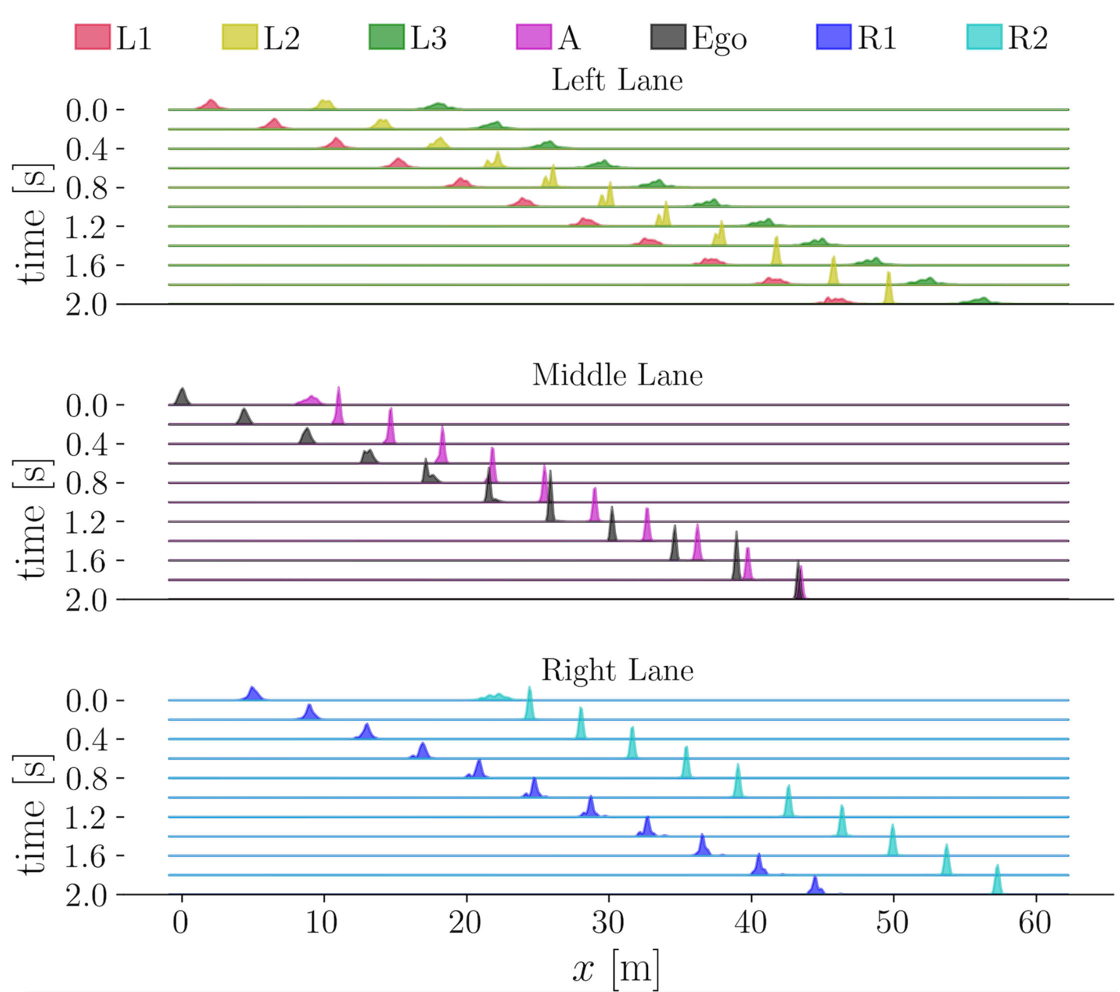
Application: Multi-lane Automated Driving



