Generalized Schrödinger Bridges

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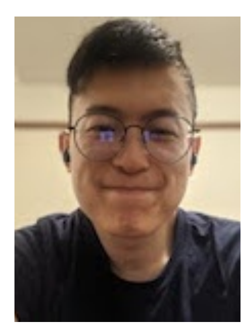
Iowa State University

Joint work with students and collaborators





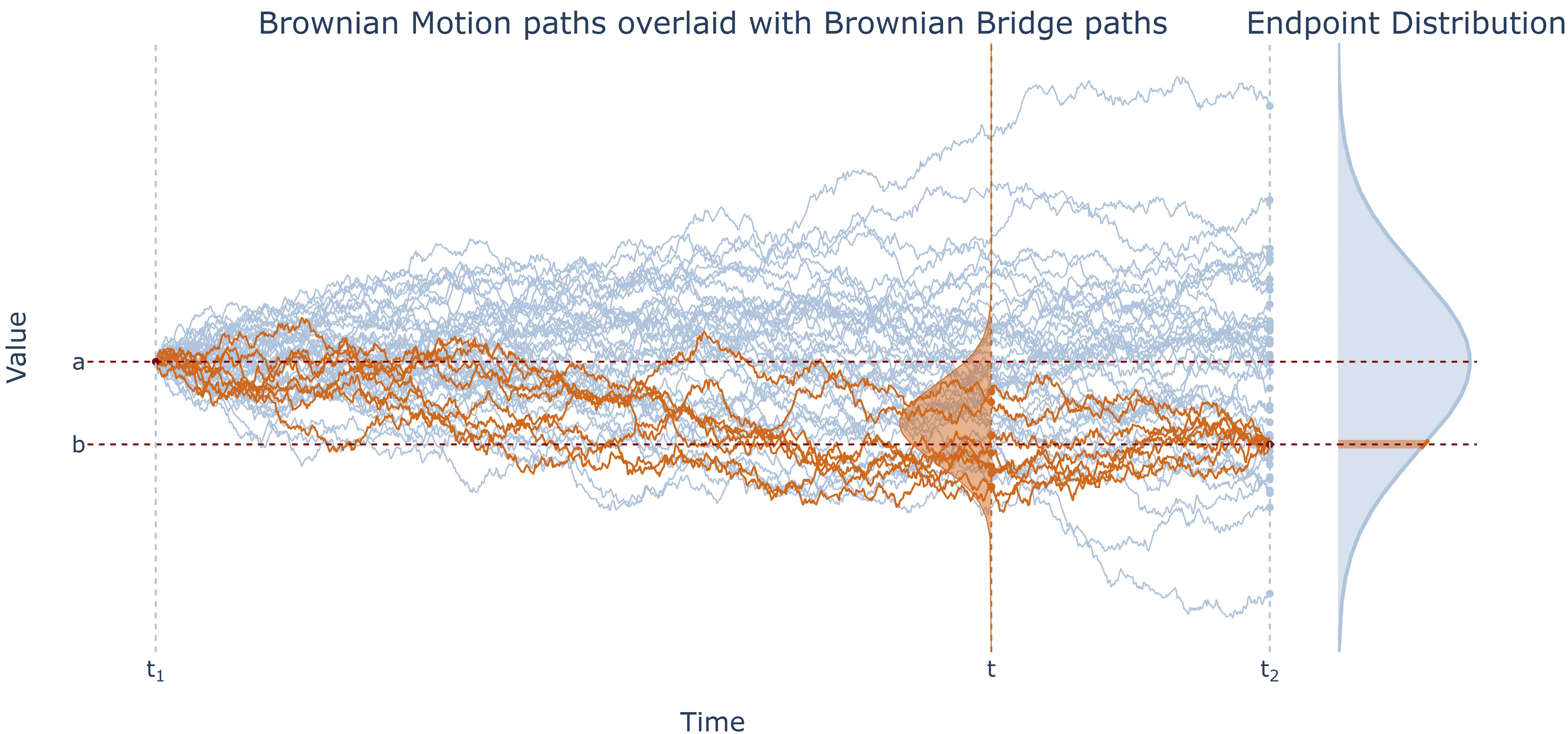




2024 Physics Informed Machine Learning Workshop, Los Alamos
October 17, 2024

What is a bridge

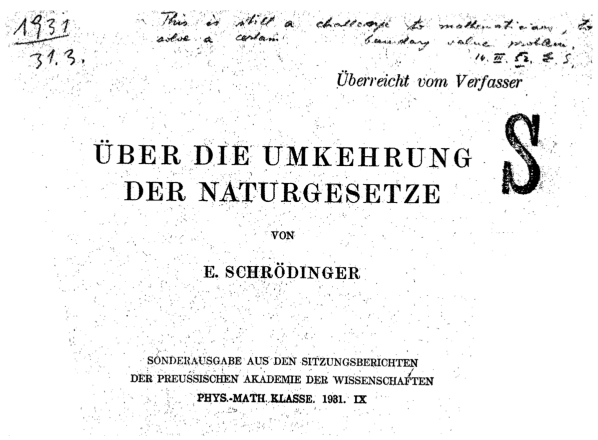
A stochastic process connecting two given states a, b in a given deadline $[t_1, t_2]$



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

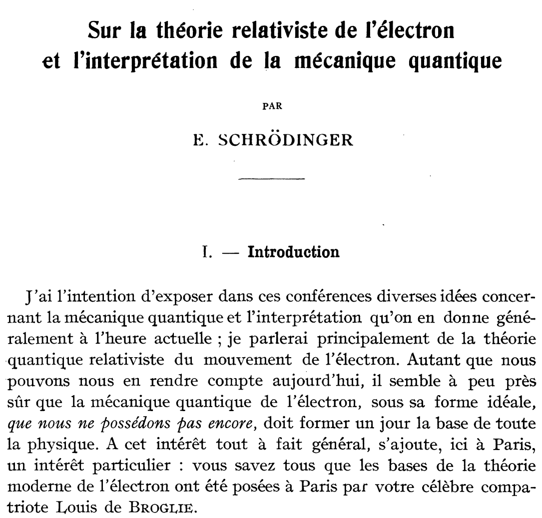
ÜBER DIE UMKEHRUNG
DER NATURGESETZE

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

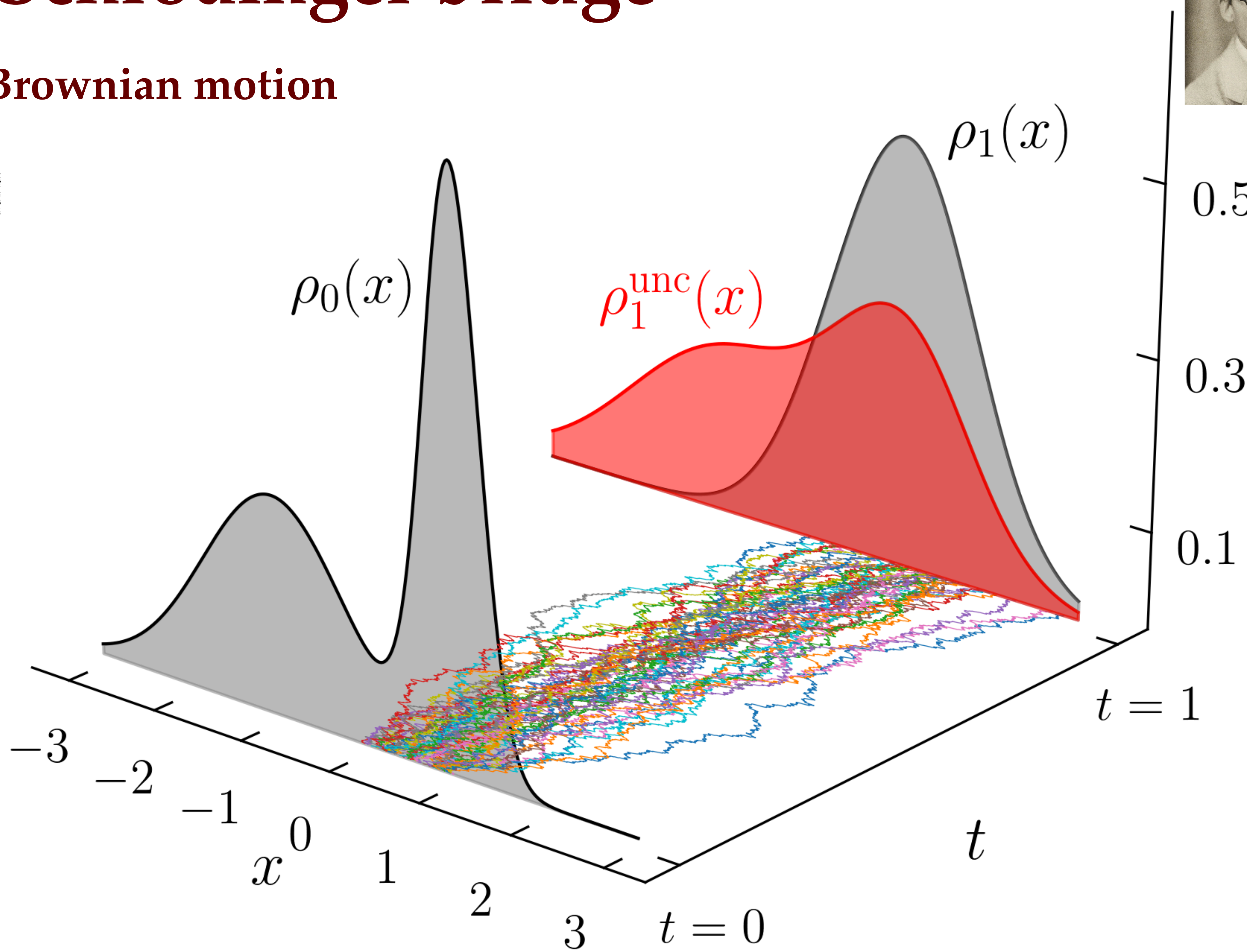
PAR

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 $\mathcal{M}(\Omega)$

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

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

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]

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

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

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

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

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

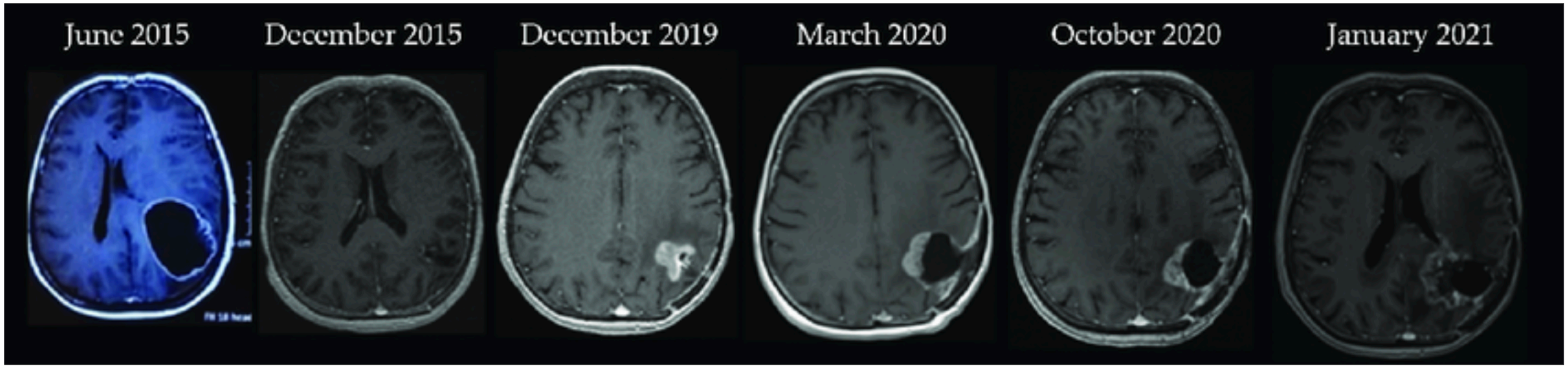
$$\mathrm{d}\boldsymbol{x}_t^u = \boldsymbol{u}(t, \boldsymbol{x}_t^u)\mathrm{d}t + \mathrm{d}\boldsymbol{w}_t$$

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

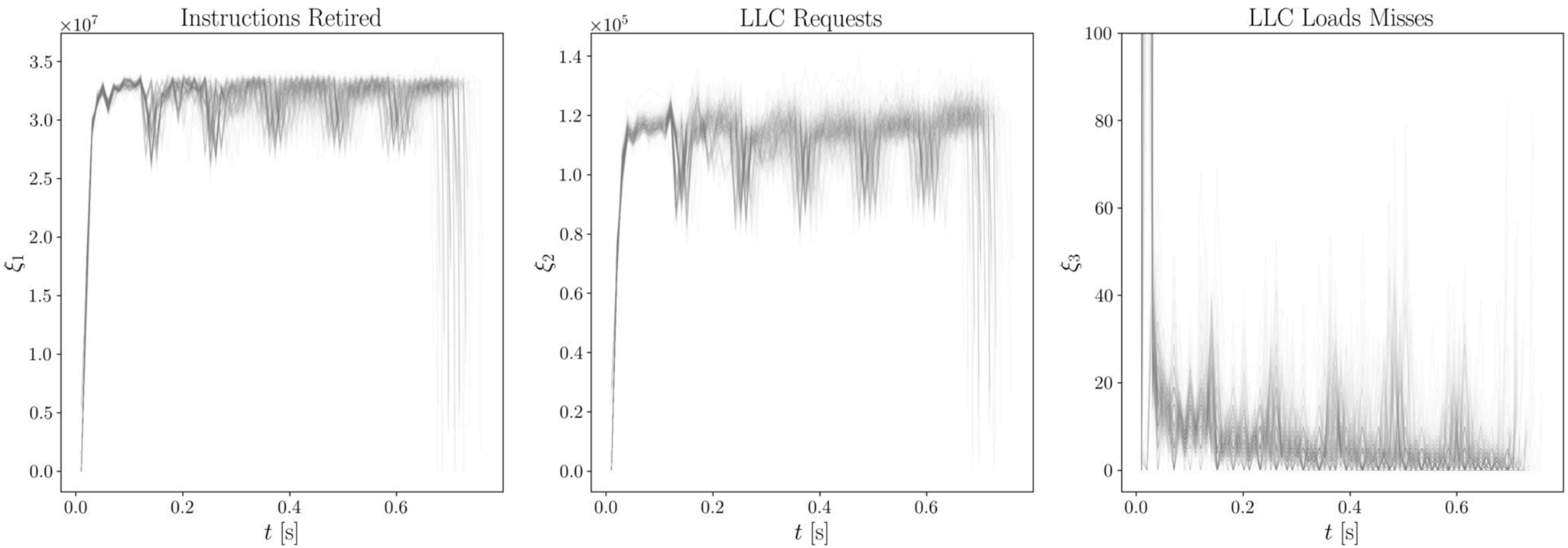
$\mathrm{d}\boldsymbol{w}_t \rightarrow$ **0** Benamou-Brenier OMT [1999]

Resurgence of Schrödinger bridge in ML/AI

Learn most likely progression of medical condition



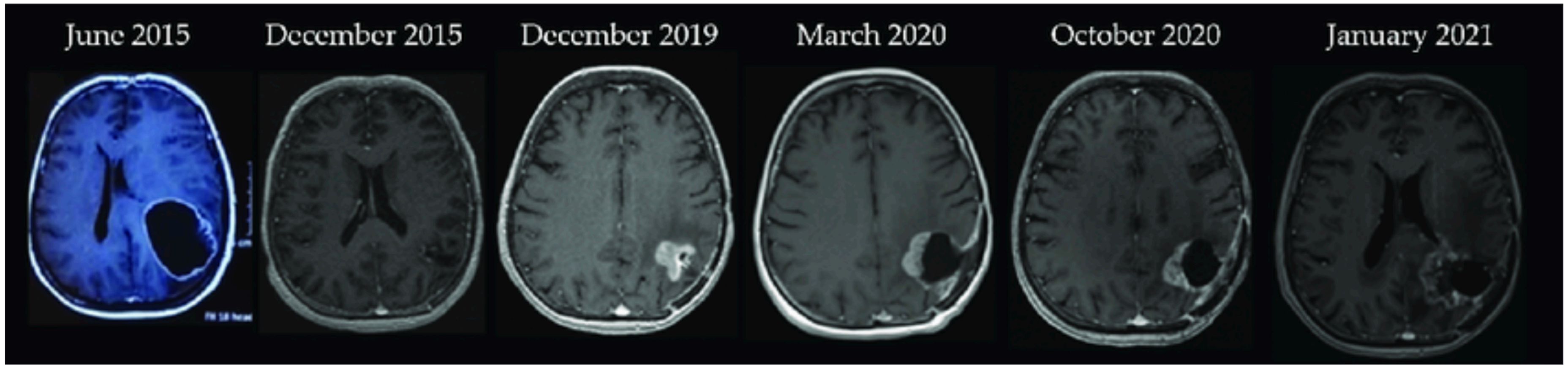
Learn joint stochastic time-varying hardware resource availability

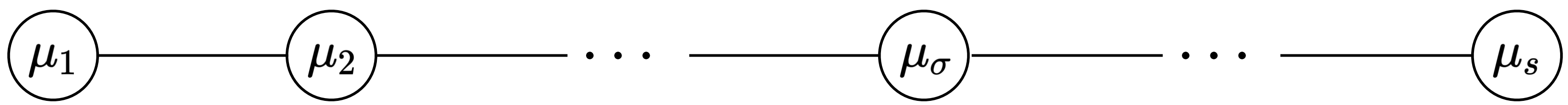


G.A. Bondar, R. Gifford, L.T.X. Phan, and A.H., ***ACC 2024,***
arXiv:2310.00604
arXiv:2405.12463

