A Distributed Algorithm for Wasserstein Proximal Operator Splitting

Abhishek Halder

Department of Aerospace Engineering, Iowa State University
Translational AI Center, Iowa State University
Department of Applied Mathematics, UC Santa Cruz

Joint work with I. Nodozi (UC Santa Cruz)

Mini-symposium on Mean Field Games and Optimal Transport with Applications in Data Science and Biology
10th ICIAM 2023, Tokyo, August 21, 2023

Topic of this talk

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

Measure-valued Optimization Problems

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

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

2-Wasserstein geodescially convex functional

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

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

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

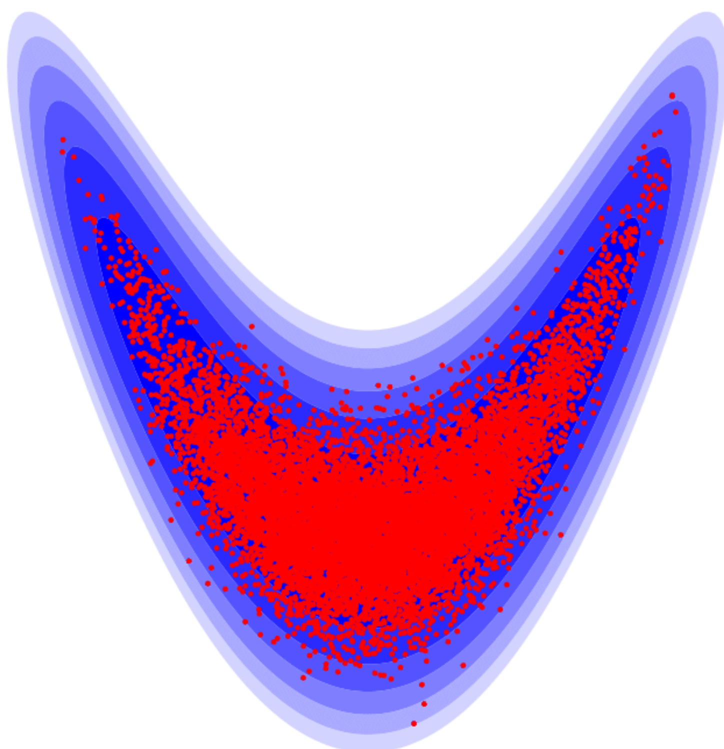
Wasserstein proximal recursion à la Jordan-Kinderlehrer-Otto (JKO) scheme

Gradient Flows

Gradient Flow in $\mathcal{X}$	Gradient Flow in $\mathcal{P}_2(\mathcal{X})$
$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = -\nabla f(\boldsymbol{x}), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0$	$\frac{\partial \mu}{\partial t} = -\nabla^W F(\mu), \quad \mu(\boldsymbol{x}, 0) = \mu_0$
Recursion:	**Recursion:**
$\begin{aligned} \boldsymbol{x}_k &= \boldsymbol{x}_{k-1} - h\nabla f(\boldsymbol{x}_k) \\ &= \underset{\boldsymbol{x}\in\mathcal{X}}{\arg\min} \left\{ \frac{1}{2}\Vert\boldsymbol{x} - \boldsymbol{x}_{k-1}\Vert_2^2 + hf(\boldsymbol{x}) \right\} \\ &=: \mathrm{prox}_{hf}^{\Vert\cdot\Vert_2}(\boldsymbol{x}_{k-1}) \end{aligned}$	$\begin{aligned} \mu_k &= \mu(\cdot, t = kh) \\ &= \underset{\mu\in\mathcal{P}_2(\mathcal{X})}{\arg\min} \left\{ \frac{1}{2} W^2(\mu, \mu_{k-1}) + hF(\mu) \right\} \\ &=: \mathrm{prox}_{hF}^{W}(\mu_{k-1}) \end{aligned}$
Convergence:	**Convergence:**
$\boldsymbol{x}_k \to \boldsymbol{x}(t = kh) \quad \text{as} \quad h \downarrow 0$	$\mu_k \to \mu(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$
f as Lyapunov function:	**F as Lyapunov functional:**
$\frac{\mathrm{d}}{\mathrm{d}t} f = -\Vert \nabla f \Vert_2^2 \leq 0$	$\frac{\mathrm{d}}{\mathrm{d}t} F = -\mathbb{E}_\mu\left[\left\Vert \nabla \frac{\delta F}{\delta \mu} \right\Vert_2^2\right] \leq 0$

