A Distributed Algorithm for Wasserstein Proximal Operator Splitting

Abhishek Halder

Department of Applied Mathematics
University of California, Santa Cruz
Santa Cruz, CA 95064

Joint work with I. Nodozi, A.M. Teter (UC Santa Cruz)

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Topic of this talk

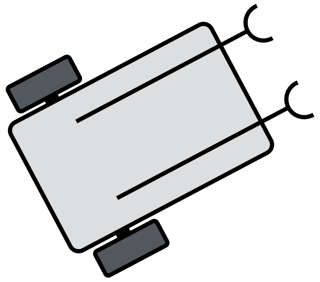
Optimization over the space of measures a.k.a. distributions

What do we mean by measure a.k.a. distribution

measure a.k.a. distribution = mass

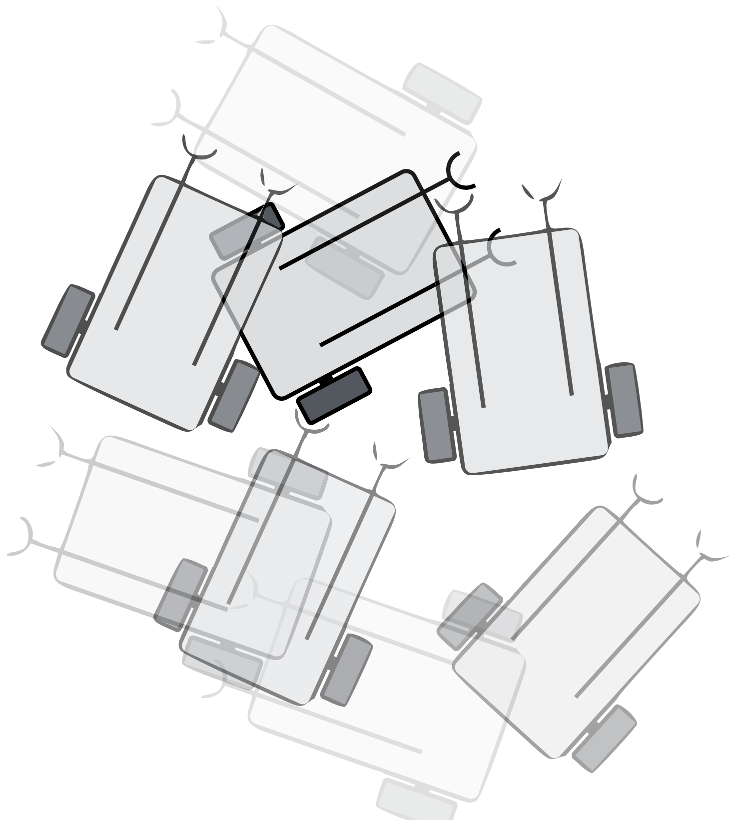
mass = density $\times$ volume

Probability Distribution



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

Probability Distribution

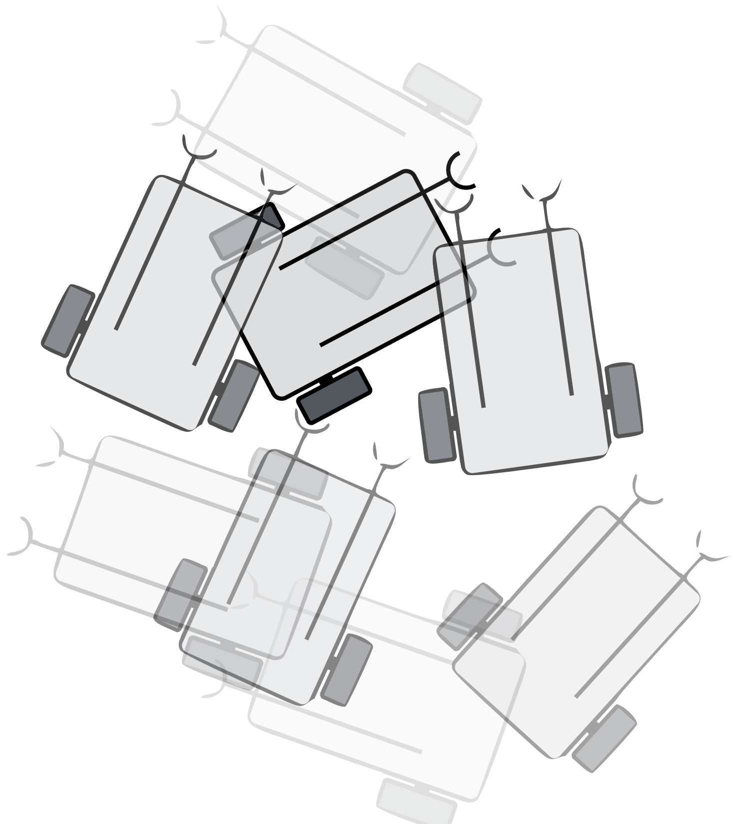


$$\boldsymbol{x}(t) = \begin{pmatrix} x \\ y \\ \theta \end{pmatrix} \in \mathcal{X} \equiv \mathbb{R}^2 \times \mathbb{S}^1$$

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

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

Probability Distribution



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probability measure probability density function

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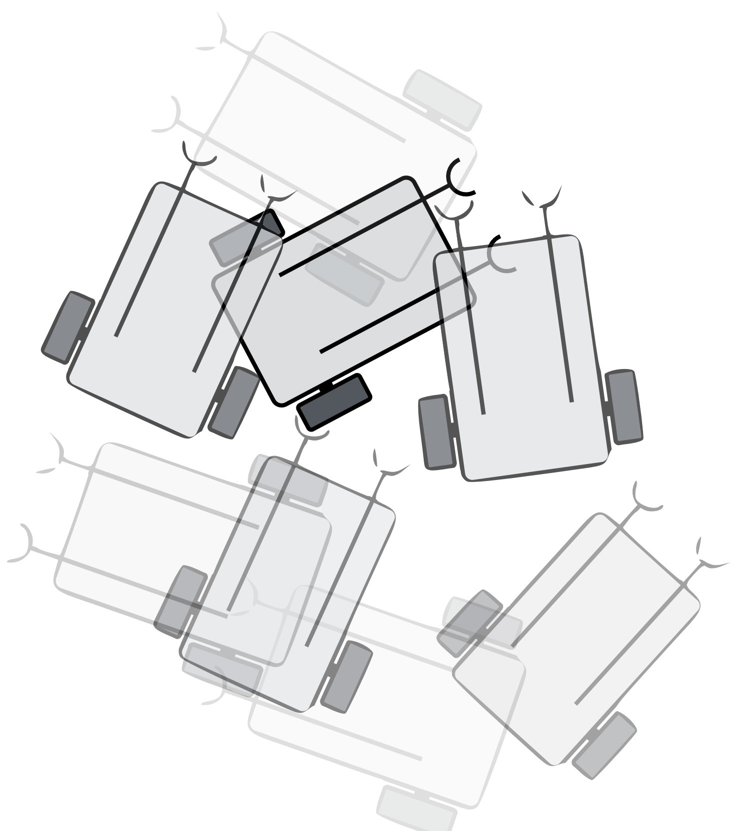
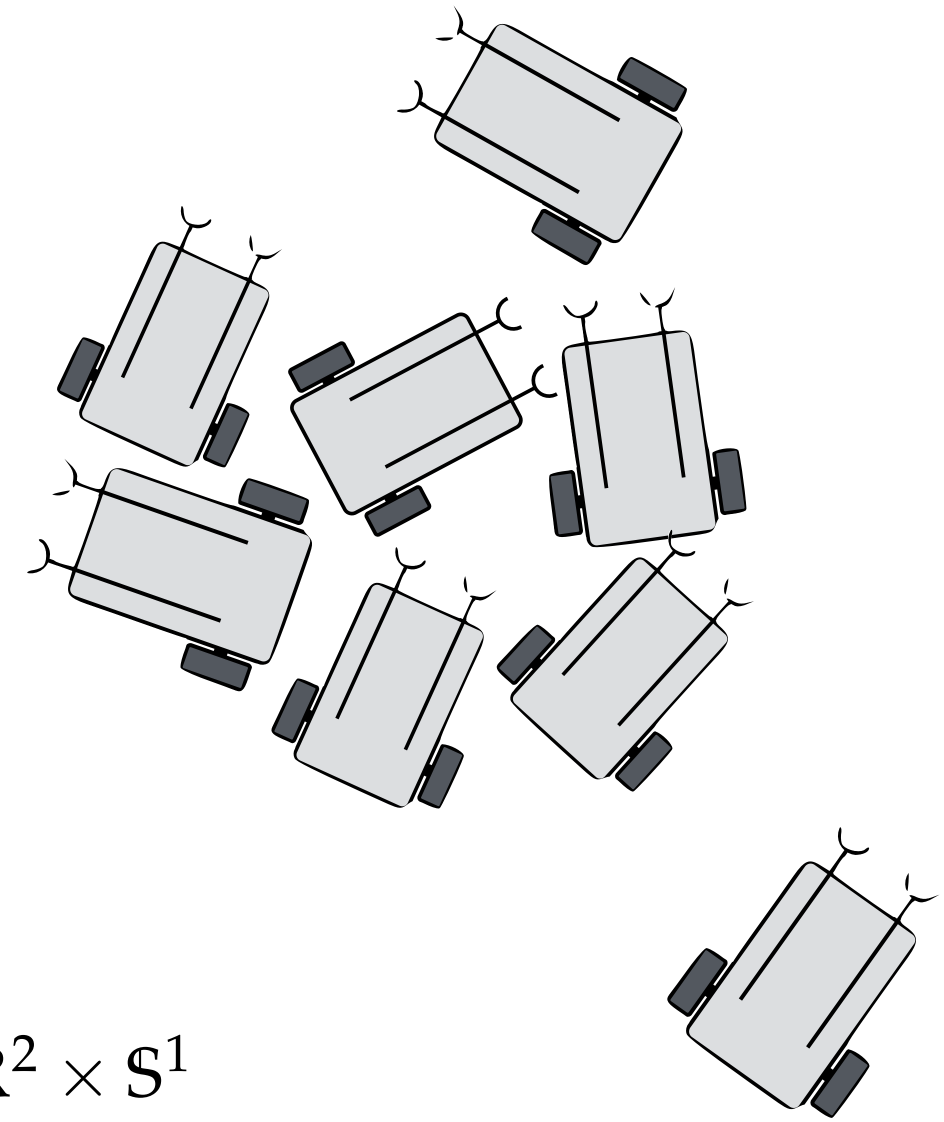
Probability Distribution   Population Distribution





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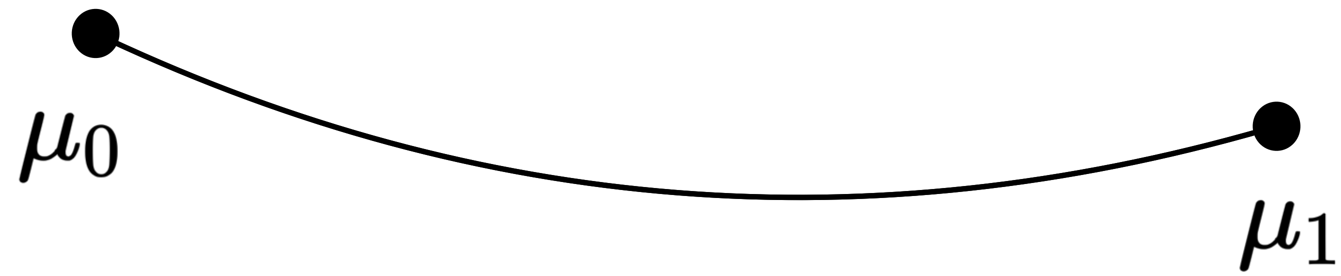
population measure   population density function

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

Geometry on the Space of Prob. Measures

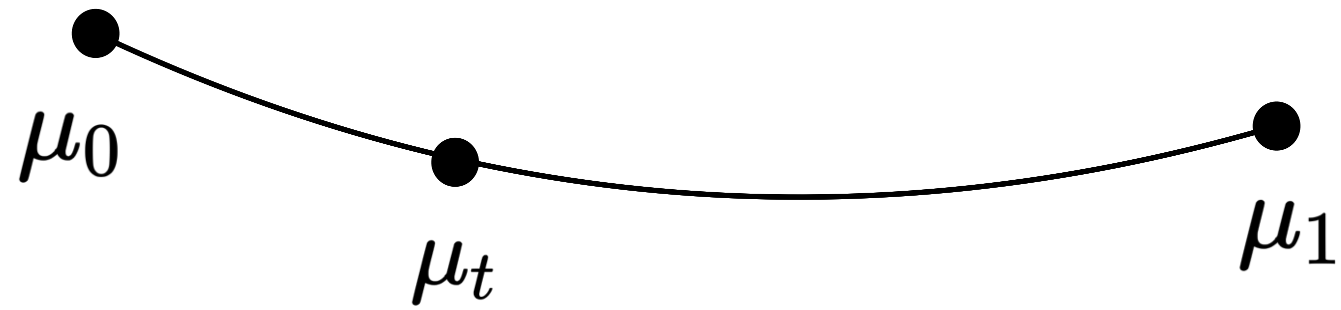


2-Wasserstein distance metric

$$W_2(\mu_0, \mu_1) := \left(\inf_{\mu, \boldsymbol{v}} \left\{ \frac{1}{2} \int_0^1 \int_{\mathcal{X}} \|\boldsymbol{v}\|^2 \mathrm{d}\mu \, \mathrm{d}t \right\} \right)^{1/2}$$

$$\text{subject to} \quad \frac{\partial \mu}{\partial t} = -\nabla \cdot (\mu \boldsymbol{v}), \ \mu(t=0, \cdot) = \mu_0, \ \mu(t=1, \cdot) = \mu_1$$