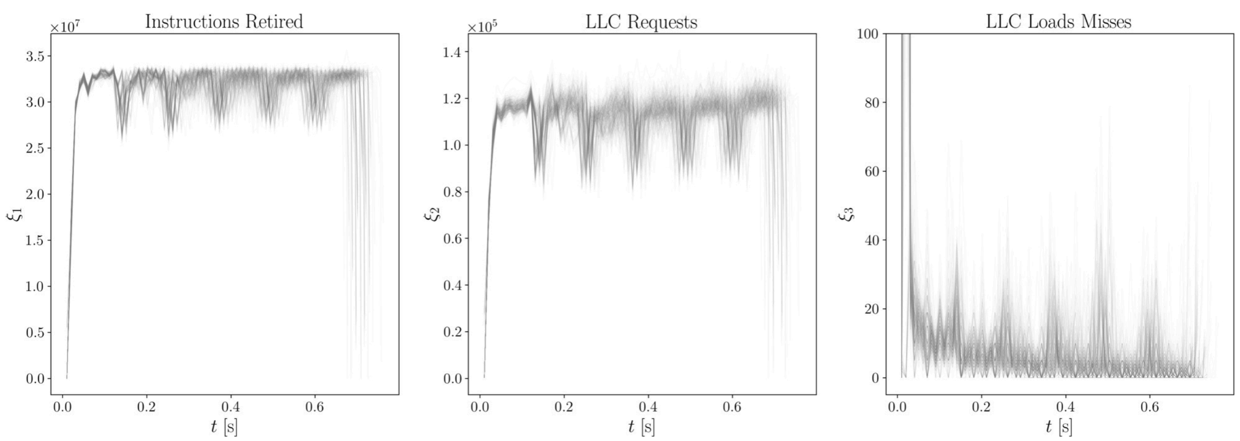
Connections with graphical models

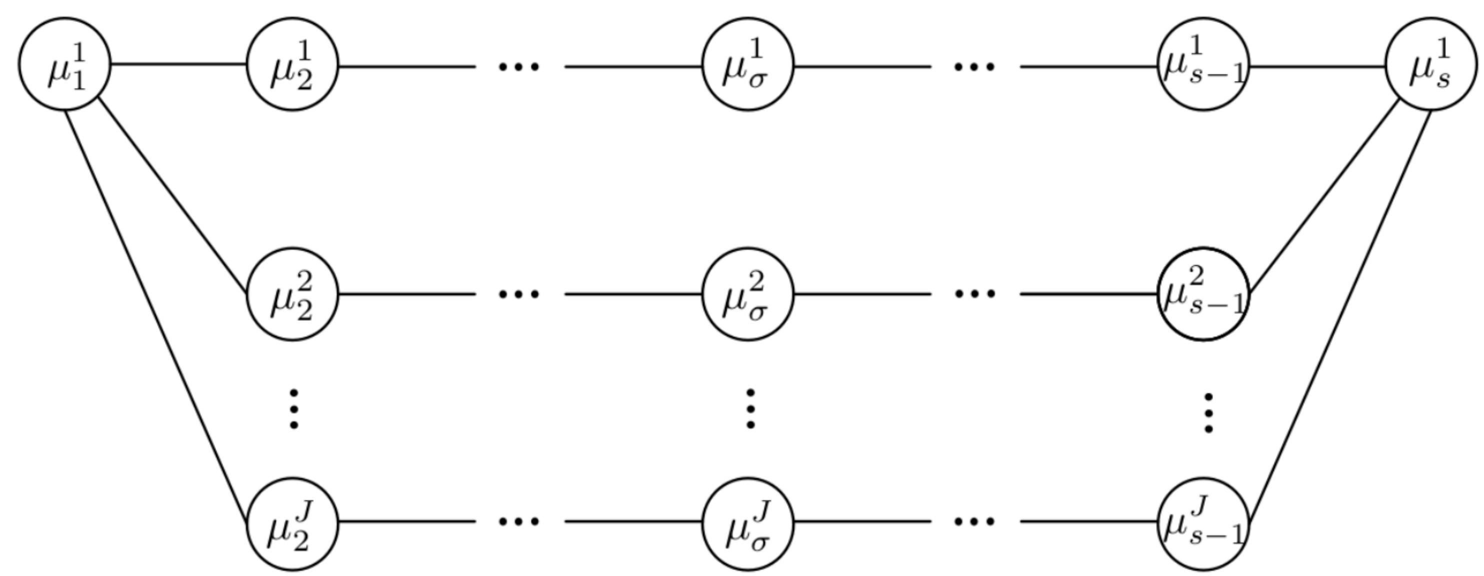
Learn most likely progression of medical condition





Learn joint stochastic time-varying hardware resource availability



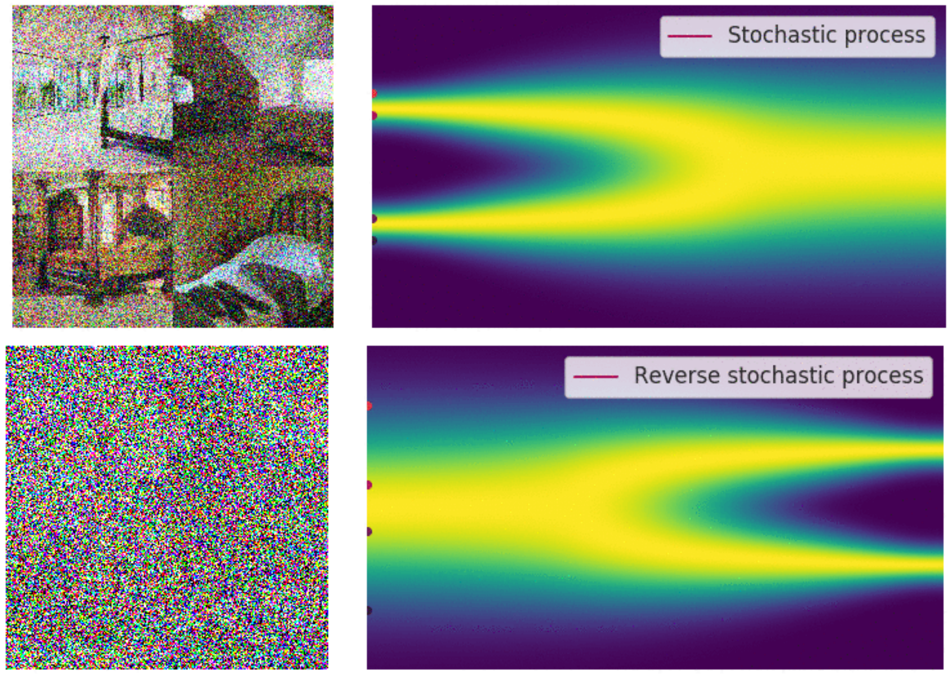


G.A. Bondar, R. Gifford, L.T.X. Phan, and A.H., *ACC 2024*,
arXiv:2310.00604
arXiv:2405.12463

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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University of Oxford, UK

James Thornton
Department of Statistics,
University of Oxford, UK

Jeremy Heng
ESSEC Business School,
Singapore

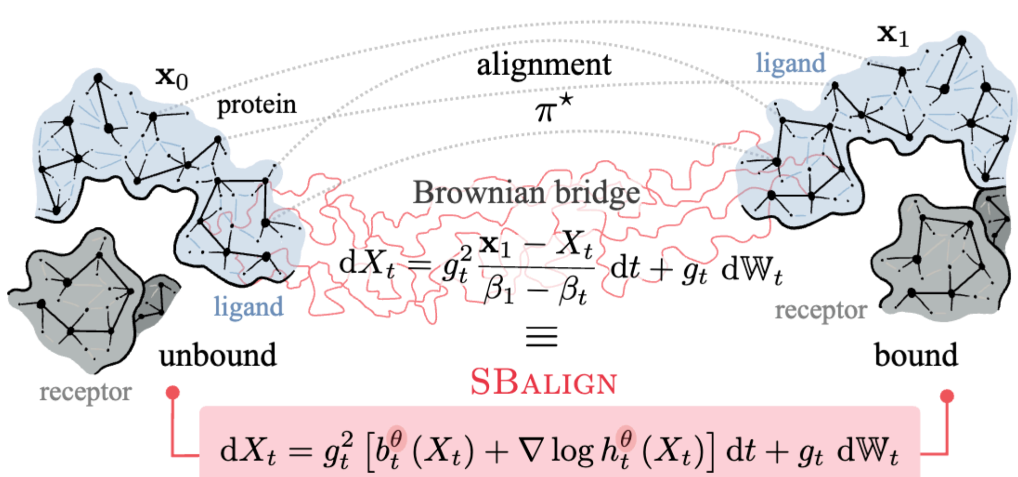
Arnaud Doucet
Department of Statistics,
University of Oxford, UK

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]

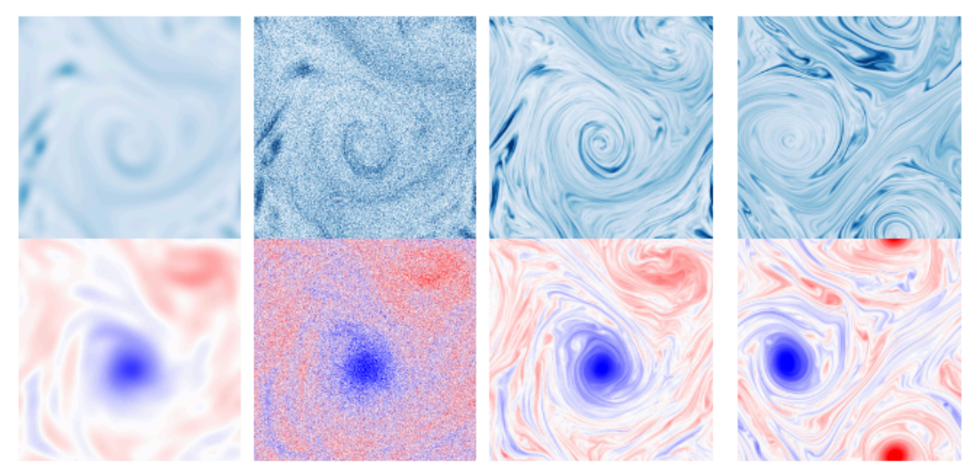
[1]Department of Computer Science, ETH Zürich
[2]IBM Research Zürich
[3]Department of Computer Science, EPFL



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

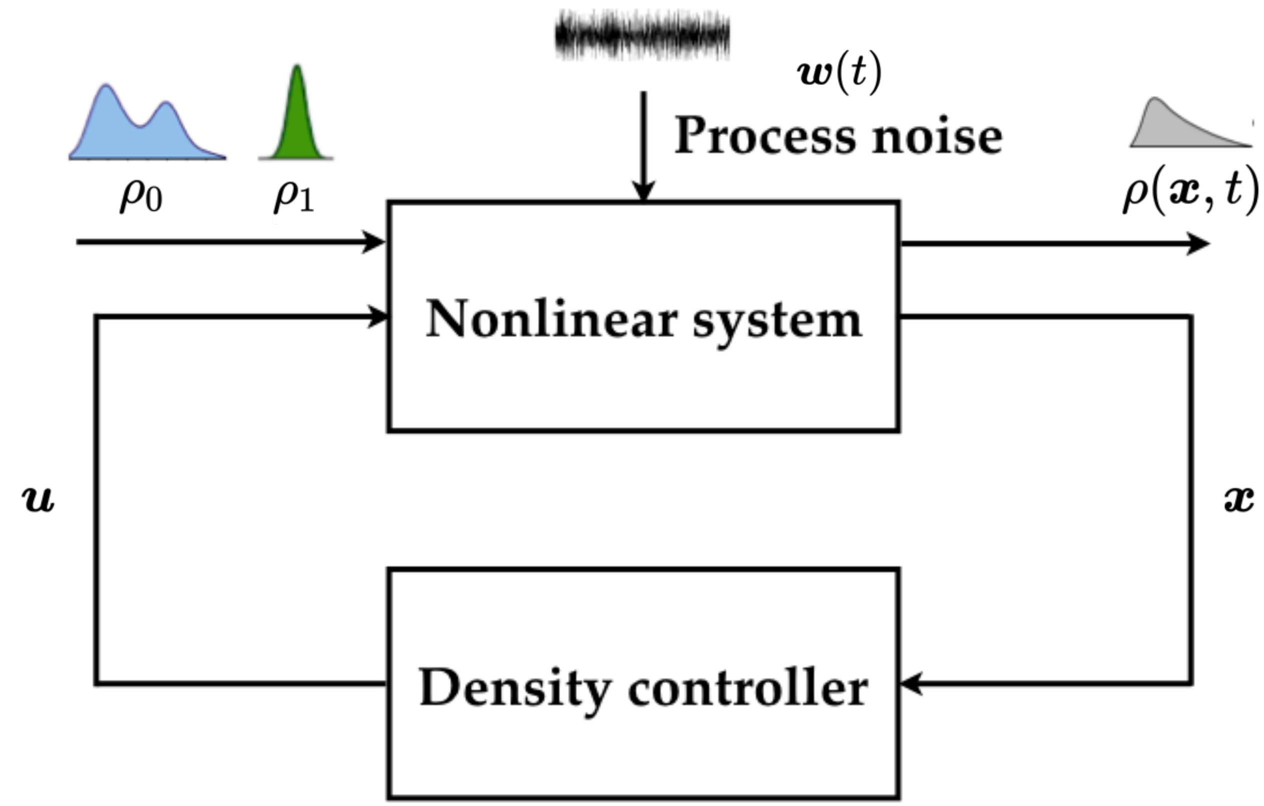
#1. general controlled dynamics

#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: $G \equiv B$

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

subject to

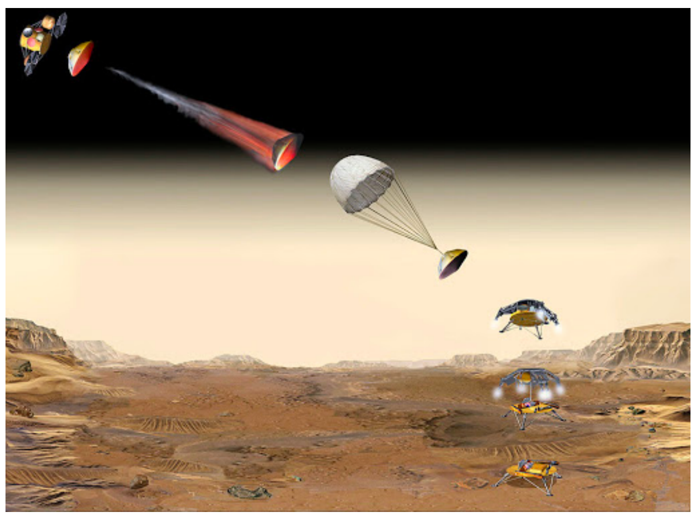
$$\mathrm{d}x_t^u = \{f(t,x_t^u) + B(t,x_t^u)u\}\mathrm{d}t + \sqrt{2}G(t,x_t^u)\mathrm{d}w_t$$

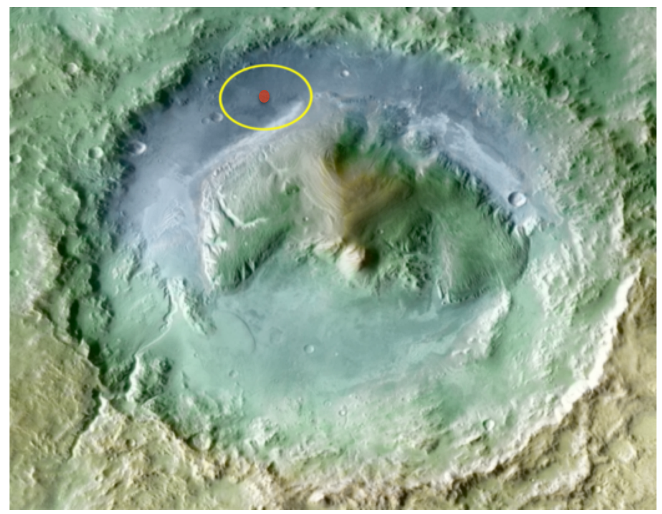
$$x_0^u := x_t^u(t=0) \sim \rho_0, \quad x_1^u := x_t^u(t=1) \sim \rho_1$$

Motivating applications

Distribution ~ Probability

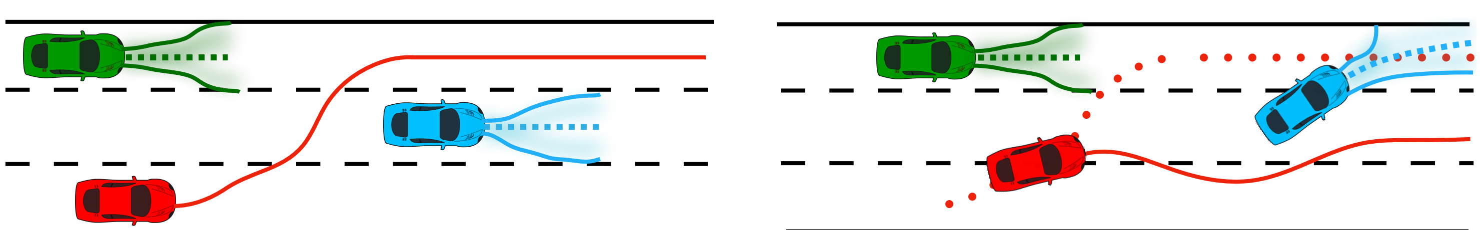
Spacecraft landing with desired statistical accuracy