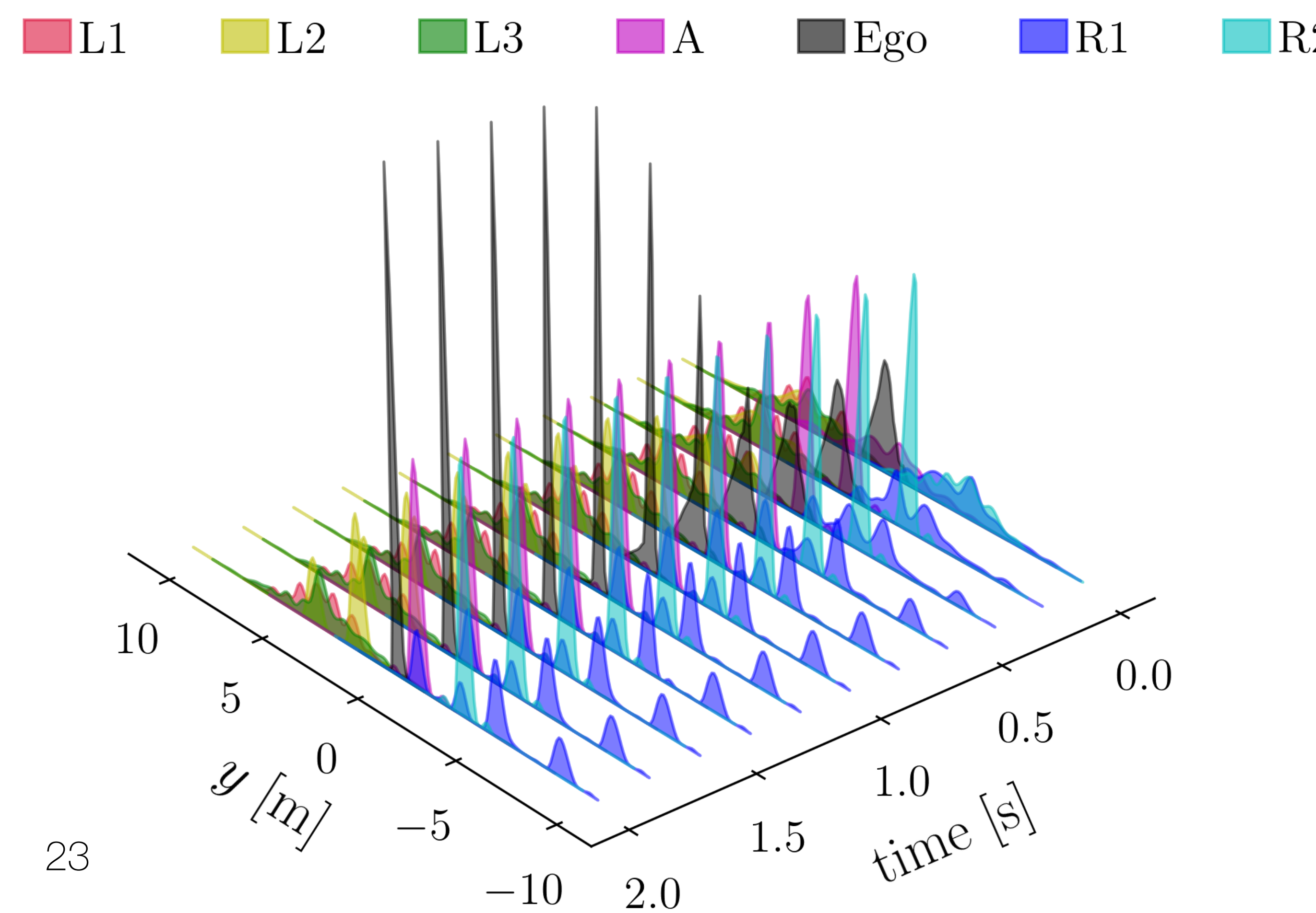


t_0 → t_1

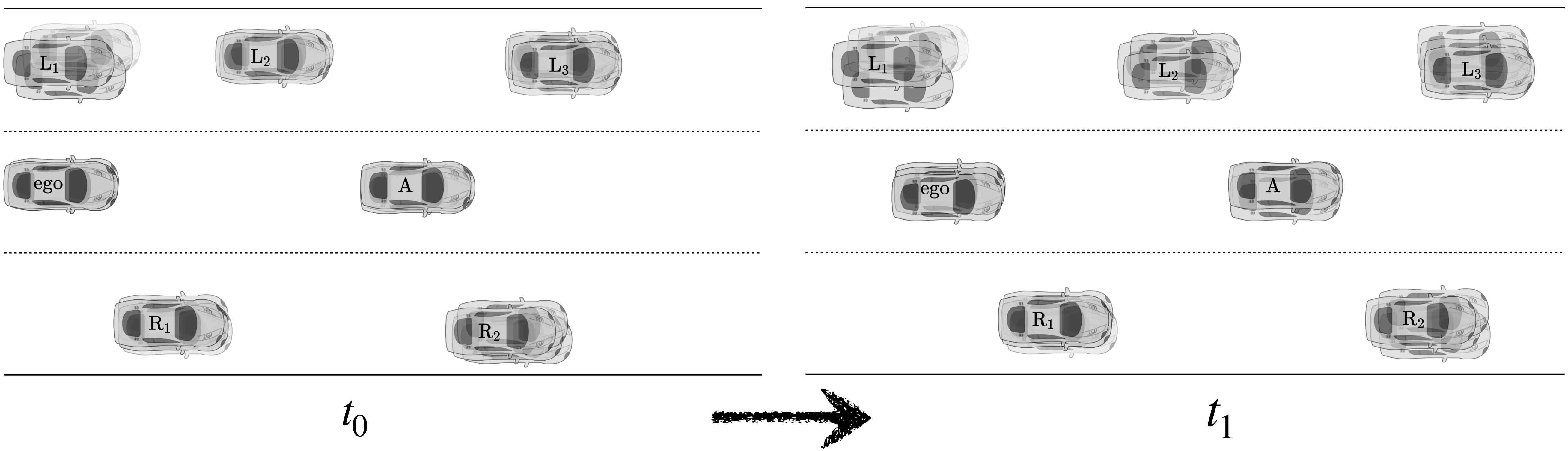
x marginals

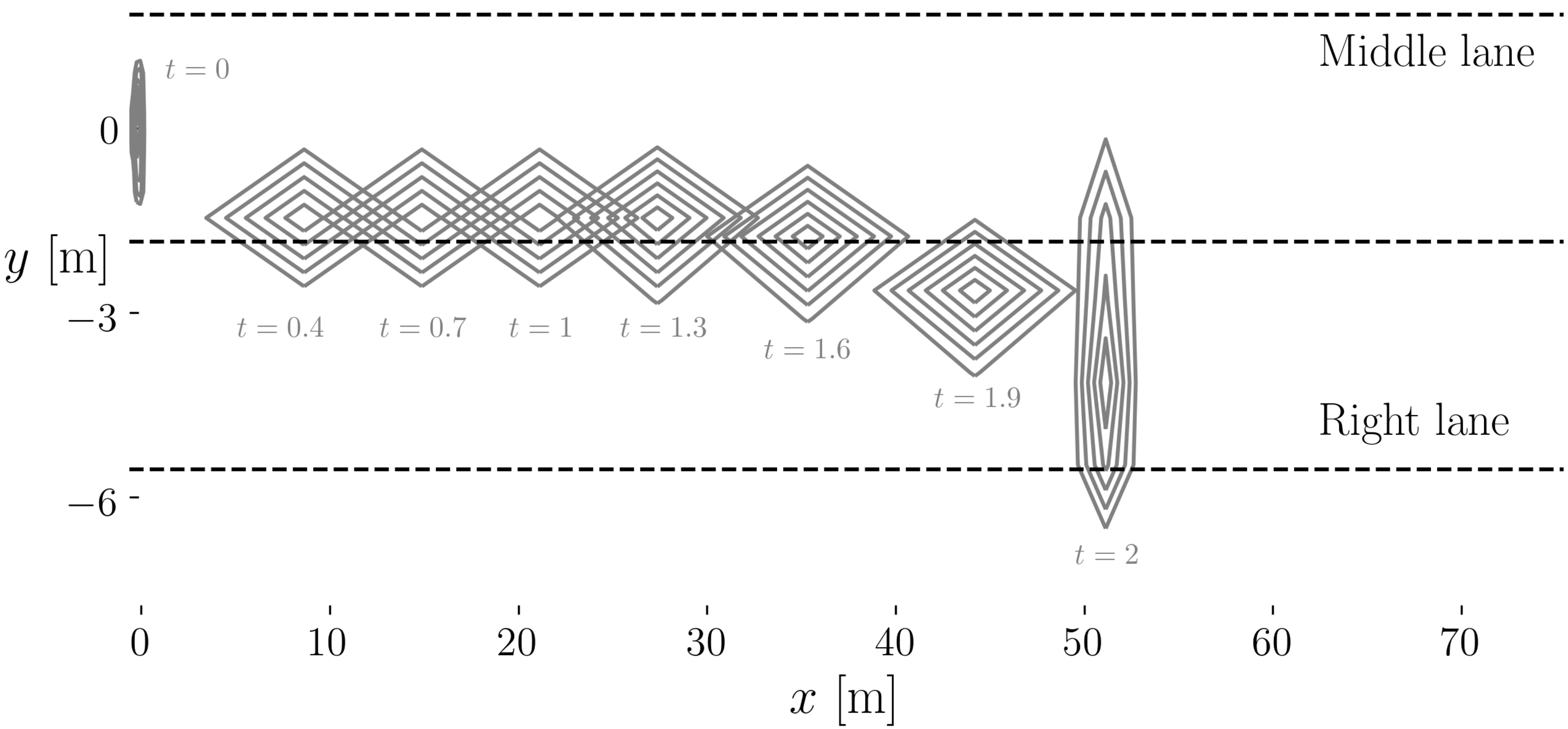


y marginals



Application: Multi-lane Automated Driving





S. Haddad, K.F. Caluya, A.H., and B. Singh, *LCSS 2020*

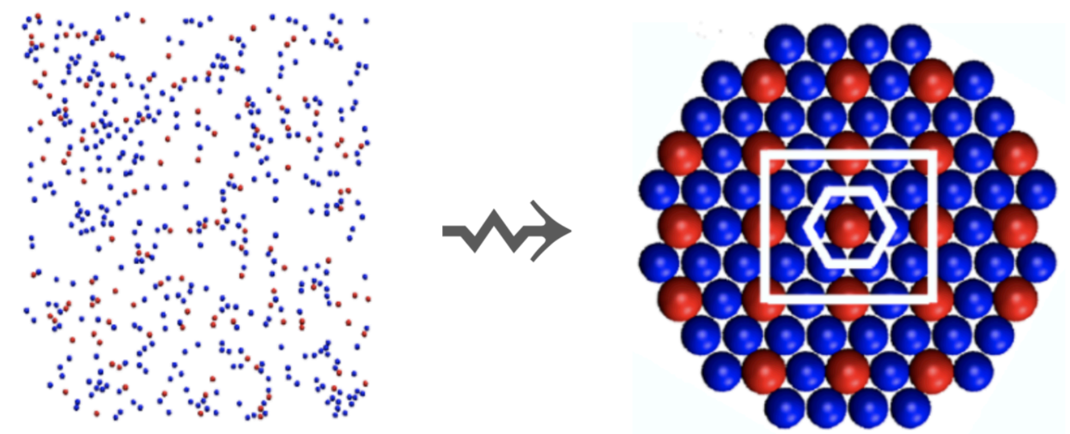
Control non-affine generalized Schrödinger bridge

No state cost: $q = 0$

Controlled SDE:

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

Controlled diffusion tensor: $\boldsymbol{G} := \boldsymbol{g}\boldsymbol{g}^\top \succeq \boldsymbol{0}$



Conditions for optimality: system of $m + 2$ coupled PDEs

$$\begin{aligned}
\frac{\partial \psi}{\partial t} &= \frac{1}{2}\|\boldsymbol{u}_{\mathrm{opt}}\|_2^2 - \langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle - \langle \boldsymbol{G}, \mathrm{Hess}(\psi)\rangle \\
\frac{\partial \rho_{\mathrm{opt}}^{\boldsymbol{u}}}{\partial t} &= -\nabla \cdot \left(\rho_{\mathrm{opt}}^{\boldsymbol{u}} \boldsymbol{f}\right) + \Delta_{\boldsymbol{G}} \rho_{\mathrm{opt}}^{\boldsymbol{u}} \\
\boldsymbol{u}_{\mathrm{opt}} &= \nabla_{\boldsymbol{u}_{\mathrm{opt}}}\left(\langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle + \langle \boldsymbol{G}, \mathrm{Hess}(\psi)\rangle\right) \\
\rho_{\mathrm{opt}}^{\boldsymbol{u}}(0, \boldsymbol{x}) &= \rho_0, \quad \rho_{\mathrm{opt}}^{\boldsymbol{u}}(T, \boldsymbol{x}) = \rho_T
\end{aligned}$$

Known $\boldsymbol{f}, \boldsymbol{g}$

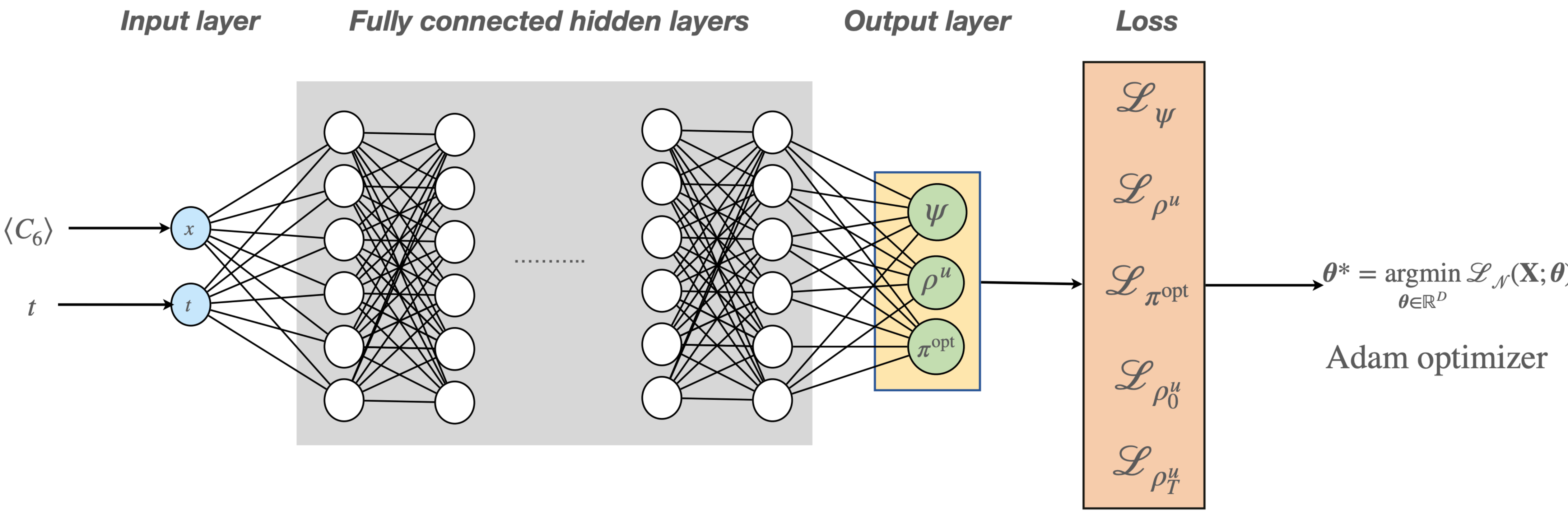
I. Nodozi, J.O'Leary, A. Mesbah, and A.H., ACC *2023*