Geometry on the Space of Prob. Measures



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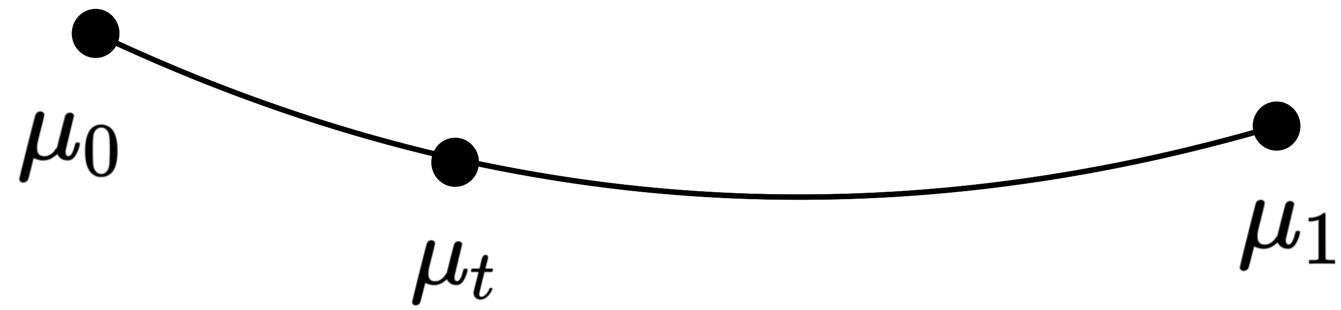
Measure-valued geodesic path for any $t \in [0,1]$

$$\mu_t = \arg\inf_{\nu\in\mathcal{P}_2(\mathcal{X})} \left\{ (1-t)W_2^2(\mu_0,\nu) + tW_2^2(\mu_1,\nu) \right\}$$

manifold of probability measures supported
on $\mathcal{X}$ with finite second moments

Geometry on the Space of Prob. Measures



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subject to $\quad \dfrac{\partial \mu}{\partial t} = -\nabla \cdot (\mu \boldsymbol{v}), \;\; \mu(t=0, \cdot) = \mu_0, \;\; \mu(t=1, \cdot) = \mu_1$

$(\mu, \boldsymbol{v}) \in \mathrm{AC}((0,1); \mathcal{P}_2(\mathcal{X})) \times L^2(\mu_t, \mathcal{X})$

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$$\mu_t = \arg\inf_{\nu \in \mathcal{P}_2(\mathcal{X})} \left\{ (1-t) W_2^2(\mu_0, \nu) + t W_2^2(\mu_1, \nu) \right\}$$

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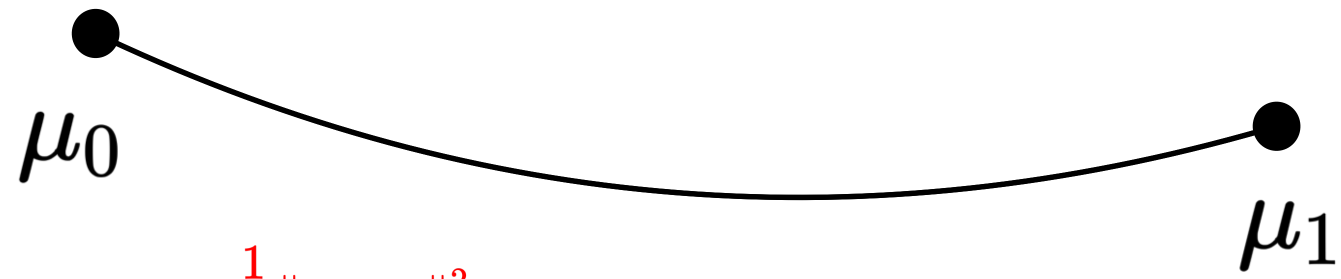
Geometry on the Space of Prob. Measures



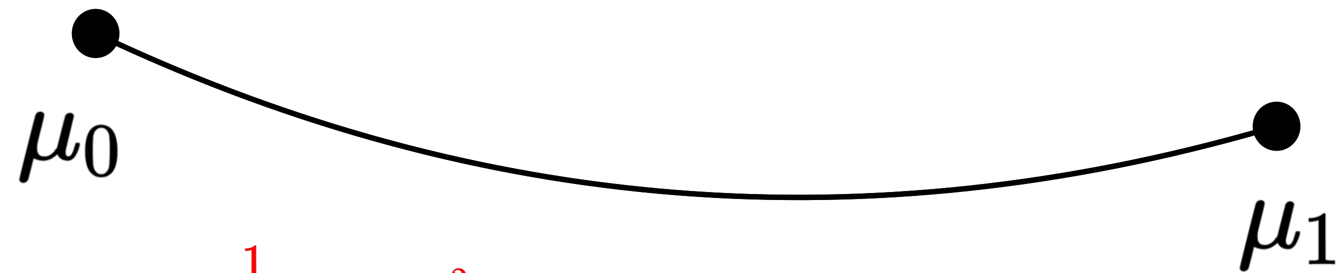
Optimal coupling formulation:

Ground cost, e.g., $\frac{1}{2}\|\boldsymbol{x}-\boldsymbol{y}\|_2^2$

$$W_2(\mu_0,\mu_1) := \left(\inf_{m} \int_{\mathcal{X}\times\mathcal{Y}} \boxed{c(\boldsymbol{x},\boldsymbol{y})}\, \mathrm{d}m(\boldsymbol{x},\boldsymbol{y})\right)^{1/2}$$

$$\text{subject to} \quad \int_{\mathcal{Y}} \mathrm{d}m = \mu_0(\mathrm{d}\boldsymbol{x}), \quad \int_{\mathcal{X}} \mathrm{d}m = \mu_1(\mathrm{d}\boldsymbol{y})$$

Geometry on the Space of Prob. Measures



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Sinkhorn divergence:

$$W_\varepsilon(\mu_0,\mu_1) := \left(\inf_m \int_{\mathcal{X}\times\mathcal{Y}} \left\{c(\boldsymbol{x},\boldsymbol{y}) + \varepsilon \log m\right\} \mathrm{d}m(\boldsymbol{x},\boldsymbol{y})\right)^{1/2}, \quad \varepsilon > 0$$

$$\text{subject to} \quad \int_{\mathcal{Y}} \mathrm{d}m = \mu_0(\mathrm{d}\boldsymbol{x}), \quad \int_{\mathcal{X}} \mathrm{d}m = \mu_1(\mathrm{d}\boldsymbol{y})$$

Measure-valued Optimization Problems

$$\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf} \; F(\mu)$$

2-Wasserstein geodescially convex functional

Space of Borel probability measures on $\mathbb{R}^d$ with finite second moments

In many applications, we have additive structure:

$$F(\mu) = F_1(\mu) + F_2(\mu) + \ldots + F_n(\mu)$$

where each $F_i : \mathscr{P}_2\left(\mathbb{R}^d\right) \mapsto (-\infty, +\infty]$ is proper, lsc, and 2-Wasserstein geodescially convex

Connection with Wasserstein Gradient Flows

$$\frac{\partial \mu}{\partial t} = -\nabla^{W_2} F(\mu) := \nabla \cdot \left(\mu \nabla \frac{\delta F}{\delta \mu} \right) \qquad (\star)$$

Wasserstein gradient

Minimizer of $\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf} F(\mu)$ $\leftsquigarrow$ Stationary solution of $(\star)$

Transient solution of $(\star)$ $\rightsquigarrow$ Discrete time-stepping realizing grad. descent of $\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf} F(\mu)$

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Transient solution of $(\,\star\,)$ $\rightsquigarrow$ Discrete time-stepping realizing grad. descent of $\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf}\; F(\mu)$

Wasserstein proximal recursion à la Jordan-Kinderlehrer-Otto (JKO) scheme

Gradient Flows

Gradient Flow in $\mathcal{X}$

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = -\nabla f(\boldsymbol{x}), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0$$

Recursion:

$$\begin{aligned}\boldsymbol{x}_k &= \boldsymbol{x}_{k-1} - h\nabla f(\boldsymbol{x}_k)\\ &= \underset{\boldsymbol{x}\in\mathcal{X}}{\arg\min}\left\{\frac{1}{2}\|\boldsymbol{x}-\boldsymbol{x}_{k-1}\|_2^2 + hf(\boldsymbol{x})\right\}\\ &=: \mathrm{prox}_{hf}^{\|\cdot\|_2}(\boldsymbol{x}_{k-1})\end{aligned}$$

Convergence:

$$\boldsymbol{x}_k \to \boldsymbol{x}(t = kh) \quad \text{as} \quad h \downarrow 0$$

f as Lyapunov function:

$$\frac{\mathrm{d}}{\mathrm{d}t} f = -\|\nabla f\|_2^2 \leq 0$$

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

$$\frac{\partial \mu}{\partial t} = -\nabla^W F(\mu), \quad \mu(\boldsymbol{x}, 0) = \mu_0$$

Recursion:

$$\begin{aligned}\mu_k &= \mu(\cdot, t = kh)\\ &= \underset{\mu\in\mathcal{P}_2(\mathcal{X})}{\arg\min}\left\{\frac{1}{2}W^2(\mu,\mu_{k-1}) + hF(\mu)\right\}\\ &=: \mathrm{prox}_{hF}^{W}(\mu_{k-1})\end{aligned}$$

Convergence:

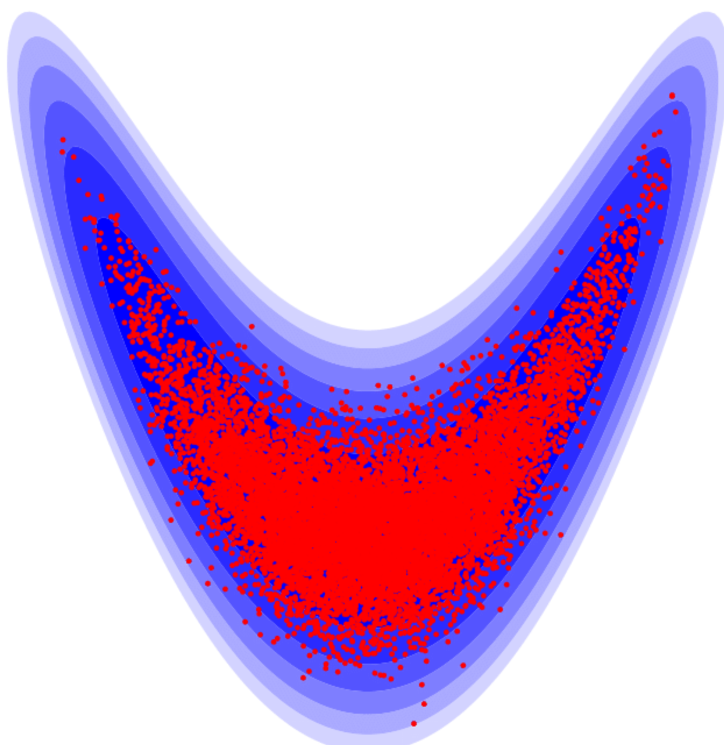
$$\mu_k \to \mu(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$$

F as Lyapunov functional:

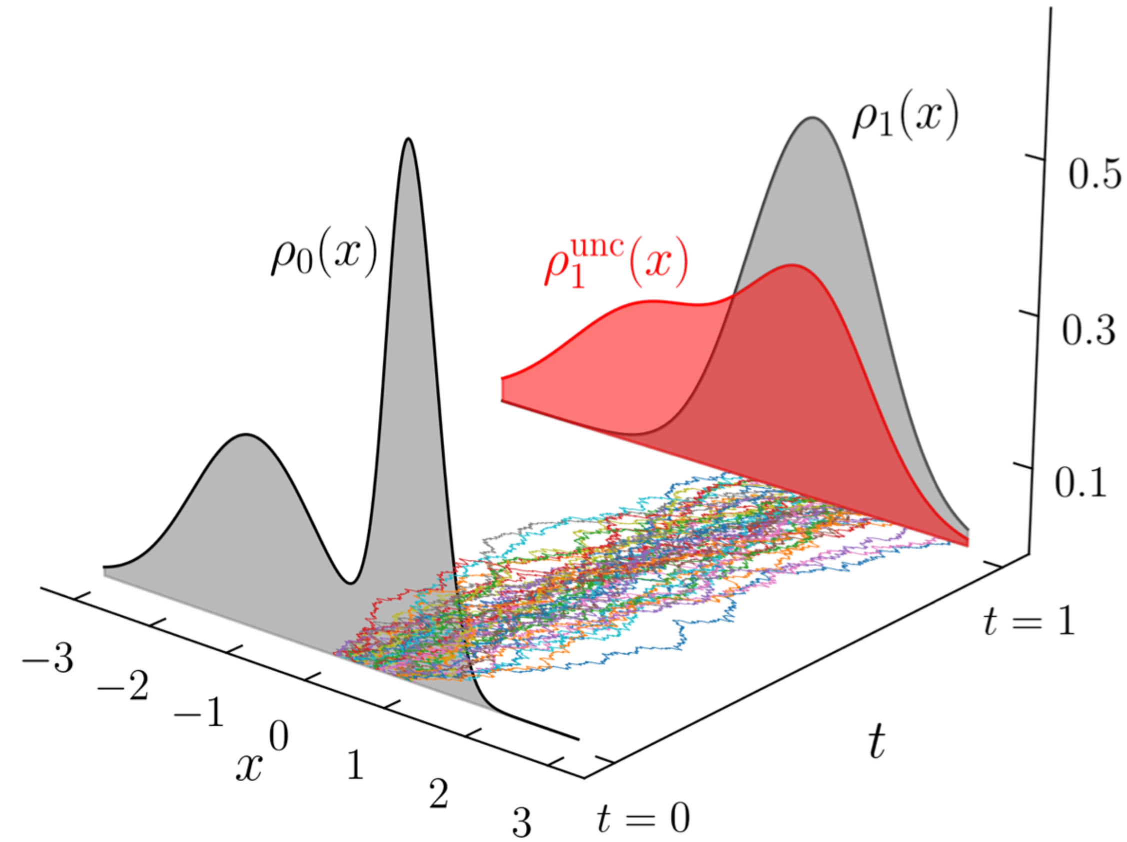
$$\frac{\mathrm{d}}{\mathrm{d}t} F = -\mathbb{E}_\mu\left[\left\|\nabla\frac{\delta F}{\delta\mu}\right\|_2^2\right] \leq 0$$