Gale Crater (4.49S, 137.42E)

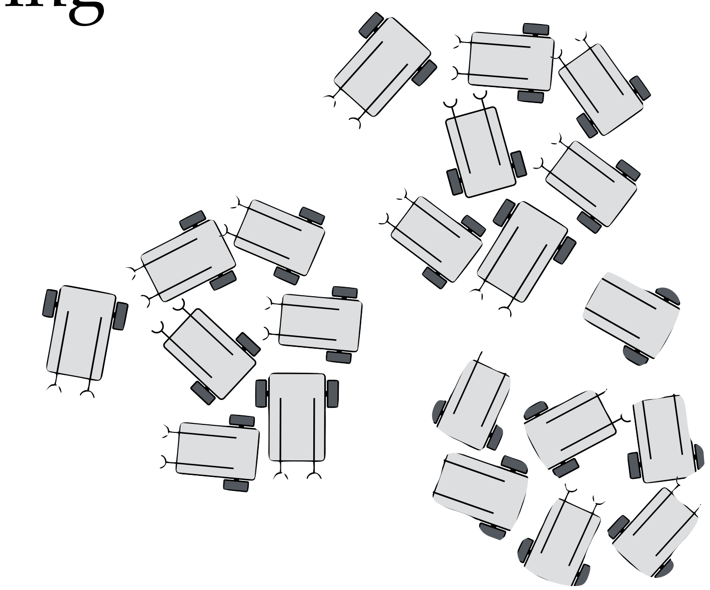
Risk management for automated driving in multi-lane highways



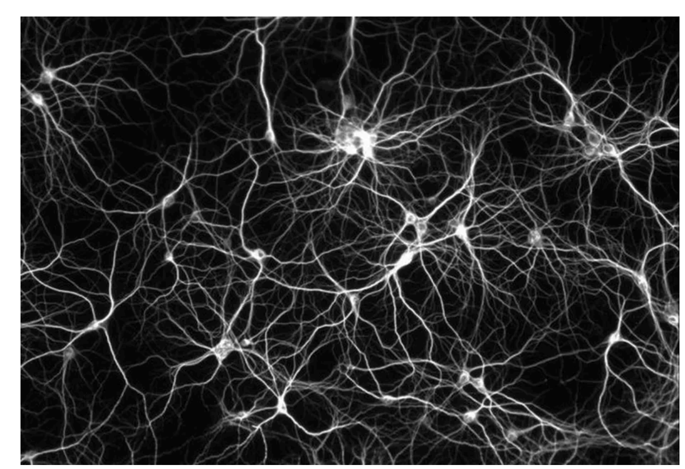
Control of uncertainties

Distribution ~ Population

Dynamic shaping of swarms



Feedback sync. and desync. of neuronal population



Control of ensemble

Generalized Schrödinger bridge

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

Hessian operator w.r.t. state: Hess

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

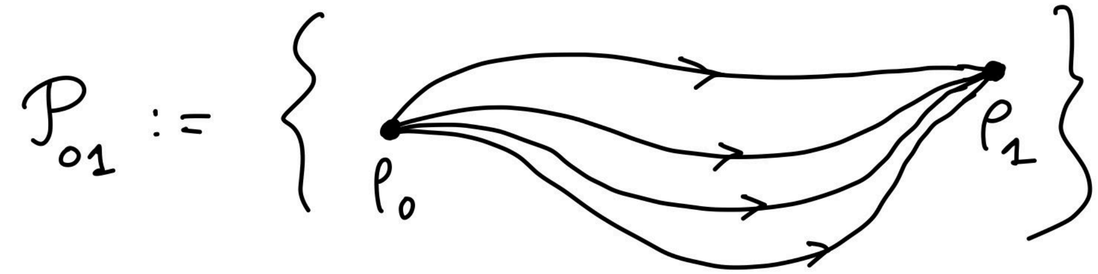
subject to

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

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

Controlled Fokker-Planck or Kolmogorov's forward PDE

Zero process noise ⇝ Generalized OMT



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

Hessian operator w.r.t. state: Hess

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subject to

$$\frac{\partial\rho}{\partial t} + \nabla\cdot((\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u})\rho) = \Delta_{\boldsymbol{D}}\rho \quad \to \mathbf{0}$$

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

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

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

Hamilton-Jacobi-Bellman-like PDE

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

Boundary conditions:

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

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

Feedback synthesis via the Schrödinger factors

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

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

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

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

2 coupled nonlinear PDEs ⟶ boundary-coupled linear PDEs!!

Uncontrolled forward-backward advection-reaction-diffusion PDEs:

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

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

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

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

What exactly are Schrödinger factors?

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

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]

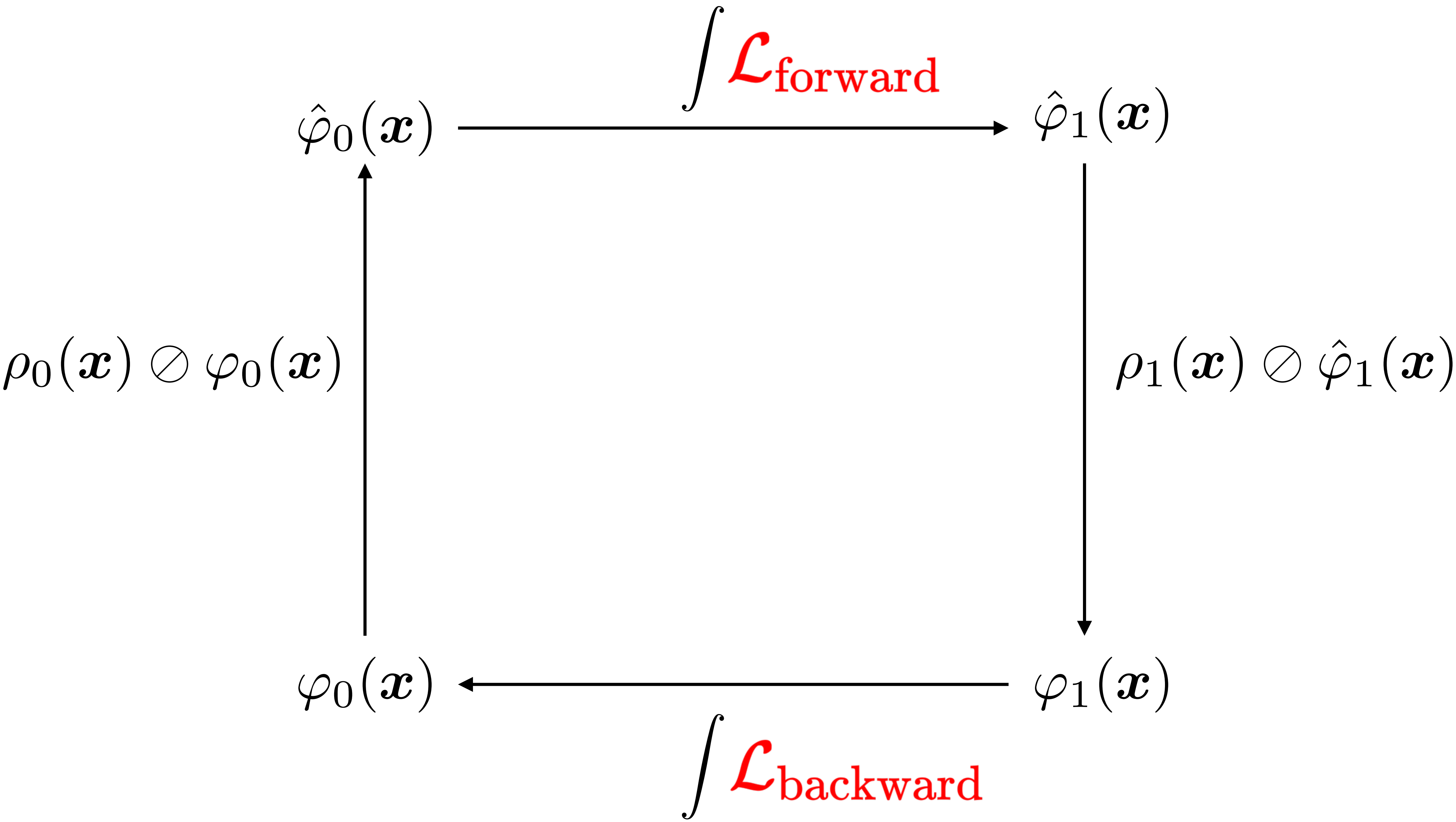
Quantum: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \Psi(\boldsymbol{x}, t)\widehat{\Psi}(\boldsymbol{x}, t)$ [Born's relation]

wave function

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

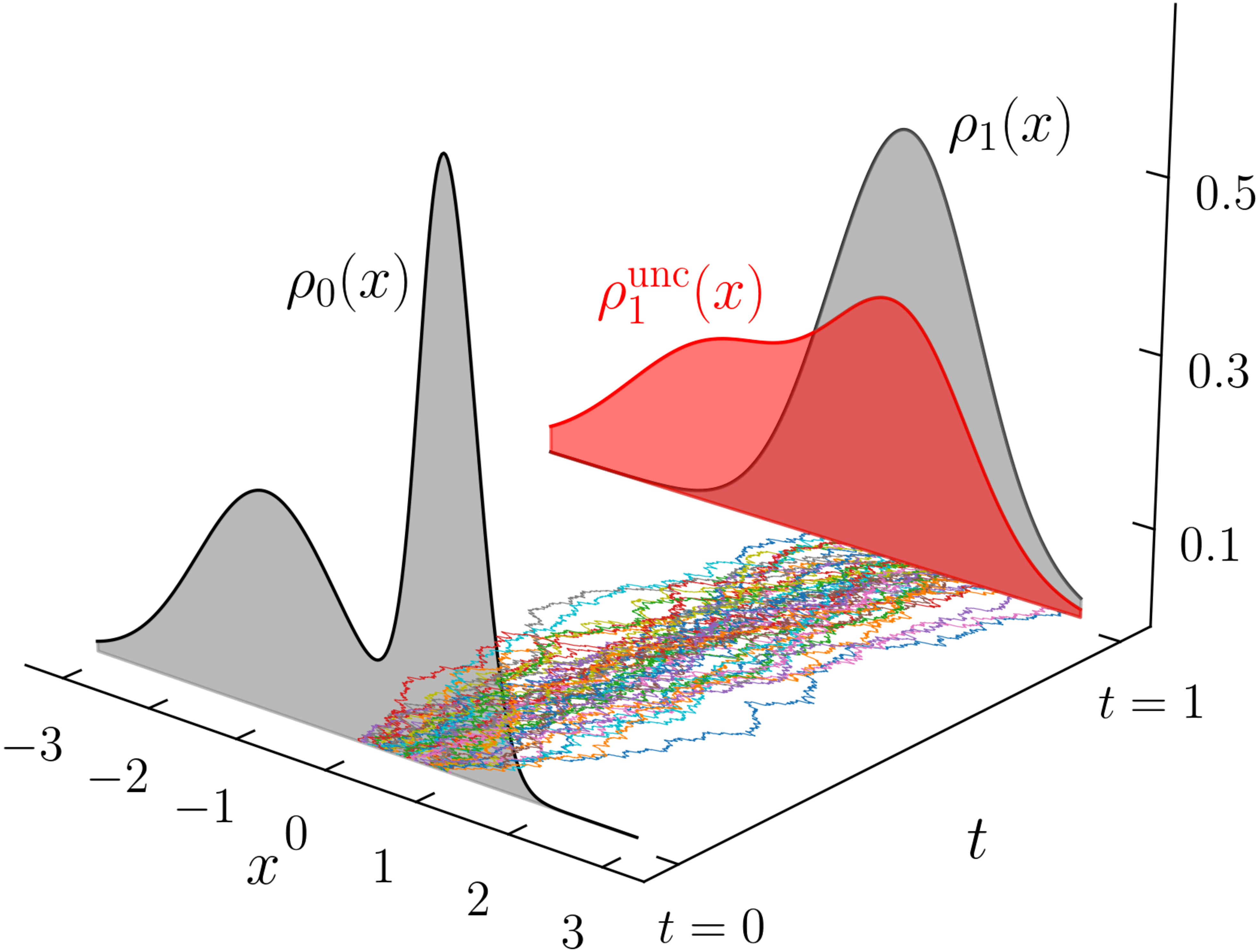
$$\left(-\sqrt{-1}\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q\right)\widehat{\Psi} = 0$$ [Adjoint Schrödinger PDE]

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



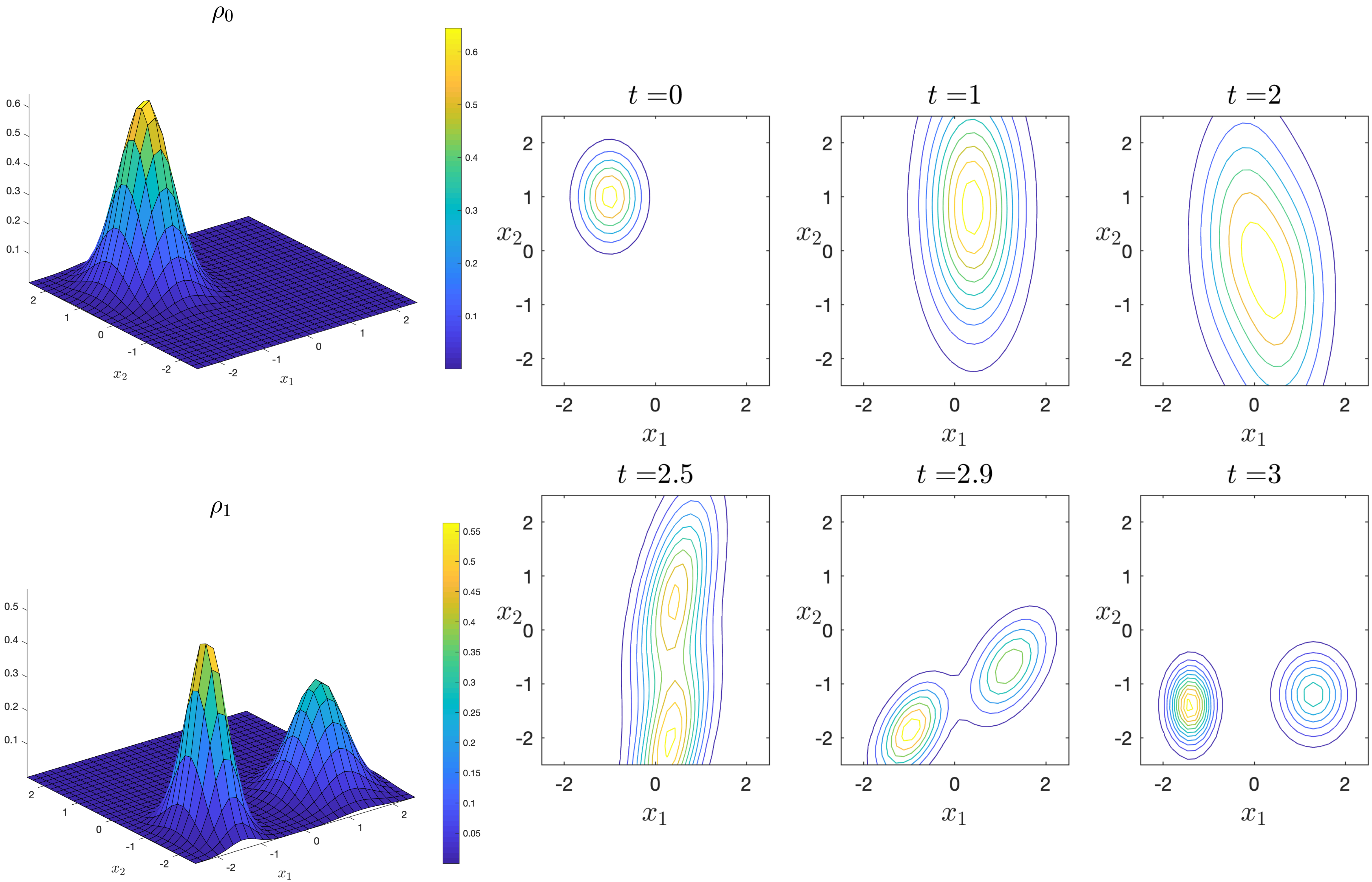
This recursion is contractive in the Hilbert's projective metric!!

