Generalized Gradient Flows for Stochastic Prediction, Filtering, Learning and Control

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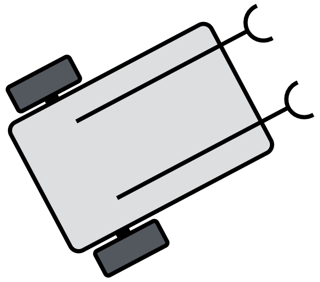
Overarching Theme

Systems-control theory and algorithms for densities

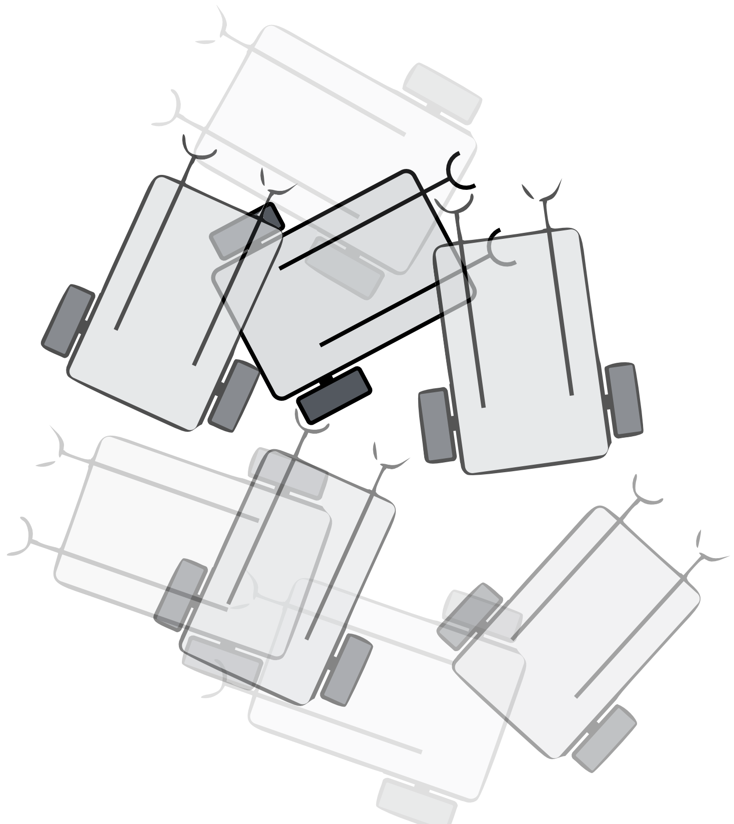
What is density?

Probability Density Fn.



$$\boldsymbol{x}(t) \in \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

Probability Density Fn.

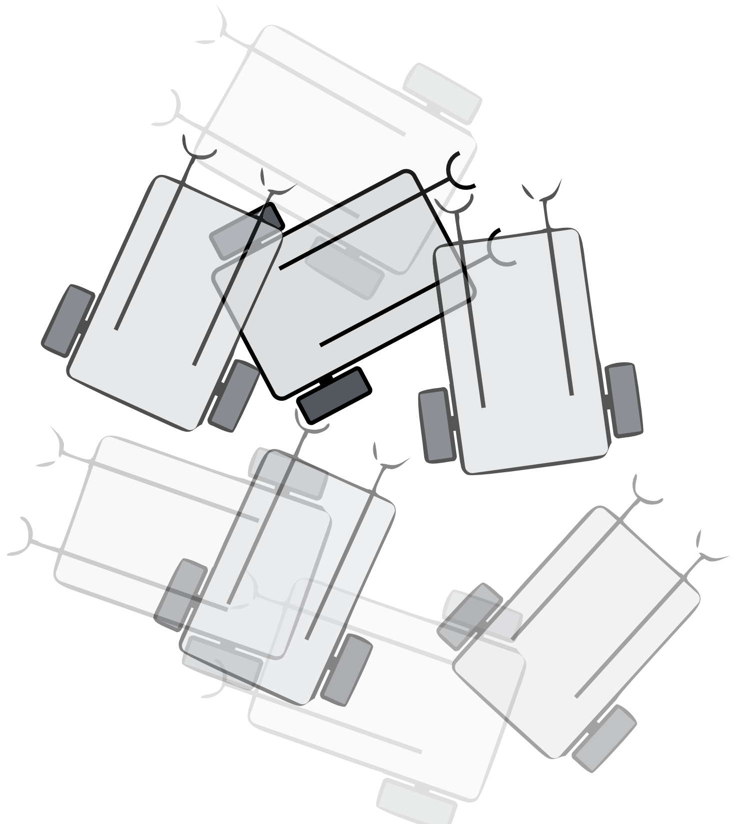


$$\boldsymbol{x}(t) \in \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

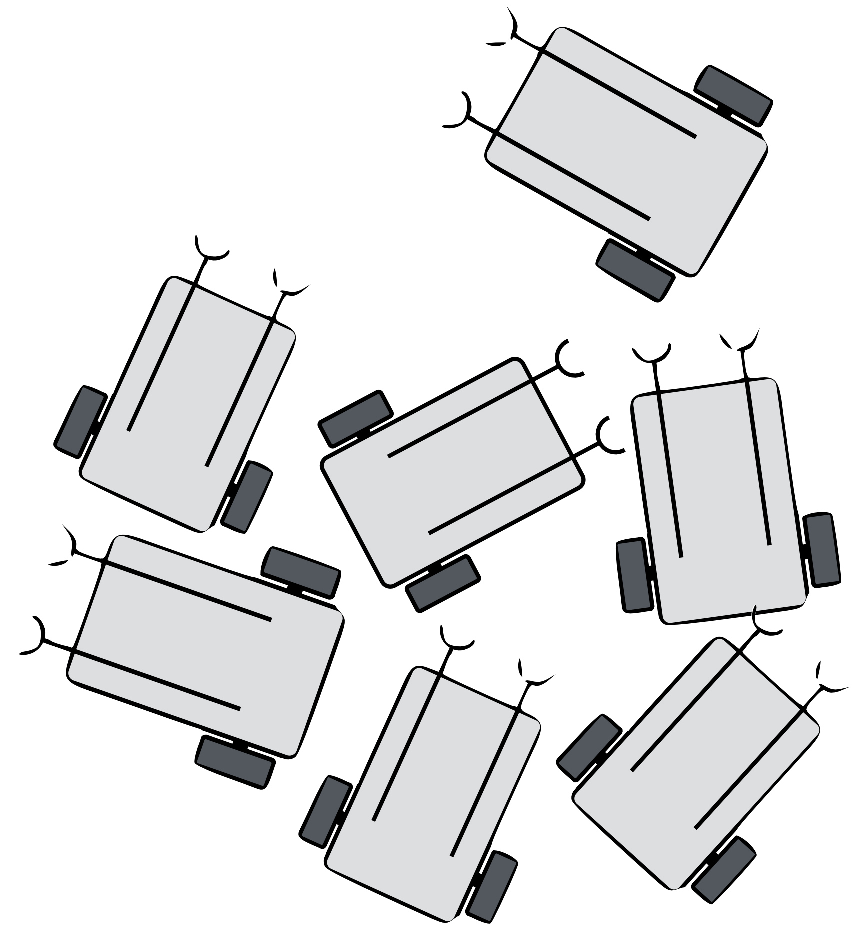
$$\rho\left(\boldsymbol{x}, t\right) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

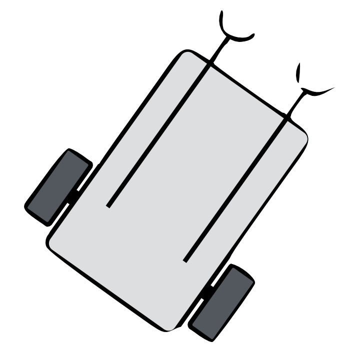
$$\int_{\mathcal{X}} \rho \, \mathrm{d}\boldsymbol{x} = 1 \quad \text{for all } t \in [0, \infty)$$

Probability Density Fn.



Population Density Fn.





$$\boldsymbol{x}(t) \in \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

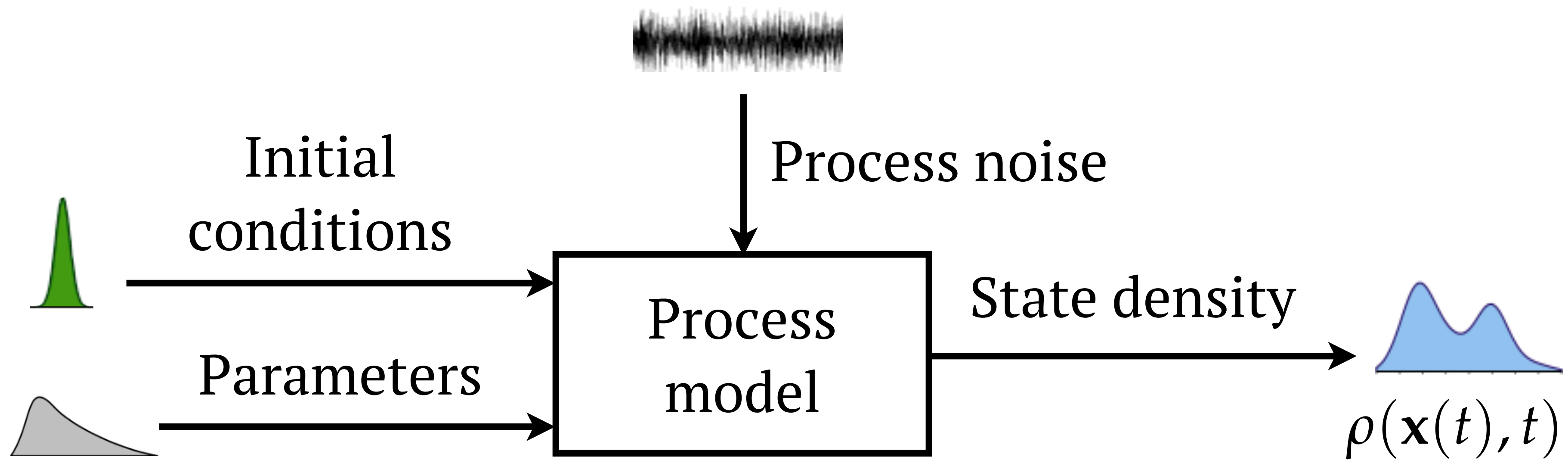
$$\rho\left(\boldsymbol{x}, t\right) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

$$\int_{\mathcal{X}} \rho \, \mathrm{d}\boldsymbol{x} = 1 \quad \text{for all } t \in [0, \infty)$$

Why care about densities?

Prediction Problem

Compute
joint state PDF
$\rho\left(x, t\right)$



Trajectory flow:

$$\mathrm{d}\mathbf{X}(t) = \mathbf{f}(\mathbf{X}, t)\,\mathrm{d}t + \mathbf{g}(\mathbf{X}, t)\,\mathrm{d}\mathbf{w}(t), \quad \mathrm{d}\mathbf{w}(t) \sim \mathcal{N}(0, \mathbf{Q}\mathrm{d}t)$$

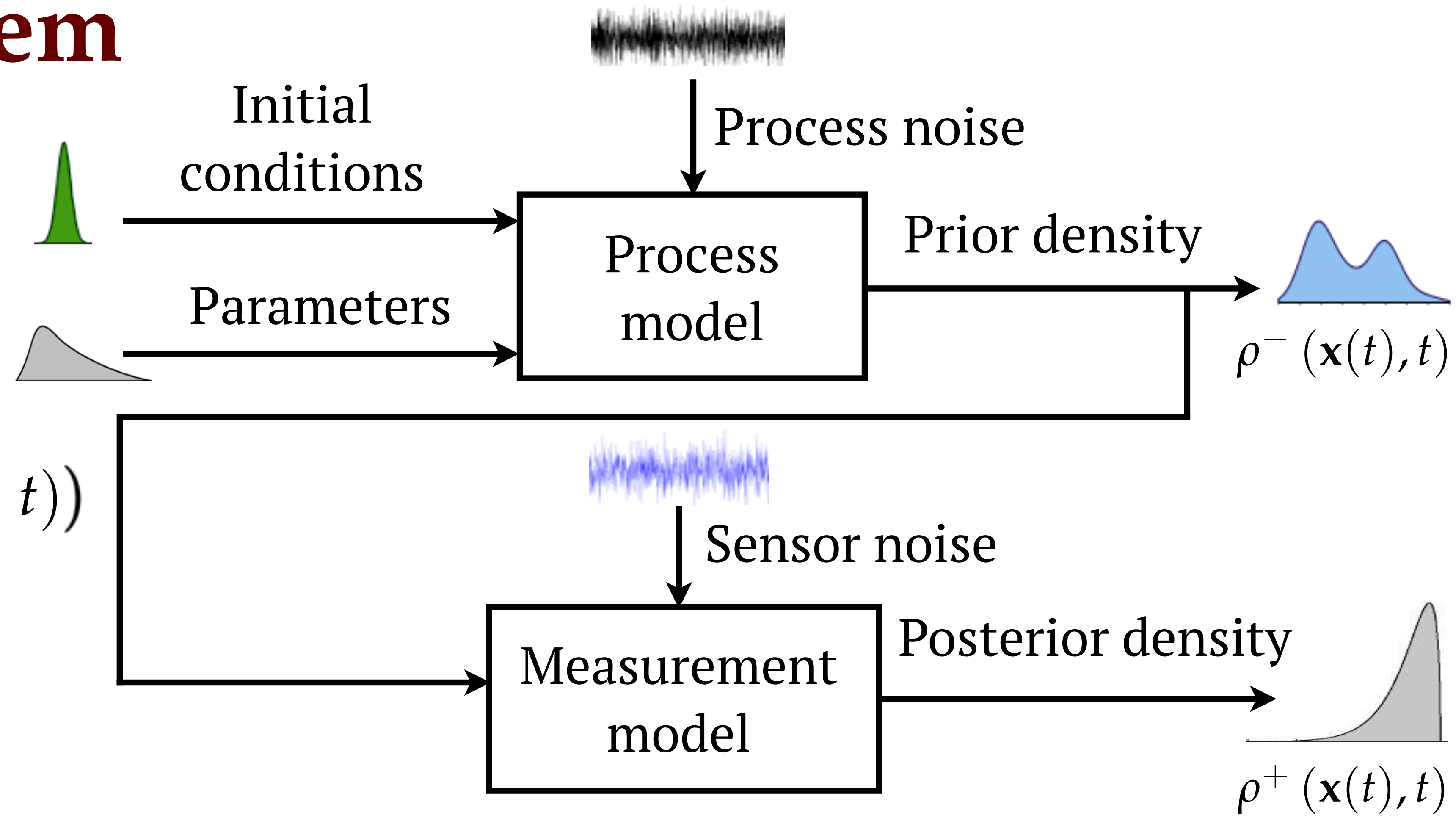
Density flow:

$$\frac{\partial \rho}{\partial t} = \mathcal{L}_{\mathrm{FP}}(\rho) := -\nabla \cdot (\rho \mathbf{f}) + \frac{1}{2} \sum_{i,j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j} \left(\left(\mathbf{g}\mathbf{Q}\mathbf{g}^{\top} \right)_{ij} \rho \right)$$

Filtering Problem

Compute conditional joint state PDF

$$\rho^+ := \rho\left(x, t \mid z(s), 0 \le s \le t\right)$$



Trajectory flow:

$$\mathrm{d}\mathbf{X}(t) = \mathbf{f}(\mathbf{X}, t)\,\mathrm{d}t + \mathbf{g}(\mathbf{X}, t)\,\mathrm{d}\mathbf{w}(t), \qquad \mathrm{d}\mathbf{w}(t) \sim \mathcal{N}(0, \mathbf{Q}\mathrm{d}t)$$

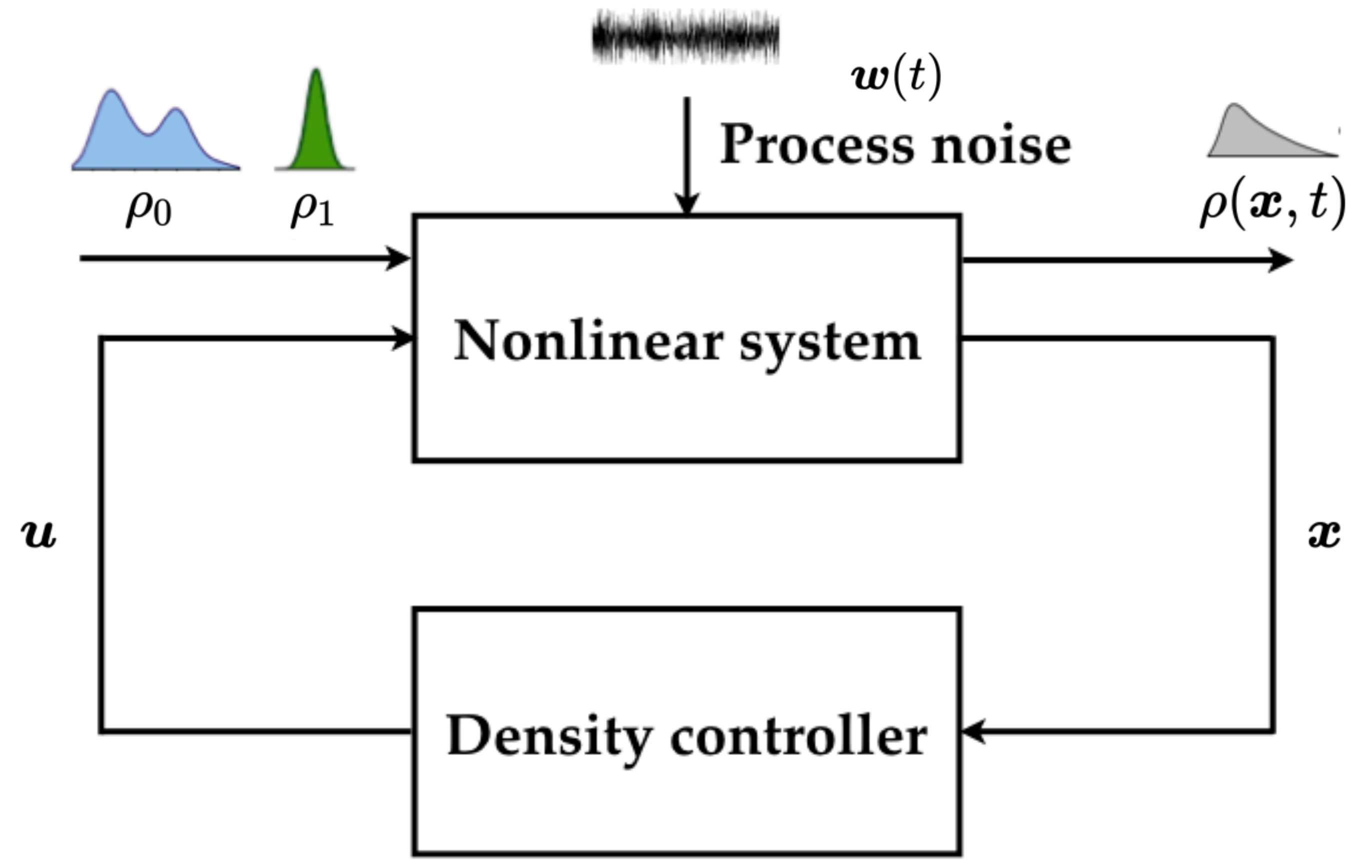
$$\mathrm{d}\mathbf{Z}(t) = \mathbf{h}(\mathbf{X}, t)\,\mathrm{d}t + \mathrm{d}\mathbf{v}(t), \qquad \mathrm{d}\mathbf{v}(t) \sim \mathcal{N}(0, \mathbf{R}\mathrm{d}t)$$