Motivating Applications

Langevin sampling from an unnormalized prior



Optimal control of distributions a.k.a. Schrödinger bridge problems



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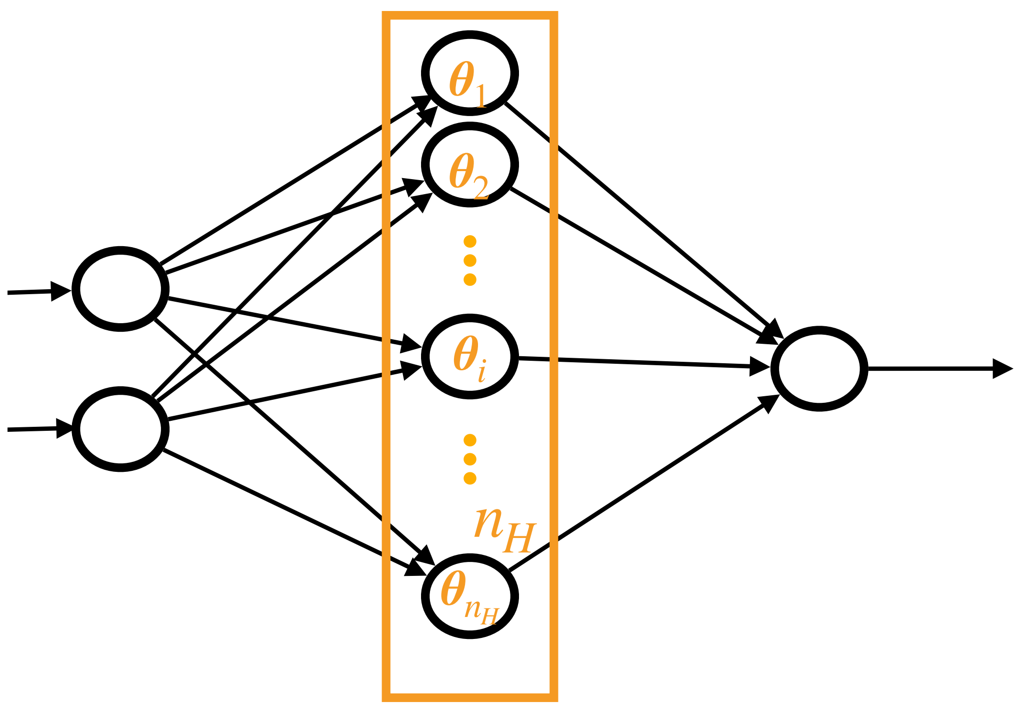
Chen, Georgiou and Pavon, *SIAM Journal on Applied Mathematics*, 2016

Chen, Georgiou and Pavon, *Journal on Optimization Theory and Applications*, 2016

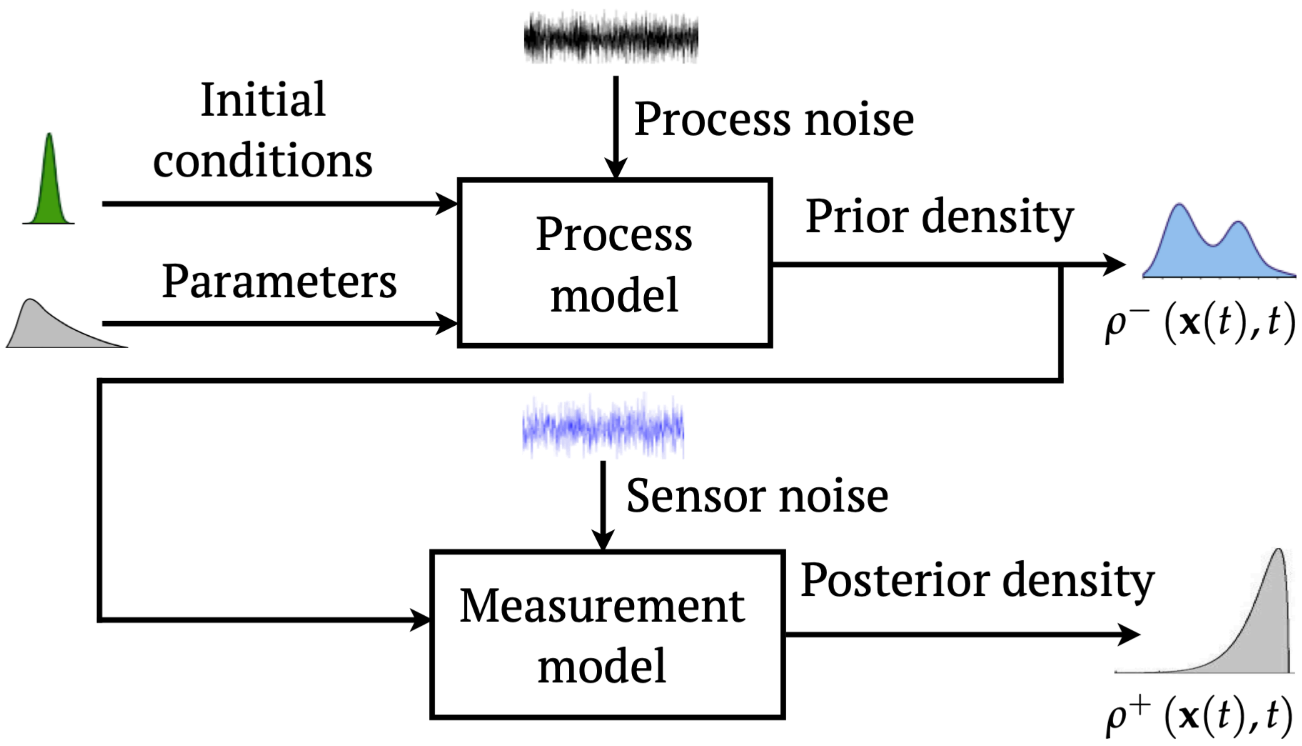
Caluya and Halder, *IEEE Transactions on Automatic Control*, 2021

Motivating Applications (contd.)

Mean field learning dynamics in neural networks



Prediction and estimation of time-varying joint state probability densities



Mei, Montanari and Nguyen, *Proceedings of the National Academy of Sciences*, 2018

Chizat and Bach, *NeurIPS*, 2018

Rotskoff and Vanden-Eijnden, *NeurIPS*, 2018

Sirignano and Spiliopoulos, *Stochastic Processes and their Applications*, 2020

Caluya and Halder, *IEEE Transactions on Automatic Control*, 2019

Halder and Georgiou, *CDC*, 2019

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Many Recently Proposed Algorithms to Solve Measure-valued Optimization Problems

Peyré, *SIAM Journal on Imaging Sciences*, 2015

Benamou, Carlier and Laborde, *ESAIM: Proceedings and Surveys*, 2016

Carlier, Duval, Peyré and Schimtzer, *SIAM Journal on Mathematical Analysis*, 2017

Karlsson and Ringh, *SIAM Journal on Imaging Sciences*, 2017

Caluya and Halder, *IEEE Transactions on Automatic Control*, 2019

Carrillo, Craig, Wang and Wei, *Foundations of Computational Mathematics*, 2021

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Alvarez-Melis, Schiff, and Mroueh, *NeurIPS*, 2021

But all require centralized computing

Centralized Computing Case Study: Mean Field SGD Dynamics in NN Classification

Free energy functional: $F(\mu) = R\Big(\hat{f}\left(\boldsymbol{x}, \mu\right)\Big)$

For quadratic loss:

$$F(\mu) = F_0 + \int_{\mathbb{R}^p} V(\boldsymbol{\theta})\mathrm{d}\mu(\boldsymbol{\theta}) + \int_{\mathbb{R}^{2p}} U(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}})\mathrm{d}\mu(\boldsymbol{\theta})\mathrm{d}\mu(\tilde{\boldsymbol{\theta}})$$

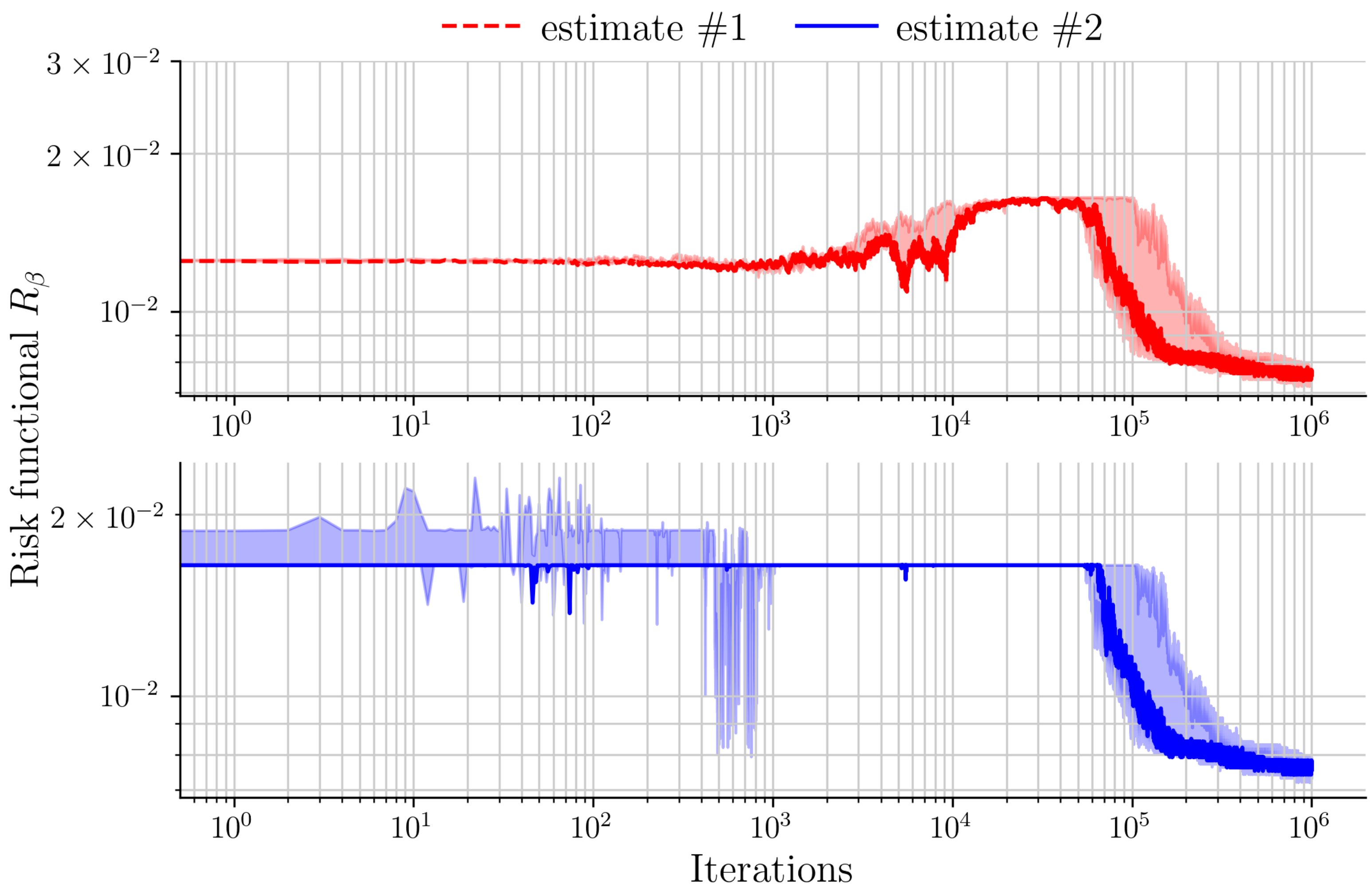
depend on activation functions of the NN