2024 O. Hugo Schuck Best Application Paper Award

Data-driven $\boldsymbol{f}, \boldsymbol{g}$

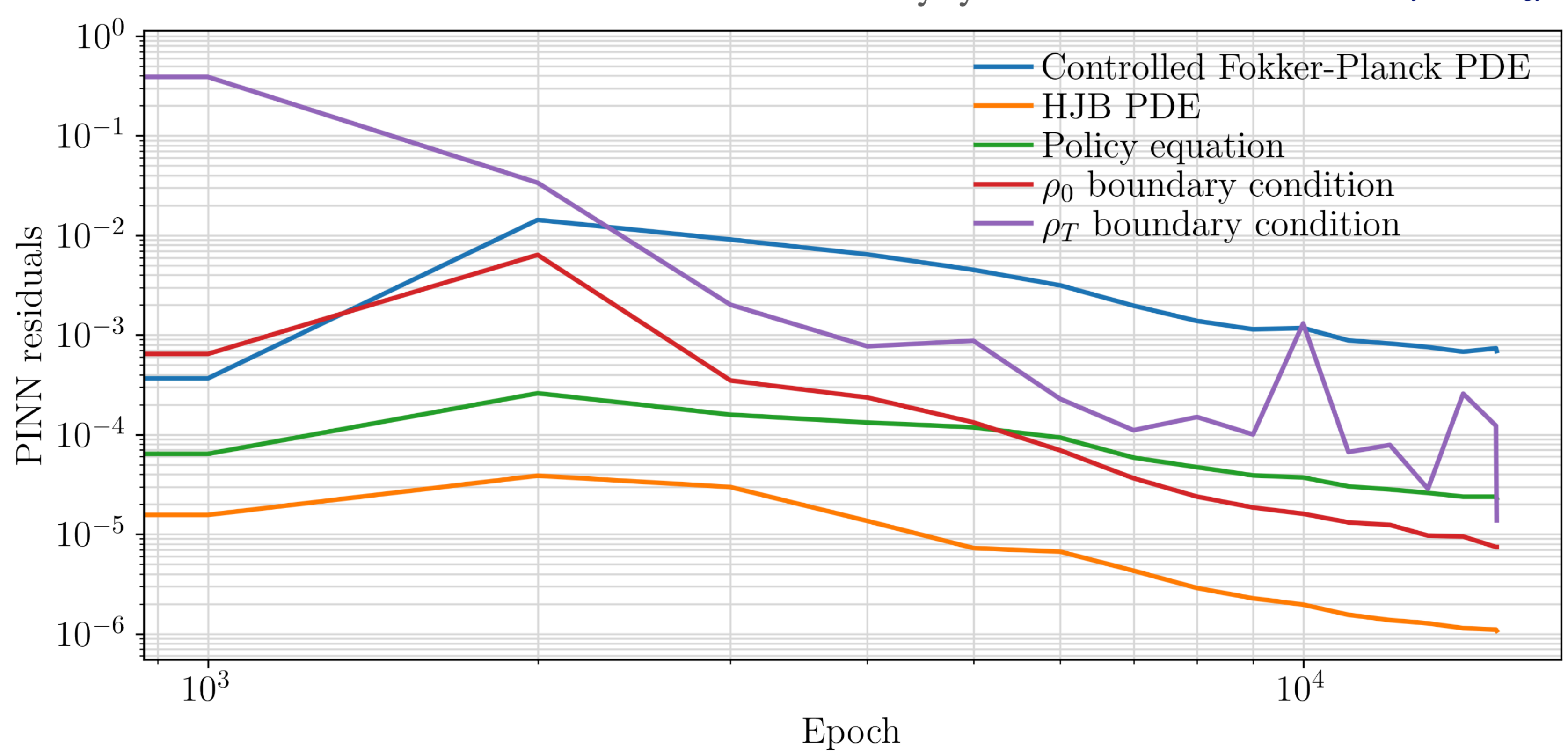
I. Nodozi, C. Yan, M. Khare, A.H., and A. Mesbah, *TCST 2024*

Control non-affine generalized Schrödinger bridge



$$\mathscr{L}_{\mathcal{N}} = \mathscr{L}_{\psi} + \mathscr{L}_{\rho^u} + \mathscr{L}_{\pi^{\text{opt}}} + \mathscr{L}_{\rho_0^u} + \mathscr{L}_{\rho_T^u}$$

Benchmark controlled self-assembly system: [Y Xue, et al, *IEEE Trans. Control Sys. Technology*, 2014]



Generalization #2: hard sample path constraints

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

K.F. Caluya, and A.H., *ACC 2021*

Reflected bridge: Schrödinger factor recursion

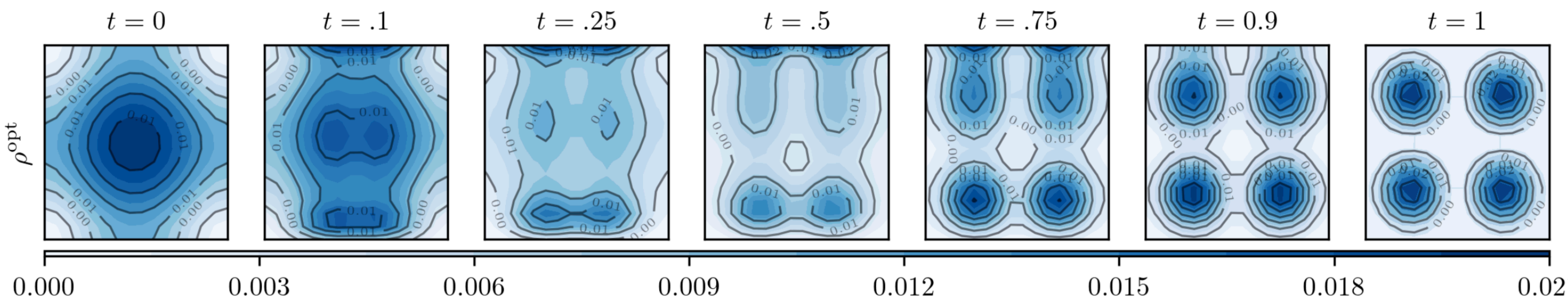
$$
\begin{tikzcd}
\hat{\varphi}_0(\boldsymbol{x}) \arrow[r, "\int \text{with b.c.} \left.\langle \boldsymbol{f}\hat{\varphi} - \theta\nabla\hat{\varphi}, \boldsymbol{n}\rangle\right|_{\partial\mathcal{X}} = 0"] & \hat{\varphi}_1(\boldsymbol{x}) \arrow[d, "\rho_1(\boldsymbol{x}) \oslash \hat{\varphi}_1(\boldsymbol{x})"]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

K.F. Caluya, and A.H., *ACC 2021*

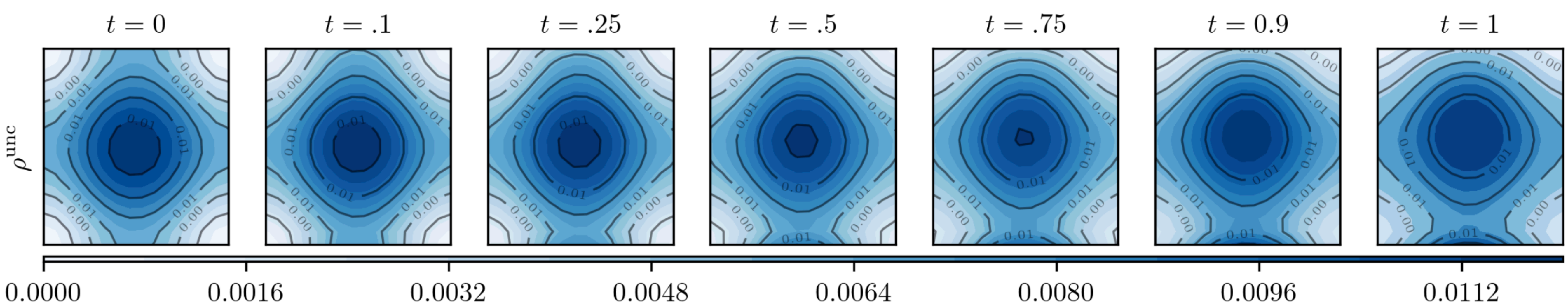
Reflected bridge: numerics with ∇V drift

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

Optimal controlled state PDFs:



Uncontrolled state PDFs:

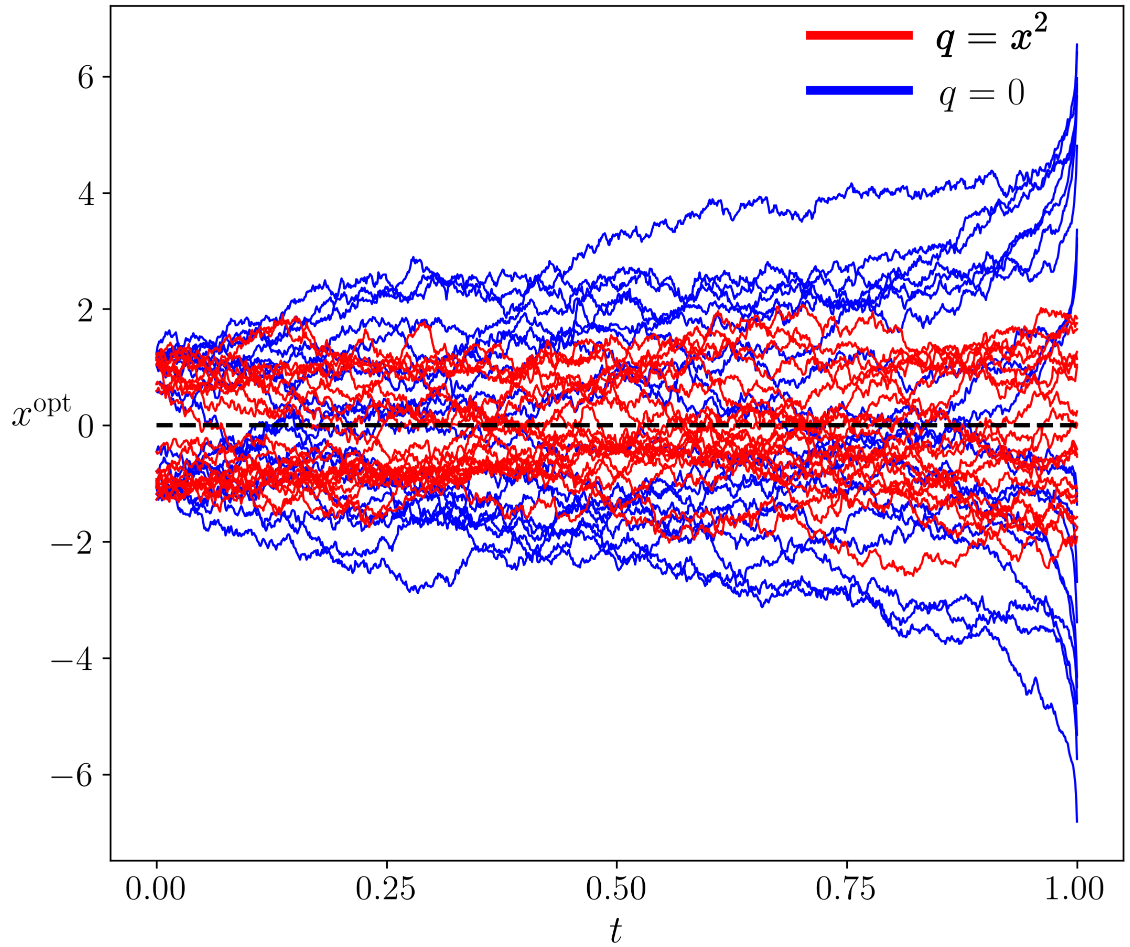


K.F. Caluya, and A.H., *ACC 2021*

Generalization #3: additive state cost ($q \neq 0$)

Question. Where does state cost come from?

Answer 1. From extra regularization (e.g., classical LQ optimal control)



Answer 2. Problem reformulation (push dynamical nonlinearity to Lagrangian)

Probabilistic Lambert Problem: Connections with Optimal Mass Transport, Schrödinger Bridge and Reaction-Diffusion PDEs*

Alexis M.H. Teter[†], Iman Nodozi[‡], and Abhishek Halder[§]

A.M. Teter, I. Nodozi, and A.H., ***arXiv:2401.07961***

Schrödinger bridge with quadratic state cost: $q(x) = x^\top Q x, Q \geq 0$

Solution: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \varphi(\boldsymbol{x}, t)\widehat{\varphi}(\boldsymbol{x}, t)$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q\right)\varphi = 0$$

[Backward reaction-diffusion PDE]

$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\varphi} = 0$$

[Forward reaction-diffusion PDE]

Schrödinger bridge with quadratic state cost: $q(x) = x^\top Q x, Q \geq 0$

We know: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \varphi(\boldsymbol{x}, t)\widehat{\varphi}(\boldsymbol{x}, t)$

$$\left(\frac{\partial}{\partial t} + \cancel{\frac{1}{2}}\Delta - q\right)\varphi = 0$$

[Backward reaction-diffusion PDE]

$$\boxed{\left(\frac{\partial}{\partial t} - \cancel{\frac{1}{2}}\Delta + q\right)\widehat{\varphi} = 0}$$

[Forward reaction-diffusion PDE]

Need kernel/Green's function $\kappa\left(0, \boldsymbol{x}; t, \boldsymbol{y}\right)$

for IVP solutions to use in Schrödinger factor recursion:

$$\frac{\partial \widehat{\varphi}}{\partial t} = \underbrace{\mathcal{L}_{\text{forward}}}_{(\Delta - \boldsymbol{x}^\top \boldsymbol{Q} x)} \widehat{\varphi}, \quad \widehat{\varphi}(t=0, \boldsymbol{x}) = \widehat{\varphi}_0 \quad \Leftrightarrow \quad \widehat{\varphi}(\boldsymbol{x}, t) = \int_{\mathbb{R}^n} \boxed{\kappa(0, \boldsymbol{x}; t, \boldsymbol{z})}\,\widehat{\varphi}_0(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$$

Schrödinger bridge with quadratic state cost: $q(x) = x^\top Q x, Q \succ 0$

Thm. Eig. decomposition: $\boldsymbol{Q} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^\top$

Then, $\widehat{\varphi}(\boldsymbol{x}, t) = \eta(\boldsymbol{y} = \boldsymbol{V}\boldsymbol{x}, t)$ where $\eta(\boldsymbol{y}, t) = \int_{\mathbb{R}^n} \kappa(0, \boldsymbol{y}; t, \boldsymbol{z})\eta_0(\boldsymbol{z})\mathrm{d}\boldsymbol{z}$

and

$$\kappa(0, \boldsymbol{y}; t, \boldsymbol{z}) = \frac{(\det(\boldsymbol{D}))^{1/4}}{\sqrt{(2\pi)^n \det\left(\sinh(2t\sqrt{\boldsymbol{D}})\right)}} \exp\left(-\frac{1}{2}(\boldsymbol{y} \quad \boldsymbol{z})\boldsymbol{M}\begin{pmatrix}\boldsymbol{y}\\ \boldsymbol{z}\end{pmatrix}\right)$$

$$\boldsymbol{M} := \begin{bmatrix}\boldsymbol{D}^{1/4} & \boldsymbol{0}_{n\times n}\\ \boldsymbol{0}_{n\times n} & \boldsymbol{D}^{1/4}\end{bmatrix}\boldsymbol{M}_1\boldsymbol{M}_2\begin{bmatrix}\boldsymbol{D}^{1/4} & \boldsymbol{0}_{n\times n}\\ \boldsymbol{0}_{n\times n} & \boldsymbol{D}^{1/4}\end{bmatrix}, \; \boldsymbol{M}_1 := \begin{bmatrix}\cosh\left(2t\sqrt{\boldsymbol{D}}\right) & -\boldsymbol{I}_n\\ -\boldsymbol{I}_n & \cosh\left(2t\sqrt{\boldsymbol{D}}\right)\end{bmatrix}, \; \boldsymbol{M}_2 := \begin{bmatrix}\operatorname{csch}\left(2t\sqrt{\boldsymbol{D}}\right) & \boldsymbol{0}\\ \boldsymbol{0} & \operatorname{csch}\left(2t\sqrt{\boldsymbol{D}}\right)\end{bmatrix}$$

$$\eta_0(\boldsymbol{y}) = \widehat{\varphi}_0(\boldsymbol{V}^\top\boldsymbol{x})$$

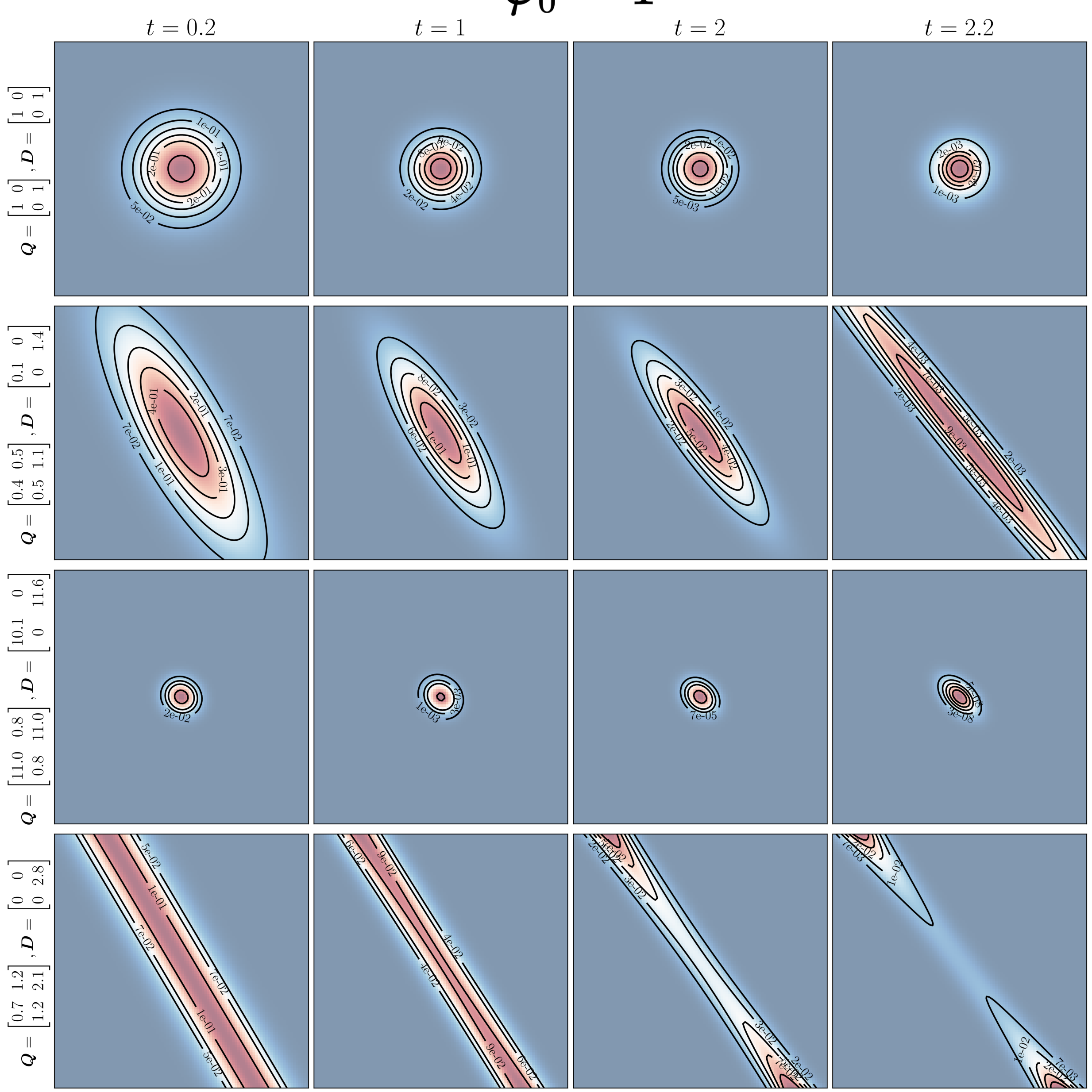
$\boldsymbol{Q} = \boldsymbol{I}$ recovers the multivariate Mehler kernel in quantum harmonic oscillator