Density flow:

$$\mathrm{d}\rho^+ = \left[\mathcal{L}_{\mathrm{FP}}\mathrm{d}t + \left(\mathbf{h}(\mathbf{x}, t) - \mathbb{E}_{\rho^+}\{\mathbf{h}(\mathbf{x}, t)\}\right)^\top \mathbf{R}^{-1}\left(\mathrm{d}\mathbf{z}(t) - \mathbb{E}_{\rho^+}\{\mathbf{h}(\mathbf{x}, t)\}\mathrm{d}t\right)\right]\rho^+$$

Control Problem

Steer joint state PDF via feedback control over finite time horizon



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

subject to

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

$$\boldsymbol{x}\left(t = 0\right) \sim \rho_0, \quad \boldsymbol{x}\left(t = 1\right) \sim \rho_1$$

Neural Network Learning Problem

Consider fully connected NN

Think "layers" as interacting population of neurons

Mean field learning problem: $$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^p)} R\left(\int \Phi(\boldsymbol{x}, \boldsymbol{\theta})\rho(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}\right)$$

PDF dynamics:

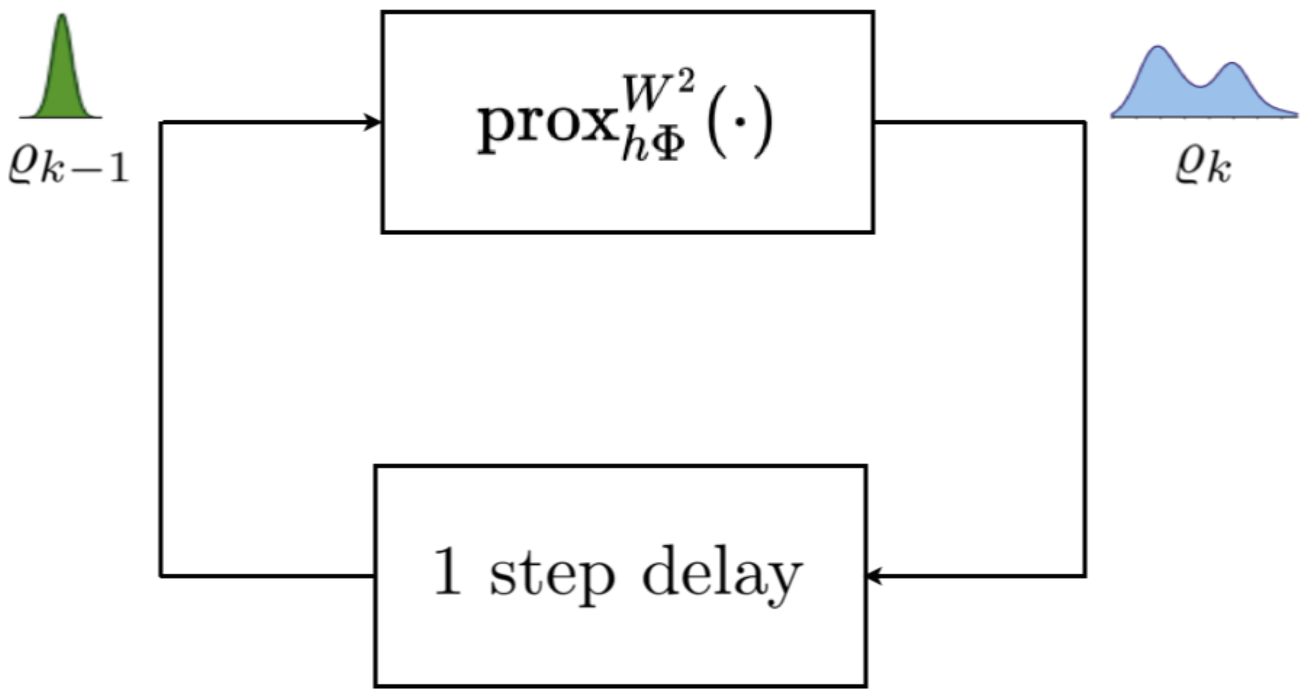
$$\frac{\partial \rho}{\partial t} = -\nabla^W R\left(\int \Phi\rho\right) = \nabla \cdot \left(\rho \nabla \frac{\delta}{\delta \rho} R\left(\int \Phi\rho\right)\right)$$

Solving prediction problem as generalized gradient flow

What's New?

Main idea: Solve $\dfrac{\partial \rho}{\partial t} = \mathcal{L}_{\mathrm{FP}}\rho, \;\; \rho(x, t=0) = \rho_0$ **as gradient flow in** $\mathcal{P}_2(\mathcal{X})$

Infinite dimensional variational recursion:



Proximal operator: $\varrho_k = \mathrm{prox}_{h\Phi}^{W^2}(\varrho_{k-1}) := \underset{\varrho \in \mathcal{P}_2(\mathcal{X})}{\arg\inf} \left\{ \dfrac{1}{2} W^2(\varrho, \varrho_{k-1}) + h\Phi(\varrho) \right\}$

Optimal transport cost: $W^2(\varrho, \varrho_{k-1}) := \displaystyle\inf_{\pi \in \Pi(\varrho, \varrho_{k-1})} \int_{\mathcal{X}\times\mathcal{X}} c(x,y)\, \mathrm{d}\pi(x,y)$

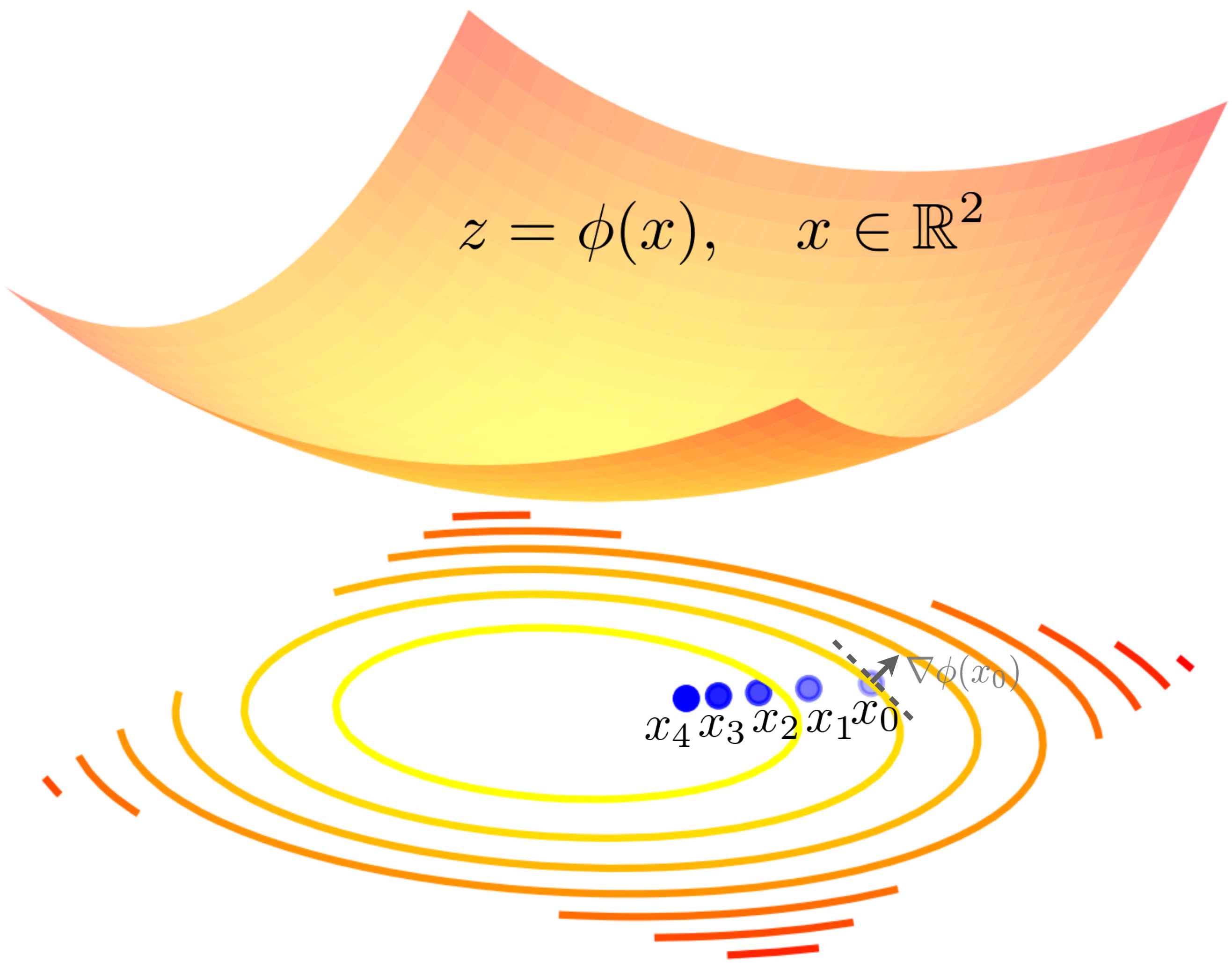
Free energy functional: $\Phi(\varrho) := \displaystyle\int_{\mathcal{X}} \psi \varrho \,\mathrm{d}x + \beta^{-1} \int_{\mathcal{X}} \varrho \log \varrho \,\mathrm{d}x$

Geometric Meaning of Gradient Flow

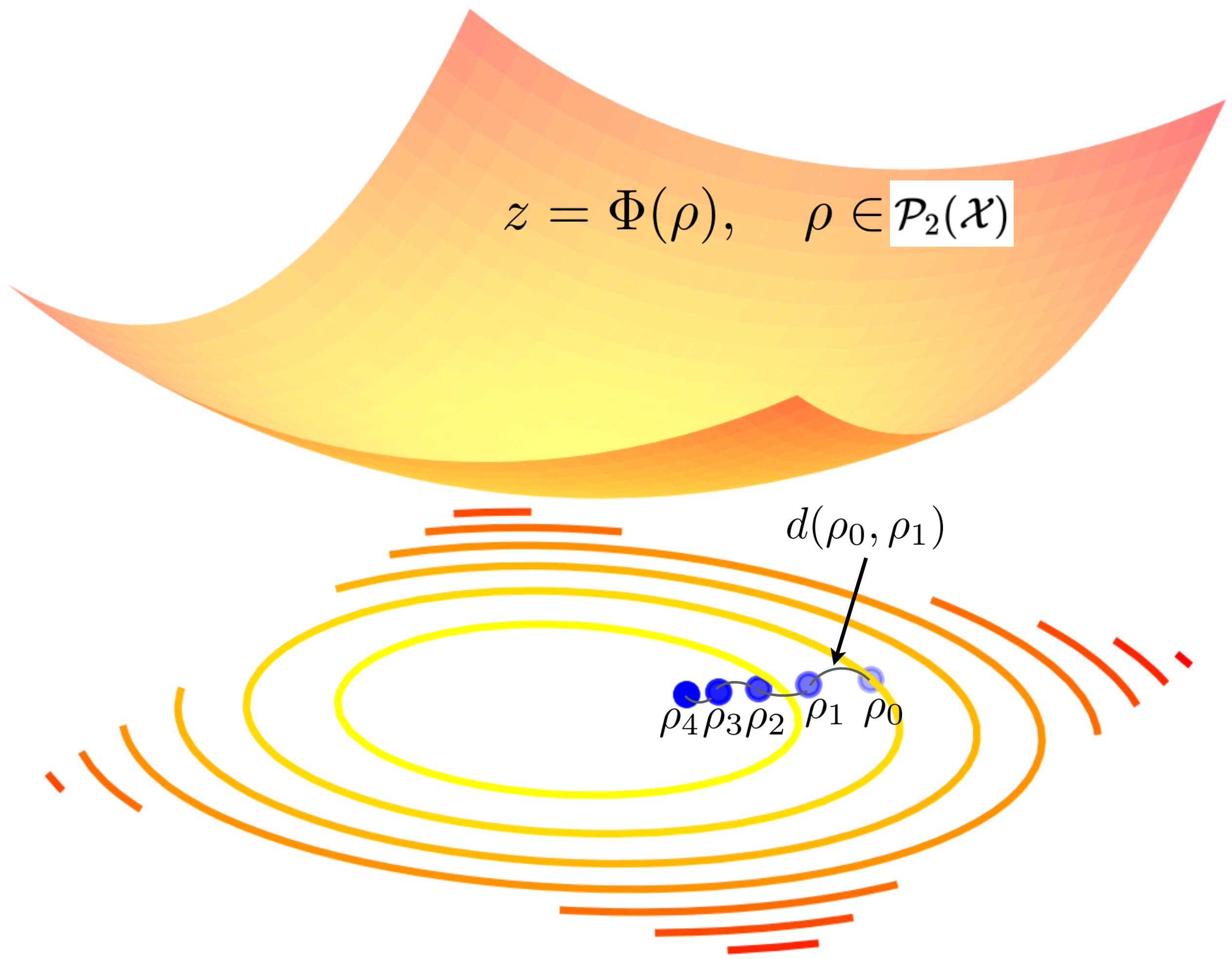
Gradient Flow in $\mathcal{X}$	Gradient Flow in $\mathcal{P}_2(\mathcal{X})$
$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = -\nabla\varphi(\boldsymbol{x}), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0$	$\frac{\partial\rho}{\partial t} = -\nabla^W \Phi(\rho), \quad \rho(\boldsymbol{x}, 0) = \rho_0$
Recursion: $\boldsymbol{x}_k = \boldsymbol{x}_{k-1} - h\nabla\varphi(\boldsymbol{x}_k) = \underset{\boldsymbol{x}\in\mathcal{X}}{\arg\min} \left\{\frac{1}{2}\\|\boldsymbol{x} - \boldsymbol{x}_{k-1}\\|_2^2 + h\varphi(\boldsymbol{x})\right\} =: \mathrm{prox}_{h\varphi}^{\\|\cdot\\|_2}(\boldsymbol{x}_{k-1})$	**Recursion:** $\rho_k = \rho(\cdot, t = kh) = \underset{\rho\in\mathcal{P}_2(\mathcal{X})}{\arg\min} \left\{\frac{1}{2}W^2(\rho, \rho_{k-1}) + h\Phi(\rho)\right\} =: \mathrm{prox}_{h\Phi}^{W^2}(\rho_{k-1})$
Convergence: $\boldsymbol{x}_k \to \boldsymbol{x}(t = kh) \quad \text{as} \quad h \downarrow 0$	**Convergence:** $\rho_k \to \rho(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$
φ as Lyapunov function: $\frac{\mathrm{d}}{\mathrm{d}t}\varphi = -\\| \nabla\varphi \\|_2^2 \leq 0$	**Φ as Lyapunov functional:** $\frac{\mathrm{d}}{\mathrm{d}t}\Phi = -\mathbb{E}_\rho\left[\left\\|\nabla\frac{\delta\Phi}{\delta\rho}\right\\|_2^2\right] \leq 0$