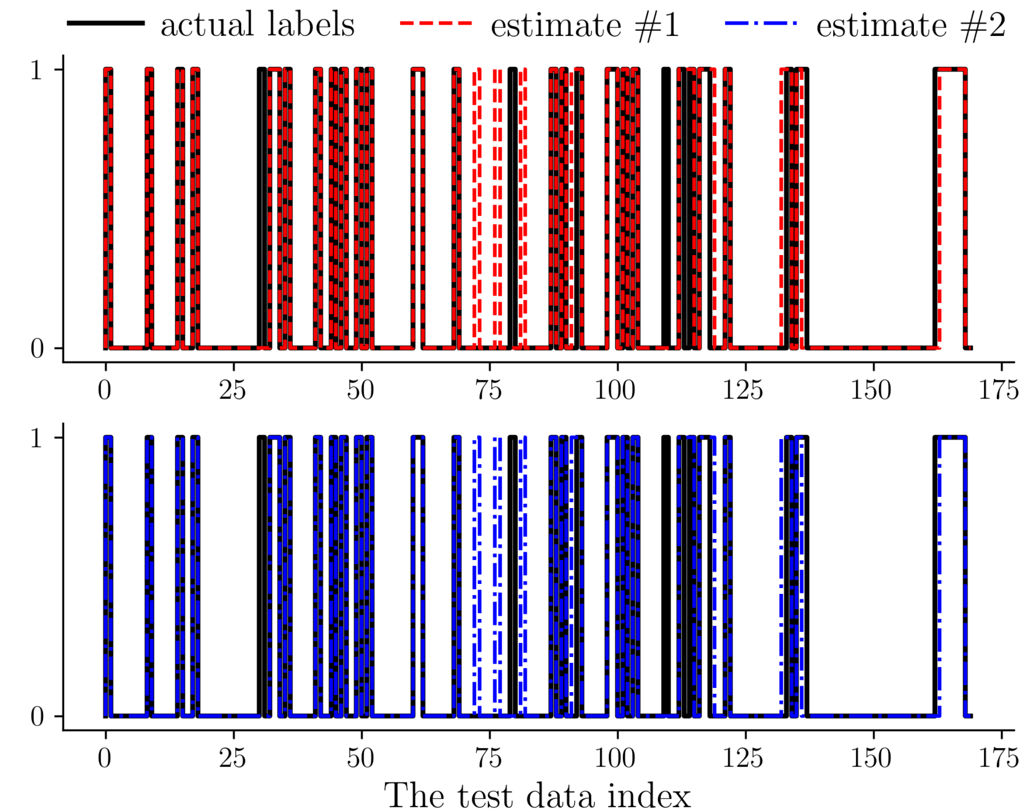
Neuronal population measure dynamics: $\dfrac{\partial \mu}{\partial t} = \nabla \cdot \left(\mu \nabla \dfrac{\delta F}{\delta \mu}\right) =: -\nabla^{W_2} F(\mu)$

Wasserstein proximal recursion: $\mu_{k+1} = \mathrm{prox}_{hF}^{W}(\mu_k)$

Centralized Computing Case Study: Mean Field SGD Dynamics in NN Classification

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%

CPU: 3.4 GHz 6 core intel i5 8GB RAM (≈ 33 hrs runtime)

GPU: Jetson TX2 NVIDIA Pascal GPU 256 CUDA cores, 64 bit NVIDIA Denver + ARM Cortex A57 CPUs (≈ 2 hrs runtime)

Teter, Nodozi and Halder, *arXiv: 2210.13879*, 2022

Our Present Work: Distributed Algorithm

$$\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf} \; F_1(\mu) + F_2(\mu) + \ldots + F_n(\mu)$$

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$$\underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf}\; F_1(\mu) + F_2(\mu) + \ldots + F_n(\mu)$$

Main idea:

$$\Big\Downarrow \text{ re-write}$$

$$\begin{aligned} \underset{(\mu_1,\ldots,\mu_n,\zeta) \in \mathcal{P}_2^{n+1}(\mathbb{R}^d)}{\arg\inf} \quad & F_1(\mu_1) + F_2(\mu_2) + \ldots + F_n(\mu_n) \\ \text{subject to} \quad & \mu_i = \zeta \quad \text{for all } i \in [n] \end{aligned}$$

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Define Wasserstein augmented Lagrangian:

$$L_\alpha(\mu_1,\ldots,\mu_n,\zeta,\nu_1,\ldots,\nu_n) := \sum_{i=1}^{n} \left\{ F_i(\mu_i) + \frac{\alpha}{2} W^2(\mu_i,\zeta) + \int_{\mathbb{R}^d} \nu_i(\boldsymbol{\theta})(\mathrm{d}\mu_i - \mathrm{d}\zeta) \right\}$$

regularization > 0 Lagrange multipliers

Proposed Consensus ADMM

$$\mu_i^{k+1} = \underset{\mu_i \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf}\, L_\alpha\big(\mu_1, \ldots, \mu_n, \zeta^k, \nu_1^k, \ldots, \nu_n^k\big)$$

$$\zeta^{k+1} = \underset{\zeta \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf}\, L_\alpha\big(\mu_1^{k+1}, \ldots, \mu_n^{k+1}, \zeta, \nu_1^k, \ldots, \nu_n^k\big)$$

$$\nu_i^{k+1} = \nu_i^k + \alpha\big(\mu_i^{k+1} - \zeta^{k+1}\big)$$

where $i \in [n]$, $k \in \mathbb{N}_0$

Proposed Consensus ADMM

$$
\begin{aligned}
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\zeta^{k+1} &= \underset{\zeta \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf}\, L_\alpha\left(\mu_1^{k+1}, \ldots, \mu_n^{k+1}, \zeta, \nu_1^k, \ldots, \nu_n^k\right) \\
\nu_i^{k+1} &= \nu_i^k + \alpha\left(\mu_i^{k+1} - \zeta^{k+1}\right) \qquad \text{where } i \in [n],\, k \in \mathbb{N}_0
\end{aligned}
$$

Define

$$
\nu_{\text{sum}}^k(\boldsymbol{\theta}) := \sum_{i=1}^n \nu_i^k(\boldsymbol{\theta}), \quad k \in \mathbb{N}_0
$$

and simplify the recursions to

$$
\begin{aligned}
\mu_i^{k+1} &= \operatorname{prox}^W_{\frac{1}{\alpha}\left(F_i(\cdot) + \int \nu_i^k \,\mathrm{d}(\cdot)\right)}\left(\zeta^k\right) \\
\zeta^{k+1} &= \underset{\zeta \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\inf} \left\{ \left(\sum_{i=1}^n W^2\left(\mu_i^{k+1}, \zeta\right) \right) - \frac{2}{\alpha} \int_{\mathbb{R}^d} \nu_{\text{sum}}^k(\boldsymbol{\theta}) \mathrm{d}\zeta \right\} \\
\nu_i^{k+1} &= \nu_i^k + \alpha\left(\mu_i^{k+1} - \zeta^{k+1}\right)
\end{aligned}
$$

Proposed Consensus ADMM (contd.)

$$\boxed{\mu_i^{k+1} = \mathrm{prox}^{W}_{\frac{1}{\alpha}\left(F_i(\cdot)+\int \nu_i^k \,\mathrm{d}(\cdot)\right)}\left(\zeta^k\right)}$$

$$\zeta^{k+1} = \underset{\zeta\in\mathcal{P}_2\left(\mathbb{R}^d\right)}{\arg\inf}\left\{\left(\sum_{i=1}^{n} W^2\left(\mu_i^{k+1},\zeta\right)\right) - \frac{2}{\alpha}\int_{\mathbb{R}^d}\nu_{\mathrm{sum}}^k(\boldsymbol{\theta})\mathrm{d}\zeta\right\}$$

$$\nu_i^{k+1} = \nu_i^k + \alpha\left(\mu_i^{k+1} - \zeta^{k+1}\right)$$

Split free energy functionals: $\Phi_i(\mu_i) := F_i(\mu_i) + \int_{\mathbb{R}^d}\nu_i^k \,\mathrm{d}\mu_i$

$\therefore$ Distributed Wasserstein prox $\approx$ time updates of $\dfrac{\partial\tilde{\mu}_i}{\partial t} = -\nabla^W\Phi_i(\tilde{\mu}_i)$

Proposed Consensus ADMM (contd.)

$$\boxed{\mu_i^{k+1} = \mathrm{prox}^{W}_{\frac{1}{\alpha}\left(F_i(\cdot)+\int \nu_i^k \,\mathrm{d}(\cdot)\right)}\left(\zeta^k\right)}$$

$$\zeta^{k+1} = \underset{\zeta\in\mathcal{P}_2\left(\mathbb{R}^d\right)}{\arg\inf}\left\{\left(\sum_{i=1}^{n} W^2\left(\mu_i^{k+1},\zeta\right)\right) - \frac{2}{\alpha}\int_{\mathbb{R}^d}\nu_{\mathrm{sum}}^k(\boldsymbol{\theta})\mathrm{d}\zeta\right\}$$

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$\therefore$ Distributed Wasserstein prox $\approx$ time updates of $\dfrac{\partial\tilde{\mu}_i}{\partial t} = -\nabla^W\Phi_i(\tilde{\mu}_i)$

Examples:

$\Phi_i(\cdot) = F_i(\cdot) + \int \nu_i^k\mathrm{d}(\cdot)$	PDE	Name
$\int_{\mathbb{R}^d}\left(V(\boldsymbol{\theta}) + \nu_i^k(\boldsymbol{\theta})\right)\mathrm{d}\mu_i(\boldsymbol{\theta})$	$\dfrac{\partial\widetilde{\mu}_i}{\partial t} = \nabla\cdot\left(\widetilde{\mu}_i\left(\nabla V + \nabla\nu_i^k\right)\right)$	Liouville equation
$\int_{\mathbb{R}^d}\left(\nu_i^k(\boldsymbol{\theta}) + \beta^{-1}\log\mu_i(\boldsymbol{\theta})\right)\mathrm{d}\mu_i(\boldsymbol{\theta})$	$\dfrac{\partial\widetilde{\mu}_i}{\partial t} = \nabla\cdot\left(\widetilde{\mu}_i\nabla\nu_i^k\right) + \beta^{-1}\Delta\widetilde{\mu}_i$	Fokker-Planck equation
$\int_{\mathbb{R}^d}\nu_i^k(\boldsymbol{\theta})\mathrm{d}\mu_i(\boldsymbol{\theta}) + \int_{\mathbb{R}^{2d}}U(\boldsymbol{\theta},\boldsymbol{\sigma})\mathrm{d}\mu_i(\boldsymbol{\theta})\mathrm{d}\mu_i(\boldsymbol{\sigma})$	$\dfrac{\partial\widetilde{\mu}_i}{\partial t} = \nabla\cdot\left(\widetilde{\mu}_i\left(\nabla\nu_i^k + \nabla\left(U\circledast\widetilde{\mu}_i\right)\right)\right)$	Propagation of chaos equation
$\int_{\mathbb{R}^d}\left(\nu_i^k(\boldsymbol{\theta}) + \frac{\beta^{-1}}{m-1}\mathbf{1}^\top\mu_i^m\right)\mathrm{d}\mu_i(\boldsymbol{\theta}), m>1$	$\dfrac{\partial\widetilde{\mu}_i}{\partial t} = \nabla\cdot\left(\widetilde{\mu}_i\nabla\nu_i^k\right) + \beta^{-1}\Delta\widetilde{\mu}_i^m$	Porous medium equation

Discrete Version of the Proposed ADMM

Euclidean distance matrix

$$\boldsymbol{\mu}_i^{k+1} = \operatorname{prox}^W_{\frac{1}{\alpha}\left(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\right)}\left(\boldsymbol{\zeta}^k\right)$$

$$= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M} \in \Pi_N\left(\boldsymbol{\mu}_i, \zeta^k\right)} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}\rangle + \frac{1}{\alpha}\left(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\right) \right\}$$

$$\boldsymbol{\zeta}^{k+1} = \operatorname*{arg\,inf}_{\zeta \in \Delta^{N-1}} \left\{ \left(\sum_{i=1}^{n} \min_{\boldsymbol{M}_i \in \Pi_N\left(\boldsymbol{\mu}_i^{k+1}, \zeta\right)} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}_i\rangle \right) - \frac{2}{\alpha}\langle \boldsymbol{\nu}_{\text{sum}}^k, \boldsymbol{\zeta}\rangle \right\}$$

$$\boldsymbol{\nu}_i^{k+1} = \boldsymbol{\nu}_i^k + \alpha\left(\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1}\right)$$

where N is the number of samples

Discrete Version of the Proposed ADMM

$$\boldsymbol{\mu}_i^{k+1} = \mathrm{prox}^{W}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle)}(\boldsymbol{\zeta}^k)$$

$$= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M}\in\Pi_N(\boldsymbol{\mu}_i,\boldsymbol{\zeta}^k)} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}\rangle + \frac{1}{\alpha}\big(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\big) \right\}$$

$$\boldsymbol{\zeta}^{k+1} = \operatorname*{arg\,inf}_{\boldsymbol{\zeta}\in\Delta^{N-1}} \left\{ \left(\sum_{i=1}^{n} \min_{\boldsymbol{M}_i\in\Pi_N(\boldsymbol{\mu}_i^{k+1},\boldsymbol{\zeta})} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}_i\rangle \right) - \frac{2}{\alpha}\langle \boldsymbol{\nu}_{\mathrm{sum}}^k, \boldsymbol{\zeta}\rangle \right\}$$

$$\boldsymbol{\nu}_i^{k+1} = \boldsymbol{\nu}_i^k + \alpha\big(\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1}\big)$$