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



Zero prior dynamics

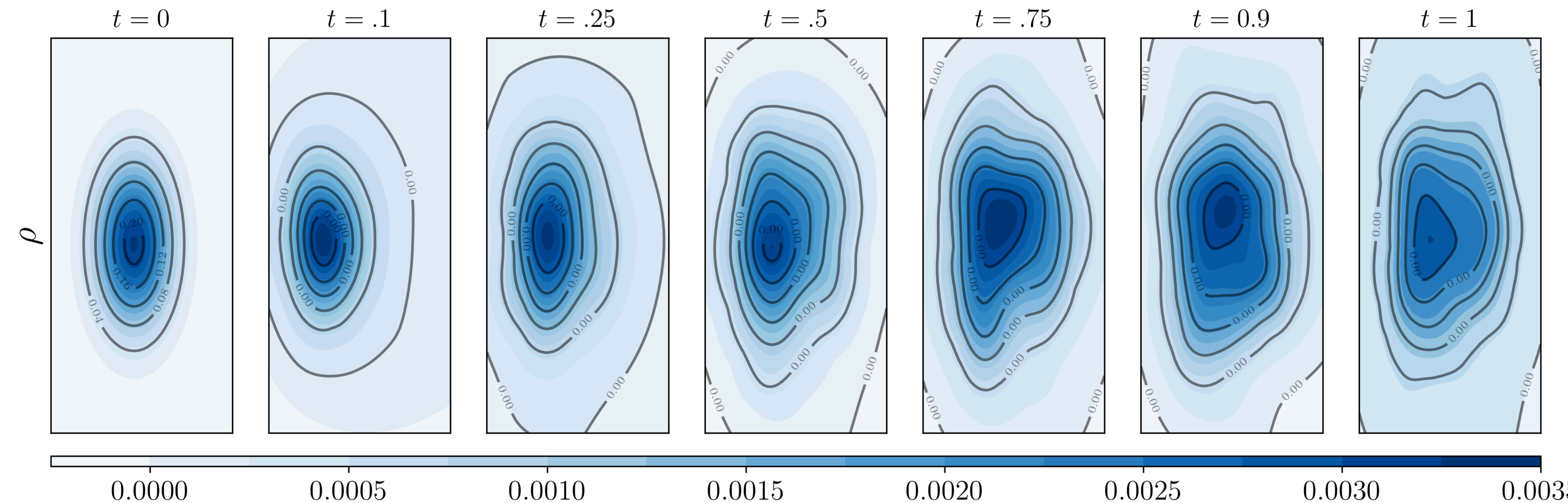
Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$



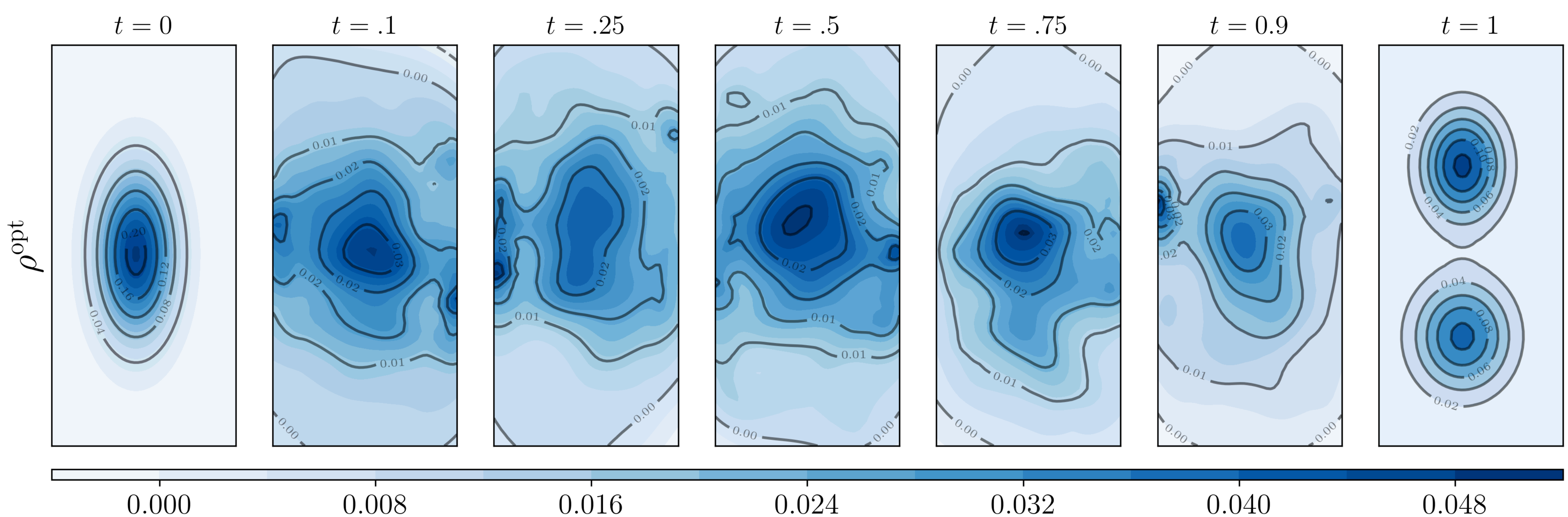
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

Uncontrolled joint PDF evolution:



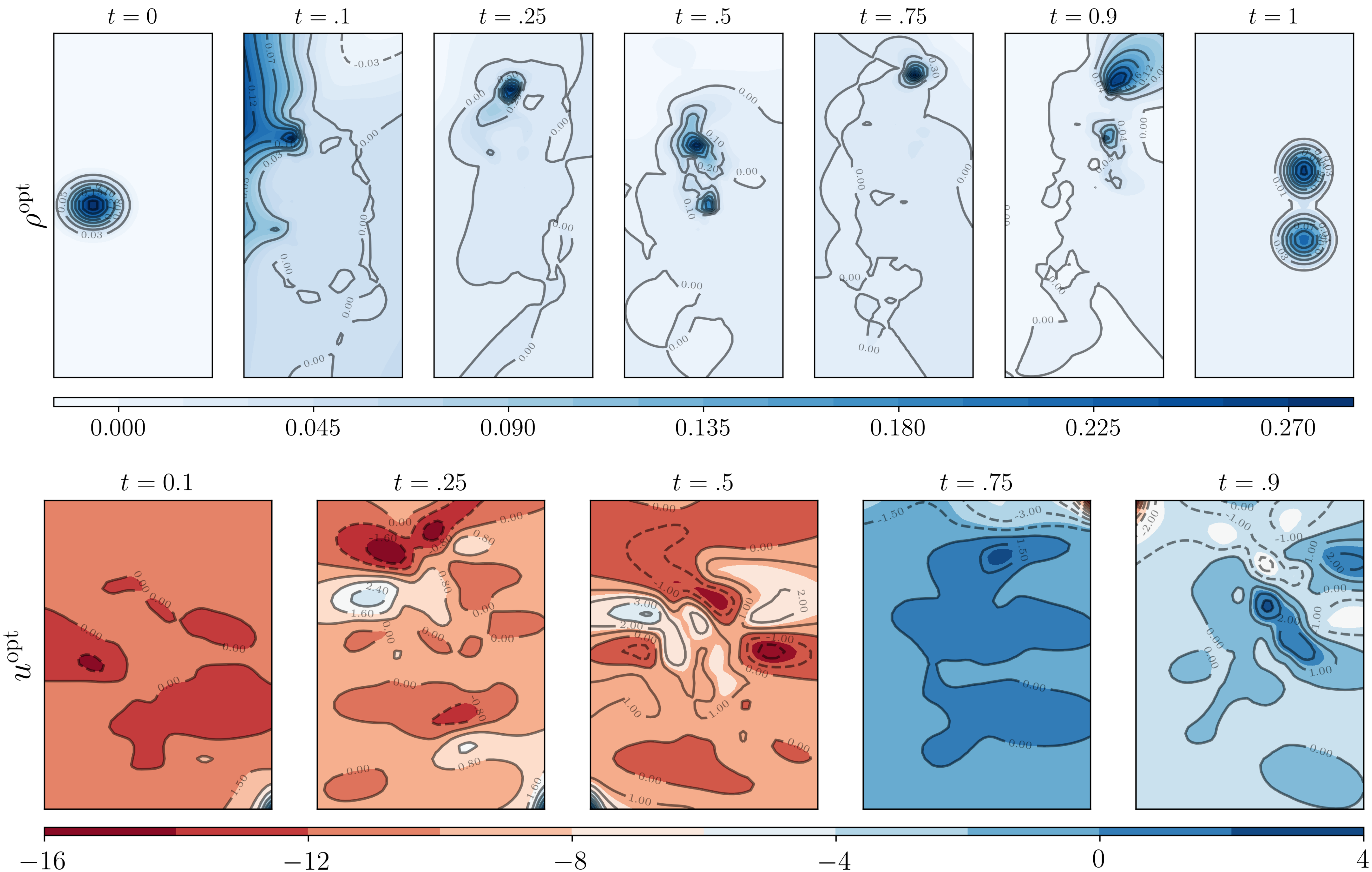
Optimal controlled joint PDF evolution:



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

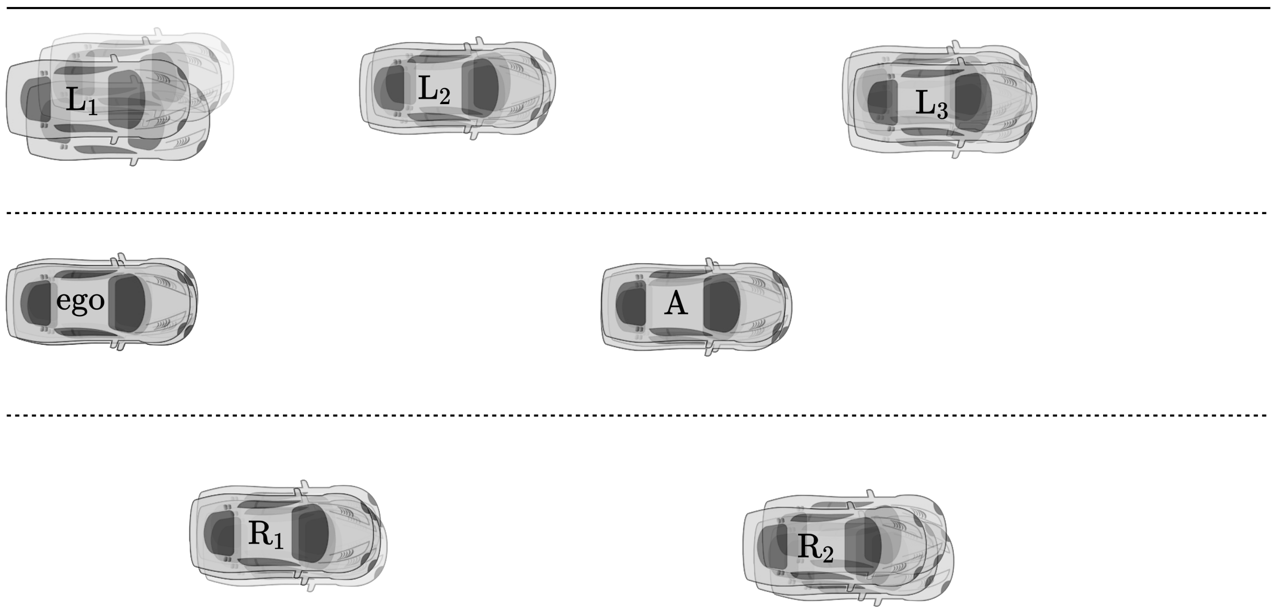
K.F. Caluya, and A.H., ***TAC 2019***

Feedback Density Control: Mixed Conservative-Dissipative Drift

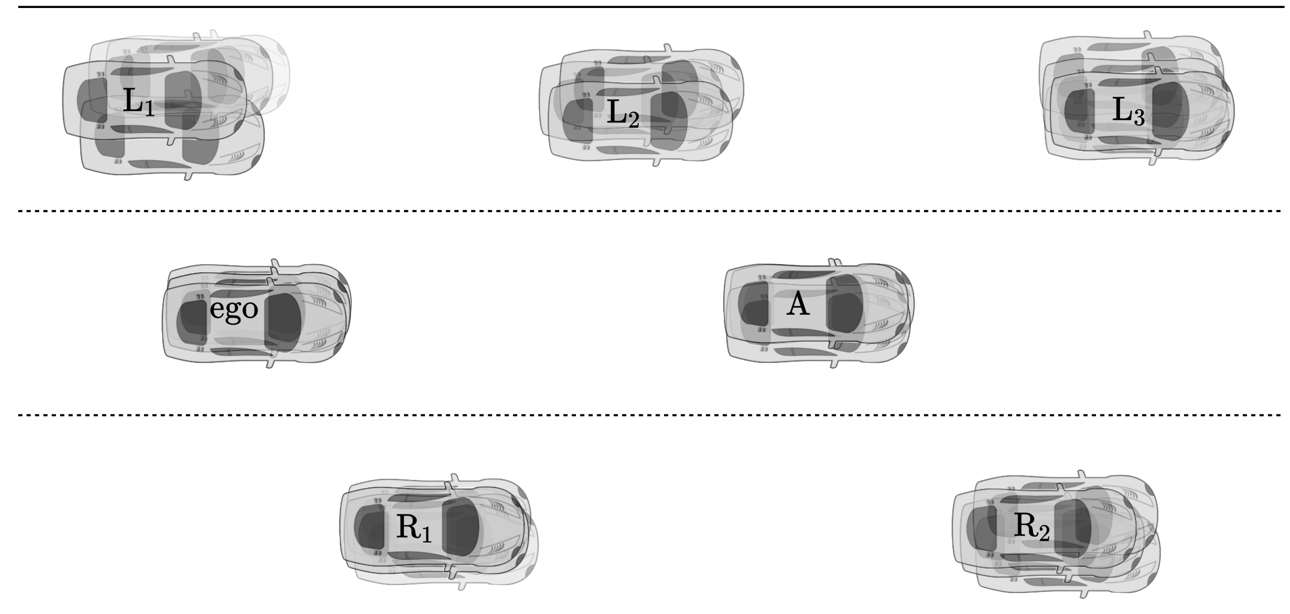


K.F. Caluya, and A.H., *TAC 2022*
K.F. Caluya, and A.H., *TAC 2019*

Application: Multi-lane Automated Driving

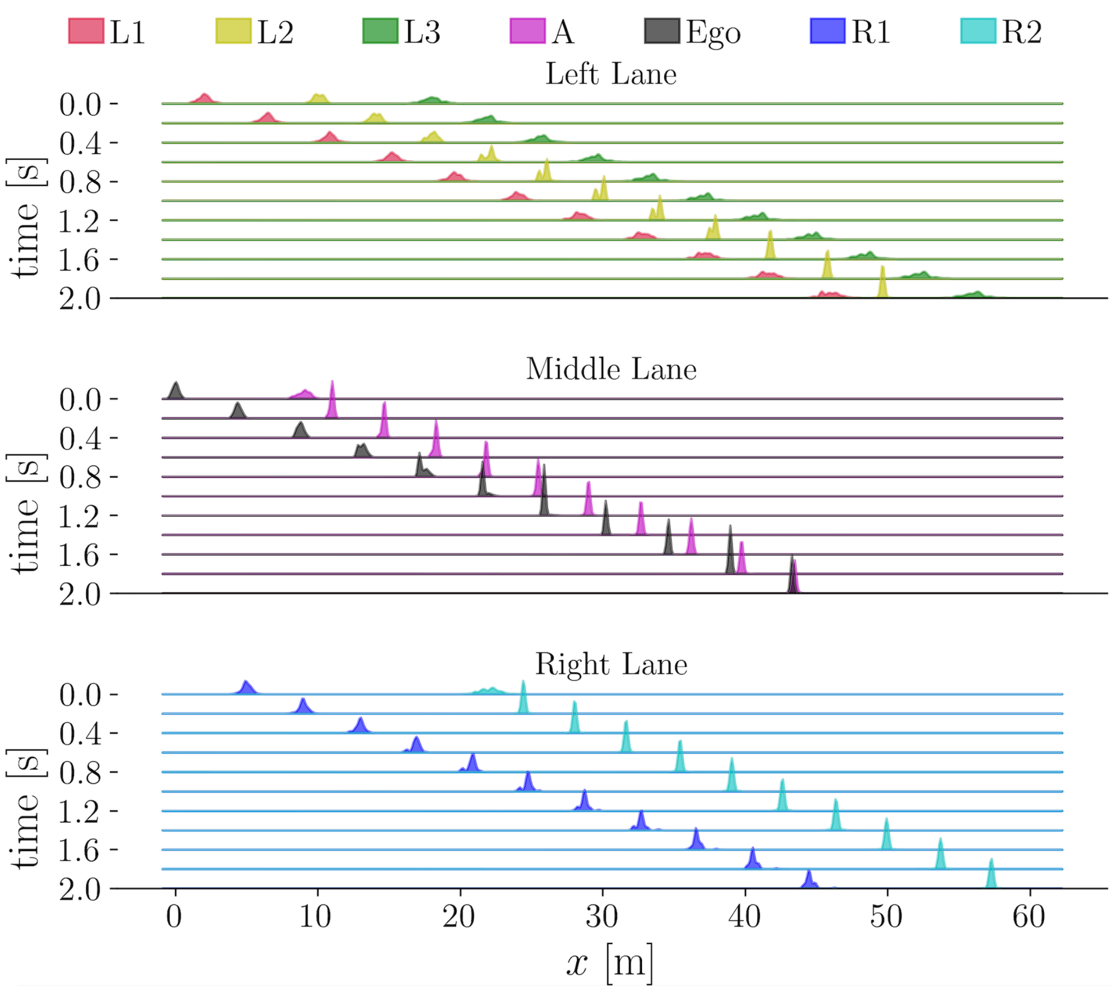


t_0

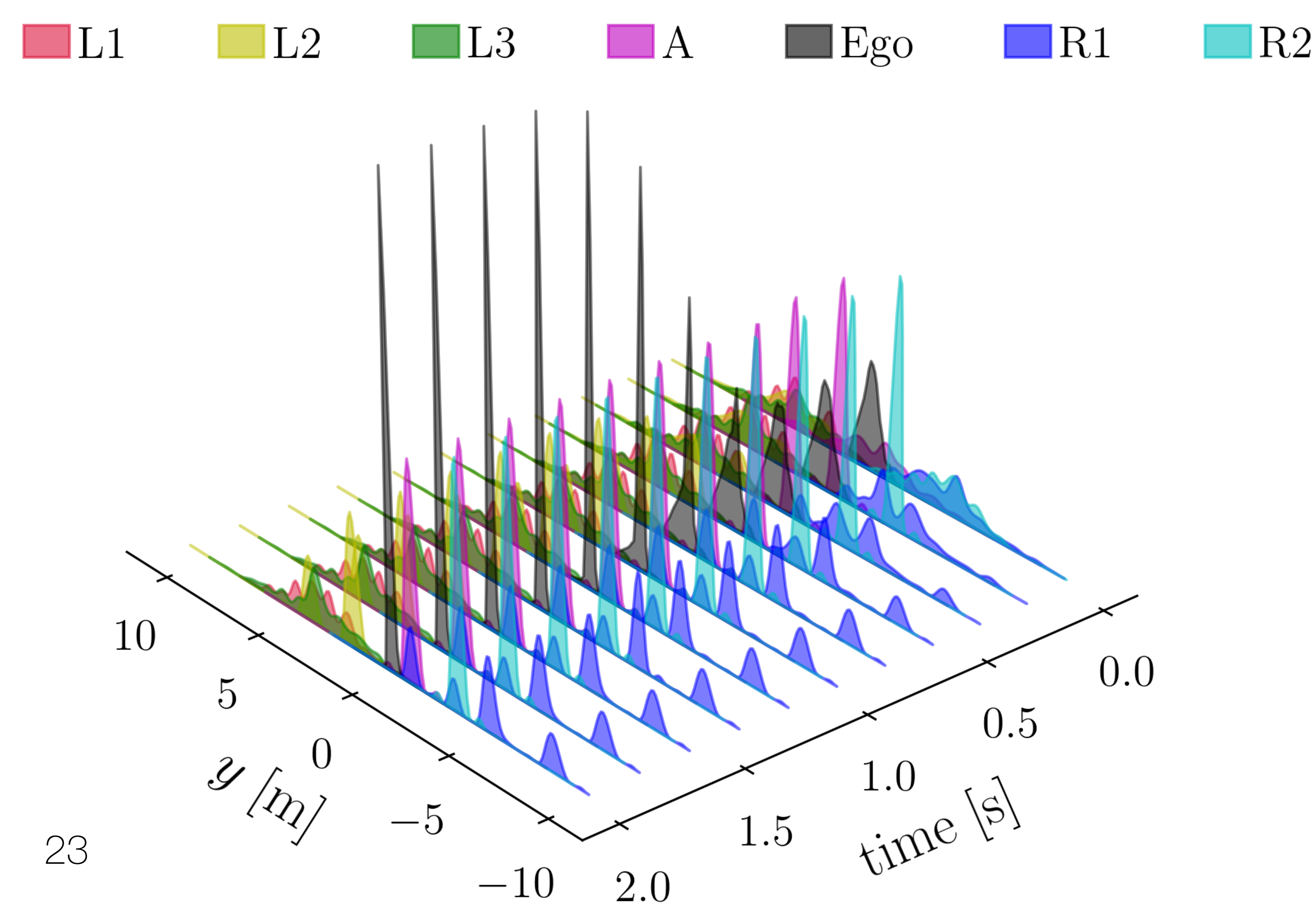


t_1

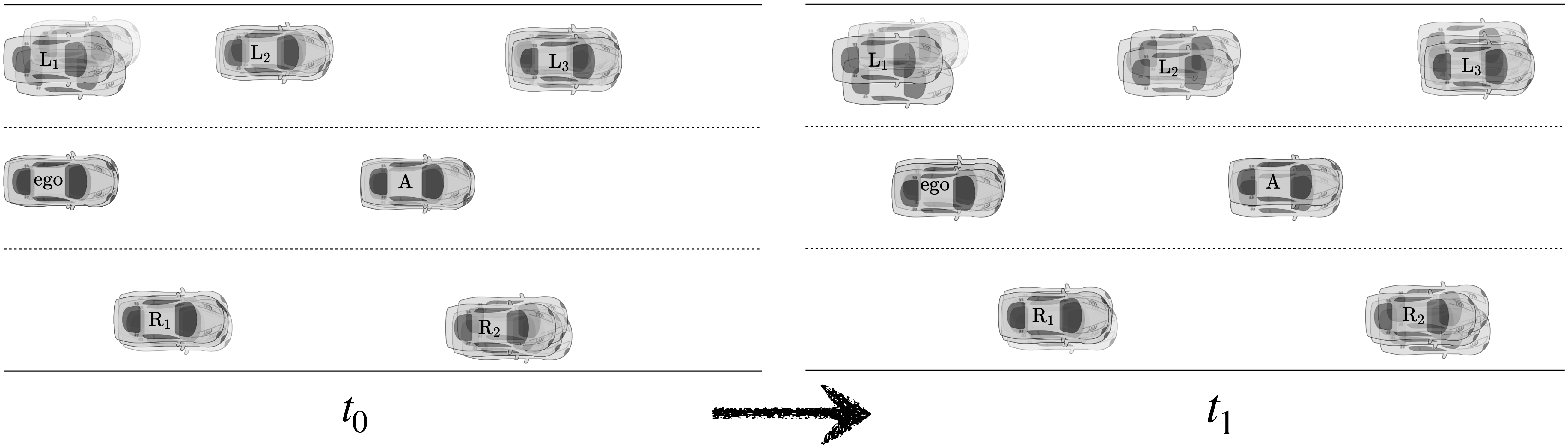
x marginals

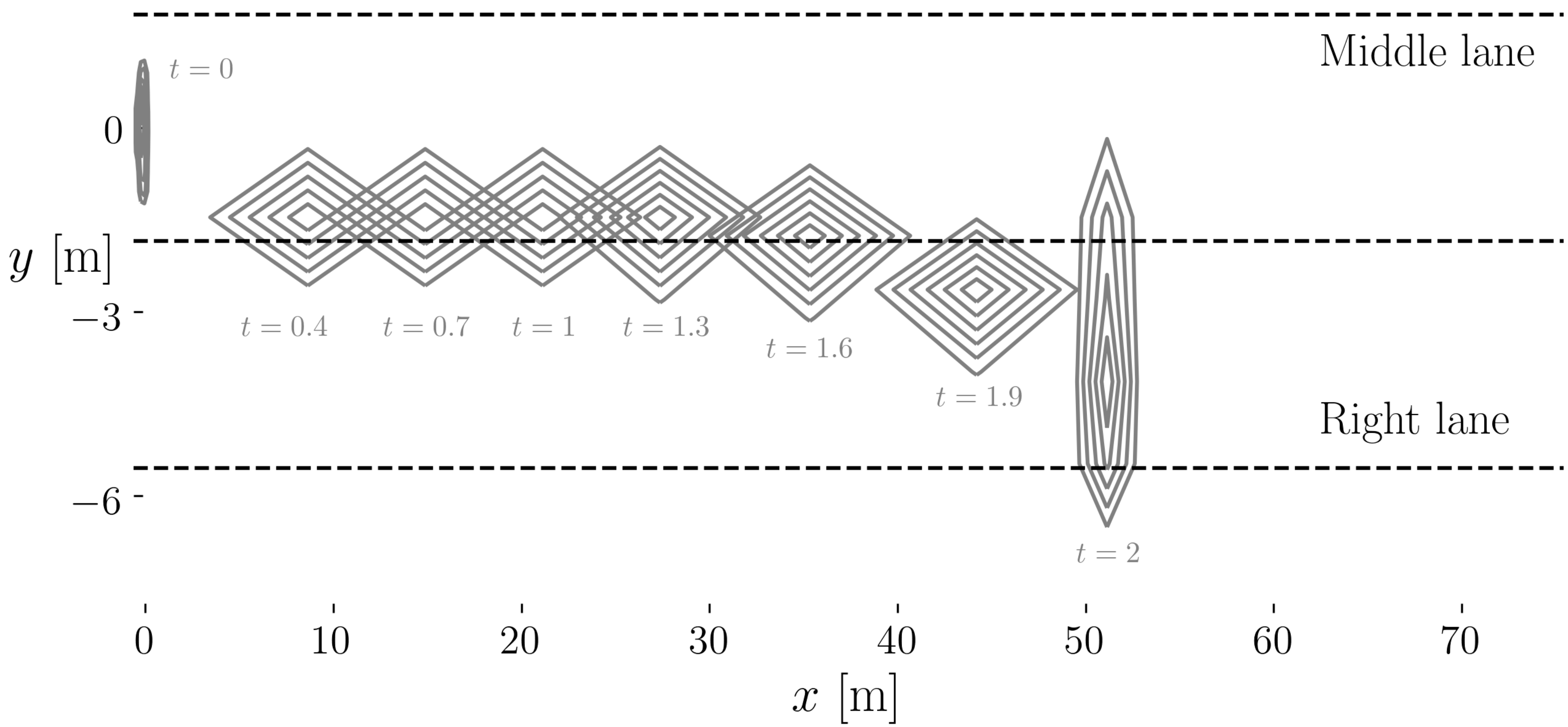


y marginals



Application: Multi-lane Automated Driving





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

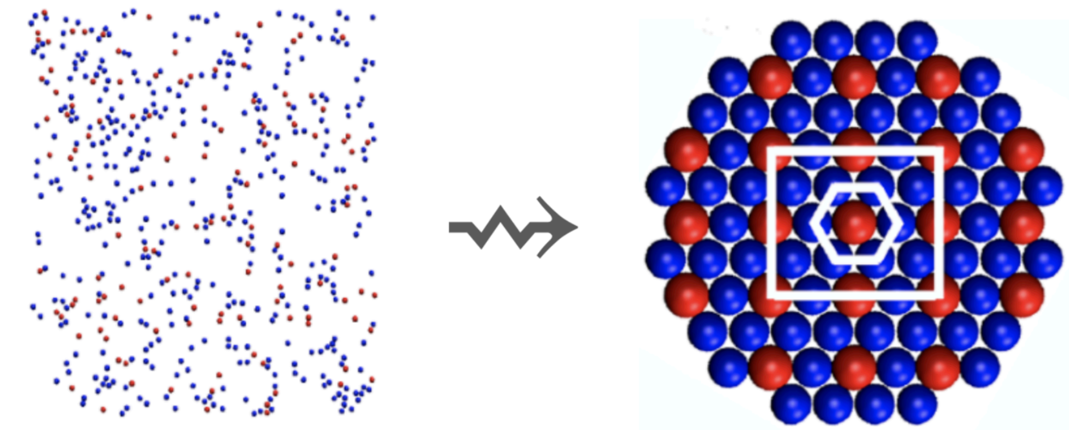
Control non-affine generalized Schrödinger bridge

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



Dispersed particles   Ordered structure

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

$$\frac{\partial \psi}{\partial t} = \frac{1}{2}\|\boldsymbol{u}_{\text{opt}}\|_2^2 - \langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle - \langle \boldsymbol{G}, \text{Hess}(\psi)\rangle$$

$$\frac{\partial \rho_{\text{opt}}^{\boldsymbol{u}}}{\partial t} = -\nabla \cdot \left(\rho_{\text{opt}}^{\boldsymbol{u}} \boldsymbol{f}\right) + \Delta_{\boldsymbol{G}} \rho_{\text{opt}}^{\boldsymbol{u}}$$

$$\boldsymbol{u}_{\text{opt}} = \nabla_{\boldsymbol{u}_{\text{opt}}}\left(\langle \nabla_{\boldsymbol{x}}\psi, \boldsymbol{f}\rangle + \langle \boldsymbol{G}, \text{Hess}(\psi)\rangle\right)$$

$$\rho_{\text{opt}}^{\boldsymbol{u}}(0, \boldsymbol{x}) = \rho_0, \quad \rho_{\text{opt}}^{\boldsymbol{u}}(T, \boldsymbol{x}) = \rho_T$$

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

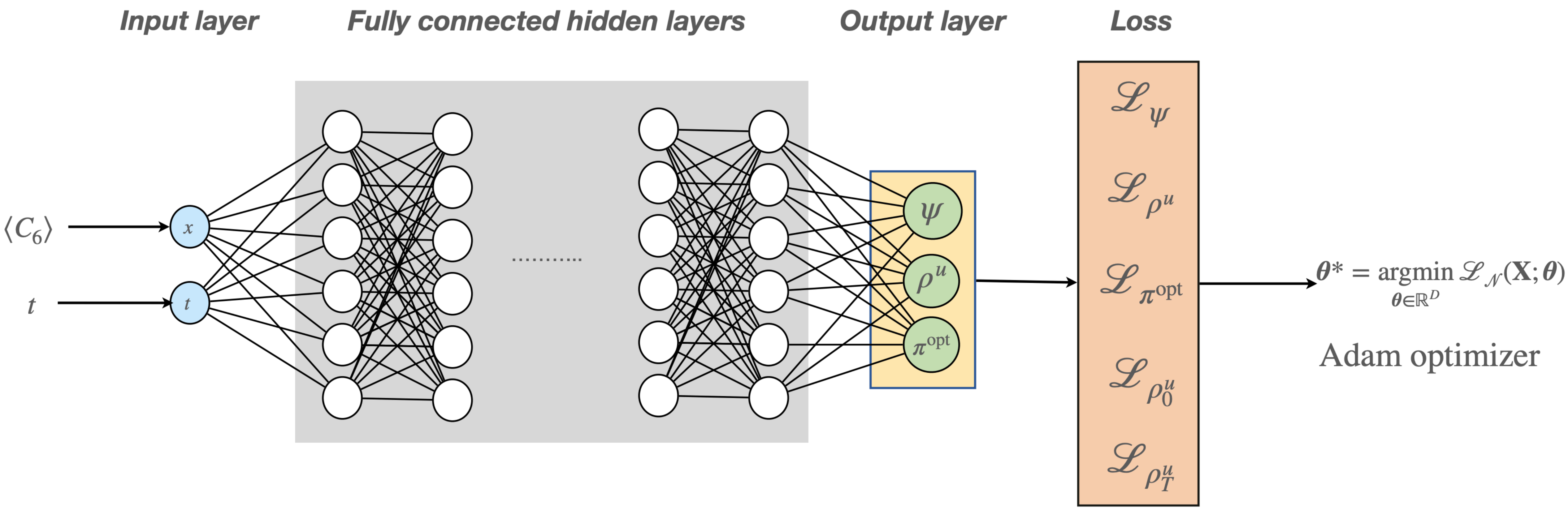
I. Nodozi, J.O'Leary, A. Mesbah, and A.H., ACC *2023*

2024 O. Hugo Schuck Best Application Paper Award

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

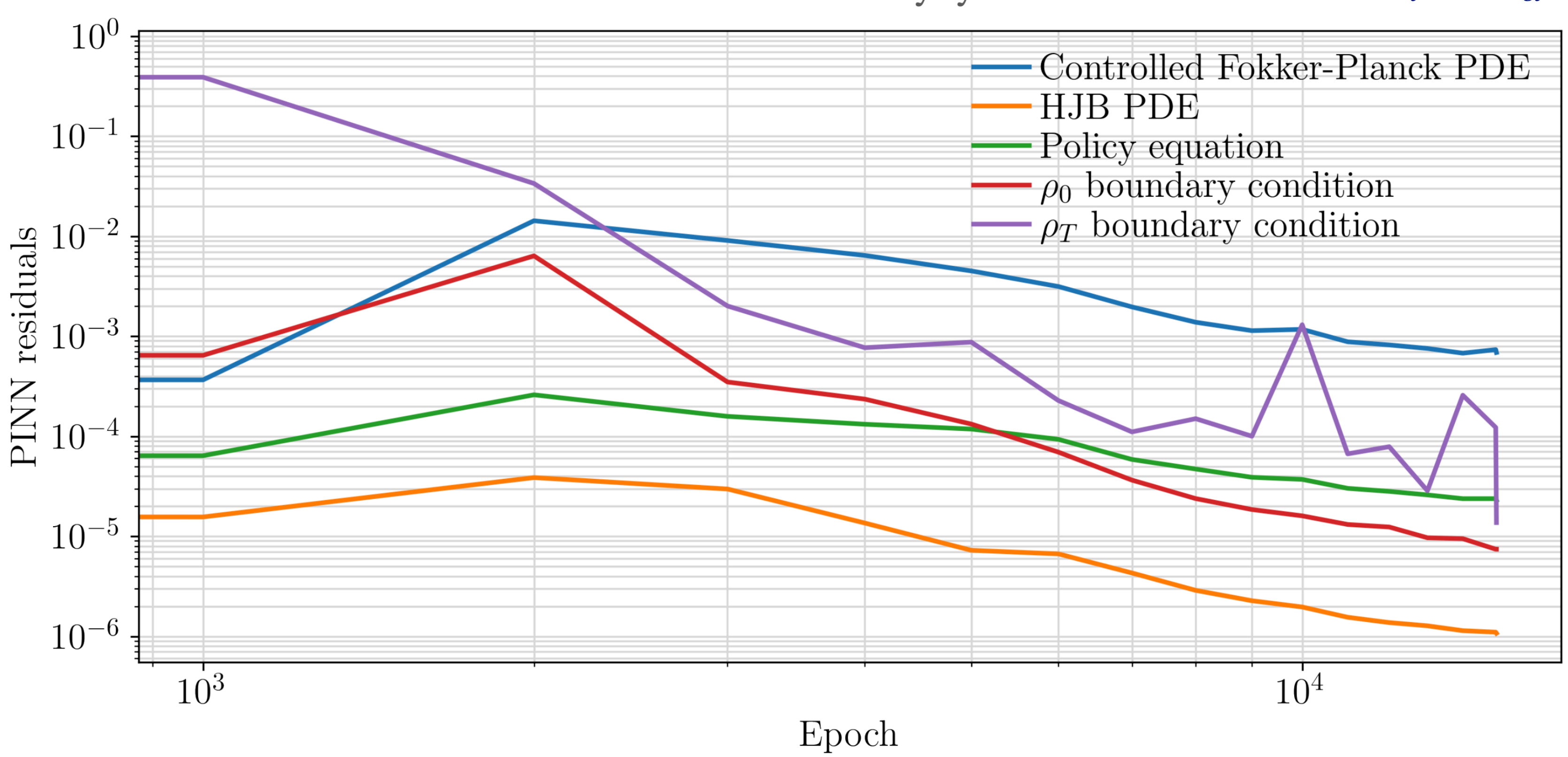
I. Nodozi, C. Yan, M. Khare, A.H., and A. Mesbah, *TCST 2024*