Geometric Meaning of Gradient Flow

Gradient Flow in $\mathcal{X}$

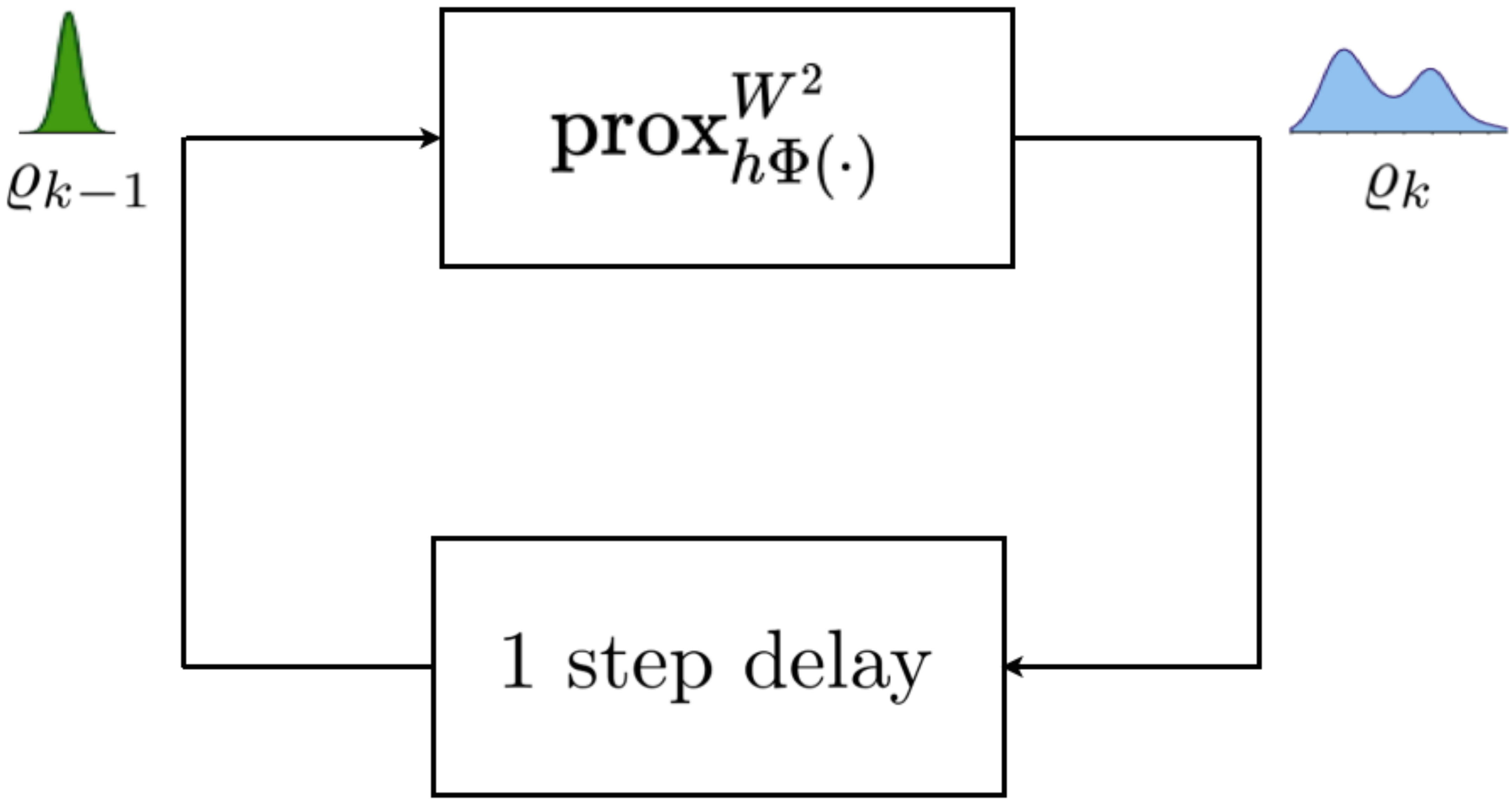


Gradient Flow in $\mathcal{P}_2(\mathcal{X})$



Algorithm: Gradient Ascent on the Dual Space

Uncertainty propagation via point clouds



No spatial discretization or function approximation

Algorithm: Gradient Ascent on the Dual Space

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\nabla \psi \rho) + \beta^{-1} \Delta \rho$$

$\Updownarrow$ **Proximal Recursion**

$$\rho_k = \rho(\boldsymbol{x}, t = kh) = \underset{\rho \in \mathcal{P}_2(\mathbb{R}^n)}{\arg\inf} \left\{ \frac{1}{2} W^2(\rho, \rho_{k-1}) + h\, \Phi(\rho) \right\}$$

$\Downarrow$ **Discrete Primal Formulation**

$$\boldsymbol{\varrho}_k = \underset{\boldsymbol{\varrho}}{\arg\min} \left\{ \min_{\boldsymbol{M} \in \Pi(\boldsymbol{\varrho}_{k-1}, \boldsymbol{\varrho})} \frac{1}{2} \langle \boldsymbol{C}_k, \boldsymbol{M} \rangle + h \left\langle \boldsymbol{\psi}_{k-1} + \beta^{-1} \log \boldsymbol{\varrho}, \boldsymbol{\varrho} \right\rangle \right\}$$

$\Downarrow$ **Entropic Regularization**

$$\boldsymbol{\varrho}_k = \underset{\boldsymbol{\varrho}}{\arg\min} \left\{ \min_{\boldsymbol{M} \in \Pi(\boldsymbol{\varrho}_{k-1}, \boldsymbol{\varrho})} \frac{1}{2} \langle \boldsymbol{C}_k, \boldsymbol{M} \rangle + \epsilon H(\boldsymbol{M}) + h \left\langle \boldsymbol{\psi}_{k-1} + \beta^{-1} \log \boldsymbol{\varrho}, \boldsymbol{\varrho} \right\rangle \right\}$$

$\Updownarrow$ **Dualization**

$$\boldsymbol{\lambda}_0^{\mathrm{opt}}, \boldsymbol{\lambda}_1^{\mathrm{opt}} = \underset{\boldsymbol{\lambda}_0, \boldsymbol{\lambda}_1 \geq 0}{\arg\max} \Big\{ \langle \boldsymbol{\lambda}_0, \boldsymbol{\varrho}_{k-1} \rangle - F^{\star}(-\boldsymbol{\lambda}_1) - \frac{\epsilon}{h} \left(\exp(\boldsymbol{\lambda}_0^{\top} h/\epsilon) \exp(-\boldsymbol{C}_k / 2\epsilon) \exp(\boldsymbol{\lambda}_1 h/\epsilon) \right) \Big\}$$

Recursion on the Cone

$$\boldsymbol{y} = e^{\frac{\boldsymbol{\lambda}_0^*}{\epsilon}} h \Big\downarrow \qquad \Big\downarrow \boldsymbol{z} = e^{\frac{\boldsymbol{\lambda}_1^*}{\epsilon}} h$$

Coupled Transcendental Equations in $\boldsymbol{y}$ and $\boldsymbol{z}$

$$\boldsymbol{\Gamma}_k = e^{\frac{-\boldsymbol{C}_k}{2\epsilon}} \longrightarrow \qquad \boldsymbol{y} \odot \boldsymbol{\Gamma}_k \boldsymbol{z} = \boldsymbol{\varrho}_{k-1}$$

$$\boldsymbol{\varrho}_{k-1} \longrightarrow \qquad \longrightarrow \boldsymbol{\varrho}_k = \boldsymbol{z} \odot \boldsymbol{\Gamma}_k^\top \boldsymbol{y}$$

$$\boldsymbol{\xi}_{k-1} = \frac{e^{-\beta \boldsymbol{\psi}_{k-1}}}{e} \longrightarrow \qquad \boldsymbol{z} \odot \boldsymbol{\Gamma}_k^\top \boldsymbol{y} = \boldsymbol{\xi}_{k-1} \odot \boldsymbol{z}^{-\beta\epsilon/2h}$$

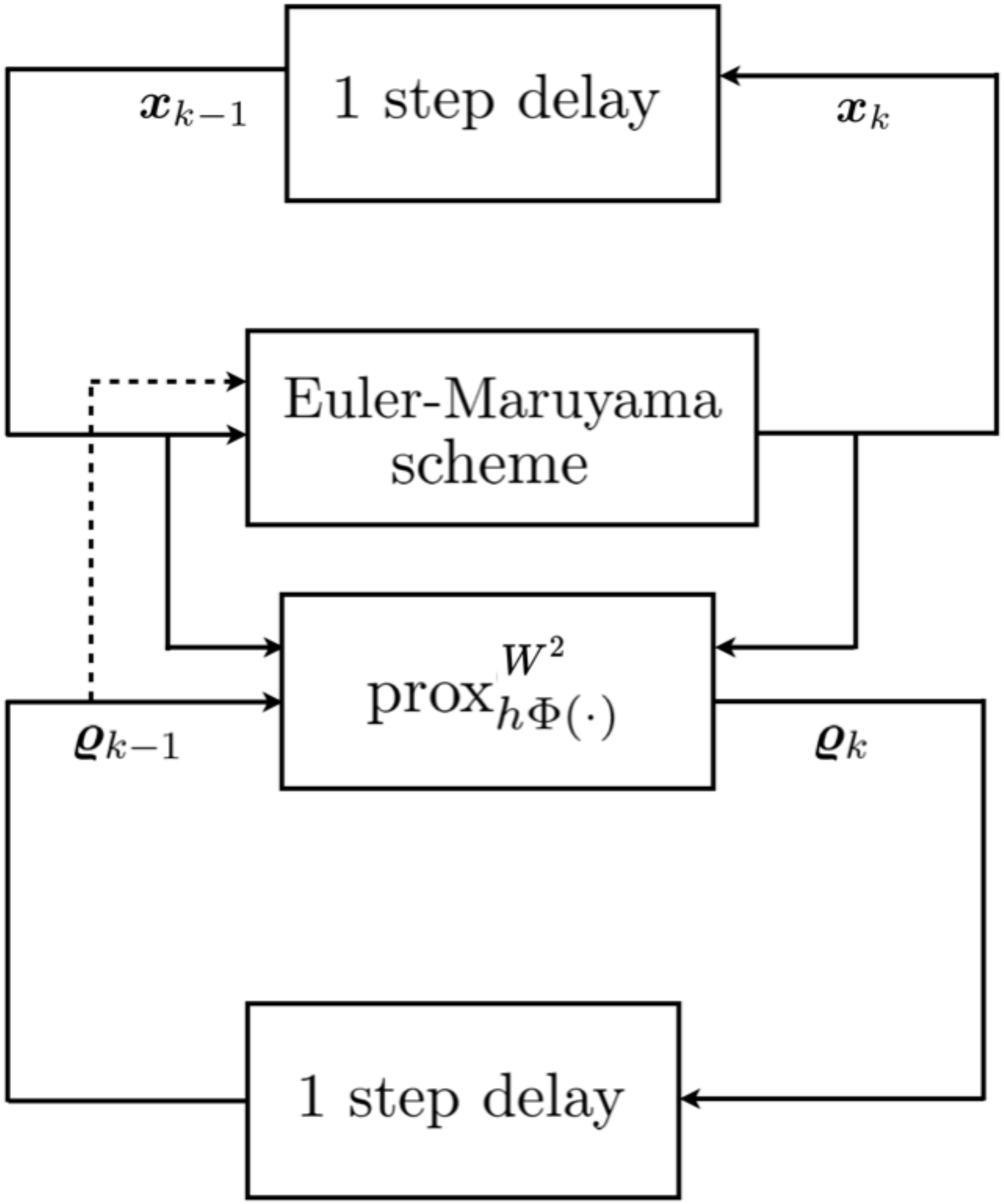
Theorem: Consider the recursion on the cone $\mathbb{R}^n_{\geq 0} \times \mathbb{R}^n_{\geq 0}$

$$\boldsymbol{y} \odot (\boldsymbol{\Gamma}_k \boldsymbol{z}) = \boldsymbol{\varrho}_{k-1}, \quad \boldsymbol{z} \odot \left(\boldsymbol{\Gamma}_k{}^\top \boldsymbol{y}\right) = \boldsymbol{\xi}_{k-1} \odot \boldsymbol{z}^{-\frac{\beta\epsilon}{h}},$$

Then the solution $(\boldsymbol{y}^*, \boldsymbol{z}^*)$ gives the proximal update $\boldsymbol{\varrho}_k = \boldsymbol{z}^* \odot (\boldsymbol{\Gamma}_k{}^\top \boldsymbol{y}^*)$

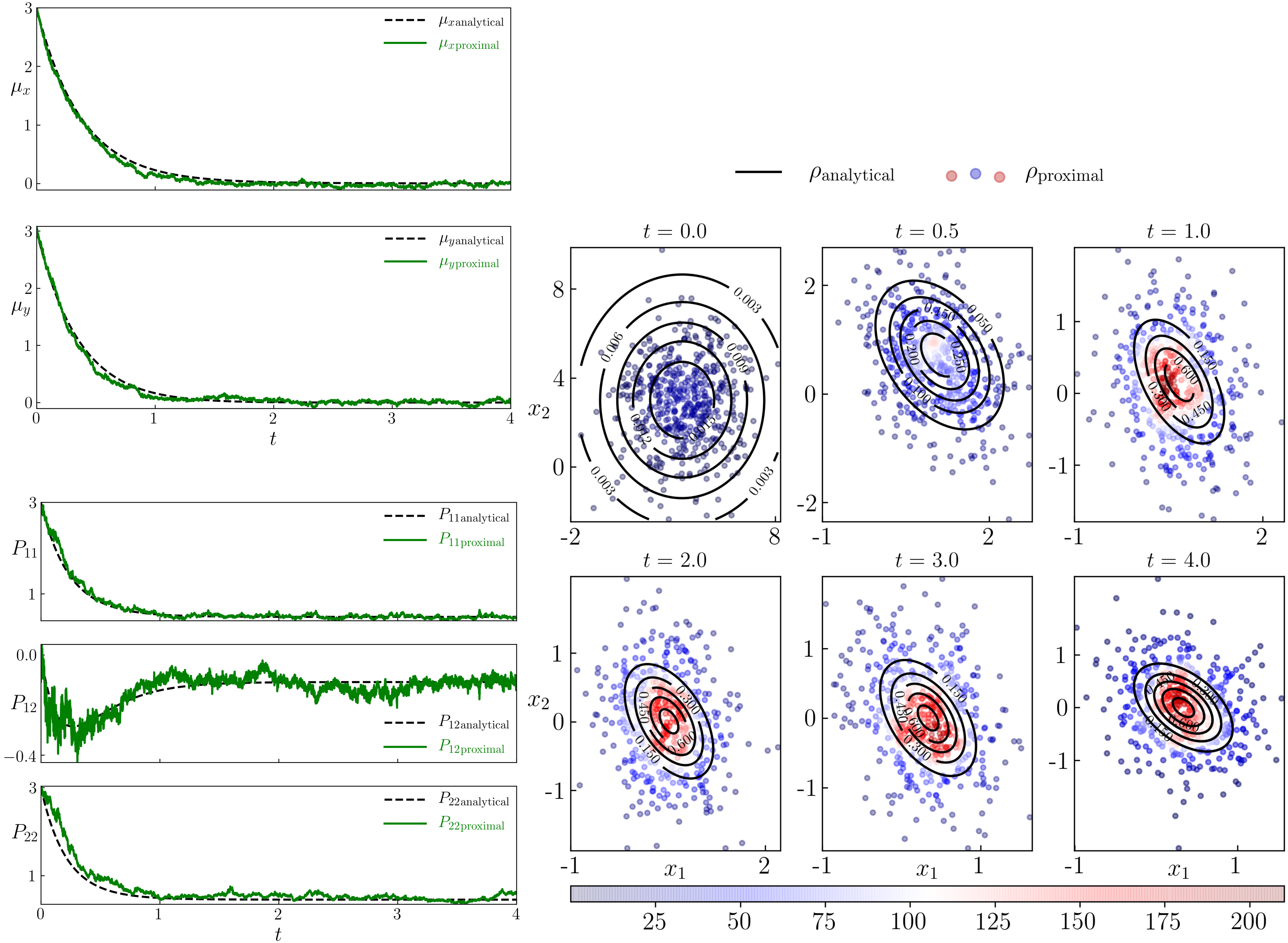
— K.F. Caluya and A.H., Gradient flow algorithms for density propagation in stochastic systems, *IEEE TAC* 2020.