With Sinkhorn regularization:

Discrete Sinkhorn divergence

$$\boldsymbol{\mu}_i^{k+1} = \mathrm{prox}^{W_\varepsilon}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle)}(\boldsymbol{\zeta}^k)$$

$$= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M}\in\Pi_N(\boldsymbol{\mu}_i,\boldsymbol{\zeta}^k)} \left\langle \frac{1}{2}\boldsymbol{C} + \varepsilon \log \boldsymbol{M}, \boldsymbol{M} \right\rangle + \frac{1}{\alpha}\big(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\big) \right\}$$

$$\boldsymbol{\zeta}^{k+1} = \operatorname*{arg\,inf}_{\boldsymbol{\zeta}\in\Delta^{N-1}} \left\{ \left(\sum_{i=1}^{n} \min_{\boldsymbol{M}_i\in\Pi_N(\boldsymbol{\mu}_i^{k+1},\boldsymbol{\zeta})} \left\langle \frac{1}{2}\boldsymbol{C} + \varepsilon \log \boldsymbol{M}_i, \boldsymbol{M}_i \right\rangle \right) - \frac{2}{\alpha}\langle \boldsymbol{\nu}_{\mathrm{sum}}^k, \boldsymbol{\zeta}\rangle \right\}$$

$$\boldsymbol{\nu}_i^{k+1} = \boldsymbol{\nu}_i^k + \alpha\big(\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1}\big)$$

Discrete Version of the Proposed ADMM

$$
\begin{aligned}
\boldsymbol{\mu}_i^{k+1} &= \mathrm{prox}^{W}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle)}(\boldsymbol{\zeta}^k) \\
&= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M} \in \Pi_N(\boldsymbol{\mu}_i, \zeta^k)} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}\rangle + \frac{1}{\alpha}\big(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\big) \right\} \\
\boldsymbol{\zeta}^{k+1} &= \operatorname*{arg\,inf}_{\zeta \in \Delta^{N-1}} \left\{ \left(\sum_{i=1}^{n} \min_{\boldsymbol{M}_i \in \Pi_N(\boldsymbol{\mu}_i^{k+1}, \zeta)} \frac{1}{2}\langle \boldsymbol{C}, \boldsymbol{M}_i\rangle \right) - \frac{2}{\alpha}\langle \boldsymbol{\nu}_{\mathrm{sum}}^k, \boldsymbol{\zeta}\rangle \right\} \\
\boldsymbol{\nu}_i^{k+1} &= \boldsymbol{\nu}_i^k + \alpha\big(\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1}\big)
\end{aligned}
$$

With Sinkhorn regularization:

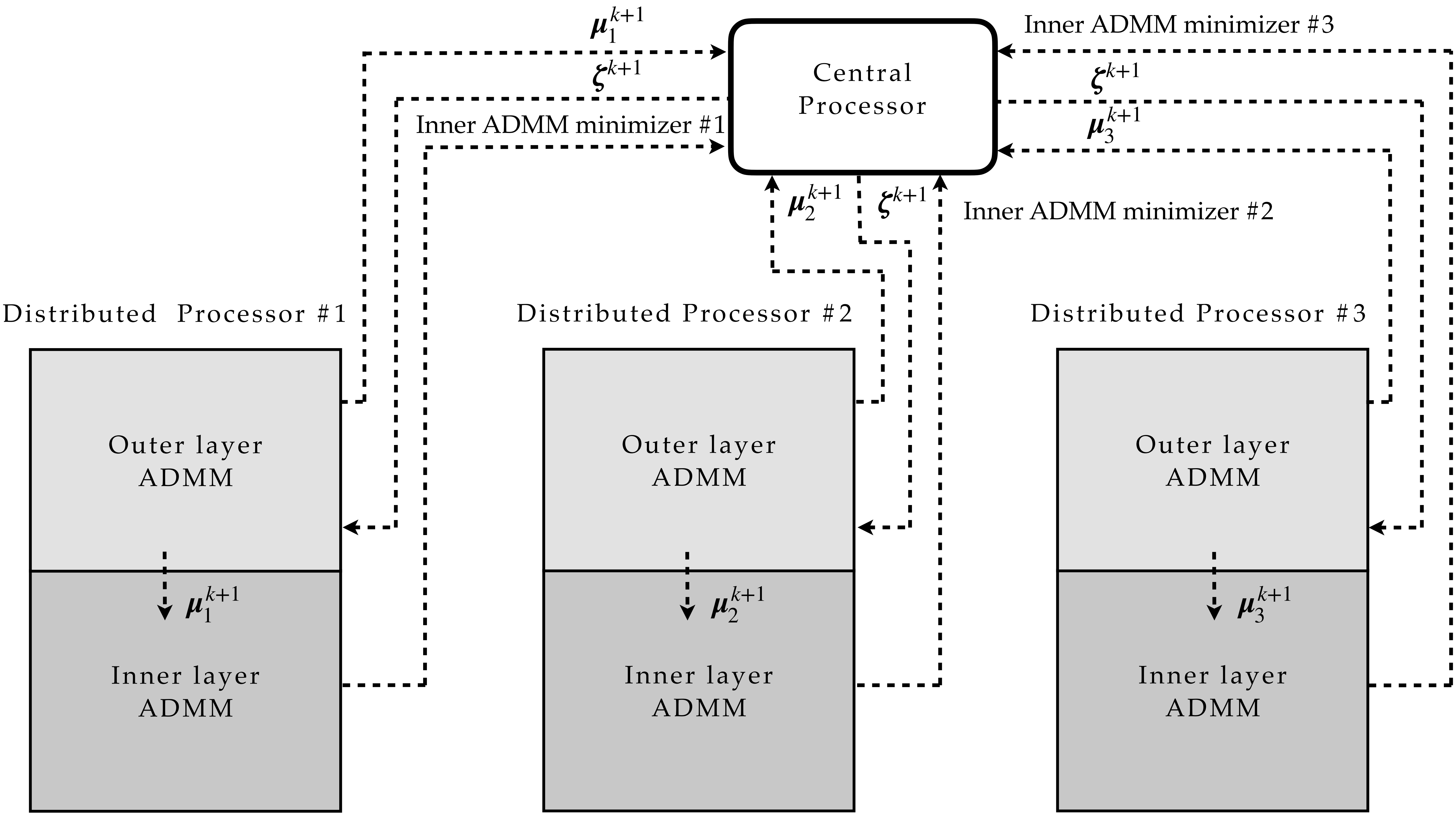
Discrete Sinkhorn divergence

Outer layer ADMM

$$
\begin{aligned}
\boldsymbol{\mu}_i^{k+1} &= \mathrm{prox}^{W_\varepsilon}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle)}(\boldsymbol{\zeta}^k) \\
&= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{M \in \Pi_N(\boldsymbol{\mu}_i, \zeta^k)} \left\langle \frac{1}{2}\boldsymbol{C} + \varepsilon \log \boldsymbol{M}, \boldsymbol{M} \right\rangle + \frac{1}{\alpha}\big(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i\rangle\big) \right\} \\
\boldsymbol{\zeta}^{k+1} &= \operatorname*{arg\,inf}_{\zeta \in \Delta^{N-1}} \left\{ \left(\sum_{i=1}^{n} \min_{\boldsymbol{M}_i \in \Pi_N(\boldsymbol{\mu}_i^{k+1}, \zeta)} \left\langle \frac{1}{2}\boldsymbol{C} + \varepsilon \log \boldsymbol{M}_i, \boldsymbol{M}_i \right\rangle \right) - \frac{2}{\alpha}\langle \boldsymbol{\nu}_{\mathrm{sum}}^k, \boldsymbol{\zeta}\rangle \right\} \\
\boldsymbol{\nu}_i^{k+1} &= \boldsymbol{\nu}_i^k + \alpha\big(\boldsymbol{\mu}_i^{k+1} - \boldsymbol{\zeta}^{k+1}\big)
\end{aligned}
$$

Inner layer ADMM

Overall Schematic



μ_i update $\rightsquigarrow$ Outer Consensus (Sinkhorn) ADMM

Example. $\Phi(\boldsymbol{\mu}) := \langle \boldsymbol{a}, \boldsymbol{\mu} \rangle$, $\boldsymbol{a} \in \mathbb{R}^N \backslash \{\mathbf{0}\}$, $\boldsymbol{\mu}, \boldsymbol{\zeta} \in \Delta^{N-1}$, $\boldsymbol{\Gamma} := \exp\left(-\boldsymbol{C}/2\varepsilon\right)$, $\varepsilon > 0$

$$\operatorname{prox}^{W_\varepsilon}_{\frac{1}{\alpha}\Phi}(\boldsymbol{\zeta}) = \exp\left(-\frac{1}{\alpha\varepsilon}\boldsymbol{a}\right) \odot \left(\boldsymbol{\Gamma}^\top \left(\boldsymbol{\zeta} \oslash \left(\boldsymbol{\Gamma} \exp\left(-\frac{1}{\alpha\varepsilon}\boldsymbol{a}\right)\right)\right)\right)$$

μ_i update $\rightsquigarrow$ Outer Consensus (Sinkhorn) ADMM

Example. $\Phi(\boldsymbol{\mu}) := \langle \boldsymbol{a}, \boldsymbol{\mu} \rangle$, $\boldsymbol{a} \in \mathbb{R}^N \setminus \{\mathbf{0}\}$, $\boldsymbol{\mu}, \boldsymbol{\zeta} \in \Delta^{N-1}$, $\boldsymbol{\Gamma} := \exp\left(-\boldsymbol{C}/2\varepsilon\right)$, $\varepsilon > 0$

$$\mathrm{prox}^{W_\varepsilon}_{\frac{1}{\alpha}\Phi}(\boldsymbol{\zeta}) = \exp\left(-\frac{1}{\alpha\varepsilon}\boldsymbol{a}\right) \odot \left(\boldsymbol{\Gamma}^\top\left(\boldsymbol{\zeta} \oslash \left(\boldsymbol{\Gamma}\exp\left(-\frac{1}{\alpha\varepsilon}\boldsymbol{a}\right)\right)\right)\right)$$

Example. $G_i(\boldsymbol{\mu_i}) := \underset{\text{Convex}}{F_i}(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle,\ \boldsymbol{\zeta}^k \in \Delta^{N-1},\ k \in \mathbb{N}_0.$

$$\boldsymbol{\mu}_i^{k+1} = \mathrm{prox}^{W_\varepsilon}_{\frac{1}{\alpha}(F_i(\boldsymbol{\mu}_i)+\langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle)}\left(\boldsymbol{\zeta}^k\right) = \exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\mathrm{opt}}}{\alpha\varepsilon}\right) \odot \left(\exp\left(-\frac{\boldsymbol{C}^\top}{2\varepsilon}\right)\exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\mathrm{opt}}}{\alpha\varepsilon}\right)\right)$$

where $\boldsymbol{\lambda}_{0i}^{\mathrm{opt}}, \boldsymbol{\lambda}_{1i}^{\mathrm{opt}} \in \mathbb{R}^N$ solve

$$\exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\mathrm{opt}}}{\alpha\varepsilon}\right) \odot \left(\exp\left(-\frac{\boldsymbol{C}}{2\varepsilon}\right)\exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\mathrm{opt}}}{\alpha\varepsilon}\right)\right) = \boldsymbol{\zeta}_k,$$

$$\mathbf{0} \in \partial_{\boldsymbol{\lambda}_{1i}^{\mathrm{opt}}} G_i^*\left(-\boldsymbol{\lambda}_{1i}^{\mathrm{opt}}\right) - \exp\left(\frac{\boldsymbol{\lambda}_{1i}^{\mathrm{opt}}}{\alpha\varepsilon}\right) \odot \left(\exp\left(-\frac{\boldsymbol{C}^\top}{2\varepsilon}\right)\exp\left(\frac{\boldsymbol{\lambda}_{0i}^{\mathrm{opt}}}{\alpha\varepsilon}\right)\right).$$

ζ update $\rightsquigarrow$ Inner (Euclidean) ADMM

Theorem.

Consider the convex problem

$$\left(\boldsymbol{u}_1^{\mathrm{opt}}, \ldots, \boldsymbol{u}_n^{\mathrm{opt}}\right) = \underset{(\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n) \in \mathbb{R}^{nN}}{\arg\min} \sum_{i=1}^{n} \left\langle \boldsymbol{\mu}_i^{k+1}, \log\left(\boldsymbol{\Gamma} \exp\left(\boldsymbol{u}_i/\varepsilon\right)\right) \right\rangle$$

$$\text{subject to} \quad \sum_{i=1}^{n} \boldsymbol{u}_i = \frac{2}{\alpha} \boldsymbol{\nu}_{\mathrm{sum}}^{k}. \qquad (\heartsuit)$$

Then

$$\zeta^{k+1} = \exp\left(\boldsymbol{u}_i^{\mathrm{opt}}/\varepsilon\right) \odot \left(\boldsymbol{\Gamma}\left(\boldsymbol{\mu}_i^{k+1} \oslash \left(\boldsymbol{\Gamma} \exp\left(\boldsymbol{u}_i^{\mathrm{opt}}/\varepsilon\right)\right)\right)\right) \in \Delta^{N-1} \quad \forall\, i \in [n].$$

ζ update $\rightsquigarrow$ Inner (Euclidean) ADMM

Theorem.