Control non-affine generalized Schrödinger bridge



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

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

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

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

$$\int \text{with b.c. } \langle \boldsymbol{f}\hat{\varphi} - \theta\nabla\hat{\varphi}, \boldsymbol{n}\rangle\big|_{\partial\mathcal{X}} = 0$$

$$\begin{array}{ccc}
\hat{\varphi}_0(\boldsymbol{x}) & \longrightarrow & \hat{\varphi}_1(\boldsymbol{x}) \\
\uparrow \; \rho_0(\boldsymbol{x}) \oslash \varphi_0(\boldsymbol{x}) & & \downarrow \; \rho_1(\boldsymbol{x}) \oslash \hat{\varphi}_1(\boldsymbol{x}) \\
\varphi_0(\boldsymbol{x}) & \longleftarrow & \varphi_1(\boldsymbol{x})
\end{array}$$

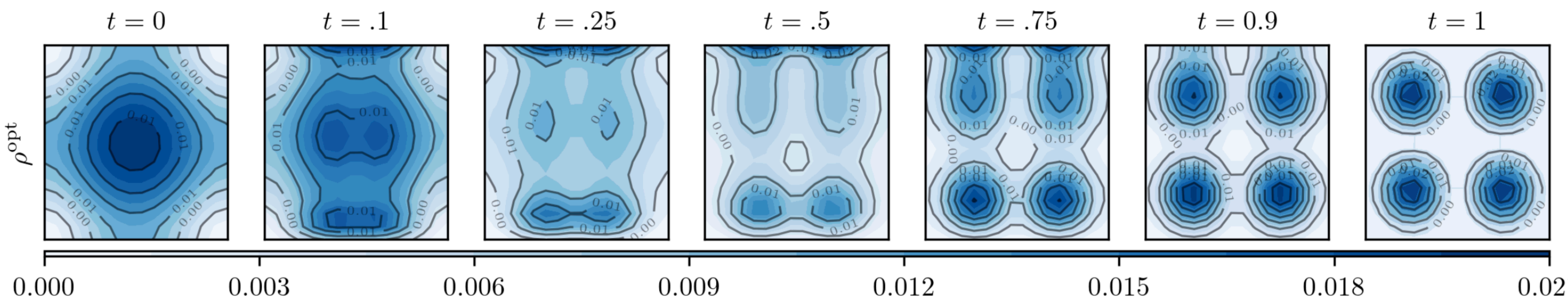
$$\int \text{with b.c. } \langle \nabla\varphi, \boldsymbol{n}\rangle\big|_{\partial\mathcal{X}} = 0$$

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

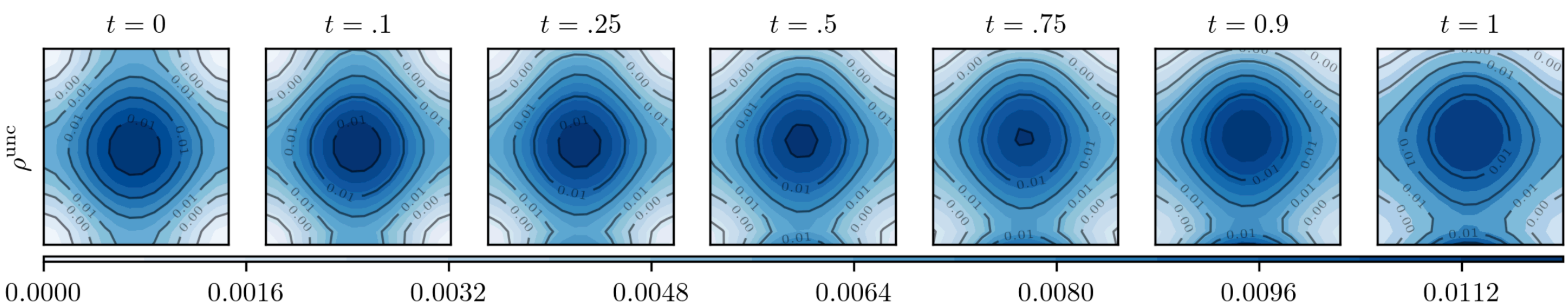
Reflected bridge: numerics with ∇V drift

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

Optimal controlled state PDFs:



Uncontrolled state PDFs:

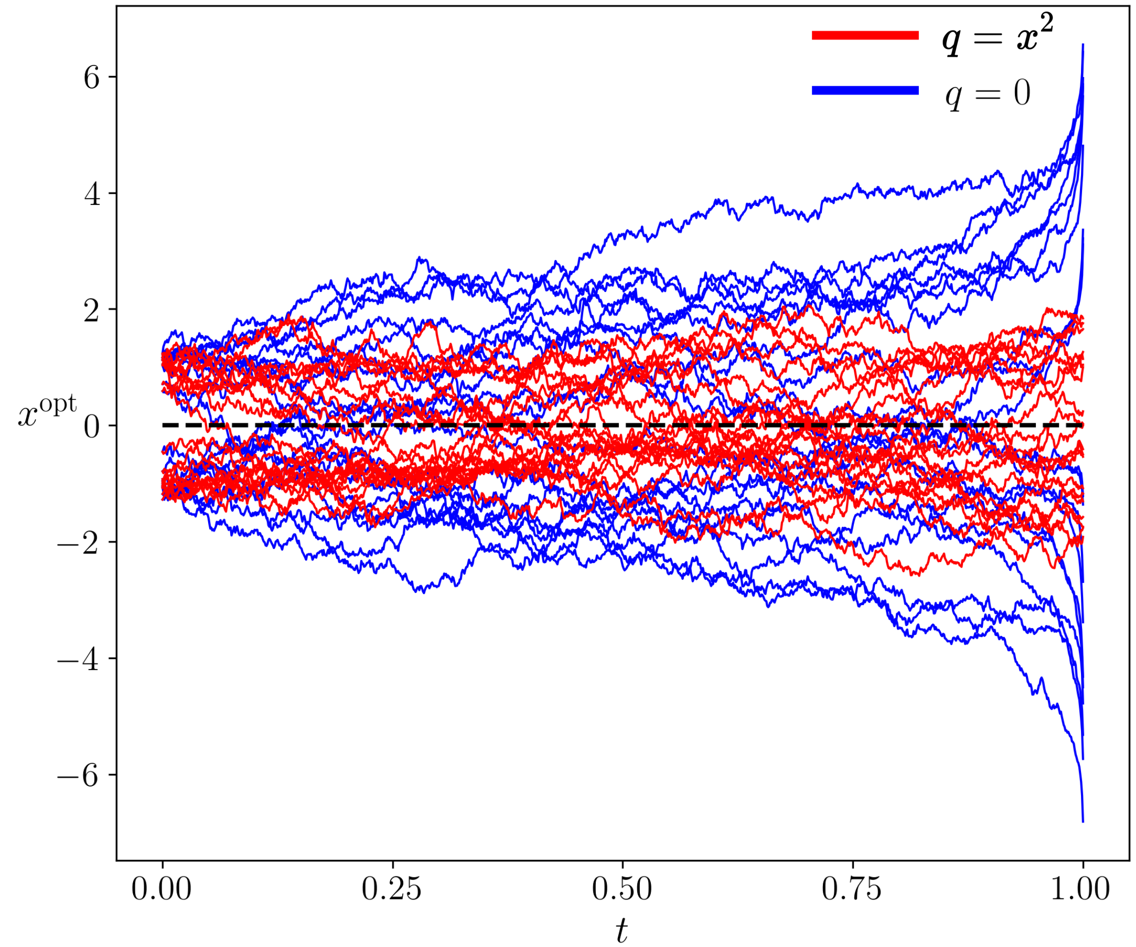


K.F. Caluya, and A.H., *ACC 2021*

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: $q(x) = x^\top Q x, Q \succeq 0$

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

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

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

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

for IVP solutions to use in Schrödinger factor recursion:

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

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

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

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

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

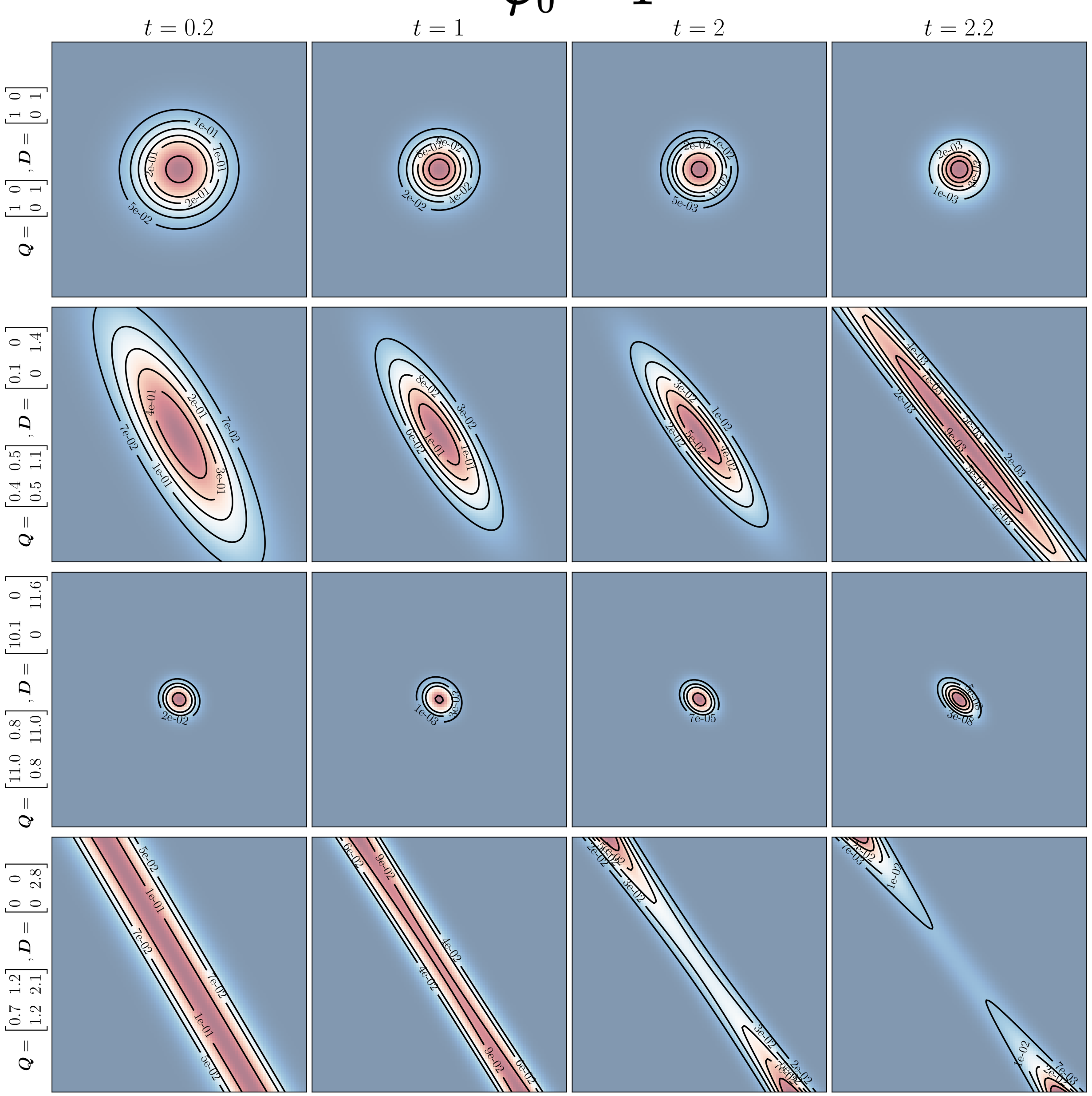
$\boldsymbol{Q} = \boldsymbol{I}$ recovers the multivariate Mehler kernel in quantum harmonic oscillator

Schrödinger bridge with quadratic state cost: $q(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x}, \boldsymbol{Q} \succeq \boldsymbol{0}$

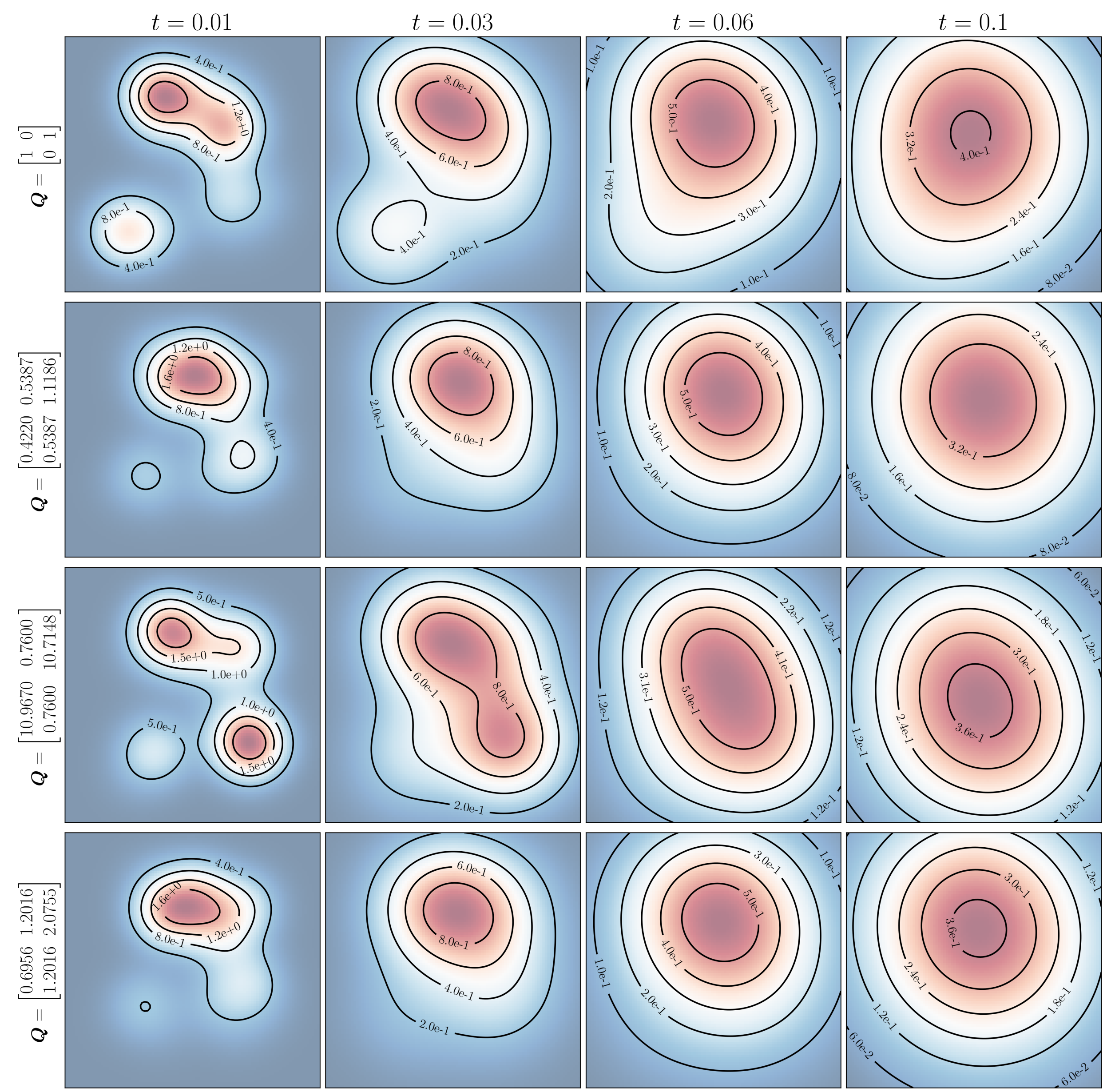
Thm. $$\kappa(0,\boldsymbol{y};t,\boldsymbol{z}) = \underbrace{\kappa_+\left(0,\boldsymbol{y}_{[i_1:i_{n-p}]};t,\boldsymbol{z}_{[i_1:i_{n-p}]}\right)}_{\text{derived pos def kernel in } n-p \text{ variables}} \underbrace{\kappa_0\left(0,\boldsymbol{y}_{[i_{n-p+1}:i_n]};t,\boldsymbol{z}_{[i_{n-p+1}:i_n]}\right)}_{\text{heat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