Algorithmic Setup

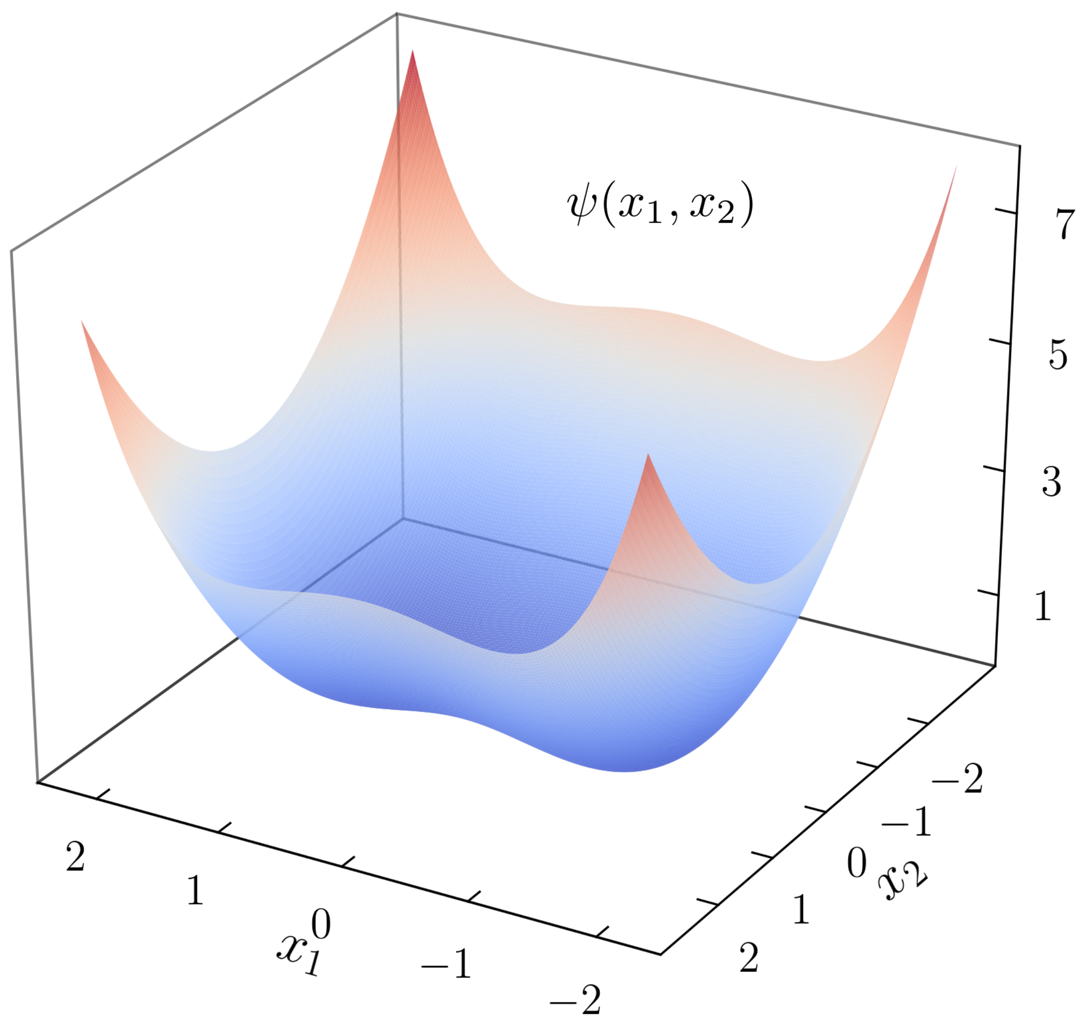


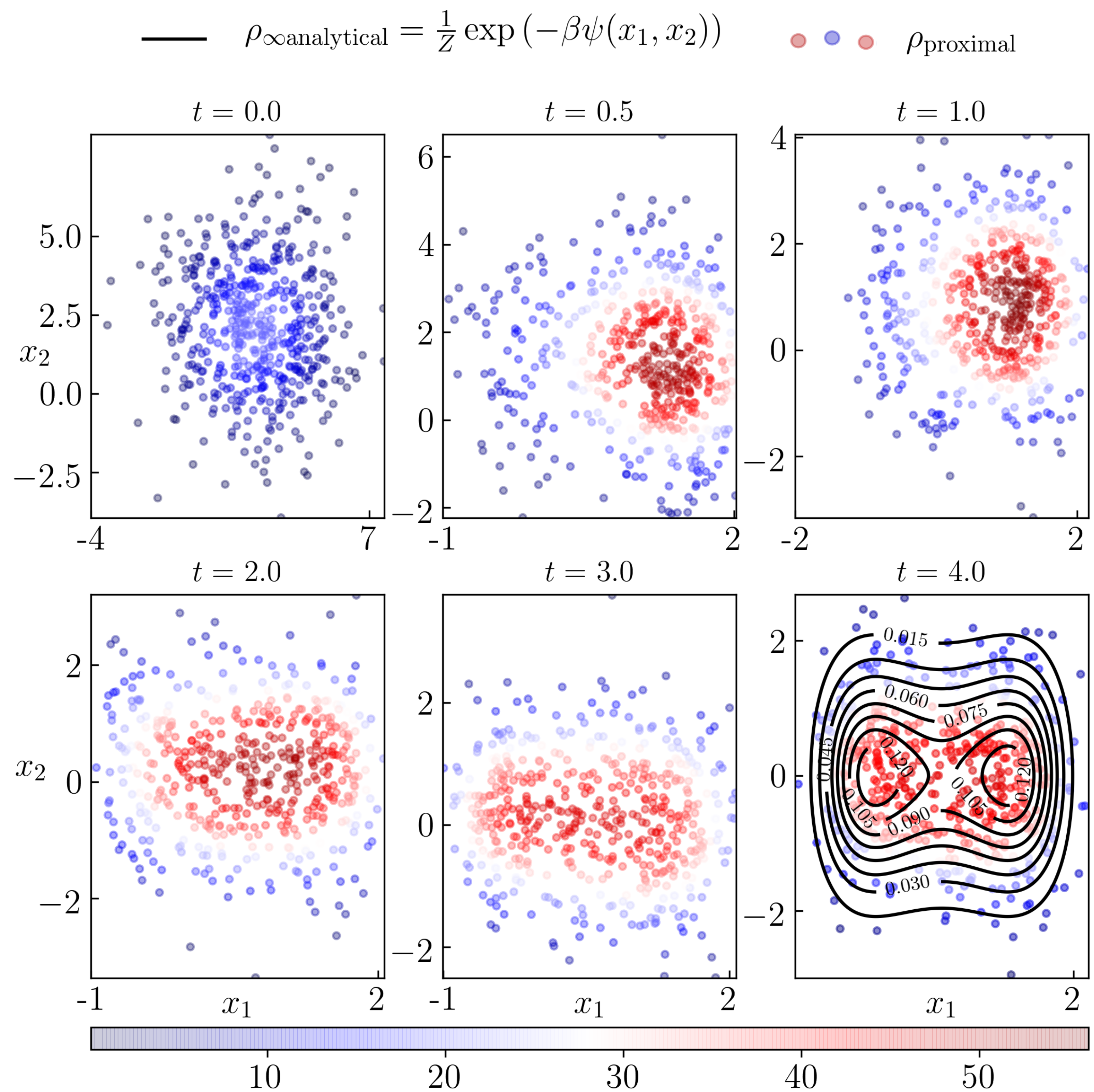
Theorem: Block co-ordinate iteration of $(\mathbf{y}, \mathbf{z})$ recursion is contractive on $\mathbb{R}^n_{>0} \times \mathbb{R}^n_{>0}$.

Proximal Prediction: 2D Linear Gaussian

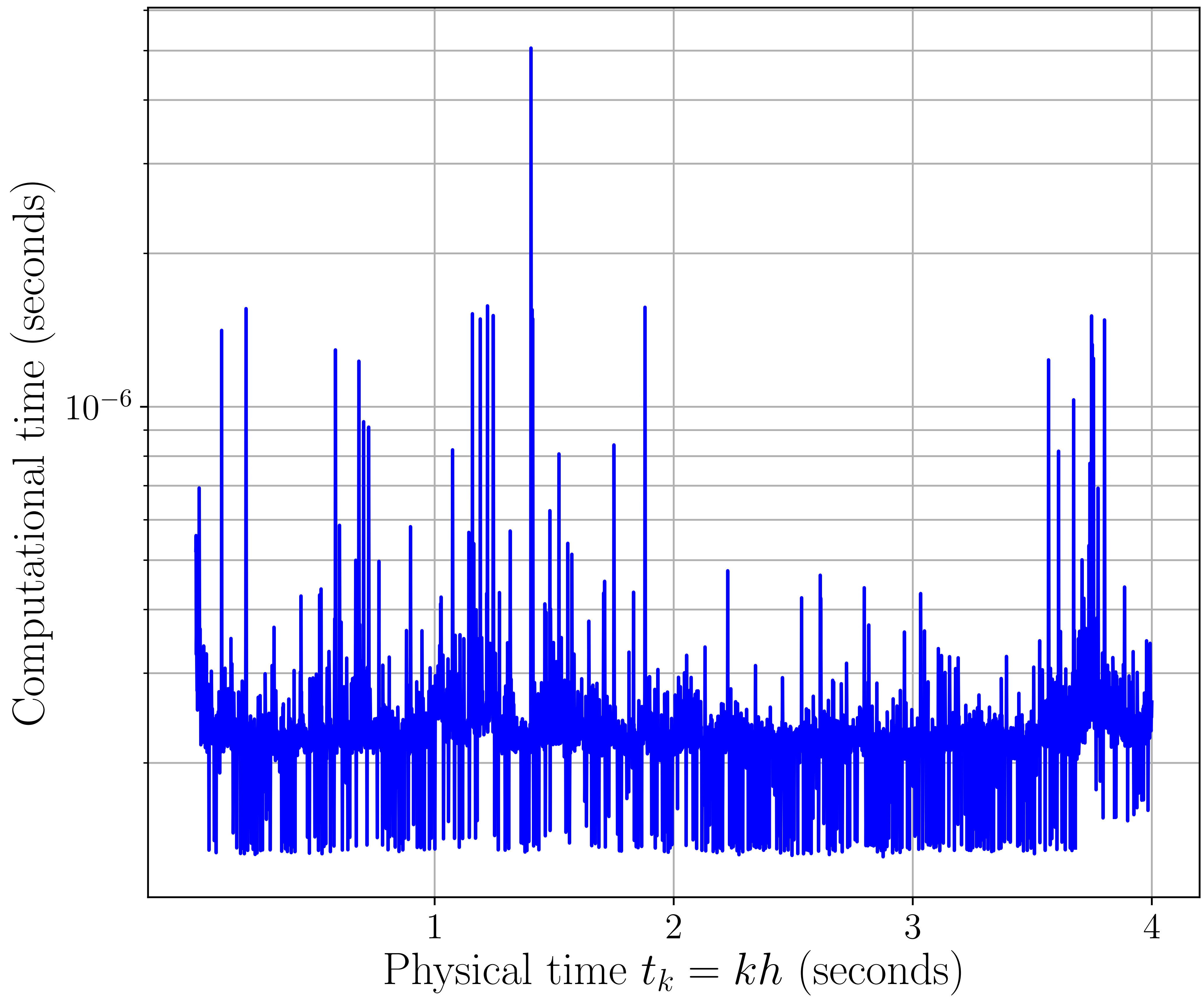


Proximal Prediction: Nonlinear Non-Gaussian





Computational Time: Nonlinear Non-Gaussian



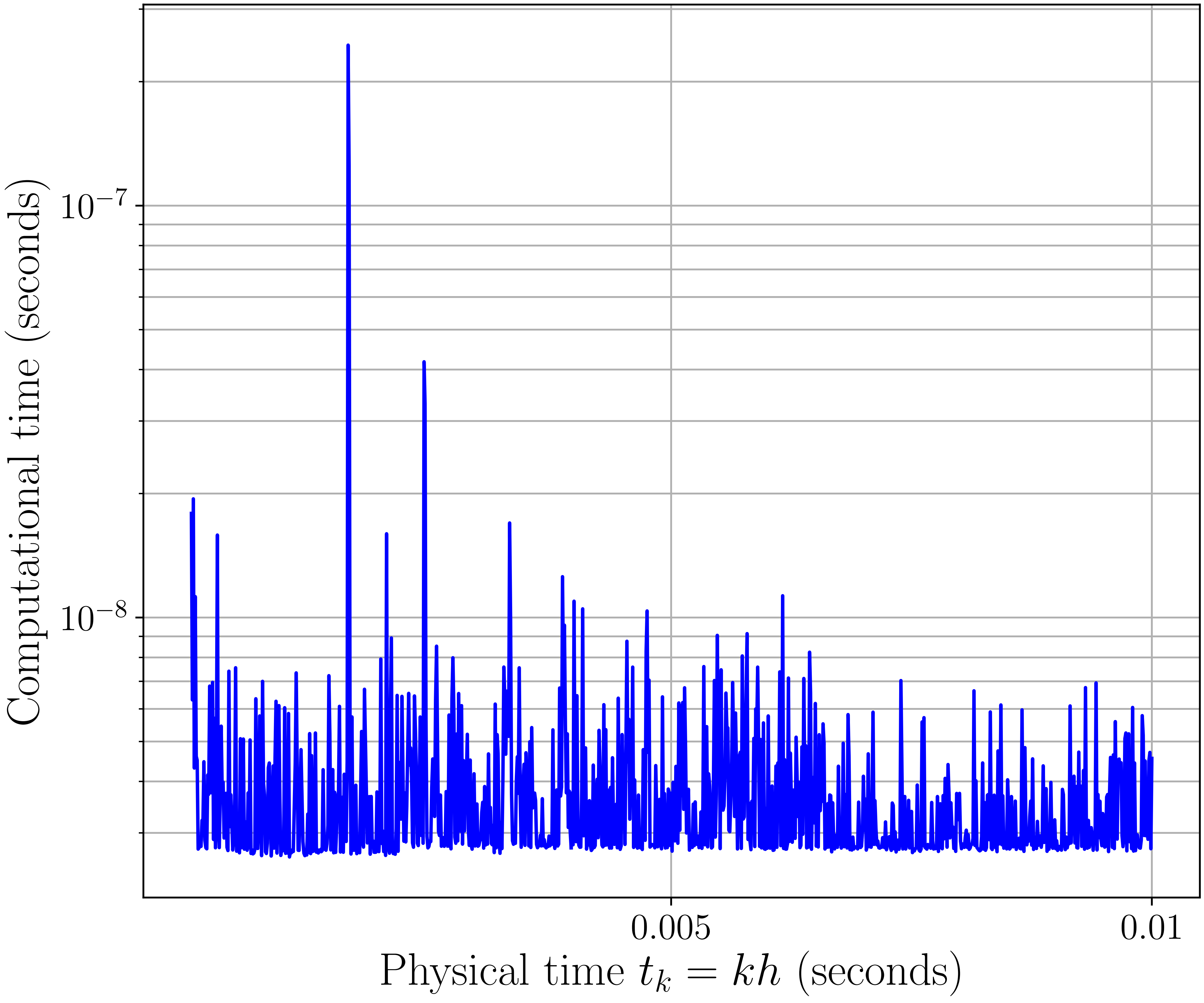
Proximal Prediction: Satellite in Geocentric Orbit

Here, $\mathcal{X} \equiv \mathbb{R}^6$

$$\begin{pmatrix} \mathrm{d}x \\ \mathrm{d}y \\ \mathrm{d}z \\ \mathrm{d}v_x \\ \mathrm{d}v_y \\ \mathrm{d}v_z \end{pmatrix} = \begin{pmatrix} v_x \\ v_y \\ v_z \\ -\dfrac{\mu x}{r^3} + (f_x)_{\text{pert}} - \gamma v_x \\ -\dfrac{\mu y}{r^3} + (f_y)_{\text{pert}} - \gamma v_y \\ -\dfrac{\mu z}{r^3} + (f_z)_{\text{pert}} - \gamma v_z \end{pmatrix} \mathrm{d}t + \sqrt{2\beta^{-1}\gamma} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \mathrm{d}w_1 \\ \mathrm{d}w_2 \\ \mathrm{d}w_3 \end{pmatrix},$$

$$\begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}_{\text{pert}} = \begin{pmatrix} s\theta\, c\phi & c\theta\, c\phi & -s\phi \\ s\theta\, s\phi & c\theta\, s\phi & c\phi \\ c\theta & -s\theta & 0 \end{pmatrix} \begin{pmatrix} \dfrac{k}{2r^4}\left(3(s\theta)^2 - 1\right) \\ -\dfrac{k}{r^5} s\theta\, c\theta \\ 0 \end{pmatrix}, k := 3J_2 R_{\mathrm{E}}^2, \mu = \text{constant}$$

Computational Time: Satellite in Geocentric Orbit



Extensions: Nonlocal Interactions

PDF dependent sample path dynamics:

$$\mathrm{d}\mathbf{x} = -\left(\nabla U\left(\mathbf{x}\right) + \nabla\rho * V\right)\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}\mathbf{w}$$

Mckean-Vlasov-Fokker-Planck-Kolmogorov integro PDE:

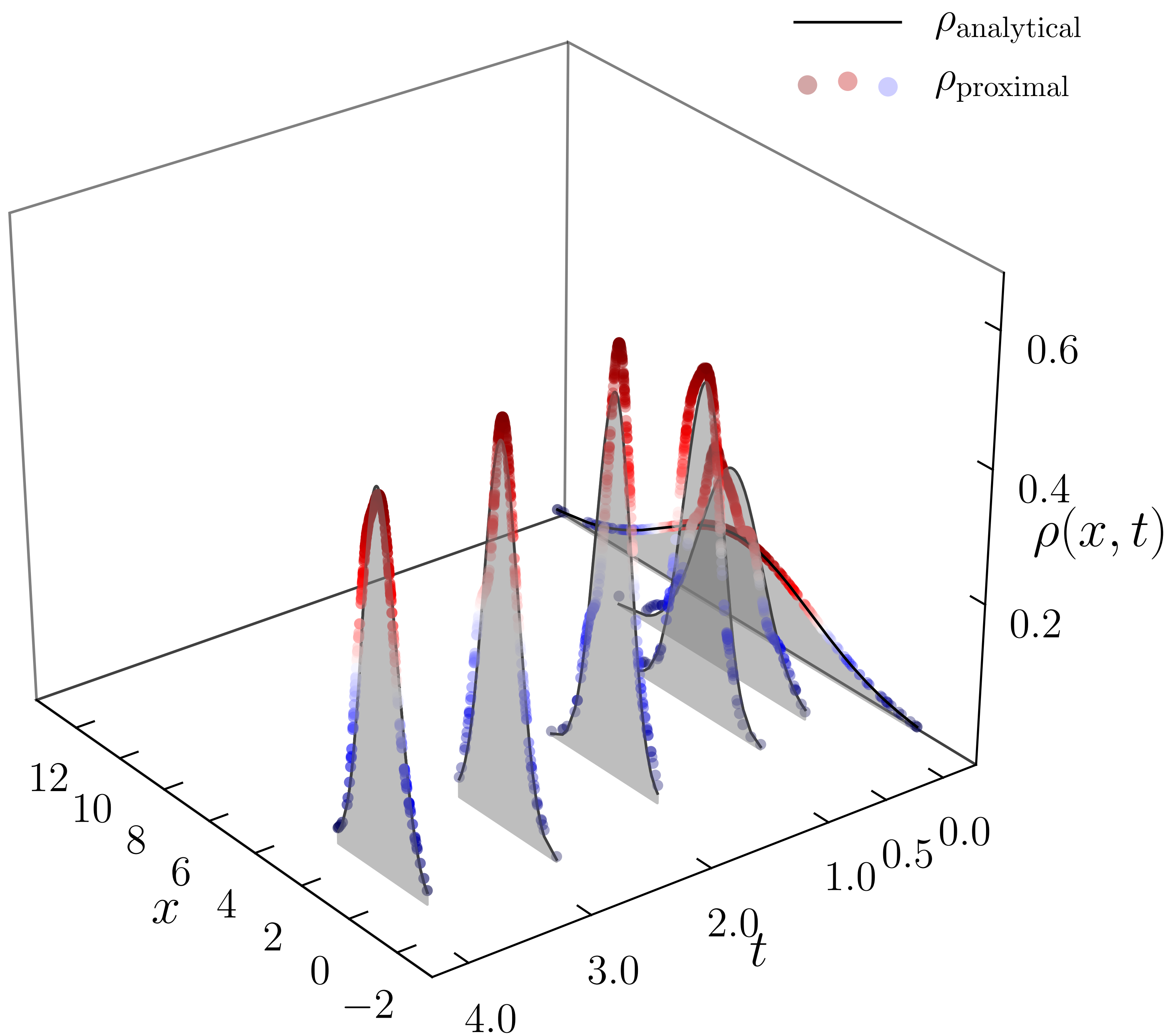
$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left(\rho\nabla\left(U + \rho * V\right)\right) + \beta^{-1}\Delta\rho$$

Free energy:

$$F(\rho) := \mathbb{E}_{\rho}\left[U + \beta^{-1}\rho\log\rho + \rho * V\right]$$