Let $f_i(\boldsymbol{u}_i) := \left\langle \boldsymbol{\mu}_i^{k+1}, \log\left(\boldsymbol{\Gamma} \exp\left(\boldsymbol{u}_i/\varepsilon\right)\right)\right\rangle, \quad \boldsymbol{u}_i \in \mathbb{R}^N, \quad$ for all $i \in [n]$,

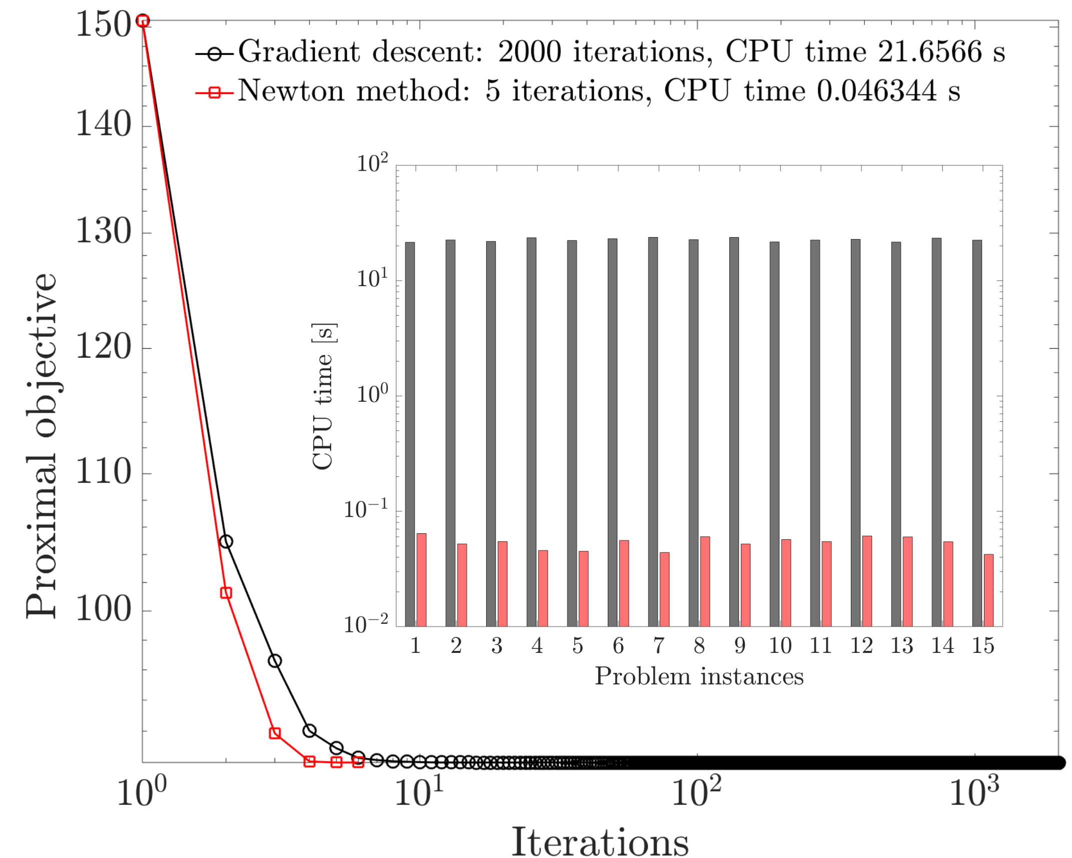
Then the following Euclidean ADMM solves (♥)

$$\boldsymbol{u}_i^{\ell+1} = \boxed{\mathrm{prox}_{\frac{1}{\tau} f_i}^{\|\cdot\|_2}\left(\boldsymbol{z}_i^{\ell} - \widetilde{\boldsymbol{\nu}}_i^{\ell}\right)}$$

No analytical solution, use e.g.,
Newton's method (has structured Hess)

$$\boldsymbol{z}_i^{\ell+1} = \left(\boldsymbol{u}_i^{\ell+1} - \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{u}_i^{\ell+1}\right) + \left(\widetilde{\boldsymbol{\nu}}_i^{\ell} - \frac{1}{n}\sum_{i=1}^{n} \widetilde{\boldsymbol{\nu}}_i^{\ell}\right) + \frac{2}{n\alpha}\boldsymbol{\nu}_{\mathrm{sum}}^{k}$$

$$\widetilde{\boldsymbol{\nu}}_i^{\ell+1} = \widetilde{\boldsymbol{\nu}}_i^{\ell} + \left(\boldsymbol{u}_i^{\ell+1} - \boldsymbol{z}_i^{\ell+1}\right)$$



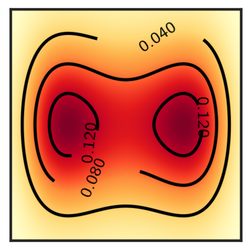
Experiment #1

Linear Fokker-Planck-Kolmogorov PDE

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

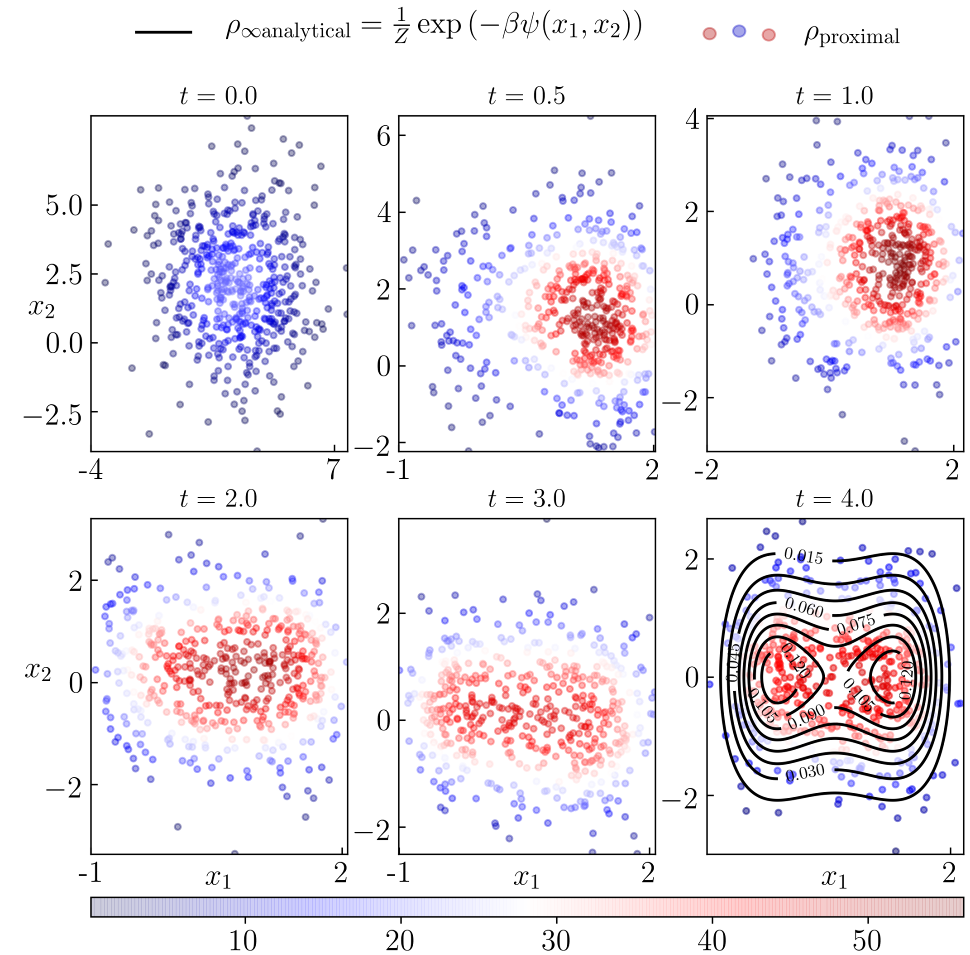
$$V(x_1, x_2) = \frac{1}{4}\left(1 + x_1^4\right) + \frac{1}{2}\left(x_2^2 - x_1^2\right)$$

$$\mu_\infty \propto \exp(-\beta V(x_1, x_2)) \mathrm{d}x_1 \mathrm{d}x_2$$



Centralized computation:

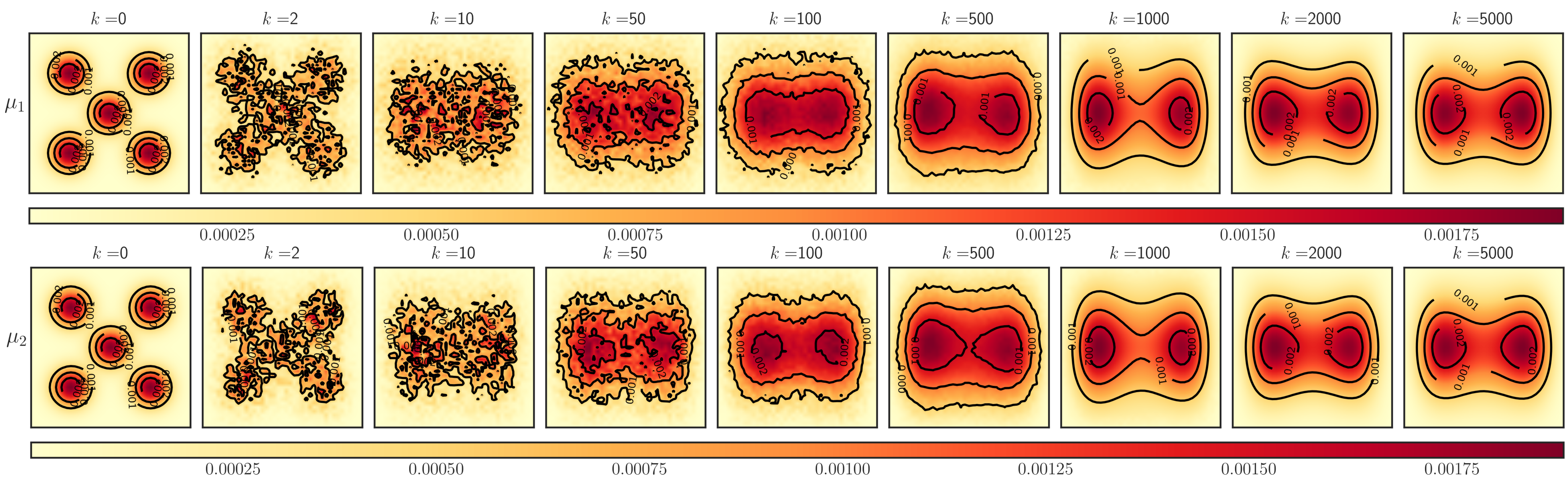
Caluya and Halder, *IEEE Trans. Automatic Control*, 2019



Runtime 99.89 s on Macbook Air 1.1 GHz intel i5 8GB RAM

Distributed computation:

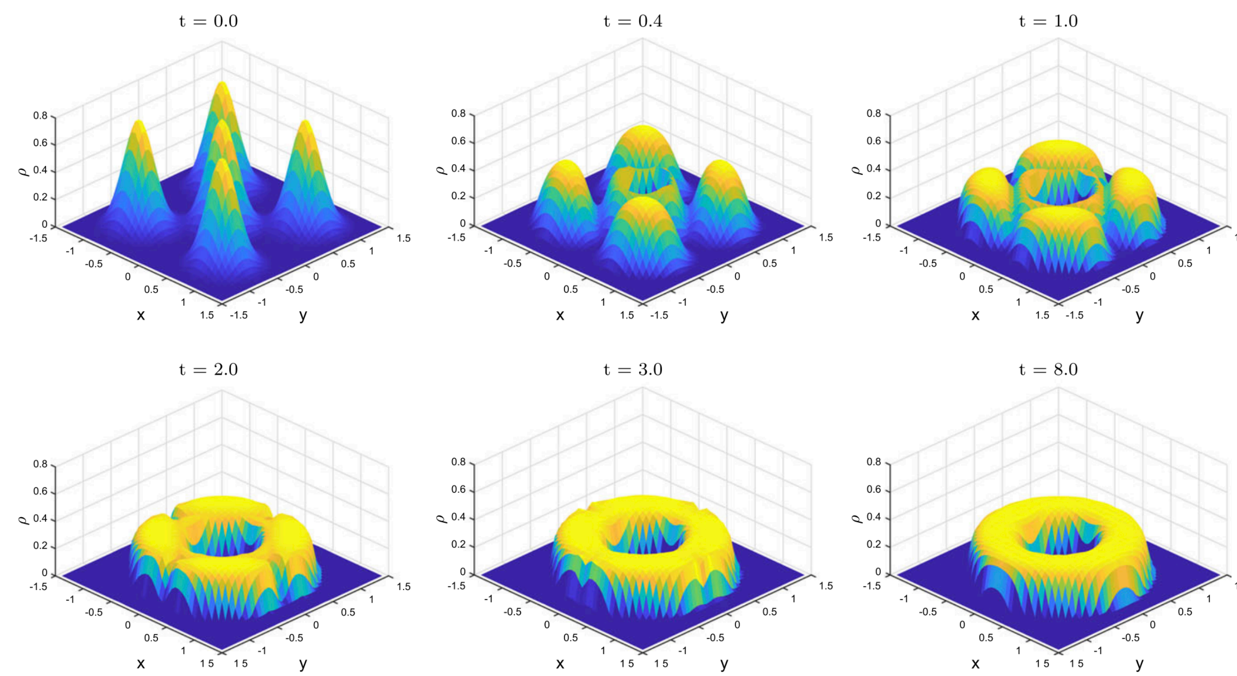
$$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle \qquad F_2(\boldsymbol{\mu}) = \left\langle \beta^{-1} \log \boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle$$