Action of kernel in $\boldsymbol{x}$ coordinates

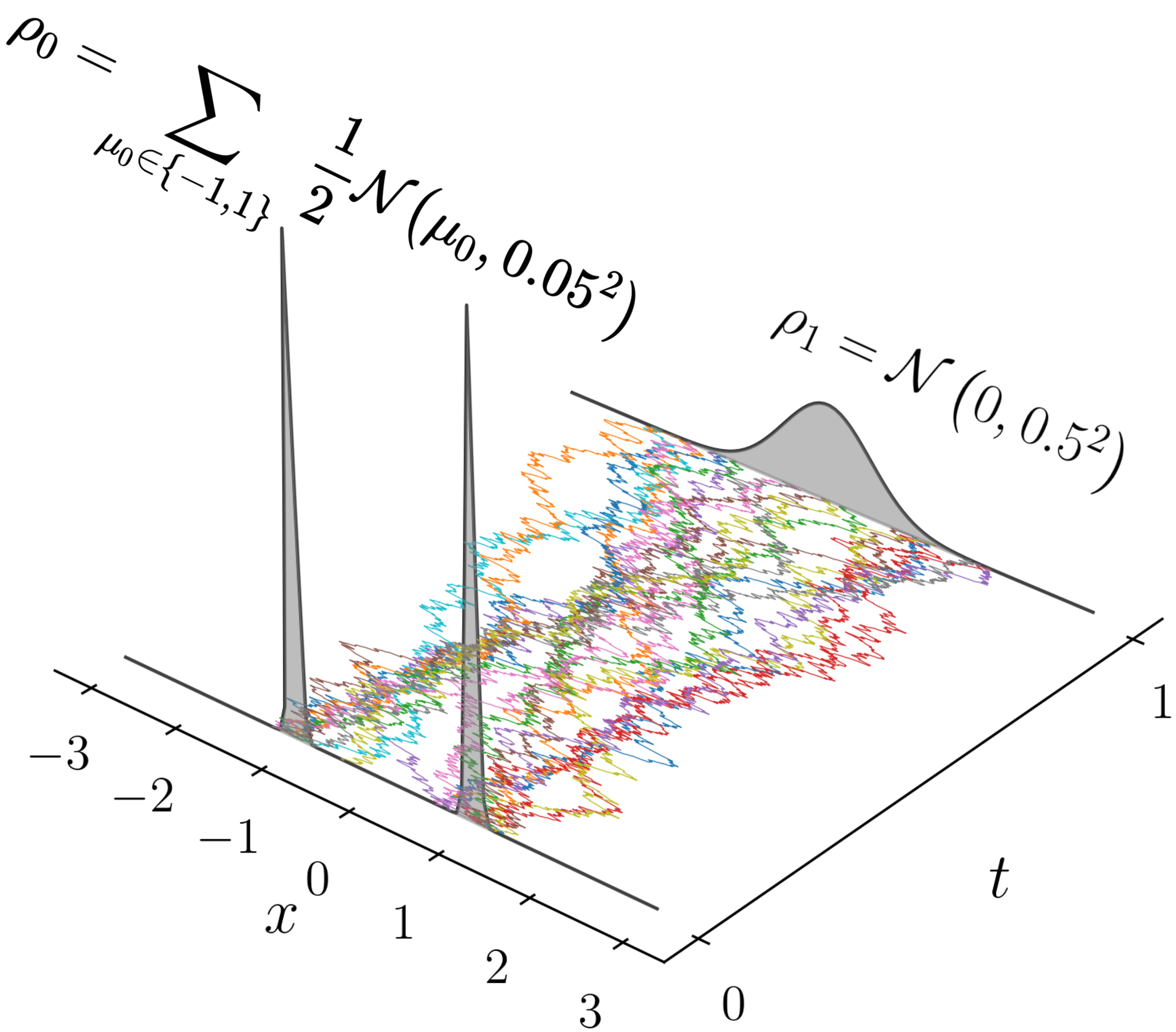
$$\varphi_0 = 1$$

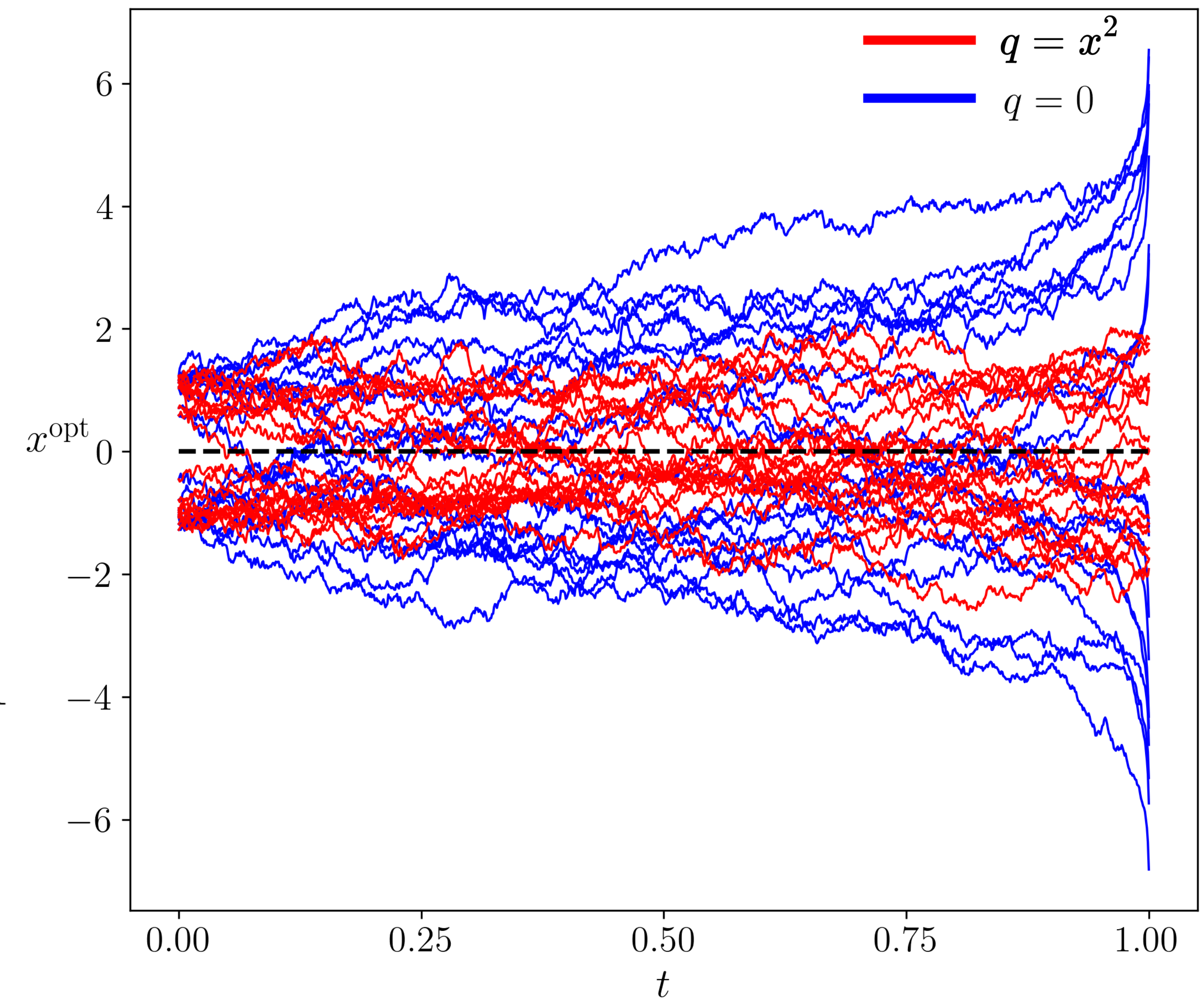


$$\varphi_0 \propto \exp\left\{-\frac{1}{25}\left(\left((10x_1-5)^2+10x_2-16\right)^2+\left(10x_1-12+(10x_2-5)^2\right)^2\right)\right\}$$



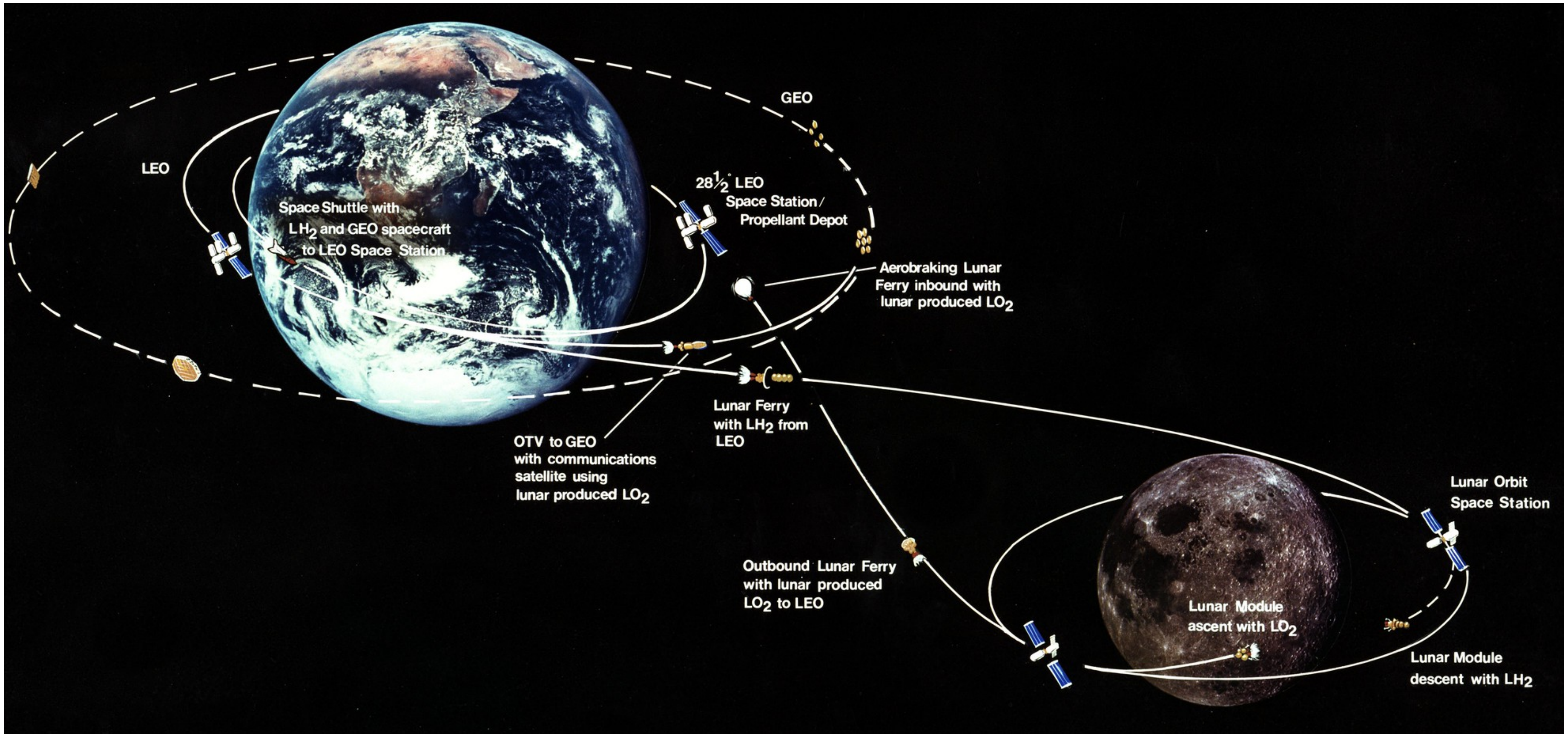
Schrödinger bridge in 1D: with vs without quadratic state cost





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

Lambert's Problem

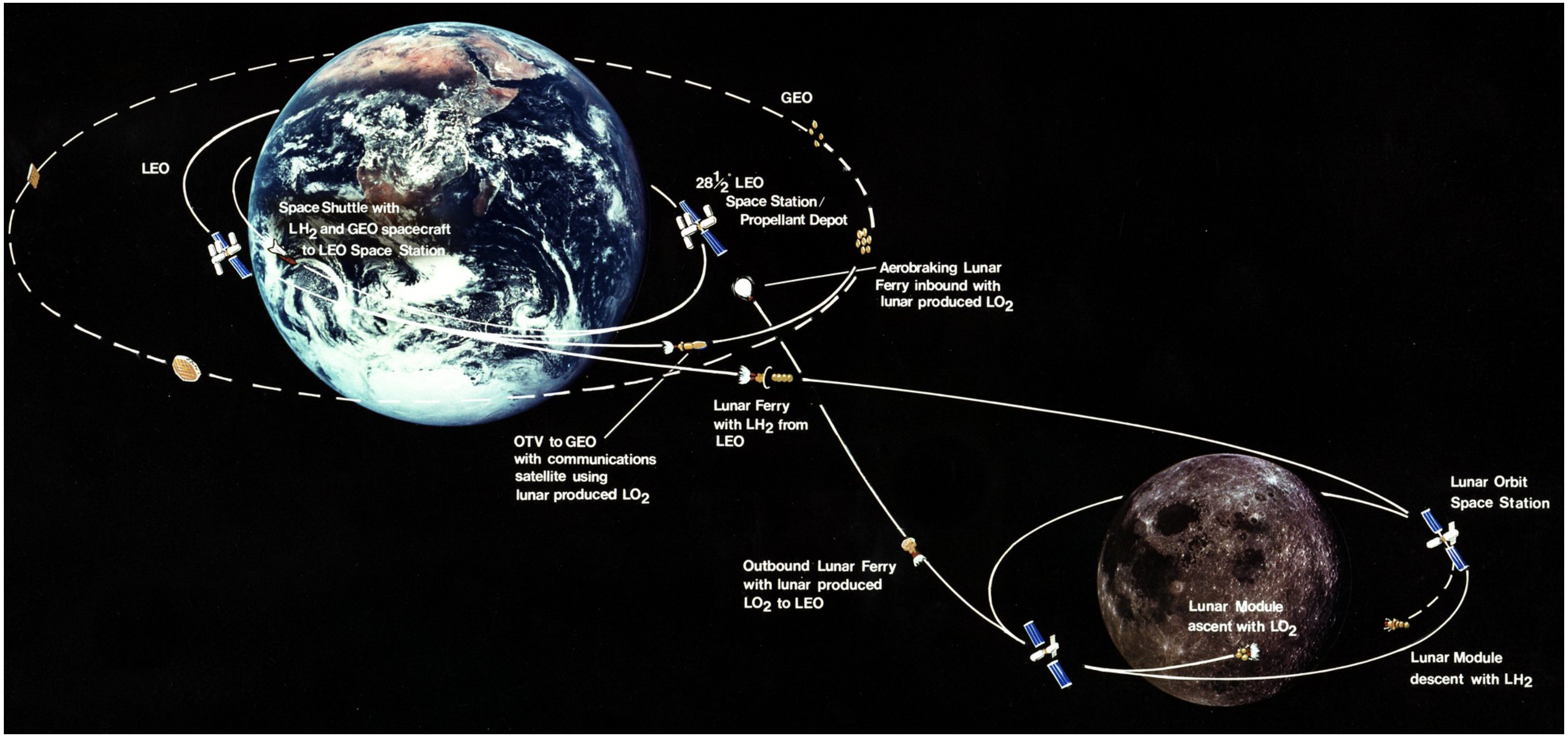


3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

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

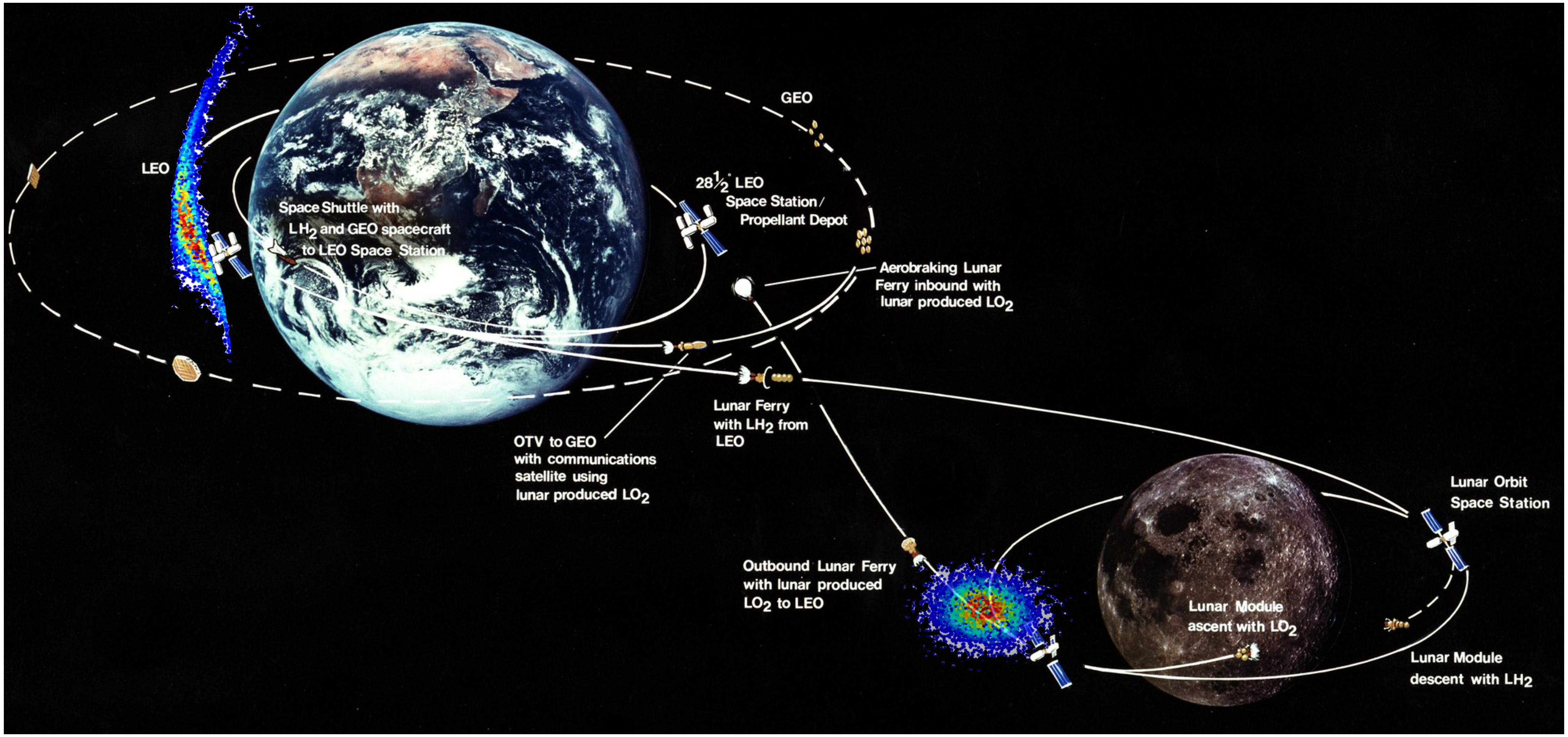
ODE is 2nd order but endpoint boundary conditions are first order