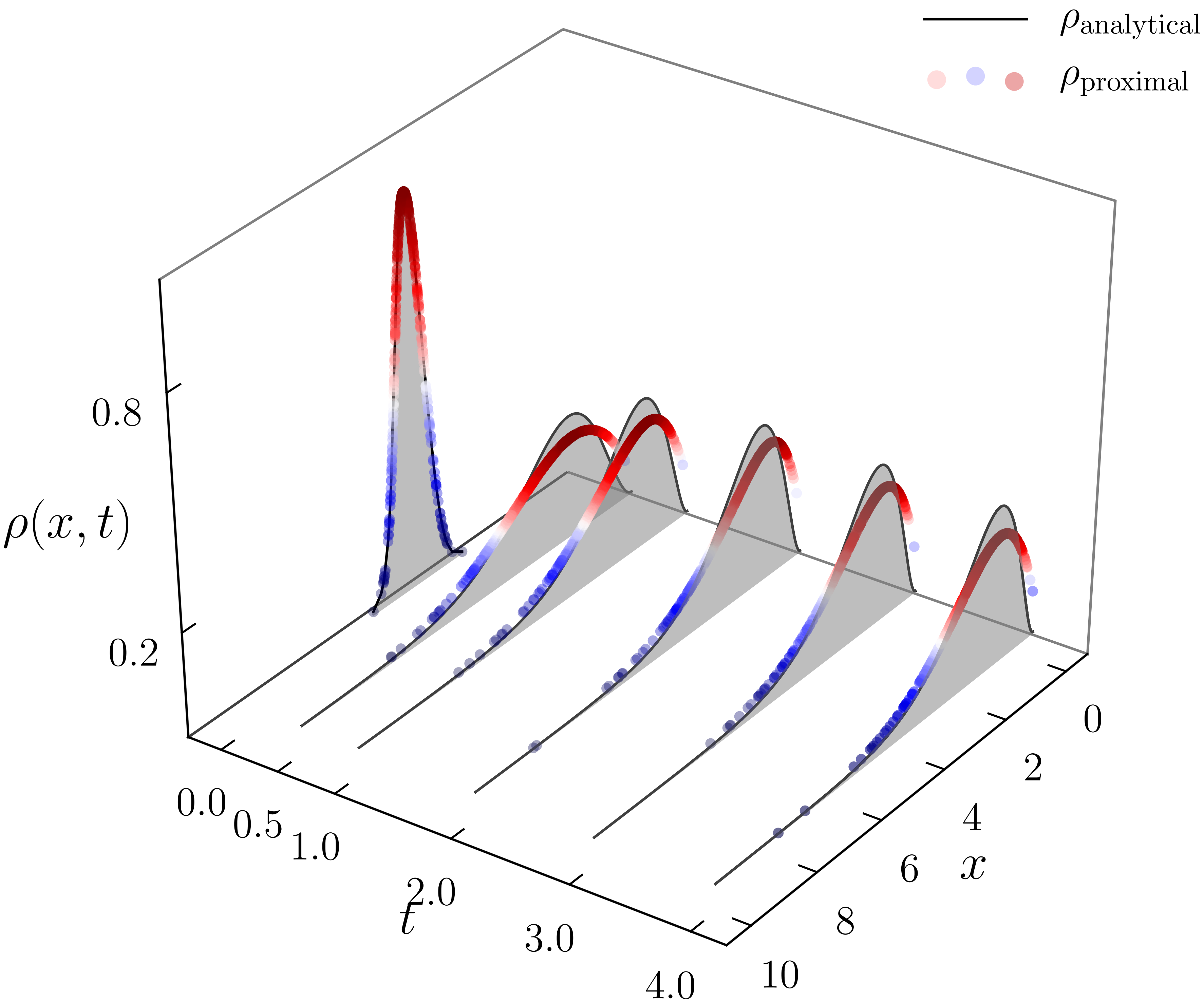
Extensions: Nonlocal Interactions

$$U(\cdot) = V(\cdot) = \| \cdot \|_2^2$$



Extensions: Multiplicative Noise

Cox-Ingersoll-Ross: $\mathrm{d}x = a\,(\theta - x)\;\mathrm{d}t + b\sqrt{x}\,\mathrm{d}w,\ 2a > b^2, \theta > 0$



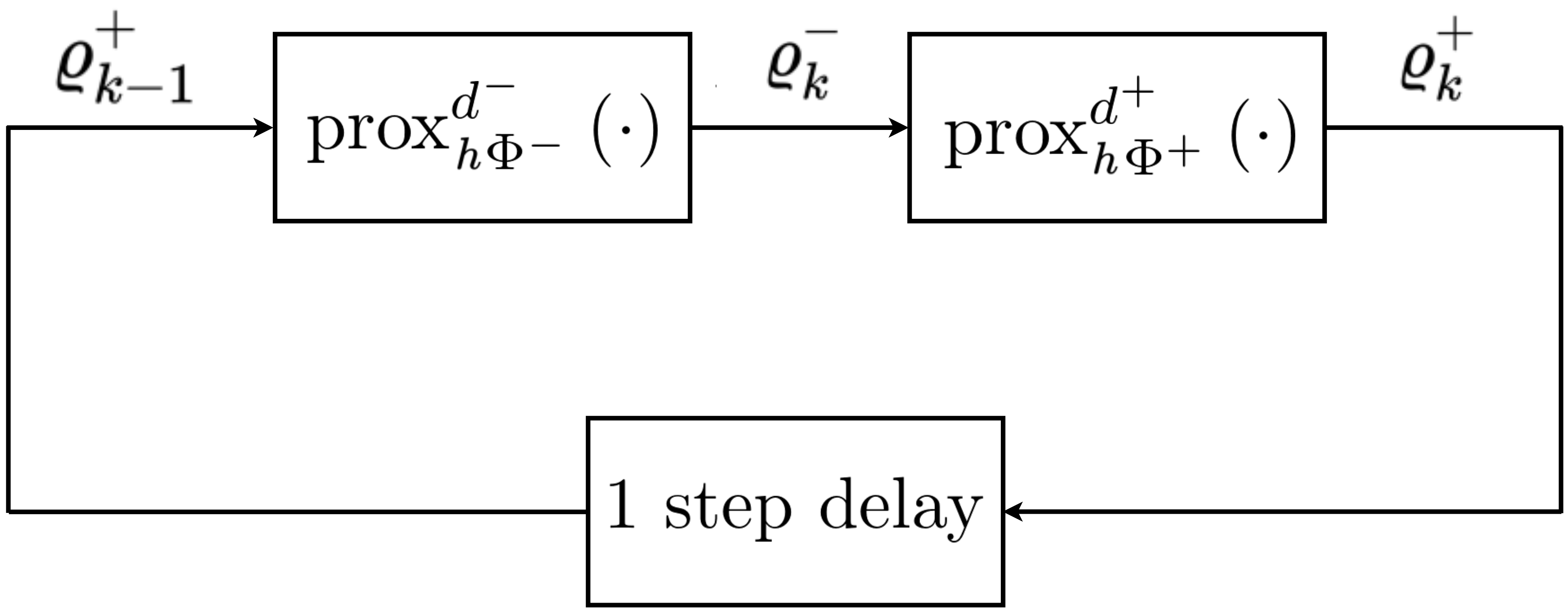
Solving filtering as generalized gradient flow

What's New?

Main idea: Solve the Kushner-Stratonovich SPDE

$\mathrm{d}\rho^{+} = \left[\mathcal{L}_{\mathrm{FP}}\mathrm{d}t + \mathcal{L}\left(\mathrm{d}z, \mathrm{d}t, \rho^{+}\right)\right]\rho^{+}, \;\; \rho(x, t=0) = \rho_0$ as gradient flow in $\mathcal{P}_2(\mathcal{X})$

Recursion of {deterministic ∘ stochastic} proximal operators:



Convergence: $\varrho_k^{+}(h) \rightarrow \rho^{+}(x, t=kh) \quad \text{as} \quad h \downarrow 0$

For prior, as before: $d^{-} \equiv W^2, \quad \Phi^{-} \equiv \mathbb{E}_{\varrho}\left[\psi + \beta^{-1}\log\varrho\right]$

For posterior: $d^{+} \equiv d_{\mathrm{FR}}^2$ or $D_{\mathrm{KL}}, \quad \Phi^{+} \equiv \dfrac{1}{2}\mathbb{E}_{\varrho^{+}}\left[(y_k - h(x))^{\top} R^{-1} (y_k - h(x))\right]$

Explicit Recovery of the Kalman-Bucy Filter

Model:

$$\mathrm{d}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t)\mathrm{d}t + \mathbf{B}\mathrm{d}\mathbf{w}(t), \quad \mathrm{d}\mathbf{w}(t) \sim \mathcal{N}(0, \mathbf{Q}\mathrm{d}t)$$

$$\mathrm{d}\mathbf{z}(t) = \mathbf{C}\mathbf{x}(t)\mathrm{d}t + \mathrm{d}\mathbf{v}(t), \quad \mathrm{d}\mathbf{v}(t) \sim \mathcal{N}(0, \mathbf{R}\mathrm{d}t)$$

Given $\mathbf{x}(0) \sim \mathcal{N}(\mu_0, \mathbf{P}_0)$, want to recover:

$$\mathrm{d}\mu^+(t) = \mathbf{A}\mu^+(t)\mathrm{d}t + \underbrace{\boxed{\mathbf{K}(t)}}_{}\!\!{}^{\mathbf{P}^+\mathbf{C}\mathbf{R}^{-1}} \left(\mathrm{d}\mathbf{z}(t) - \mathbf{C}\mu^+(t)\mathrm{d}t\right),$$

$$\dot{\mathbf{P}}^+(t) = \mathbf{A}\mathbf{P}^+(t) + \mathbf{P}^+(t)\mathbf{A}^\top + \mathbf{B}\mathbf{Q}\mathbf{B}^\top - \mathbf{K}(t)\mathbf{R}\mathbf{K}(t)^\top.$$

— A.H. and T.T. Georgiou, Gradient Flows in Uncertainty Propagation and Filtering of Linear Gaussian Systems, *CDC 2017*.

— A.H. and T.T. Georgiou, Gradient Flows in Filtering and Fisher-Rao Geometry, *ACC 2018*.

Explicit Recovery of the Wonham Filter

Model:

$$x(t) \sim \mathrm{Markov}(Q),$$
$$\mathrm{d}z(t) = h(x(t))\, \mathrm{d}t \; + \; \sigma_v(t)\mathrm{d}v(t)$$

J.SIAM Control
Ser. A, Vol. 2, No. 3
Printed in U.S.A., 1965

SOME APPLICATIONS OF STOCHASTIC DIFFERENTIAL EQUATIONS TO OPTIMAL NONLINEAR FILTERING*

W. M. WONHAM†

State space: $\Omega := \{a_1, \ldots, a_m\}$

Posterior $\pi^+(t) := \{\pi_1^+(t), \ldots, \pi_m^+(t)\}$ **solves the nonlinear SDE:**

$$\mathrm{d}\pi^+(t) = \pi^+(t)Q\; \mathrm{d}t \; + \; \frac{1}{(\sigma_v(t))^2}\pi^+(t)\Big(H - \widehat{h}(t)I\Big)\Big(\mathrm{d}z(t) - \widehat{h}(t)\mathrm{d}t\Big),$$

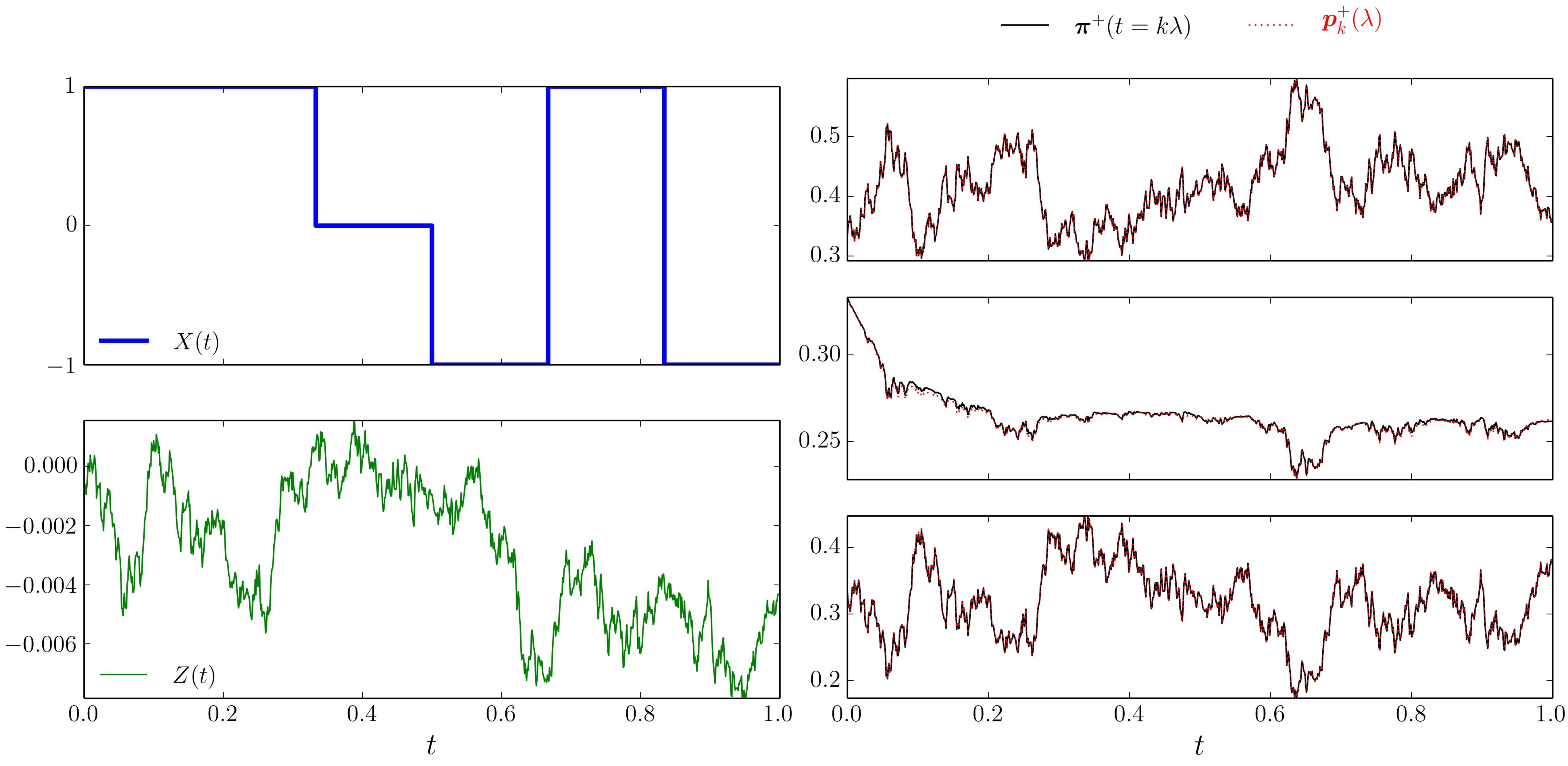
where $H := \mathrm{diag}(h(a_1), \ldots, h(a_m)), \quad \widehat{h}(t) := \sum_{i=1}^{m} h(a_i)\pi_i^+(t),$

Initial condition: $\pi^+(t=0) = \pi_0,$

By defn. $\pi^+(t) = \mathbb{P}(x(t) = a_i \mid z(s), 0 \le s \le t)$

— A.H. and T.T. Georgiou, Proximal Recursion for the Wonham Filter, *CDC 2019*.

Numerical Results for the Wonham Filter

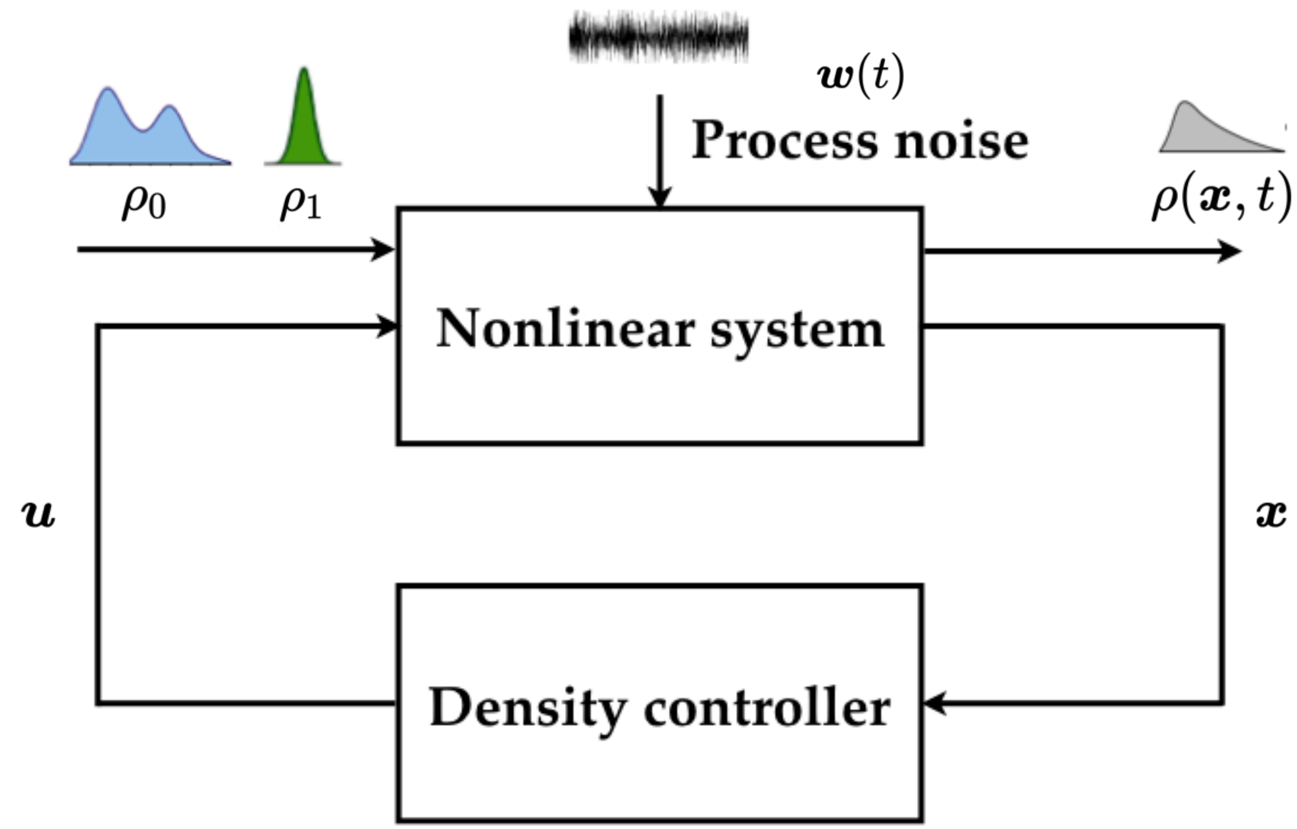


— A.H. and T.T. Georgiou, Proximal Recursion for the Wonham Filter, *CDC 2019*.