Experiment #2

Centralized computation:

Carrillo, Craig, Wang and Wei, *FOCM*, 2021



$$\lim_{\beta^{-1}\downarrow 0} \mu_\infty = \mathrm{Unif}\left(\mathscr{A}\right)$$

Annulus with inner radius $1/2$ and outer radius $\sqrt{5}/2$

Aggregation-drift-diffusion nonlinear PDE

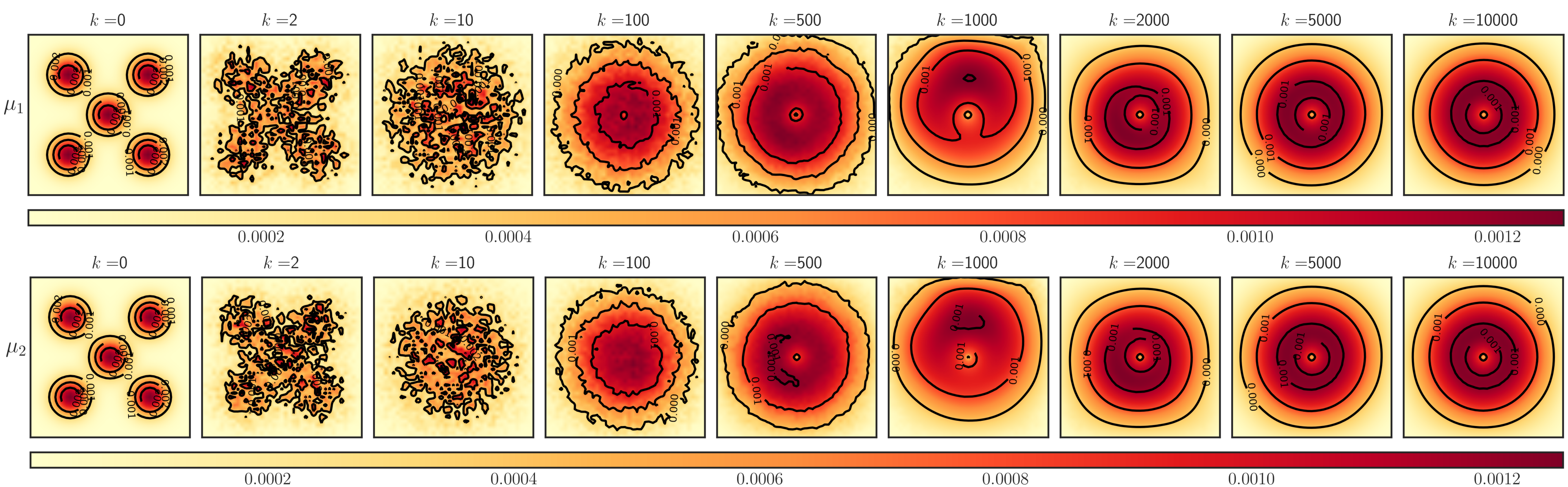
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

$$U(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{x}\|_2^2 - \ln \|\boldsymbol{x}\|_2$$

$$V(\boldsymbol{x}) = -\frac{1}{4}\ln \|\boldsymbol{x}\|_2$$

Distributed computation:

$$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}, \boldsymbol{\mu} \rangle \qquad F_2(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k + \beta^{-1} \log \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$$



Experiment #2 (contd.)

Aggregation-drift-diffusion nonlinear PDE

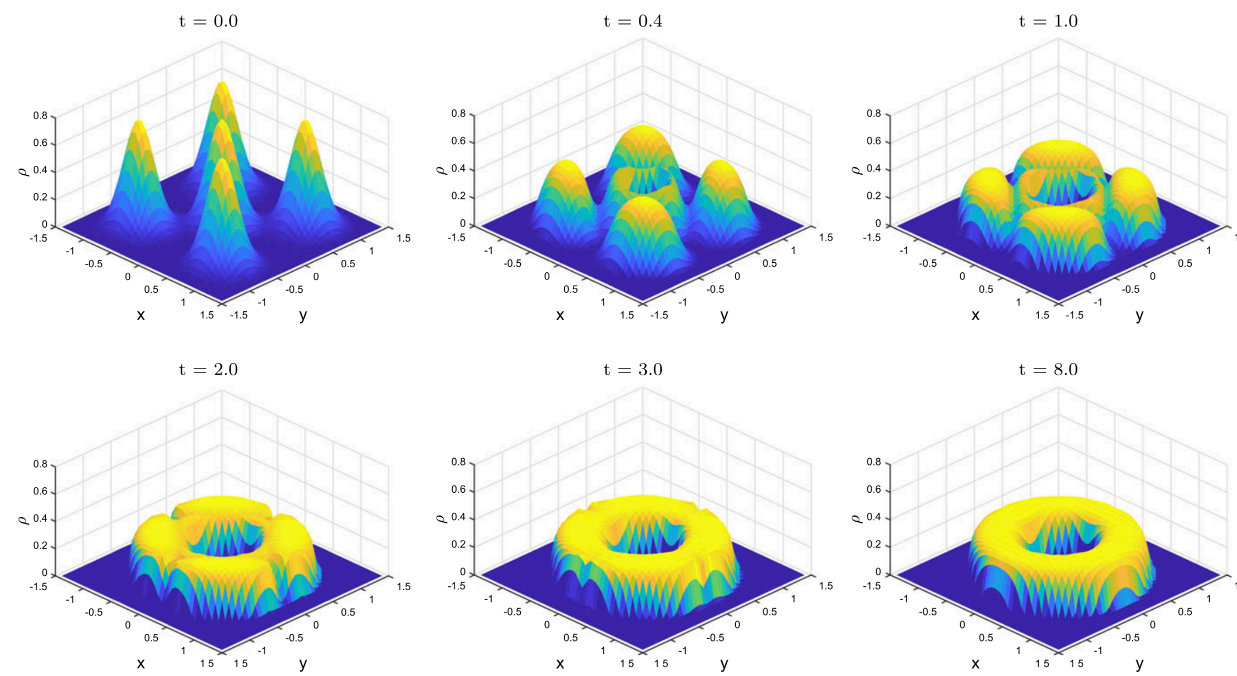
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

$$U(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{x}\|_2^2 - \ln \|\boldsymbol{x}\|_2$$

$$V(\boldsymbol{x}) = -\frac{1}{4}\ln \|\boldsymbol{x}\|_2$$

Centralized computation:

Carrillo, Craig, Wang and Wei, *FOCM*, 2021

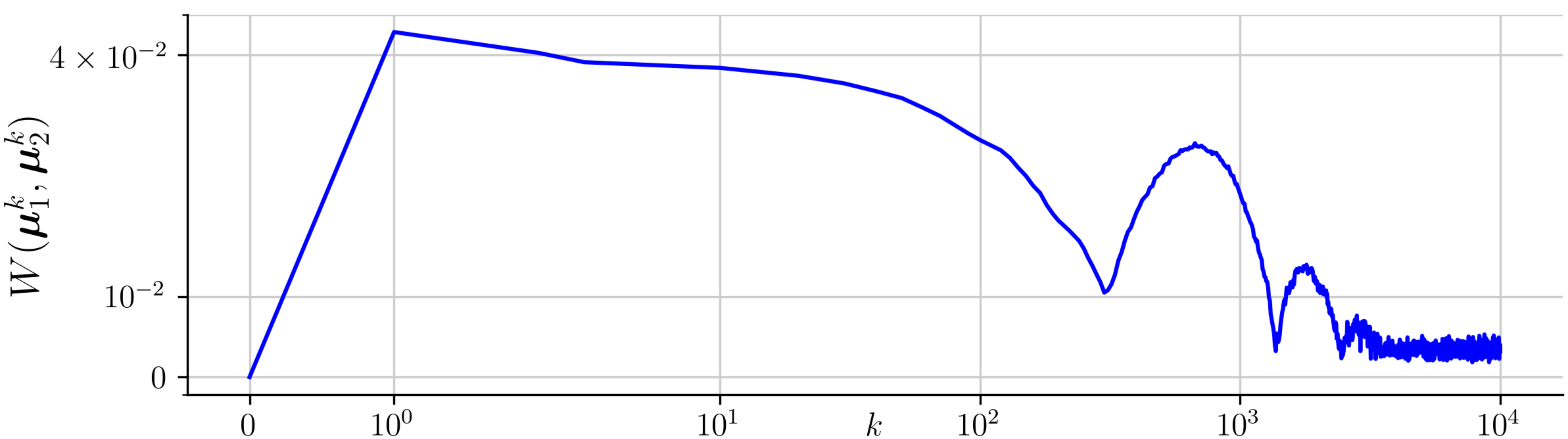


$$\lim_{\beta^{-1}\downarrow 0} \mu_\infty = \mathrm{Unif}\,(\mathscr{A})$$

Annulus with inner radius $1/2$ and outer radius $\sqrt{5}/2$

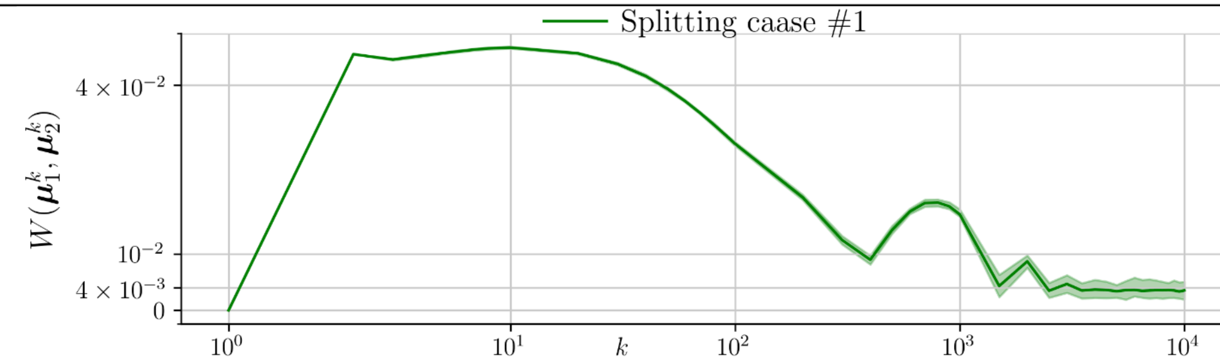
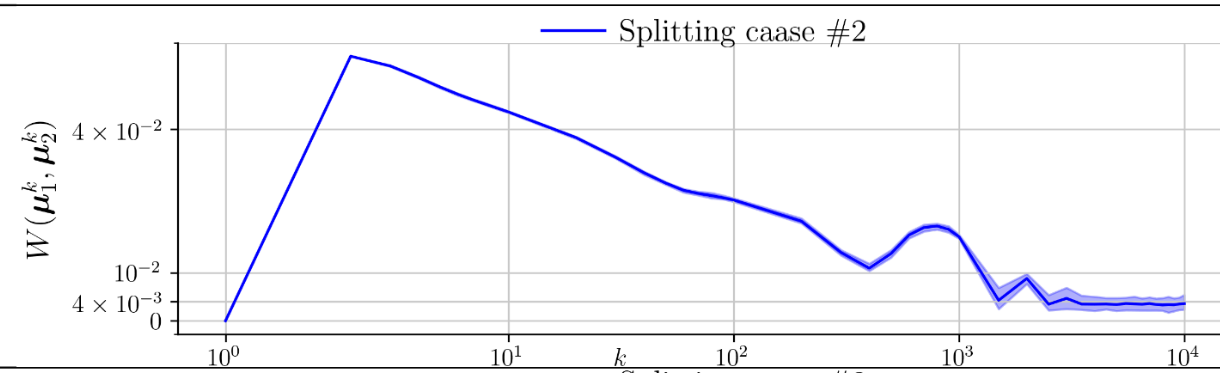
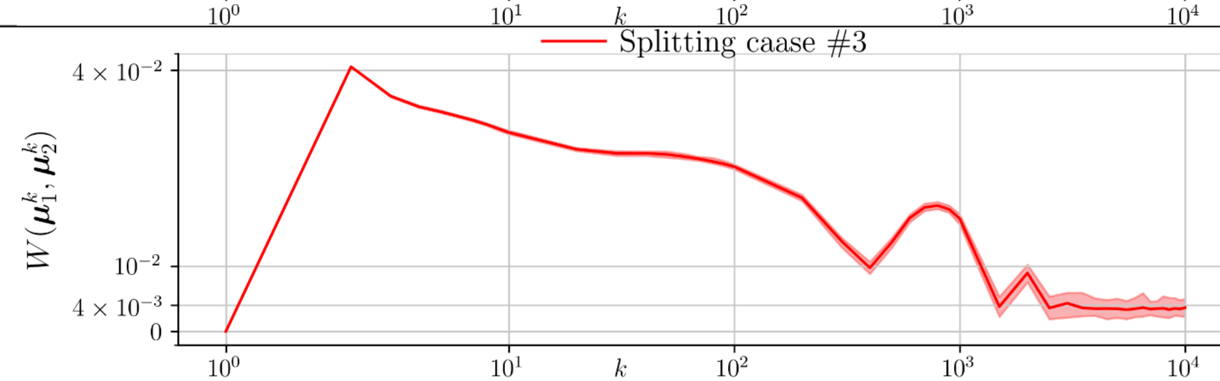
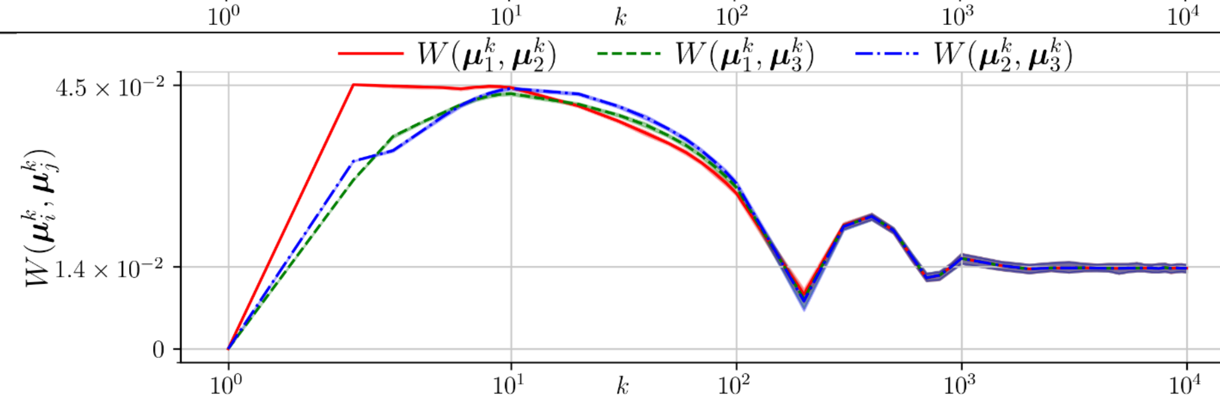
Distributed computation:

$$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}, \boldsymbol{\mu} \rangle \qquad F_2(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k + \beta^{-1} \log \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$$