Schrödinger bridge with quadratic state cost: $q(x) = x^\top Q x, Q \geq 0$

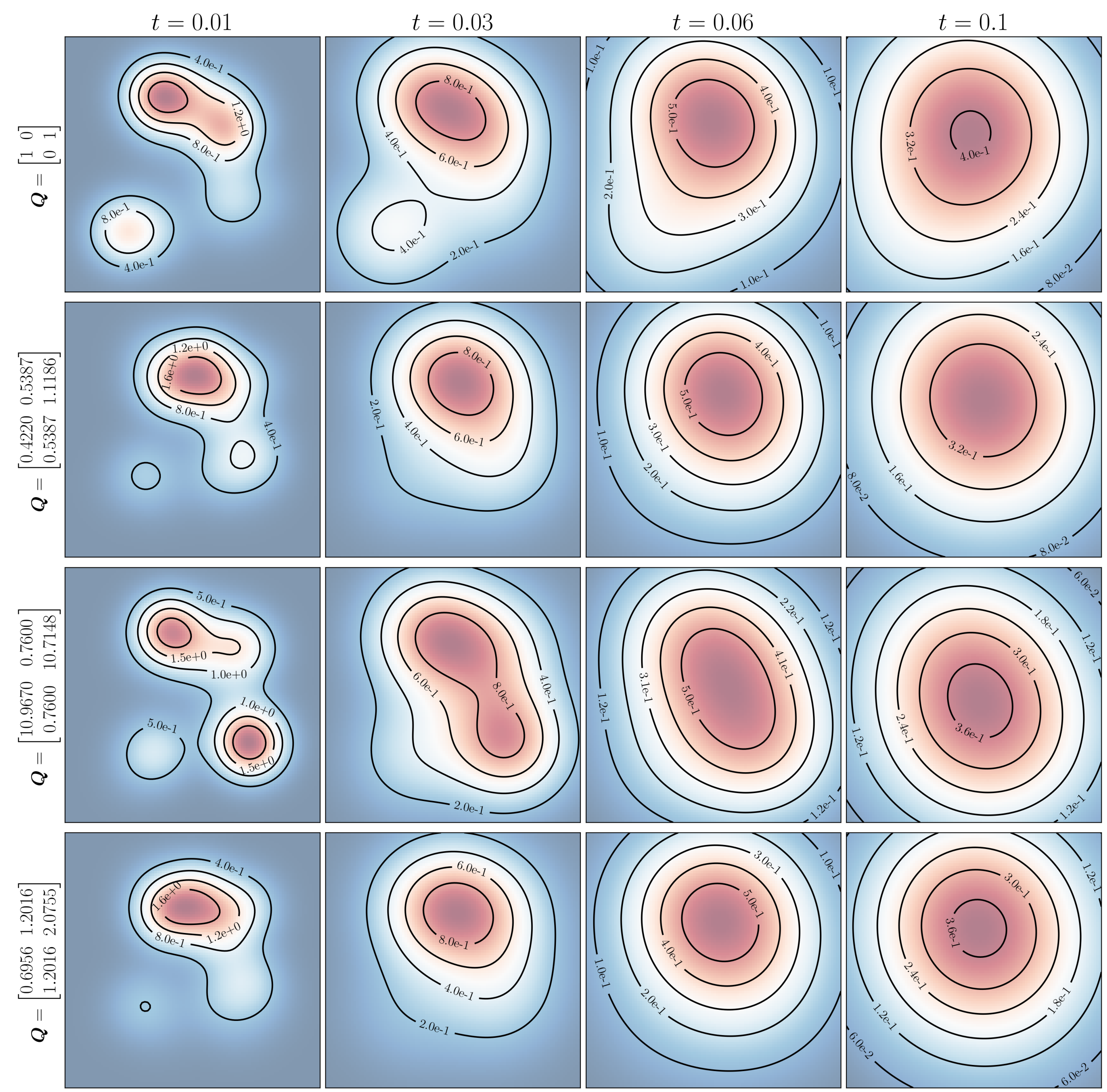
Thm. $$\kappa(0, \boldsymbol{y}; t, \boldsymbol{z}) = \underbrace{\kappa_+\left(0, \boldsymbol{y}_{[i_1:i_{n-p}]}; t, \boldsymbol{z}_{[i_1:i_{n-p}]}\right)}_{\text{derived pos def kernel in } n-p \text{ variables}} \underbrace{\kappa_0\left(0, \boldsymbol{y}_{[i_{n-p+1}:i_n]}; t, \boldsymbol{z}_{[i_{n-p+1}:i_n]}\right)}_{\text{heat kernel in } p \text{ variables}}$$