⇝ 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

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

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)

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

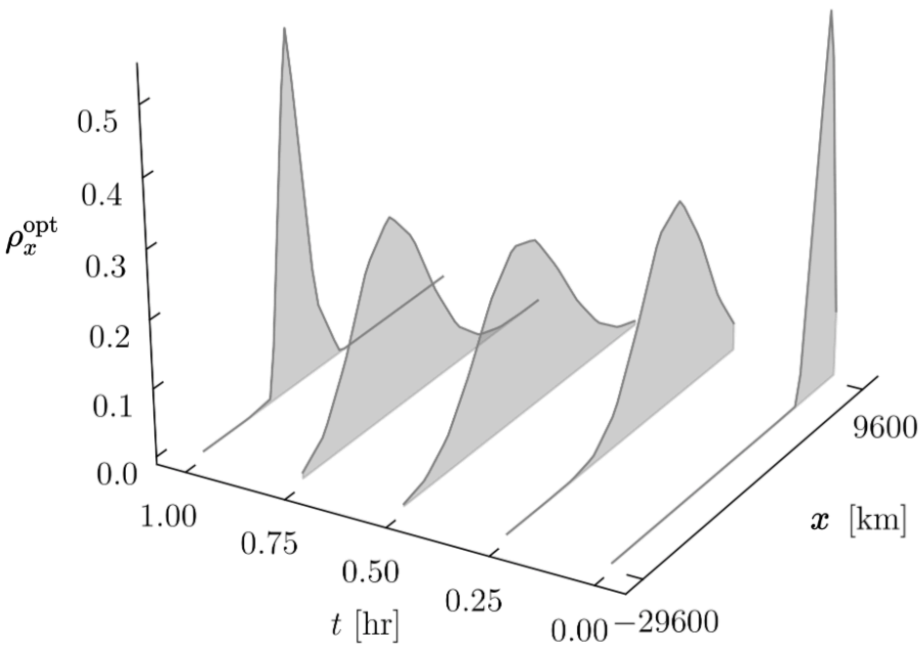
Regularization > 0

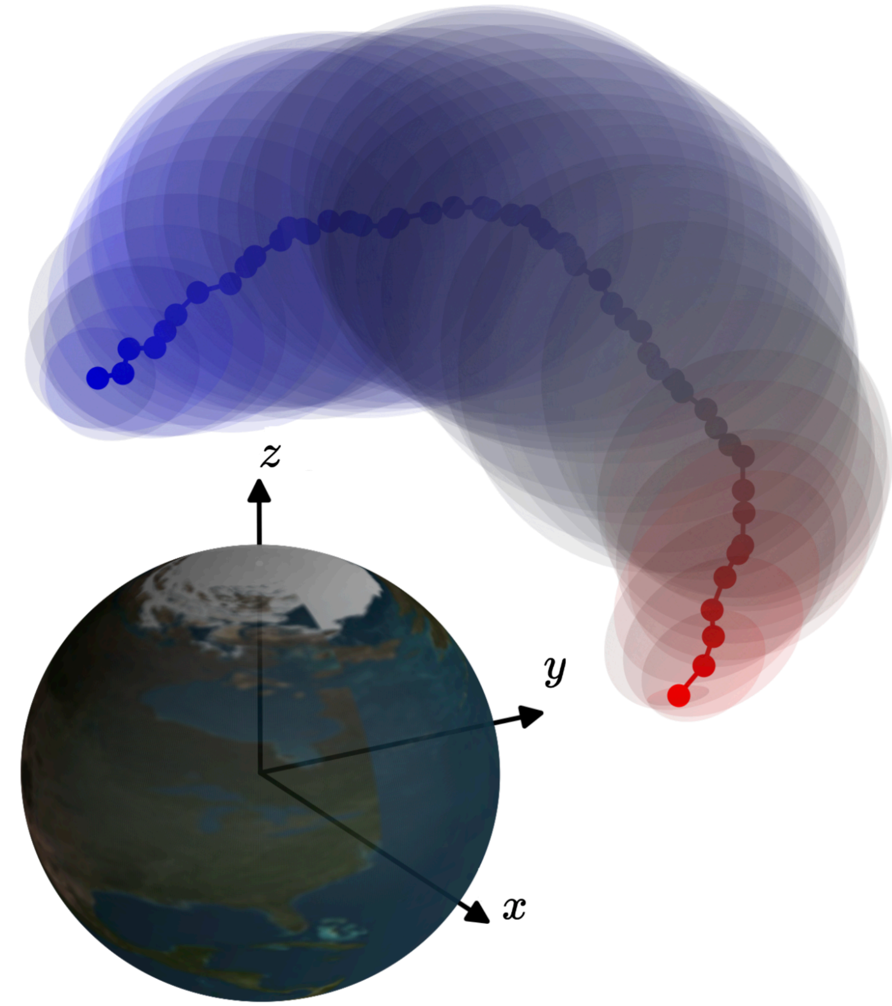
$$\frac{\partial\rho}{\partial t}+\nabla_{\boldsymbol{r}}\cdot(\rho\boldsymbol{v})=\varepsilon\Delta_{\boldsymbol{r}}\rho,$$ — Fokker-Planck-Kolmogorov PDE

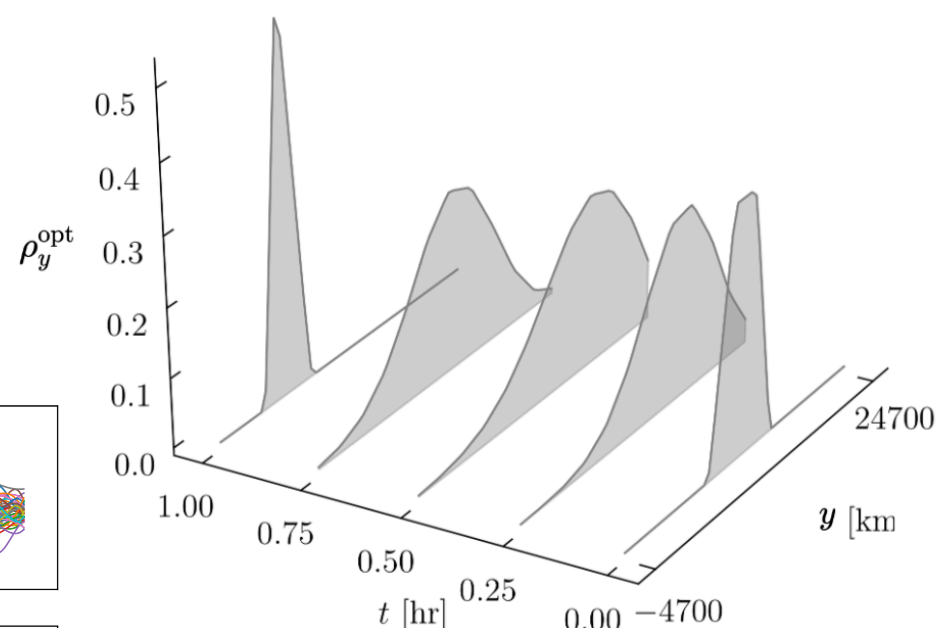
$$\rho(t=t_0,\cdot)=\rho_0,\quad \rho(t=t_1,\cdot)=\rho_1$$

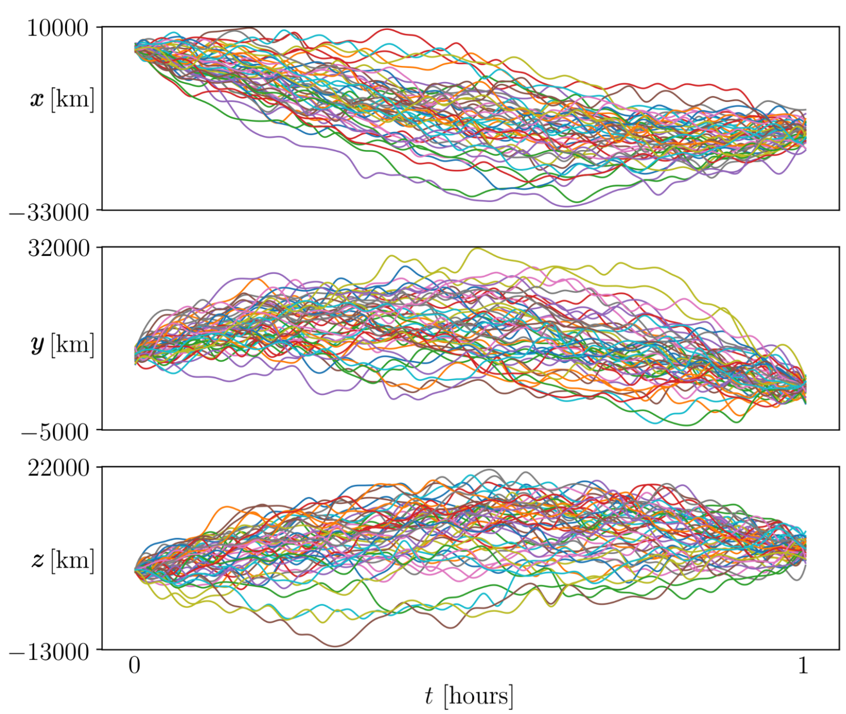
Numerical Case Study

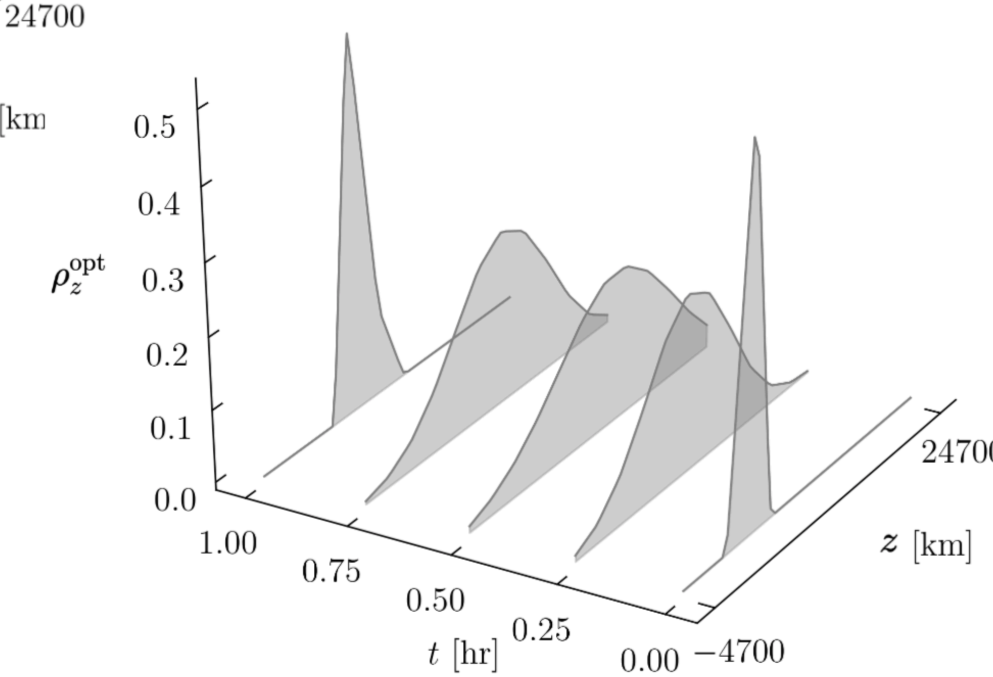
Univariate marginals for optimally controlled joint PDFs











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: control, statistics, differential geometry, analysis, AI/ML, information theory, robotics, biology

Thank You

Support: NSF CITRIS PEOPLE AND ROBOTS Ford

Backup Slides

The Beginning of Lambert's Problem

Named after polymath **Johann Heinrich Lambert (1728 - 1777)**

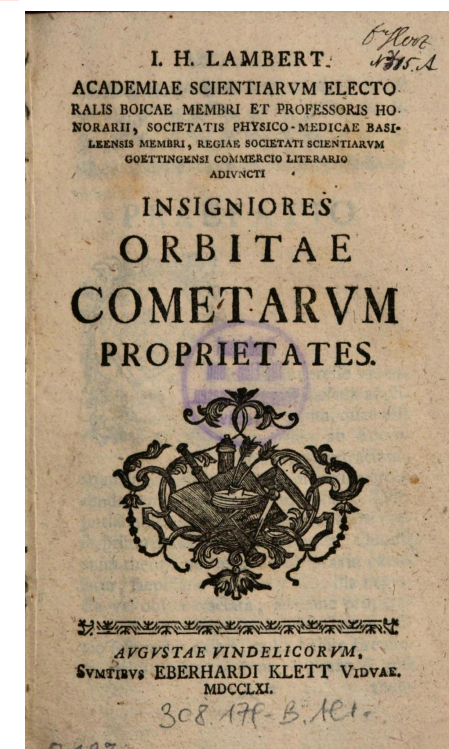
- known for first proof of irrationality of π, W function, area of a hyperbolic triangle

- special cases solved by Euler in 1743

- Lambert mentions this problem in letter to Euler in 1761

- solves the problem for parabolic, elliptic and hyperbolic Keplerian arcs in 1761 book

$$V(\boldsymbol{r}) = -\frac{\mu}{|\boldsymbol{r}|}$$


I. H. LAMBERT.
ACADEMIAE SCIENTIARVM ELECTORALIS BOICAE MEMBRI ET PROFESSORIS HONORARII, SOCIETATIS PHYSICO-MEDICAE BASILEENSIS MEMBRI, REGIAE SOCIETATI SCIENTIARVM GOETTINGENSI COMMERCIO LITERARIO ADIVNCTI
INSIGNIORES ORBITAE COMETARVM PROPRIETATES.
AVGVSTAE VINDELICORVM,
SVMTIBVS EBERHARDI KLETT VIDVAE.
MDCCLXI.

- book receives high praise from Euler in 3 response letters

- alternative proofs by Lagrange (1780), Laplace (1798), Gauss (1809)

Modern History of Lambert's Problem

- Sustained interests for spacecraft guidance, missile interception
- 20th century astrodynamics research: fast computational algorithm, J2 effect in V

$$V(\boldsymbol{x}) = -\frac{\mu}{|\boldsymbol{x}|}\left(1 + \frac{J_2 R_{\text{Earth}}^2}{2|\boldsymbol{x}|^2}\left(1 - \frac{3z^2}{|\boldsymbol{x}|^2}\right)\right) \longrightarrow \text{Bounded and negative for } |\boldsymbol{x}|^2 \geq \mathrm{R}_{\text{Earth}}^2$$

- 21st century interests in aerospace community: probabilistic Lambert's problem
- Endpoint uncertainties due to estimation errors, statistical performance
- State-of-the-art: approx. dynamics (linearization) + approx. statistics (covariance)
- Our contribution: connections with OMT and SBP
- Formulation/computation: non-parametric, well-posedness, optimality certificate

Connection with Optimal Control Problem (OCP)

Lambert Problem ⇔ Deterministic OCP

Idea: use classical Hamiltonian mechanics to reformulate as deterministic OCP

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

$$\Updownarrow$$

$$\arg\inf_{\boldsymbol{v}} \int_{t_0}^{t_1} \left(\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right) \mathrm{d}t$$

Gravitational potential pushed from dynamics to Lagrangian

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

$$\boldsymbol{r}(t=t_0) = \boldsymbol{r}_0 \text{ (given)}, \quad \boldsymbol{r}(t=t_1) = \boldsymbol{r}_1 \text{ (given)}$$