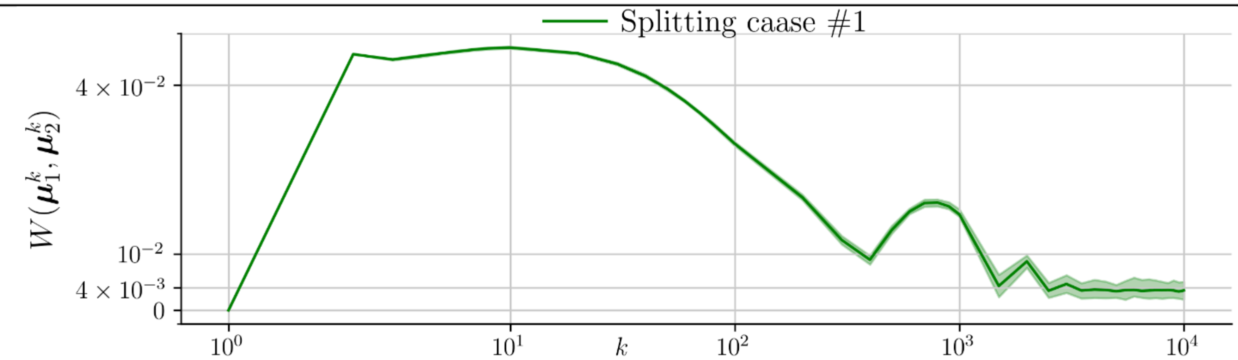
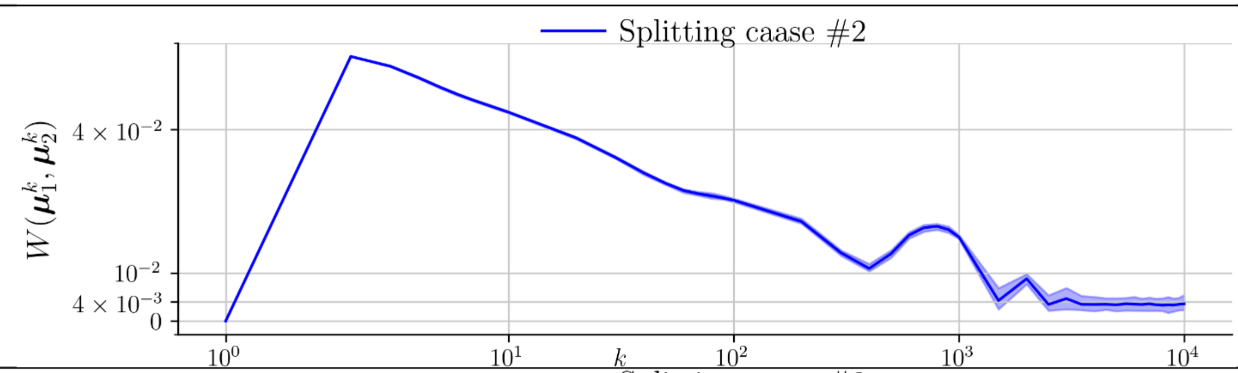
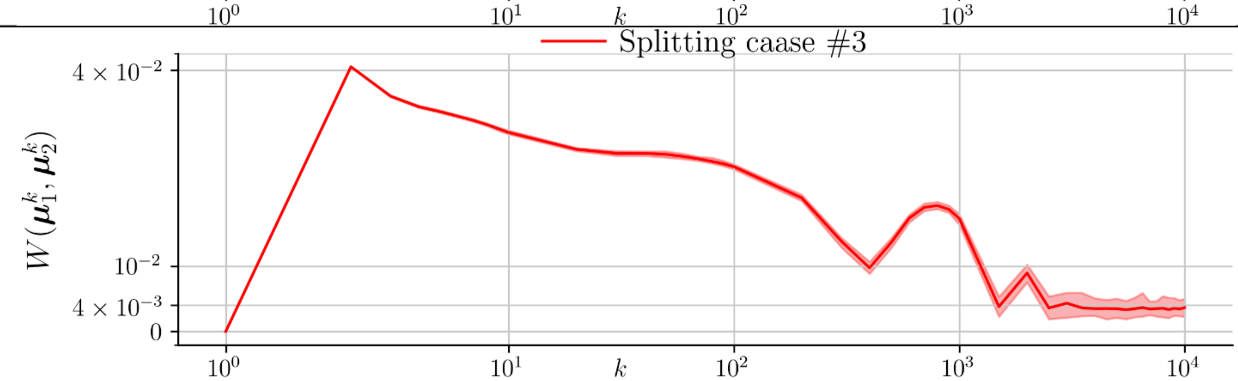
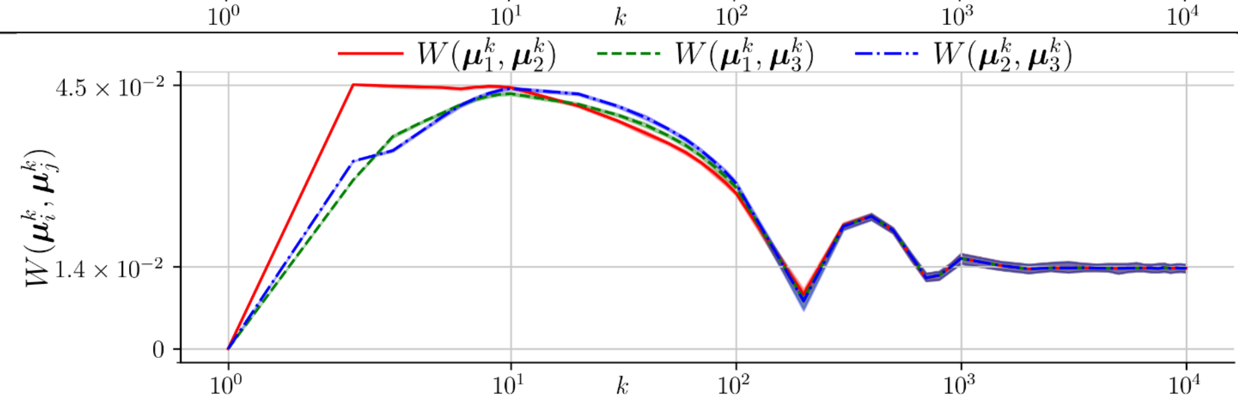
Experiment # 2 (contd.)

100 run statistics for each of the 4 ways of splitting: ($2^n - n - 1$ ways in general)

Splitting case	Functionals	Wasserstein distance
#1	$F_1(\boldsymbol{\mu}) = \left\langle \boldsymbol{V}_k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \right\rangle$	
#2	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}^k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle$	
#3	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}^k + \boldsymbol{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle$	
#4	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k \right\rangle,$ $F_3(\boldsymbol{\mu}) = \left\langle \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle$	

Experiment # 2 (contd.)

100 run for statistics each of the 4 ways of splitting: ($2^n - n - 1$ ways in general)

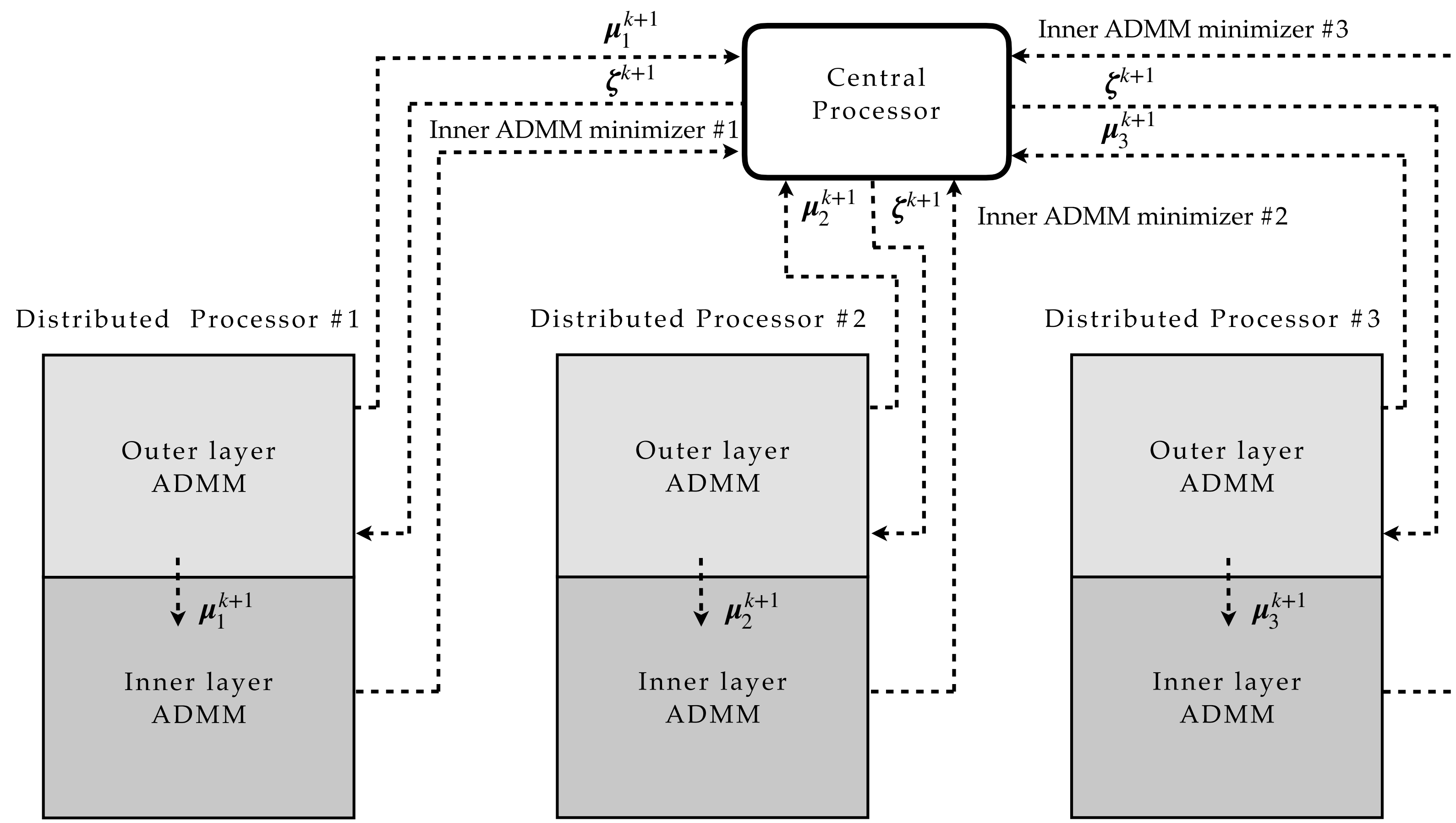
Splitting case	Functionals	Wasserstein distance
#1	$F_1(\boldsymbol{\mu}) = \left\langle \boldsymbol{V}_k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \right\rangle$ av. runtime = 294.06 s	
#2	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}^k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle$ av. runtime = 285.32 s	
#3	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}^k + \boldsymbol{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle$ av. runtime = 289.87 s	
#4	$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k \right\rangle,$ $F_3(\boldsymbol{\mu}) = \left\langle \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle$ av. runtime = 108.99 s	

Summary

Distributed computation for measure-valued optimization

Realizes measure-valued operator splitting

Takes advantage of the existing proximal and JKO type algorithms



Ongoing

Convergence guarantees for the overall scheme

High dimensional case studies

Thank You