Action of kernel in x coordinates

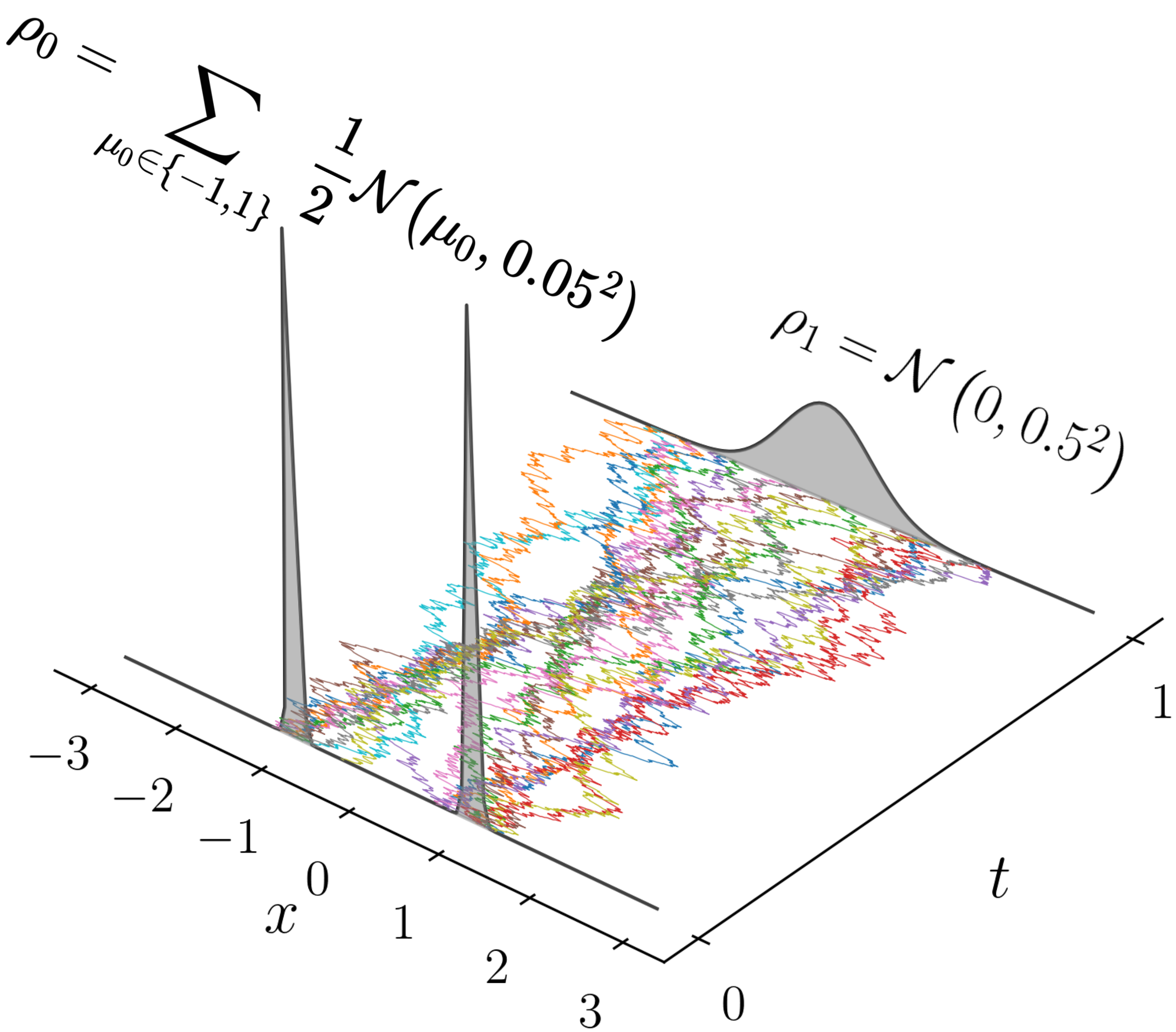
$\varphi_0 = 1$

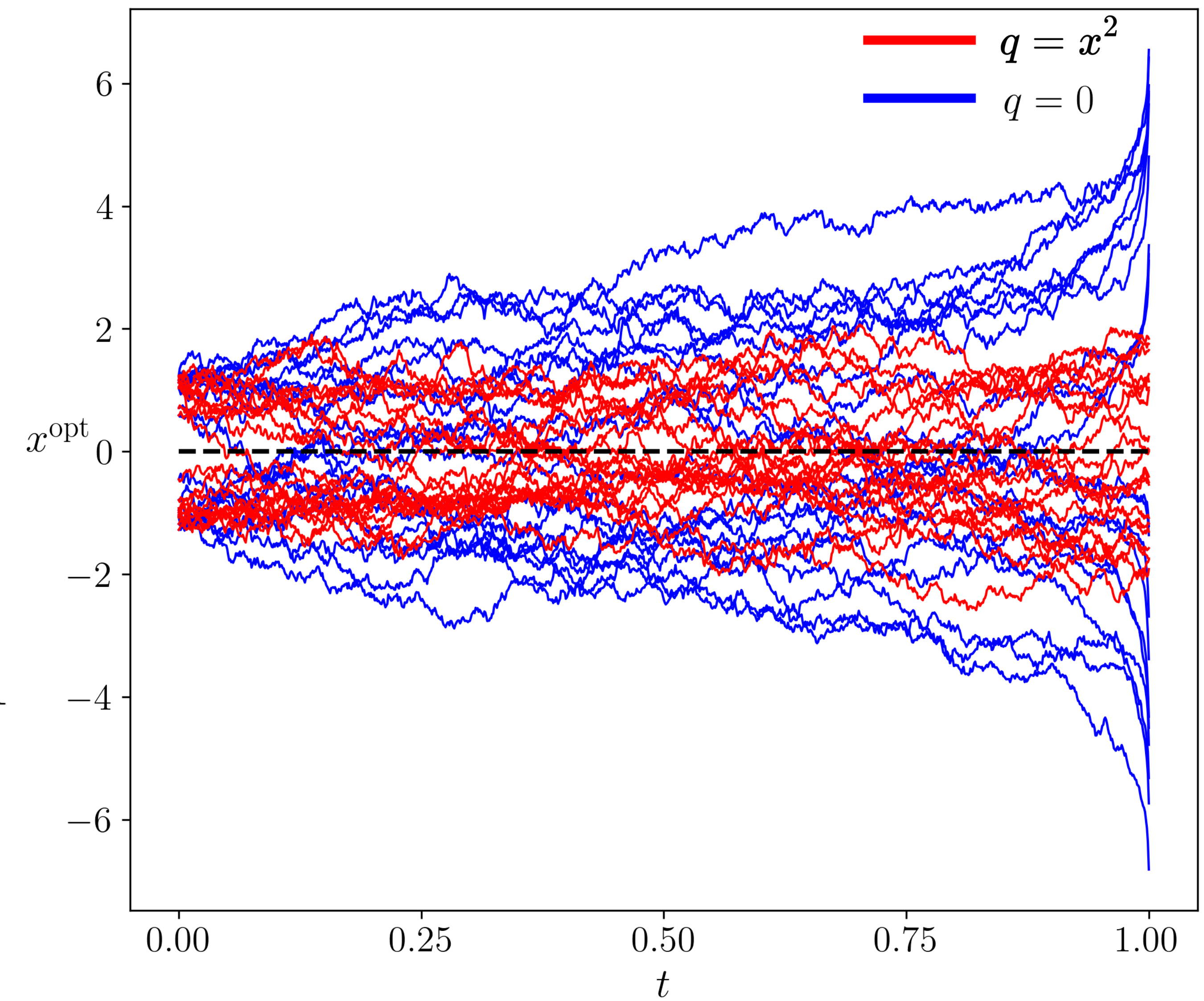


$$\varphi_0 \propto \exp\left\{-\frac{1}{25}\left(\left((10x_1-5)^2 + 10x_2 - 16\right)^2 + \left(10x_1 - 12 + (10x_2-5)^2\right)^2\right)\right\}$$



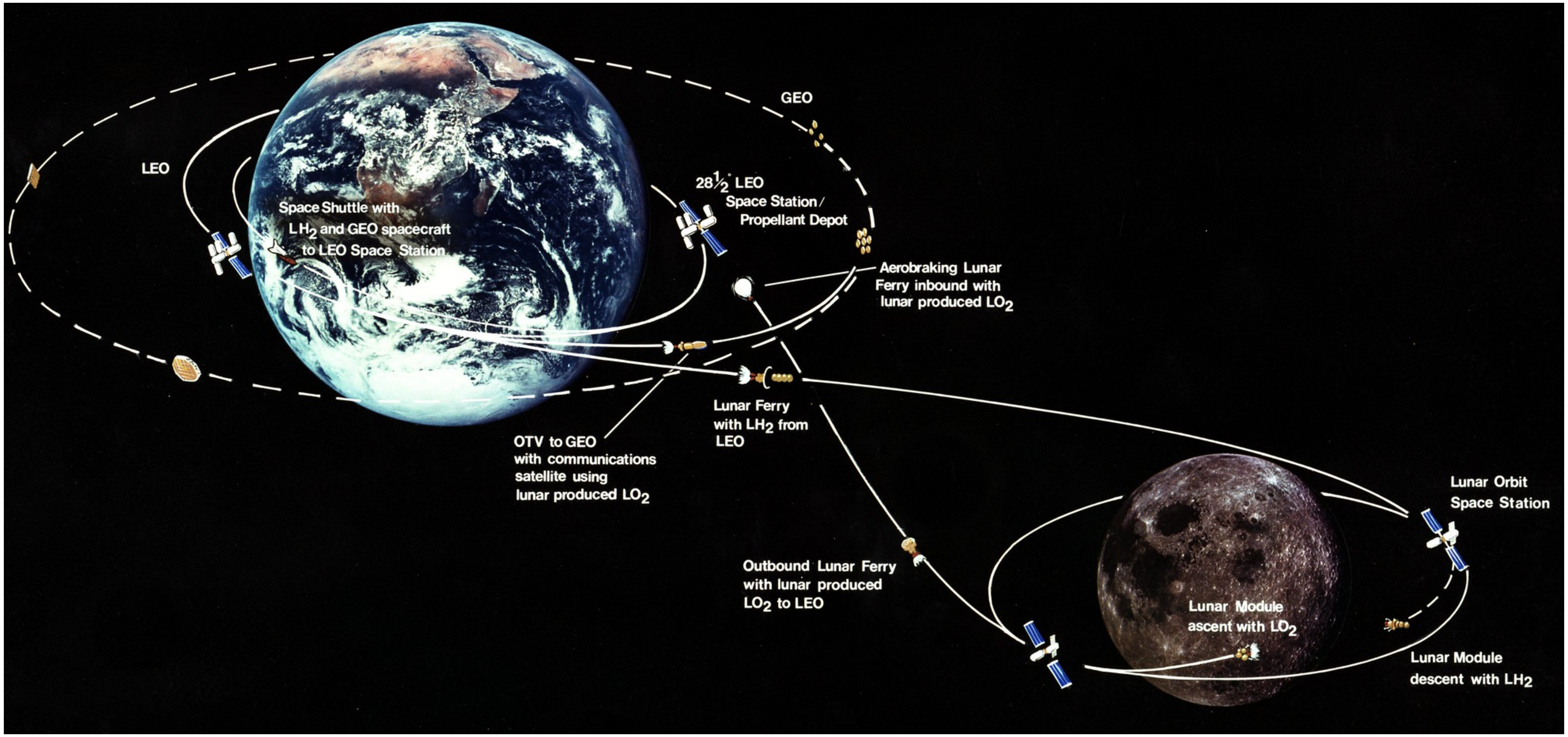
Schrödinger bridge in 1D: with vs without quadratic state cost