Solving density control as generalized gradient flow

State Feedback Density Steering

Steer joint state PDF via feedback control over finite time horizon



Common scenario: $\boldsymbol{G} \equiv \boldsymbol{B}$

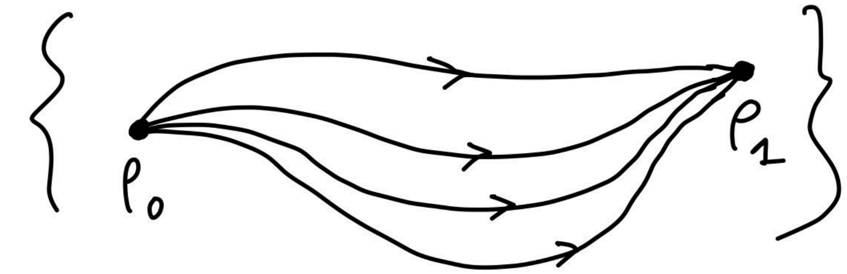
$$\underset{u \in \mathcal{U}}{\text{minimize}} \quad \mathbb{E}\left[\int_0^1 \left(\frac{1}{2}\|\boldsymbol{u}(t, \boldsymbol{x}_t^u)\|_2^2 + q(t, \boldsymbol{x}_t^u)\right) \mathrm{d}t\right]$$

subject to

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

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

Optimal Control Problem over PDFs

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

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

Hessian operator w.r.t. state: Hess

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

subject to

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\left(\left(\boldsymbol{f}+\boldsymbol{B}\boldsymbol{u}\right)\rho\right) = \langle \mathrm{Hess}, \boldsymbol{D}\rho\rangle$$

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

Optimal Control Problem over PDFs

Existence-uniqueness needs regularity assumptions

Are known to hold for many practical classes of nonlinearities

This talk: will focus on a few important classes

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

Coupled nonlinear PDEs + linear boundary conditions

Controlled Fokker-Planck or Kolmogorov's forward PDE

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

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 System

1931
31.3.

This is still a challenge to mathematicians, to solve a certain boundary value problem.
14.III.52. E.S.

Überreicht vom Verfasser

S

ÜBER DIE UMKEHRUNG
DER NATURGESETZE

VON

E. SCHRÖDINGER

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

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

PAR

E. SCHRÖDINGER

I. — **Introduction**

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

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

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

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

$$\varphi(x,t) = \exp\left(\psi\left(x,t\right)\right) \qquad \text{for all} \qquad (x,t) \in \mathbb{R}^n \times [0,1]$$

Feedback Synthesis via the Schrödinger System

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

Uncontrolled forward-backward Kolmogorov PDEs:

$$\frac{\partial \widehat{\varphi}}{\partial t} = -\nabla \cdot (\widehat{\varphi} \boldsymbol{f}) + \langle \text{Hess}, \boldsymbol{D}\widehat{\varphi} \rangle - q\widehat{\varphi}, \qquad \widehat{\varphi}_0 \varphi_0 = \rho_0,$$

$$\frac{\partial \varphi}{\partial t} = -\langle \nabla \varphi, \boldsymbol{f} \rangle - \langle \text{Hess}(\varphi), \boldsymbol{D} \rangle + q\varphi, \qquad \widehat{\varphi}_1 \varphi_1 = \rho_1,$$

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

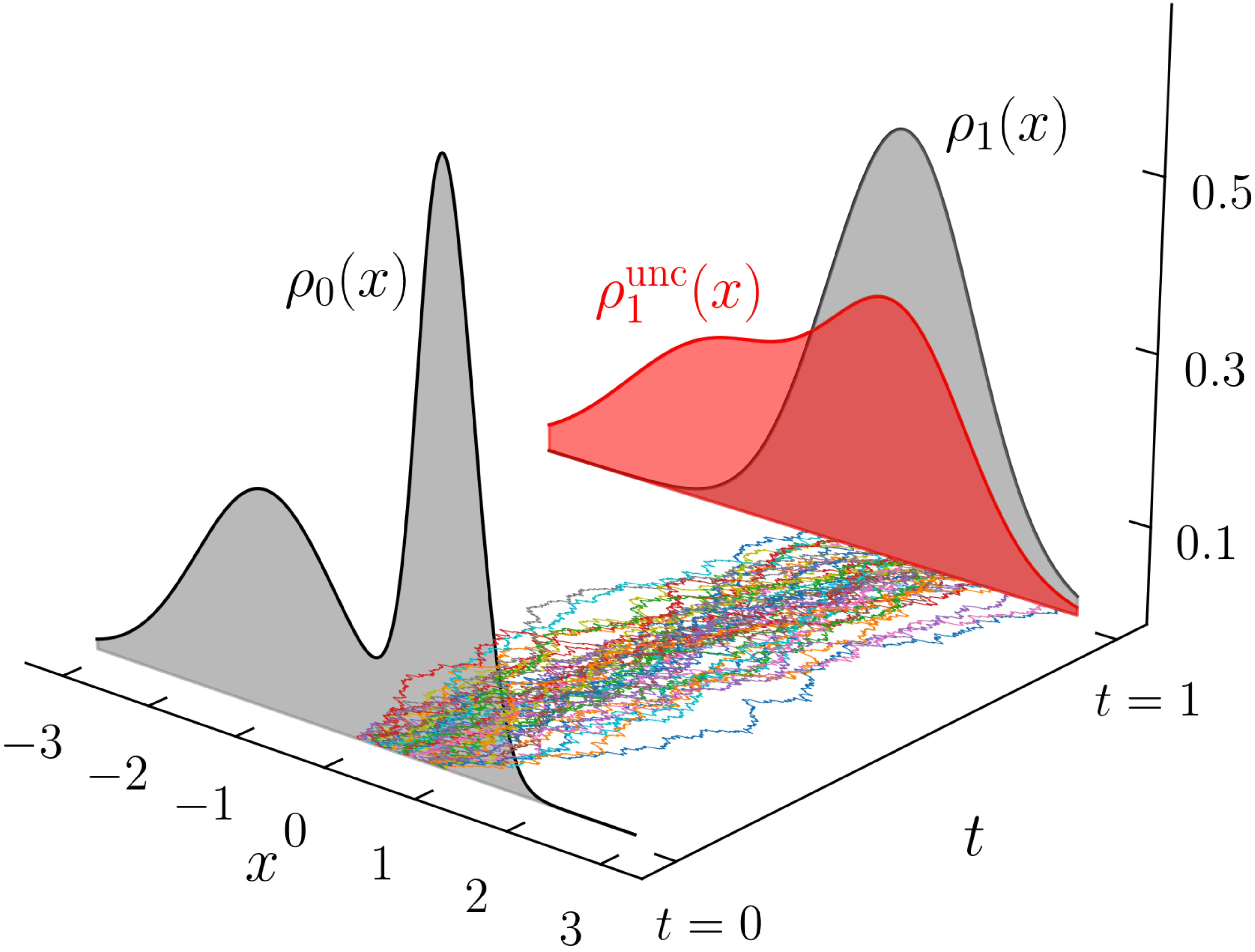
Optimal control: $\boldsymbol{u}^{\text{opt}}(\boldsymbol{x}, t) = 2\boldsymbol{B}^{\top} \nabla_{\boldsymbol{x}} \log \varphi(\boldsymbol{x}, t)$

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

$$\begin{tikzcd}
\hat{\varphi}_0(x) \arrow[r, "\int"] & \hat{\varphi}_1(x) \arrow[d, "\rho_1(x)/\hat{\varphi}_1(x)"] \\
\varphi_0(x) \arrow[u, "\rho_0(x)/\varphi_0(x)"] & \varphi_1(x) \arrow[l, "\int"]
\end{tikzcd}$$

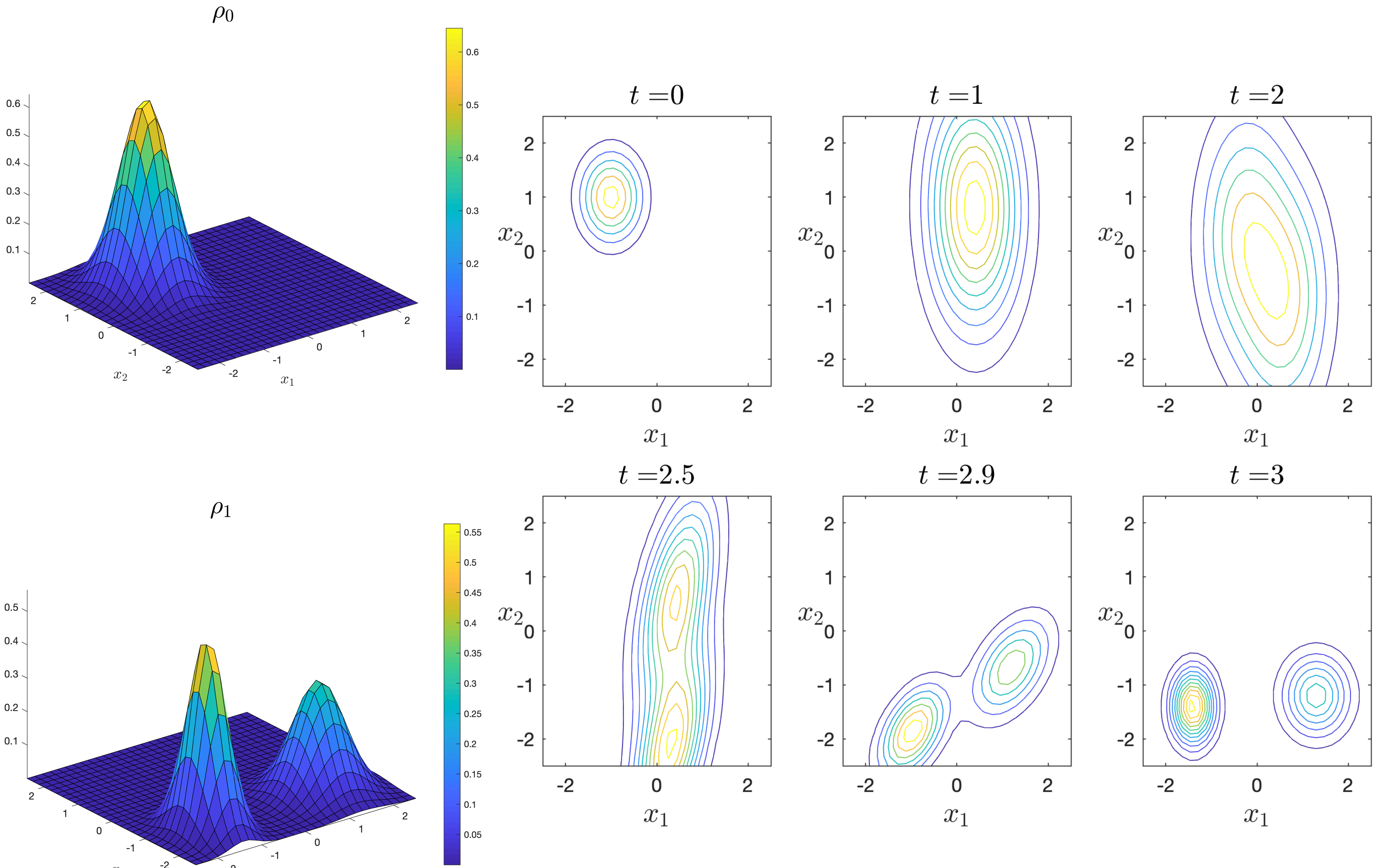
This recursion is contractive in the Hilbert metric!!

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



Zero prior dynamics

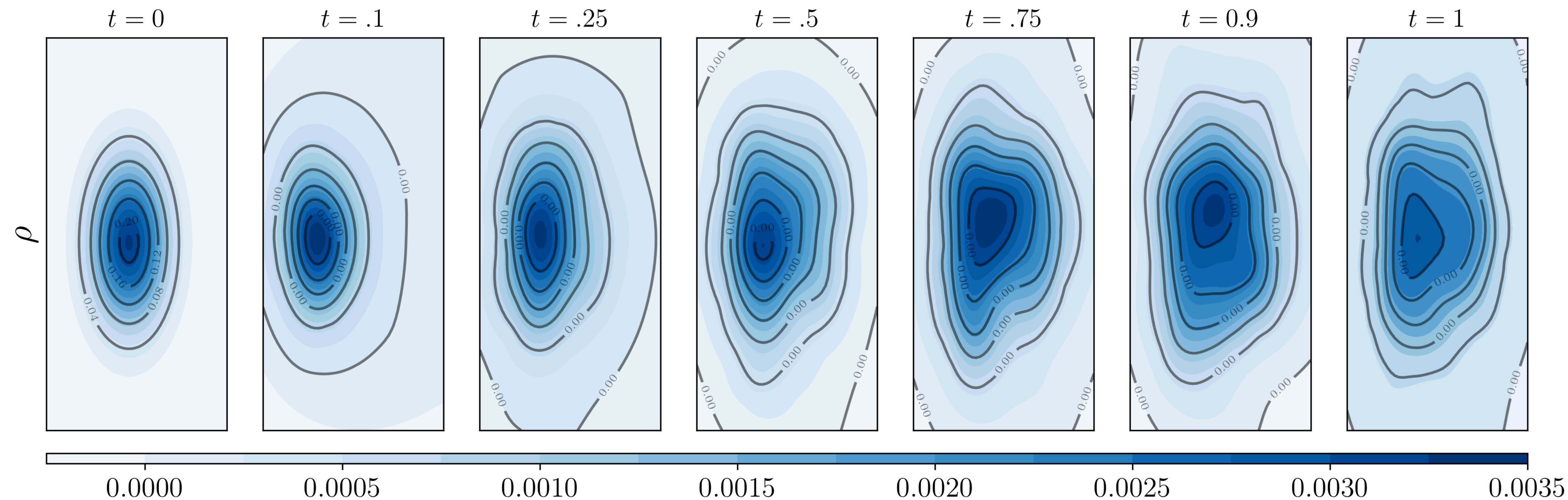
Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$



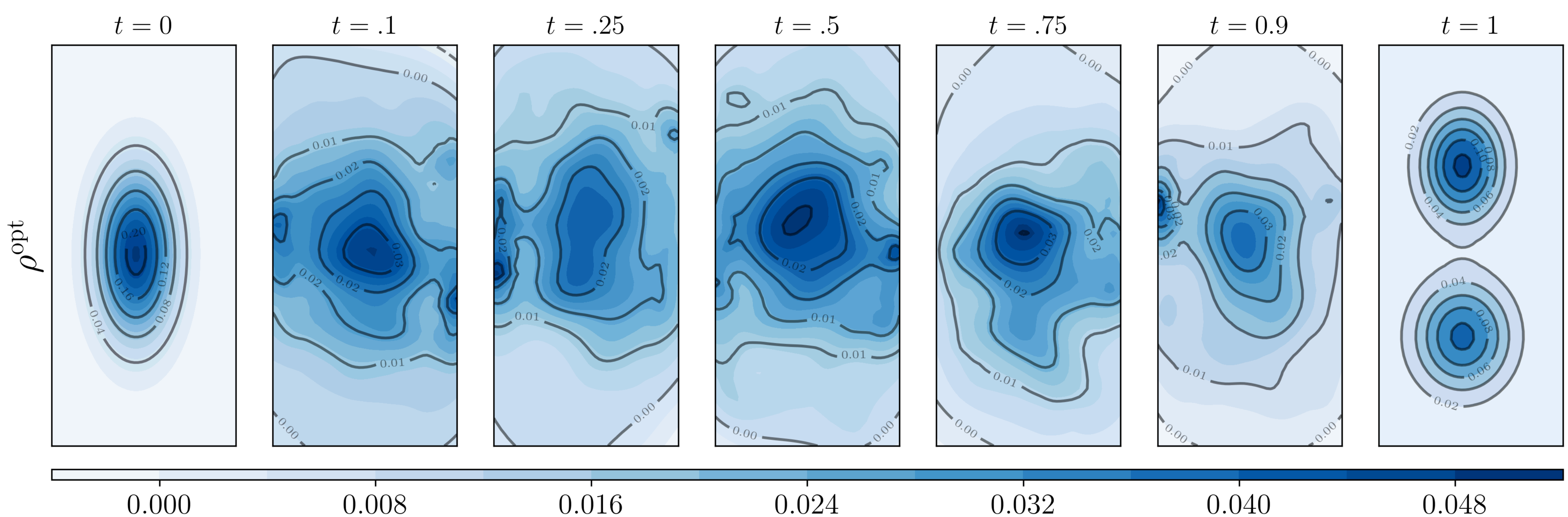
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