A.M. Teter, W. Wang, and A.H.,
arXiv:2406.00503
arXiv:2407.15245

Lambert's Problem

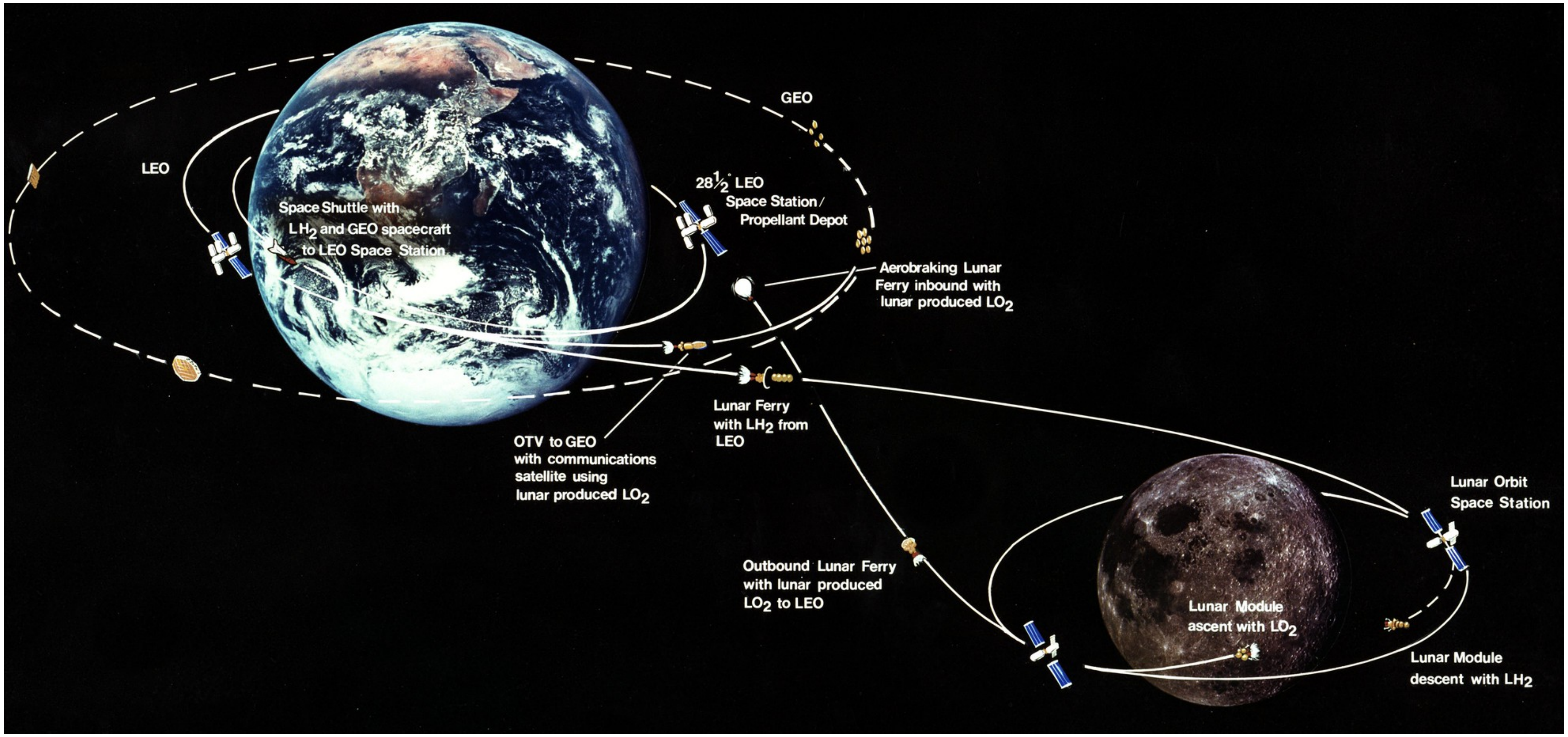


3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

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

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) = \boldsymbol{r}_0(\text{ given }), \quad \boldsymbol{r}(t = t_1) = \boldsymbol{r}_1(\text{ given })}$$

Lambert's Problem



3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

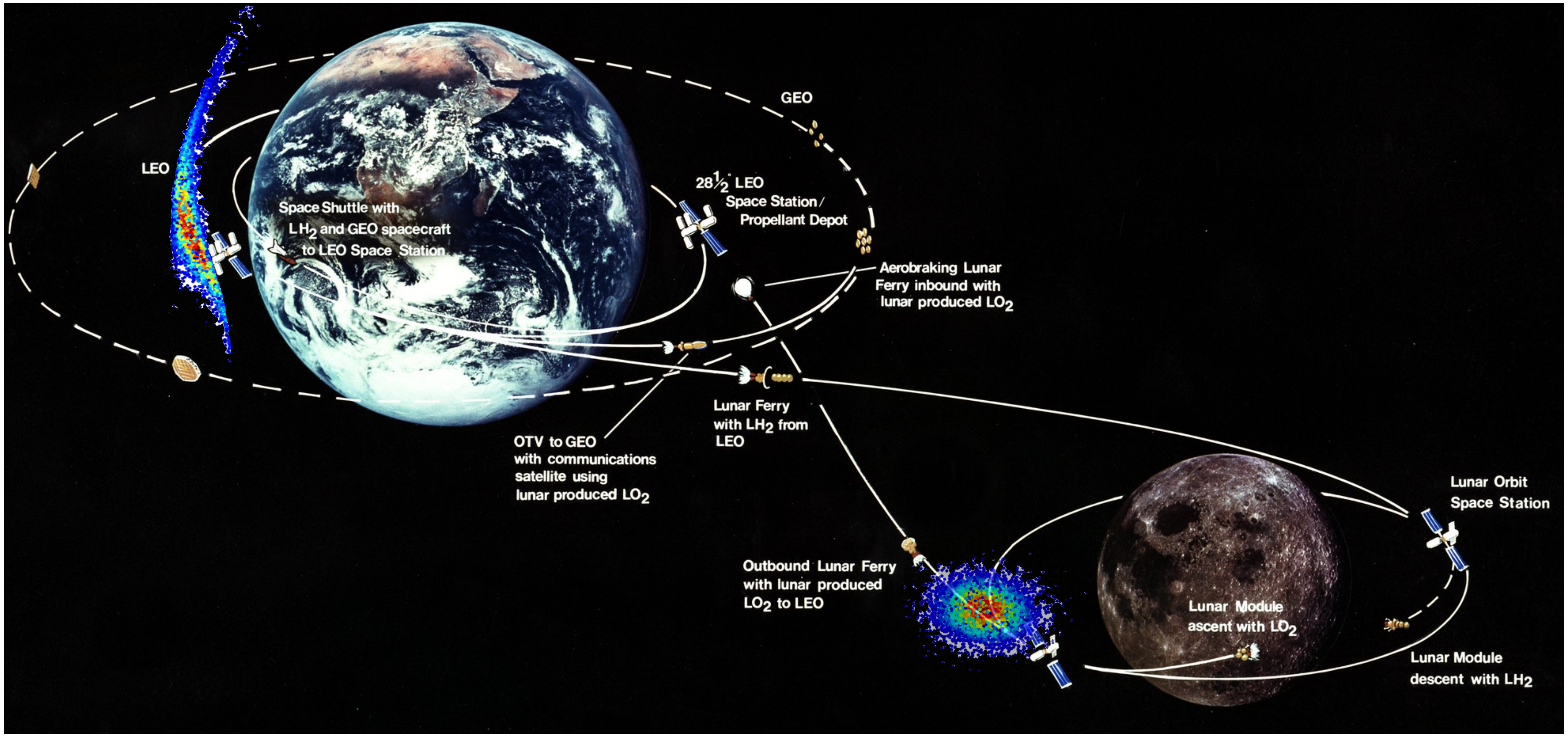
ODE is 2nd order but endpoint boundary conditions are first order

$\rightsquigarrow$ partially specified TPBVP

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

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) = \boldsymbol{r}_0(\text{ given }), \quad \boldsymbol{r}(t = t_1) = \boldsymbol{r}_1(\text{ given })}$$

Probabilistic Lambert's Problem



3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

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

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \boldsymbol{r}(t = t_1) \sim \rho_1 \text{ (given)}}$$

Probabilistic Lambert problem is OMT

$$\underset{(\rho,\boldsymbol{v})}{\arg\inf} \quad \int_{t_0}^{t_1} \mathbb{E}_{\rho}\left[\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right] \mathrm{d}t$$

$$\dot{\boldsymbol{r}} = \boldsymbol{v},$$

$$\boldsymbol{r}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \boldsymbol{r}(t = t_1) \sim \rho_1 \text{ (given)}$$

$$\Updownarrow$$

$$\underset{(\rho,\boldsymbol{v})}{\arg\inf} \quad \int_{t_0}^{t_1} \mathbb{E}_{\rho}\left[\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right] \mathrm{d}t$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}) = 0,$$ — **Liouville PDE**

$$\rho(t = t_0, \cdot) = \rho_0, \quad \rho(t = t_1, \cdot) = \rho_1$$

Connection to SBP with state cost

$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\arg\inf}\int_{t_0}^{t_1}\int_{\mathbb{R}^n}\left(\frac{1}{2}|\boldsymbol{v}|^2 - V(\boldsymbol{x})\right)\rho(\boldsymbol{x},t)\,d\boldsymbol{x}dt$$

$$\frac{\partial\rho}{\partial t}+\nabla_{\boldsymbol{r}}\cdot(\rho\boldsymbol{v})=0,$$ **— Liouville PDE**

$$\rho(t=t_0,\cdot)=\rho_0,\quad \rho(t=t_1,\cdot)=\rho_1$$

Lambertian SBP (L-SBP)

$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\arg\inf}\int_{t_0}^{t_1}\int_{\mathbb{R}^n}\left(\frac{1}{2}|\boldsymbol{v}|^2 - V(\boldsymbol{x})\right)\rho(\boldsymbol{x},t)\,d\boldsymbol{x}dt$$