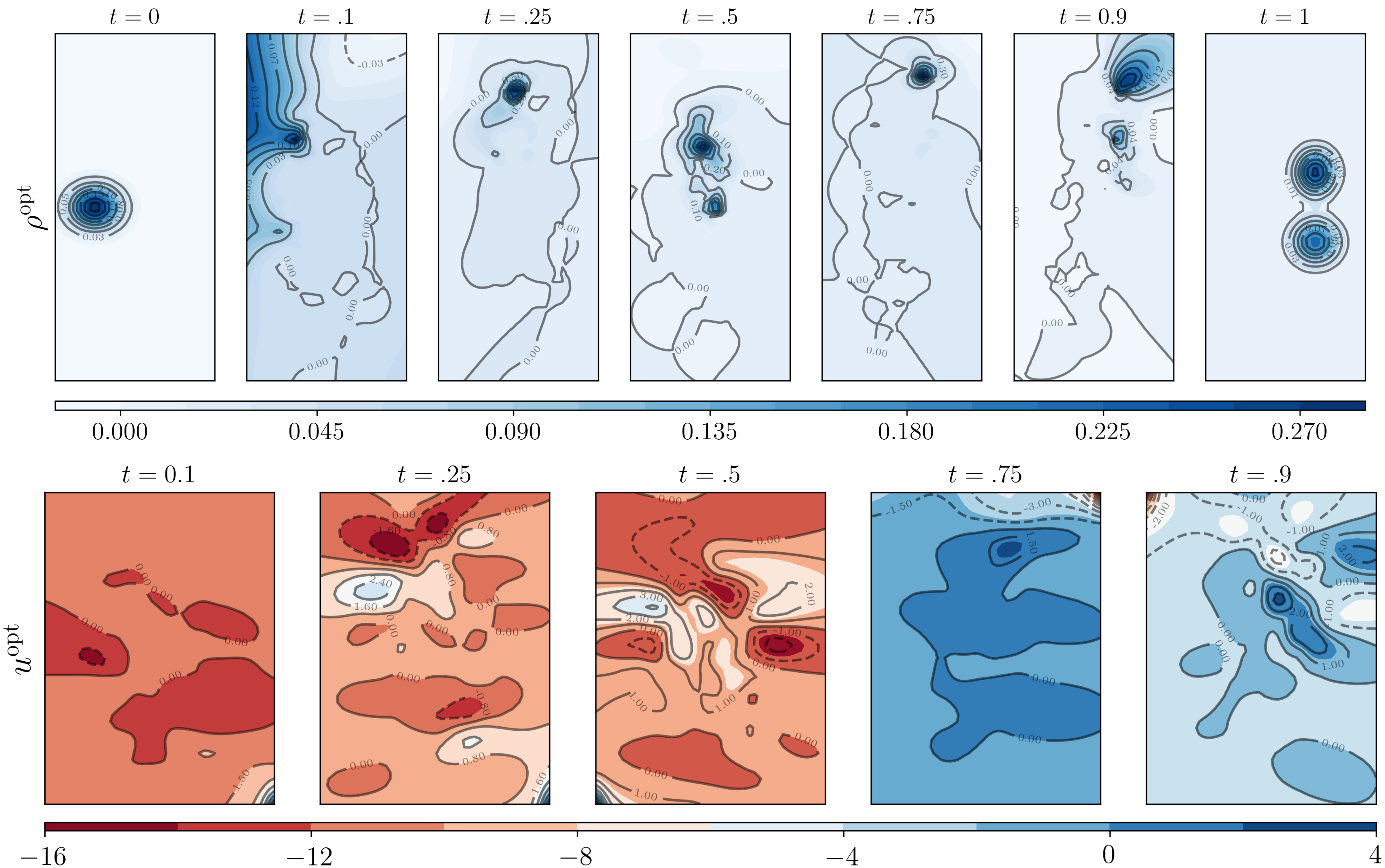
Uncontrolled joint PDF evolution:



Optimal controlled joint PDF evolution:

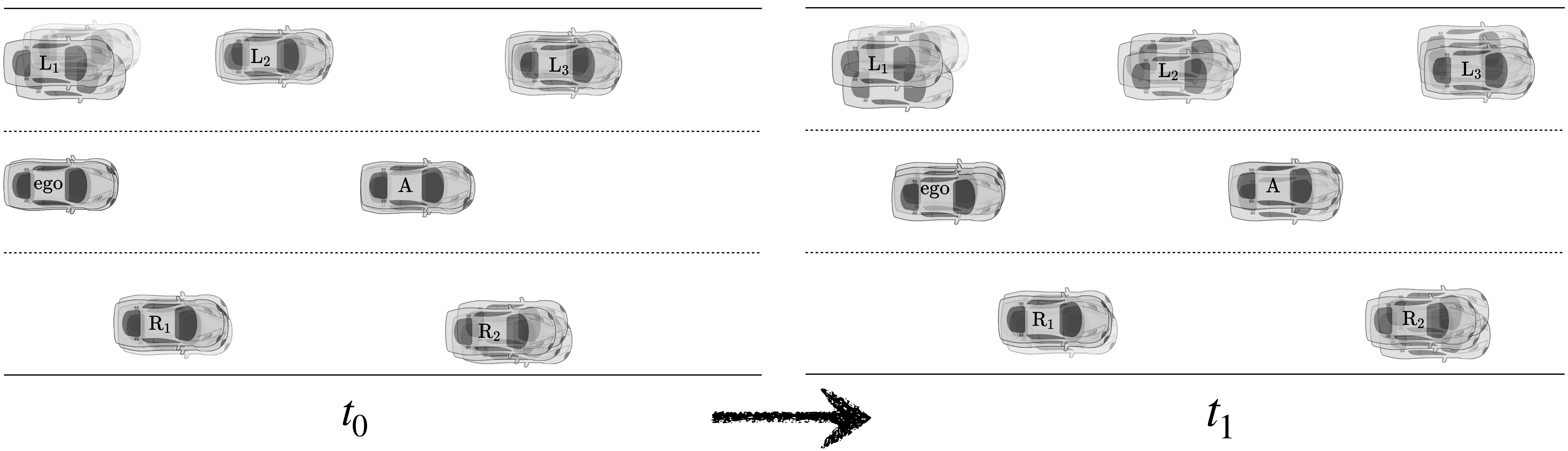


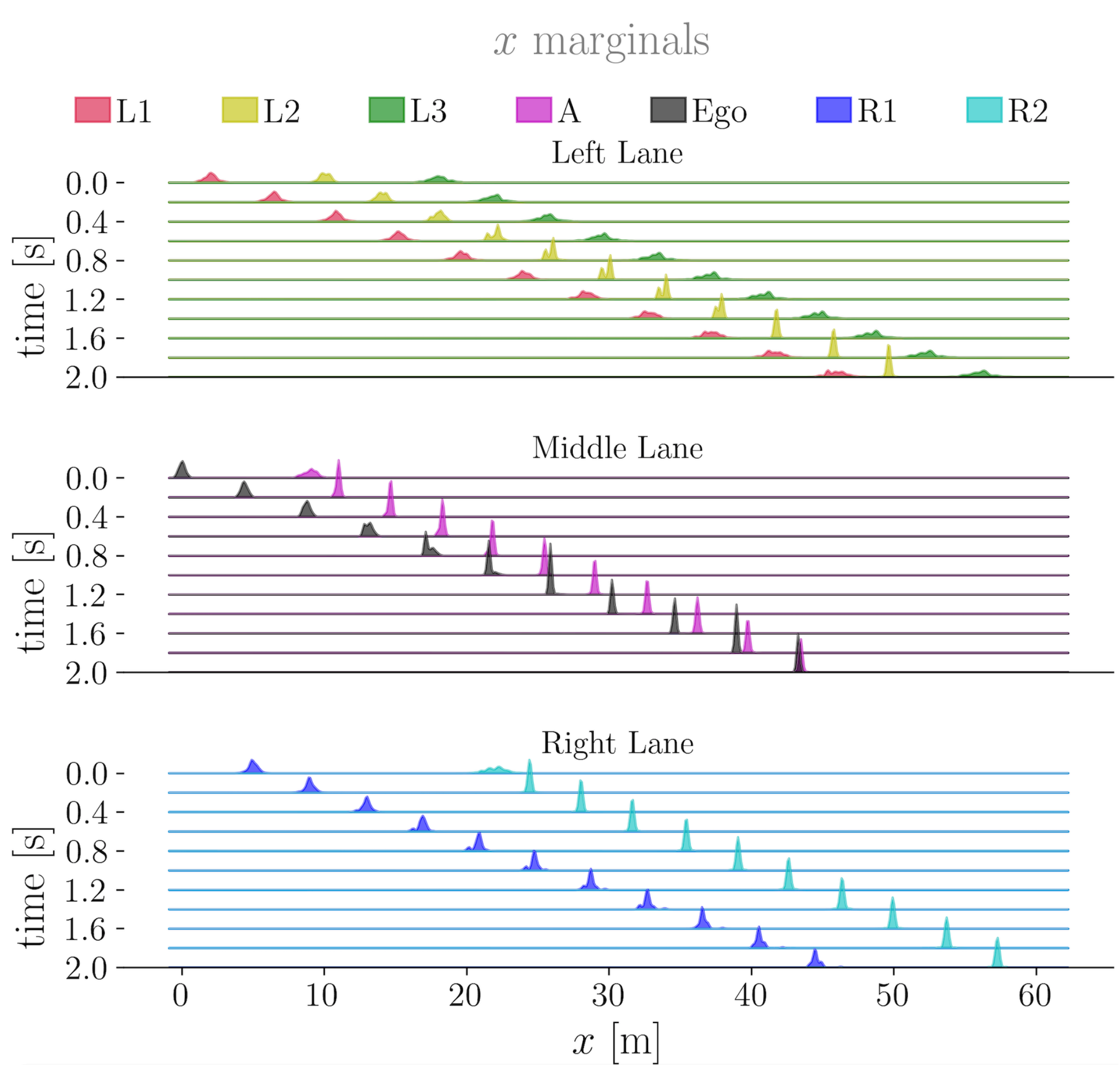
Feedback Density Control: Mixed Conservative-Dissipative Drift

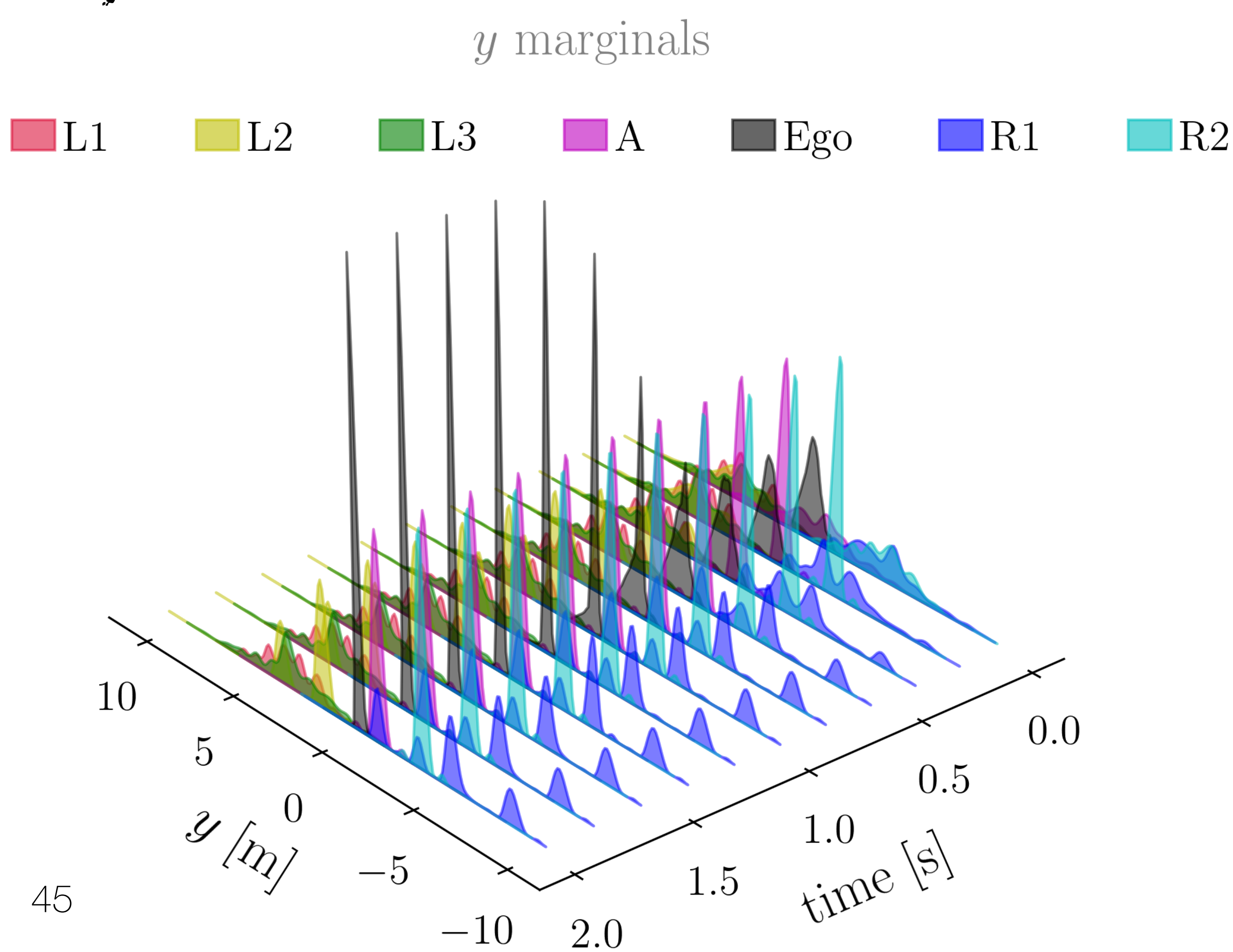


— K.F. Caluya and A.H., Wasserstein proximal algorithms for the Schrodinger bridge problem: density control with nonlinear drift, *IEEE TAC* 2021.

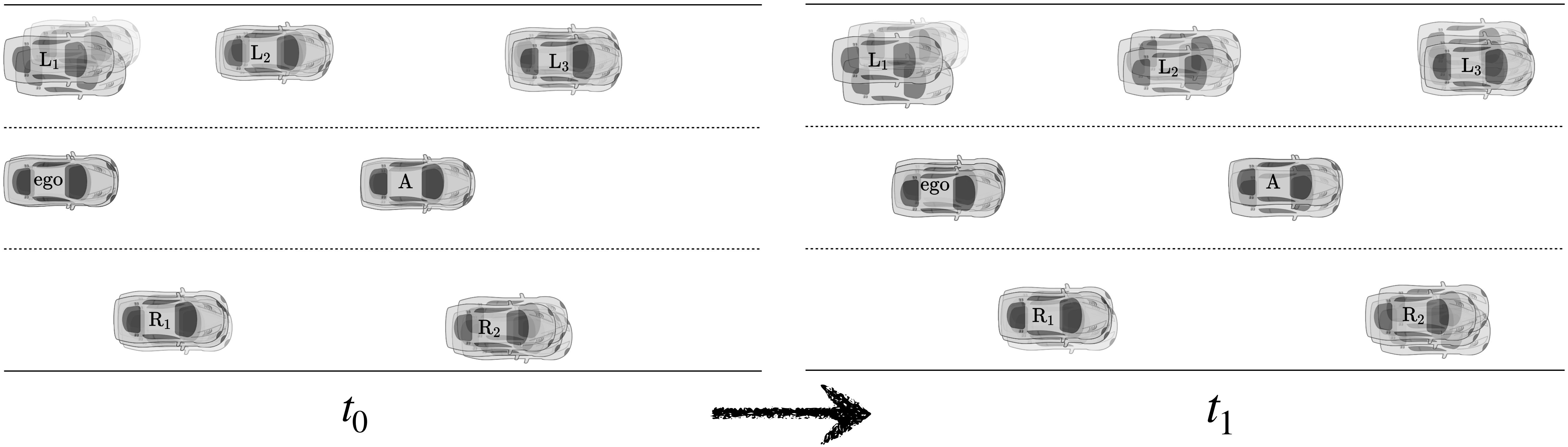
Density Prediction for Safe Automated Driving

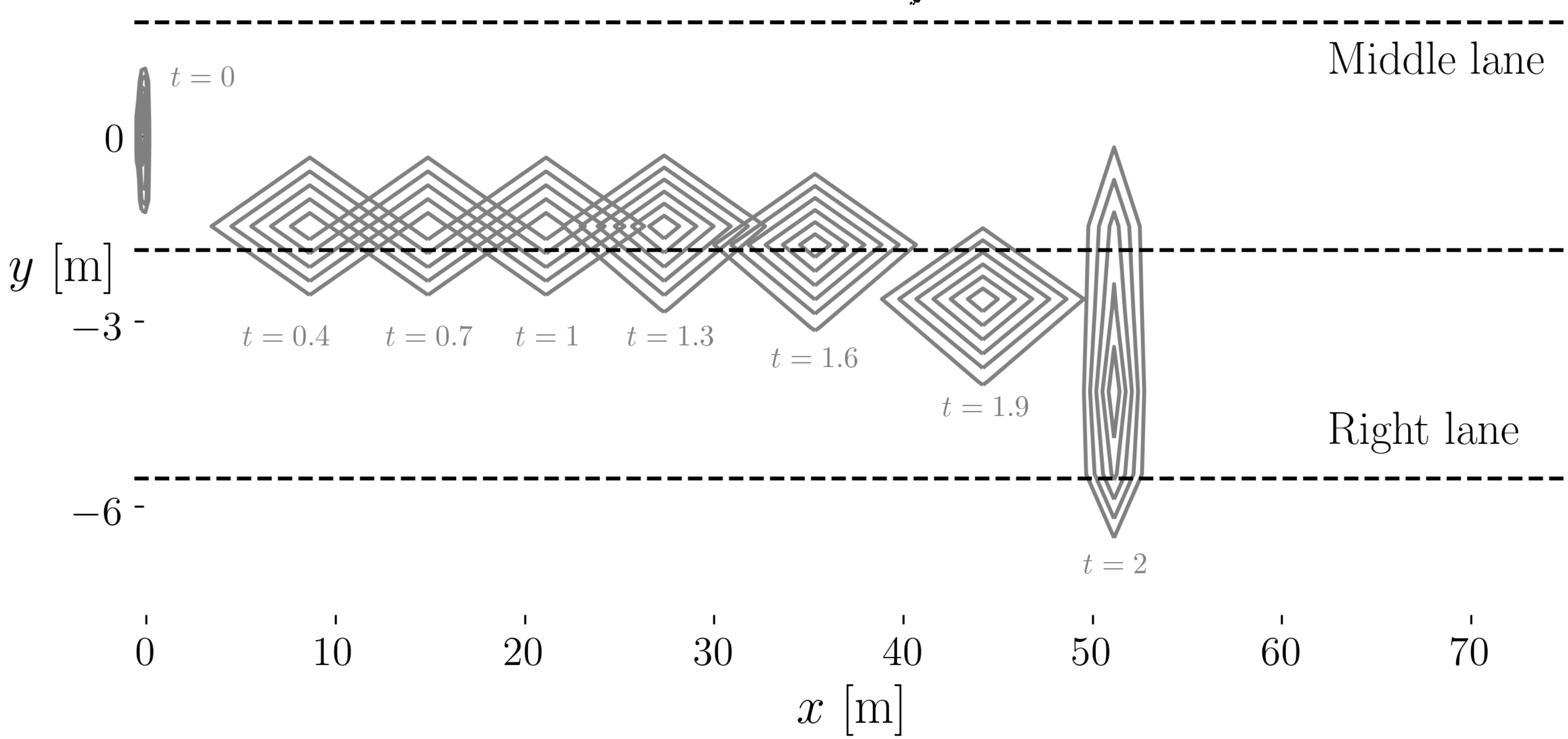






Density Control for Safe Automated Driving





Application to Safe Automated Driving

S. Haddad, A.H., and B. Singh, Density-based stochastic reachability computation for occupancy prediction in automated driving, *IEEE Transactions on Control Systems Technology*, 2022.

S. Haddad, K.F. Caluya, A.H., and B. Singh, Prediction and optimal feedback steering of probability density functions for safe automated driving, *IEEE Control Systems Letters*, 2021.

Learning a neural network as generalized gradient flow

Learning Neural Network from Data

(feature vector, label) $= (\boldsymbol{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}, \quad i = 1, \ldots, n$

Consider shallow NN: 1 hidden layer with n_{H} neurons

NN parameter vector $\boldsymbol{\theta} := (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_{n_{\mathrm{H}}})^\top \in \mathbb{R}^{p n_{\mathrm{H}}}$

Approximating function:

$$\hat{f}(\boldsymbol{x}, \boldsymbol{\theta}) = \frac{1}{n_{\mathrm{H}}} \sum_{i=1}^{n_{\mathrm{H}}} \Phi(\boldsymbol{x}, \boldsymbol{\theta}_i), \quad \text{example: } \Phi(\boldsymbol{x}, \boldsymbol{\theta}_i) = a_i \sigma\left(\boldsymbol{w}_i^\top \boldsymbol{x} + b_i\right)$$

Population risk functional:

$$R(\hat{f}) = \mathbb{E}_{(\boldsymbol{x}, y)}\left[\left(y - \hat{f}(\boldsymbol{x}, \boldsymbol{\theta})\right)^2\right] \approx \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \hat{f}(\boldsymbol{x}_i, \boldsymbol{\theta})\right)^2$$

Learning problem: $\underset{\boldsymbol{\theta} \in \mathbb{R}^{p n_{\mathrm{H}}}}{\text{minimize}} \; R(\hat{f})$

Mean Field Density Dynamics of SGD

Free energy functional: $F(\rho) := R(\hat{f}(\boldsymbol{x}, \rho))$

For quadratic loss:

$$F(\rho) = \underbrace{F_0}_{\text{independent of } \rho} + \underbrace{\int_{\mathbb{R}^p} V(\boldsymbol{\theta})\, \rho(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta}}_{\text{advection potential energy, linear in } \rho} + \underbrace{\int_{\mathbb{R}^p}\int_{\mathbb{R}^p} U(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}})\, \rho(\boldsymbol{\theta})\rho(\tilde{\boldsymbol{\theta}}) \mathrm{d}\boldsymbol{\theta} \mathrm{d}\tilde{\boldsymbol{\theta}}}_{\text{interaction potential energy, nonlinear in } \rho},$$

where

$$F_0 := \mathbb{E}_{(\boldsymbol{x},y)}\left[y^2\right], \qquad V(\boldsymbol{\theta}) := \mathbb{E}_{(\boldsymbol{x},y)}\left[-2y\Phi(\boldsymbol{x}, \boldsymbol{\theta})\right],$$

PDF dynamics for SGD:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \nabla (\underbrace{V + U \circledast \rho}_{\frac{\delta F}{\delta \rho}})), \text{ where } (U \circledast \rho)(\boldsymbol{\theta}) := \int_{\mathbb{R}^p} U(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}})\rho(\tilde{\boldsymbol{\theta}}) \mathrm{d}\tilde{\boldsymbol{\theta}}$$

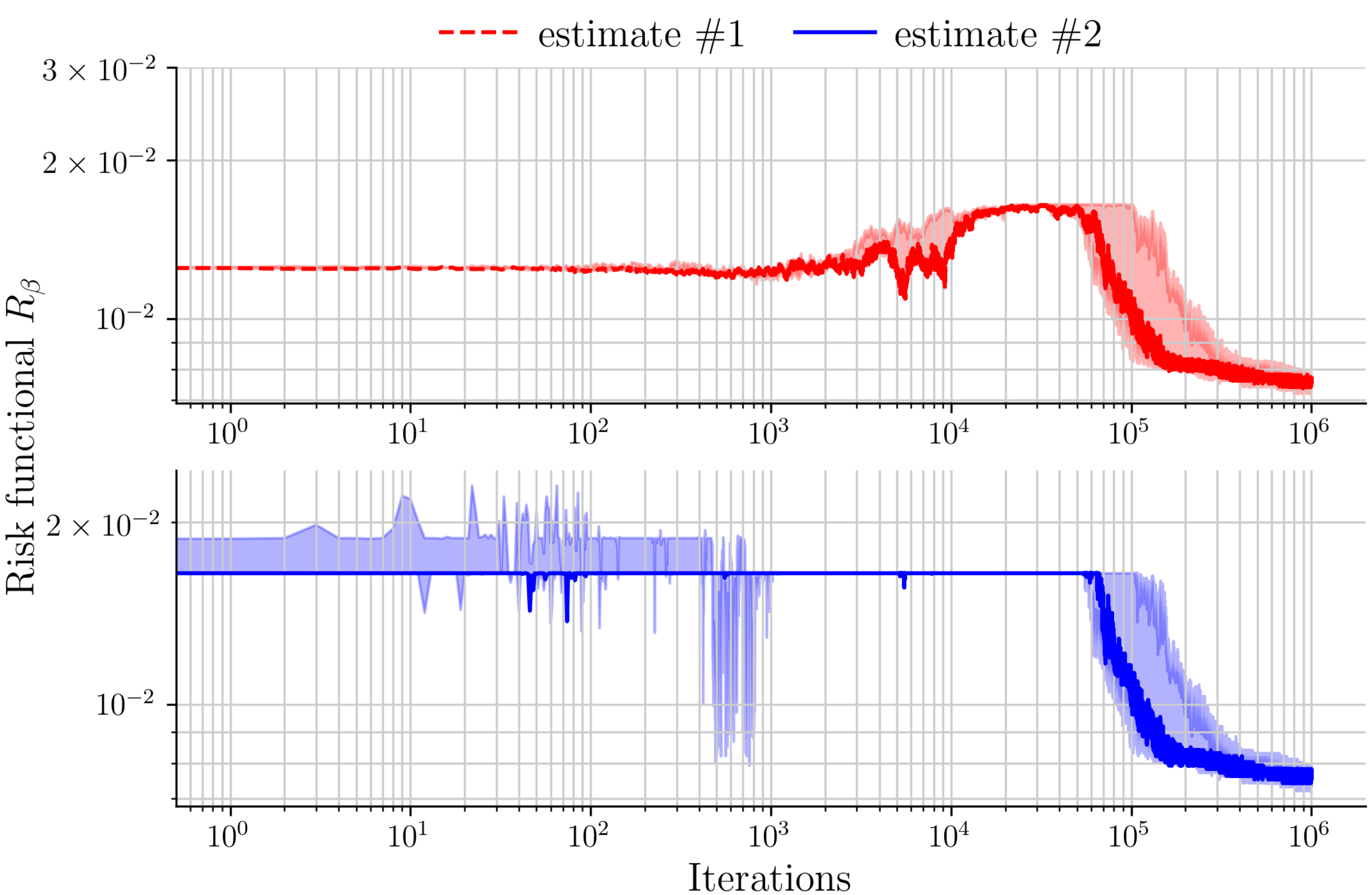
This PDE is the gradient flow of functional F w.r.t. the Wasserstein metric W

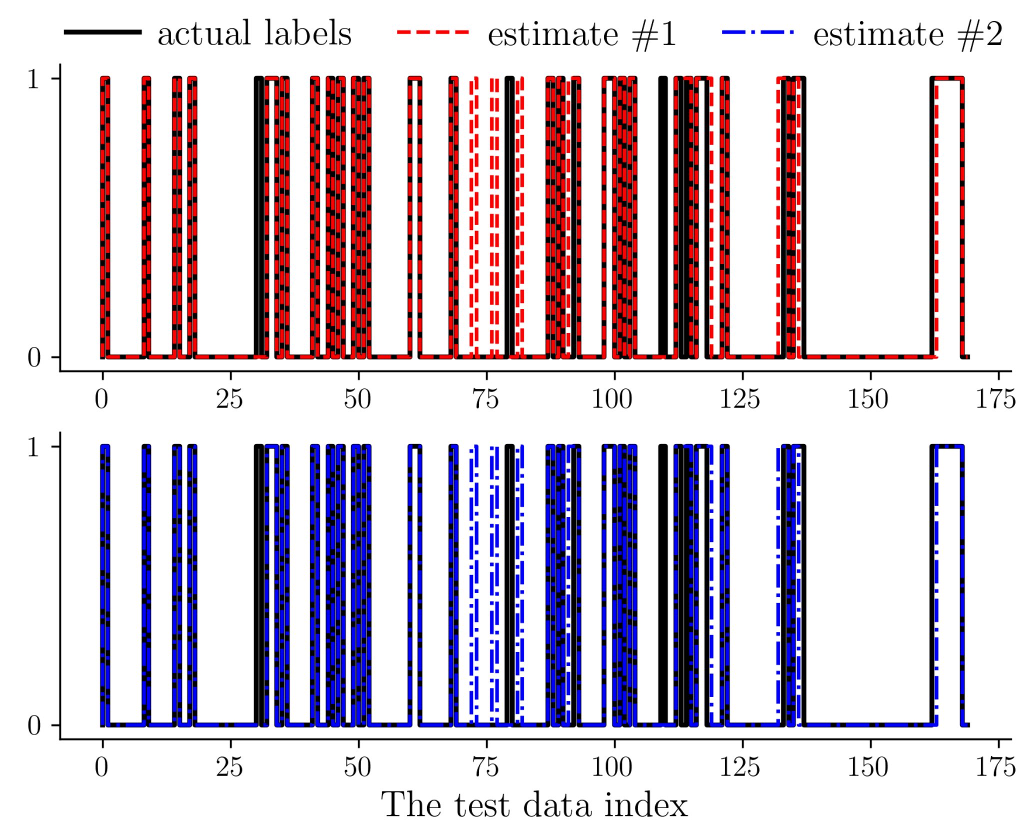
Proximal Recursion for SGD Training of NN

$$\varrho_k(\tau,\boldsymbol{\theta}) = \underset{\varrho\in\mathcal{P}(\mathbb{R}^p)}{\arg\min}\ \frac{1}{2}\left(W\left(\varrho(\boldsymbol{\theta}),\varrho_{k-1}(\tau,\boldsymbol{\theta})\right)\right)^2 + \tau\, F(\varrho(\boldsymbol{\theta}))$$

$$= \mathrm{prox}_{\tau F}^{W}\left(\varrho_{k-1}\right)$$

Case study: Wisconsin Breast Cancer (Diagnostic) Data Set

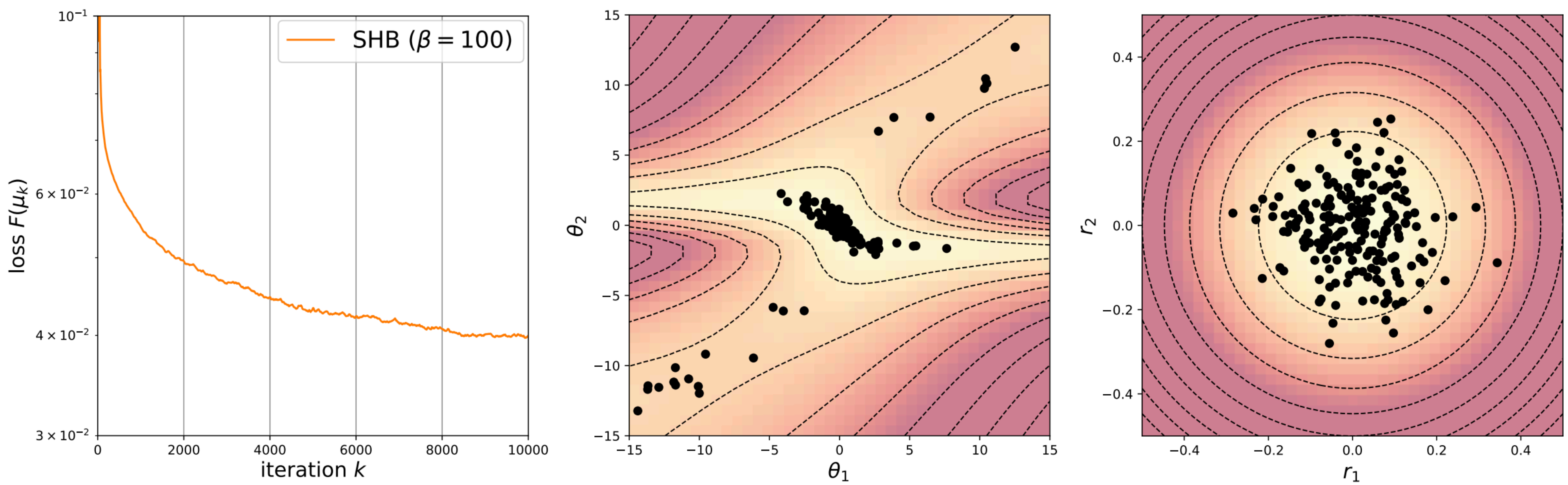




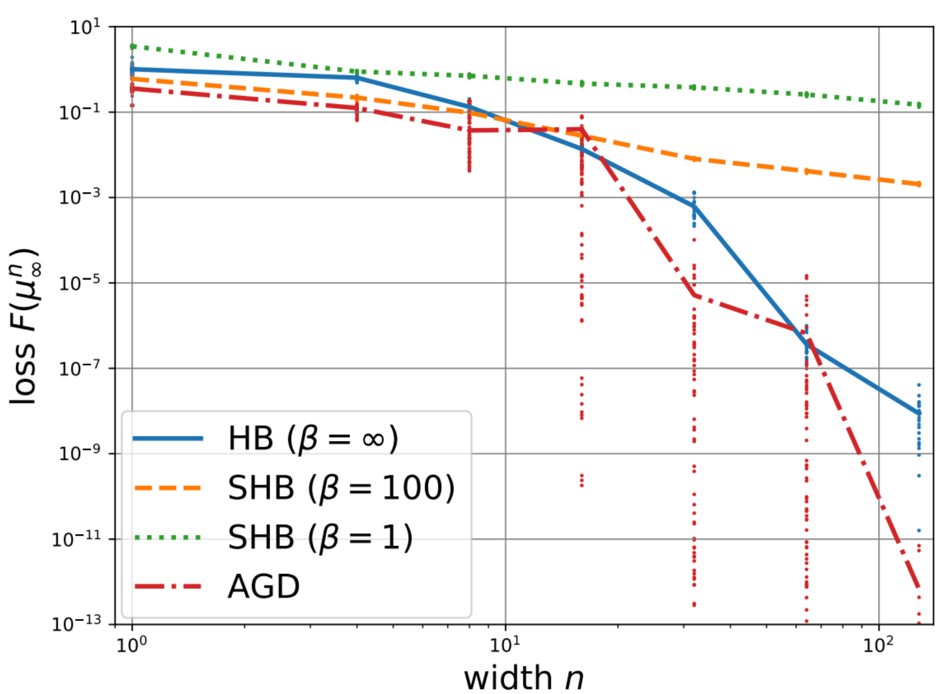
Classification accuracy for the WBDC dataset		
β	Estimate #1	Estimate #2
0.03	91.17%	92.35%
0.05	92.94%	92.94%
0.07	78.23%	92.94%

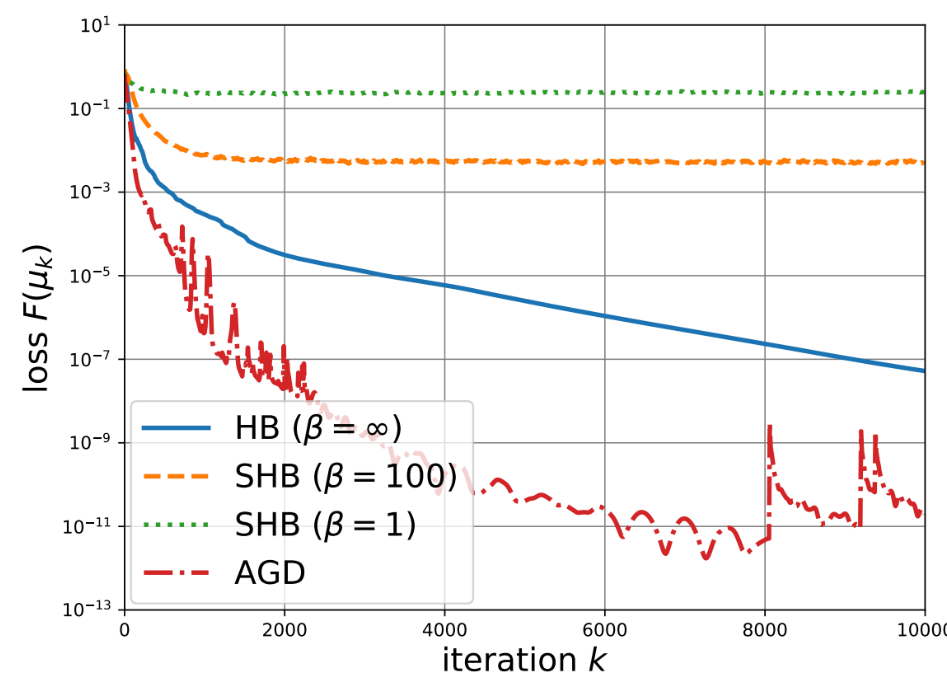
Mean Field Density Dynamics of Stoc. Heavy Ball

$$\partial_t \mu_t = -\nabla . \left[\mu_t . \begin{pmatrix} r \\ -\nabla F'([\mu_t]^\theta) - \gamma r \end{pmatrix} \right] + \gamma \beta^{-1} \Delta_r \mu_t$$



(a) Loss $F(\mu_k^n)$ (b) θ marginal (c) r marginal





Summary

Thank You

Support: CITRIS PEOPLE AND ROBOTS