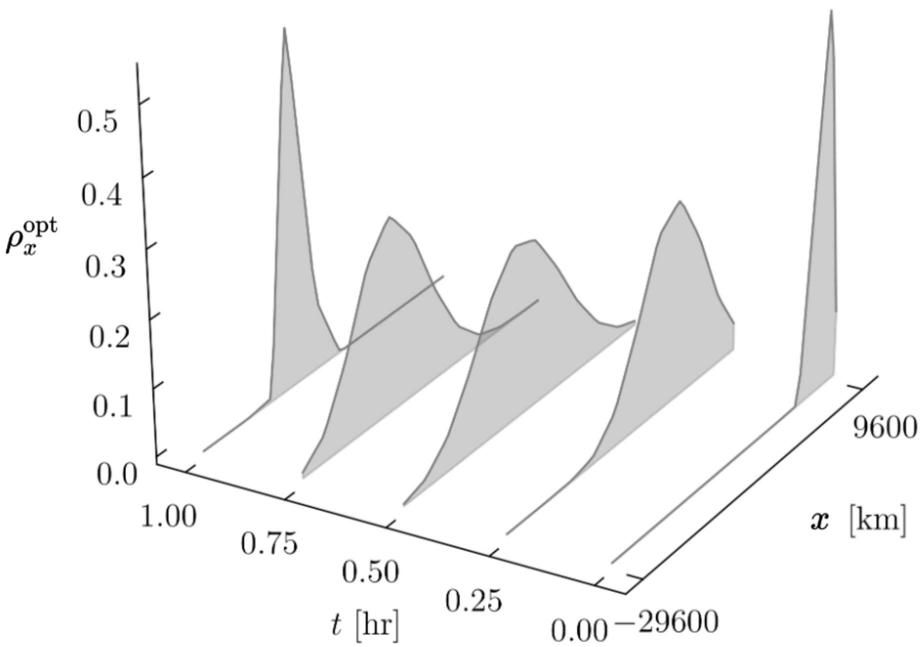
Regularization > 0

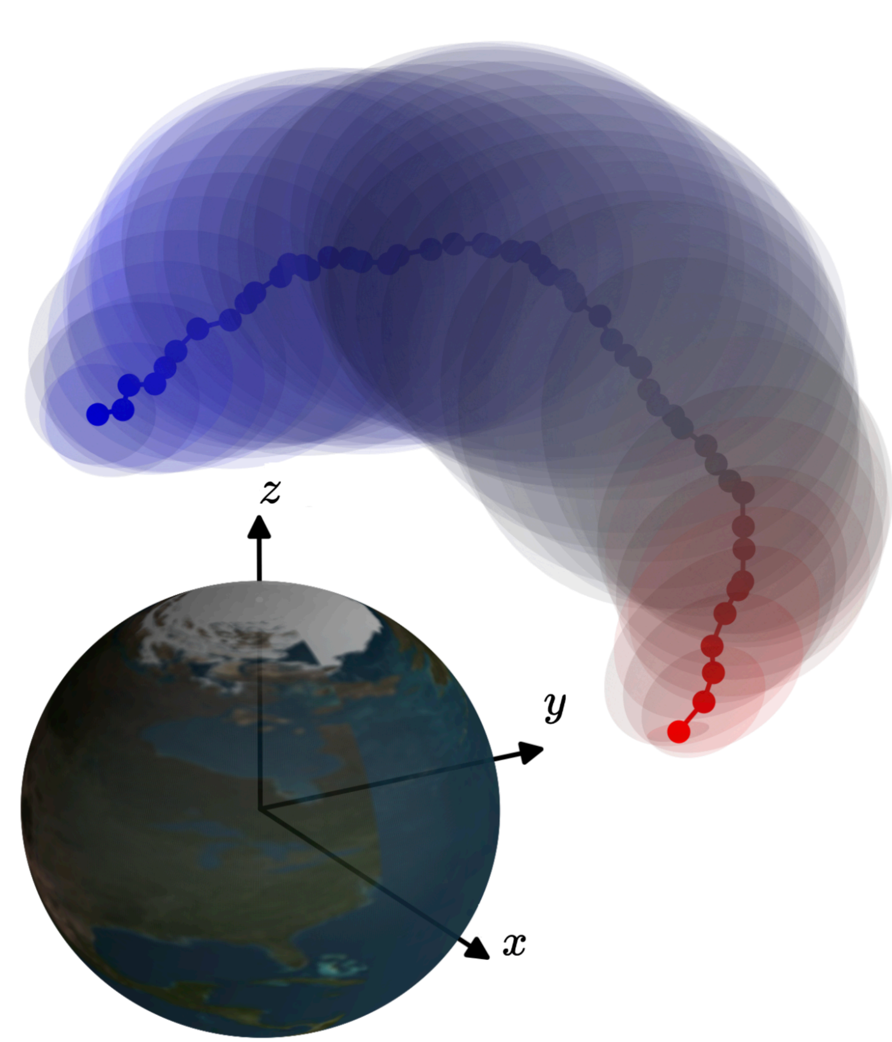
$$\frac{\partial\rho}{\partial t}+\nabla_{\boldsymbol{r}}\cdot(\rho\boldsymbol{v})=\varepsilon\Delta_{\boldsymbol{r}}\rho,$$ **— Fokker-Planck-Kolmogorov PDE**

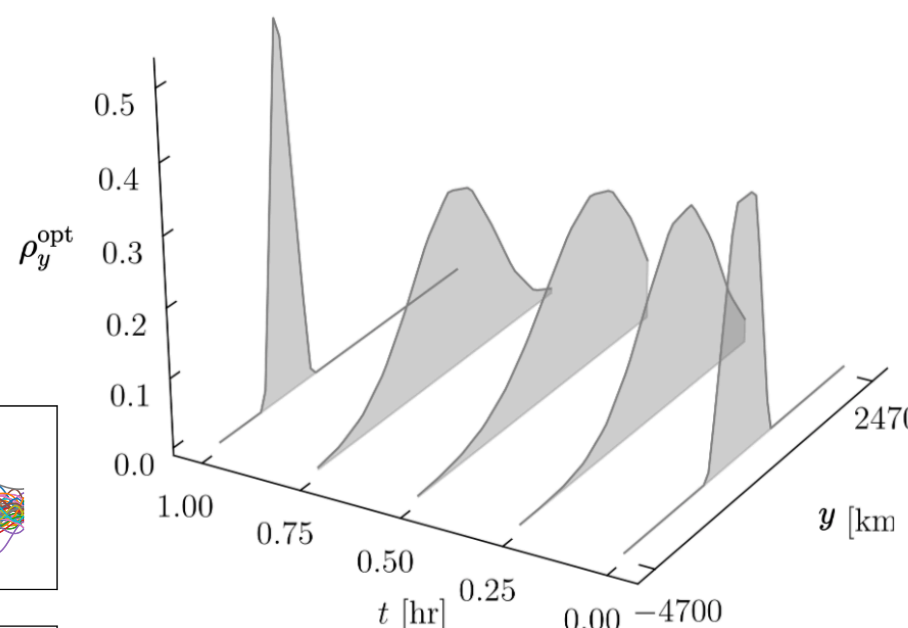
$$\rho(t=t_0,\cdot)=\rho_0,\quad \rho(t=t_1,\cdot)=\rho_1$$

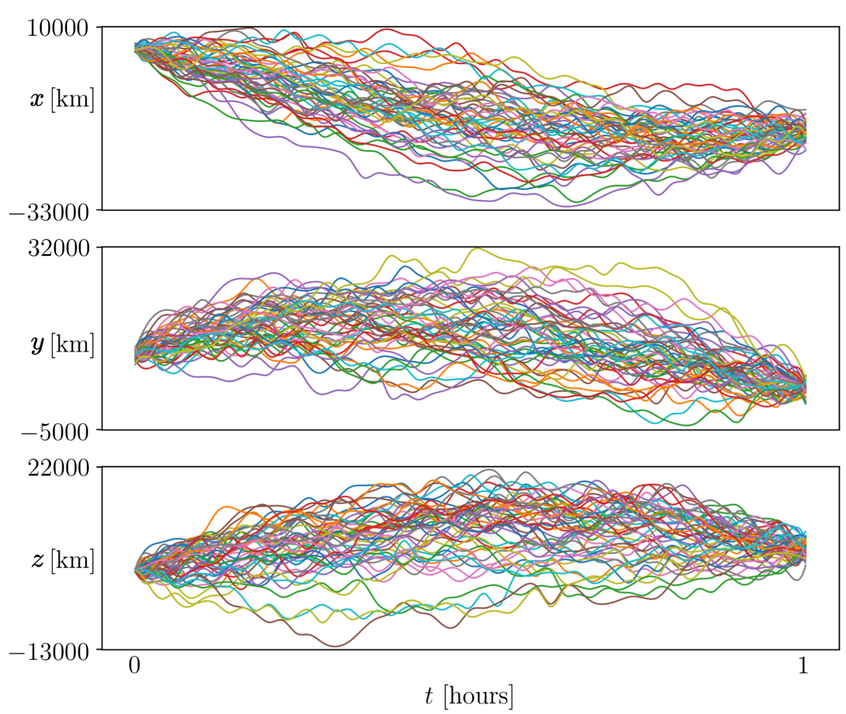
Numerical Case Study

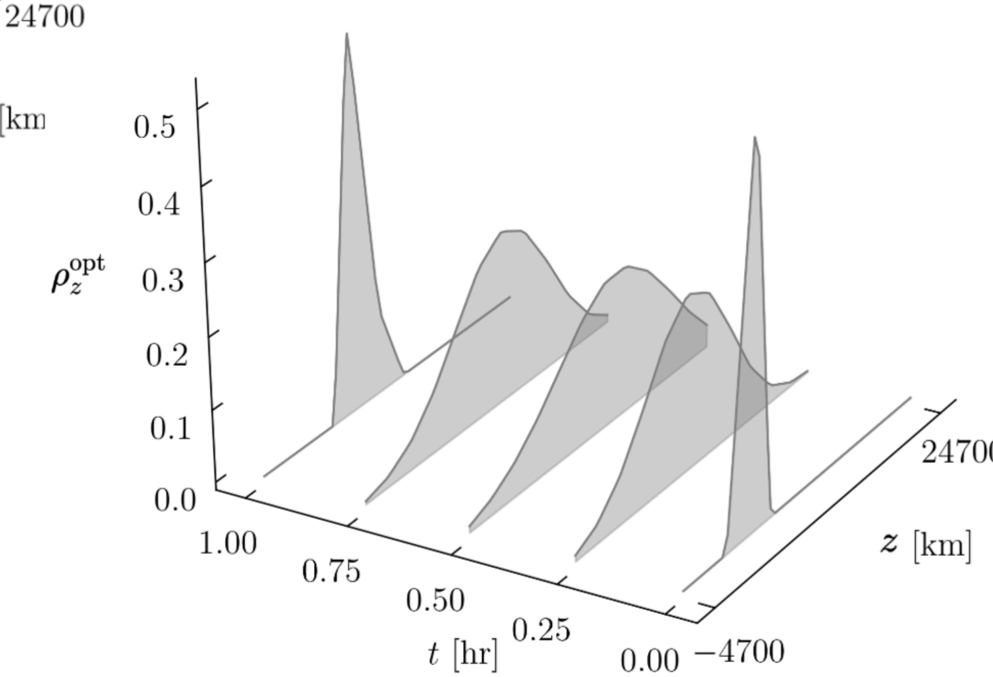
Univariate marginals for optimally controlled joint PDFs











Outlook

- Theory and applications of Schrödinger bridge are undergoing rapid developments

- Lots of mathematics, algorithms, and applications to be done

- Growing interdisciplinary community

- Strong intersections with: physics, control, probability/statistics, PDE, AI/ML, information theory, signal processing, robotics, biology

Thank You

Support: NSF CITRIS PEOPLE AND ROBOTS Ford