Motivating Applications

Langevin sampling from an unnormalized prior



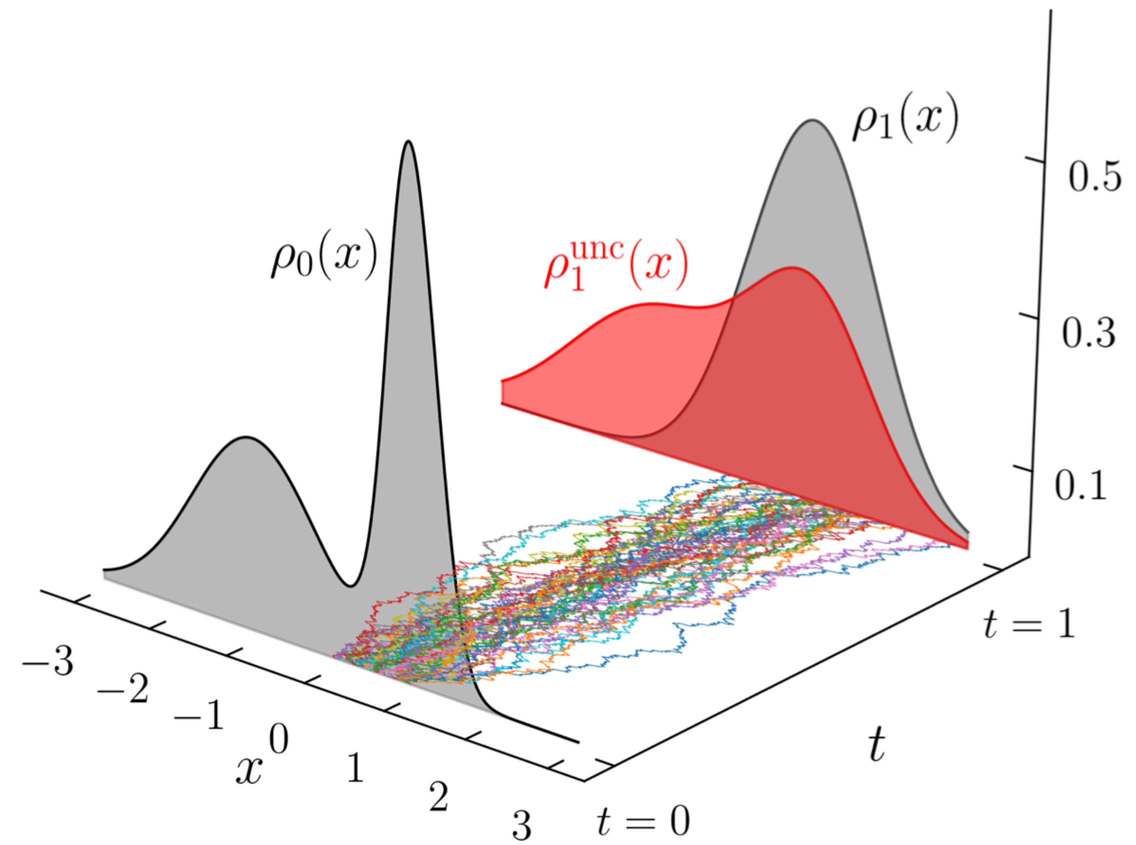
Stramer and Tweedie, *Methodology and Computing in Applied Probability*, 1999

Jarner and Hansen, *Stochastic Processes and their Applications*, 2000

Roberts and Stramer, *Methodology and Computing in Applied Probability*, 2002

Vempala and Wibisino, *NeurIPS*, 2019

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



Chen, Georgiou and Pavon, *SIAM Review*, 2021

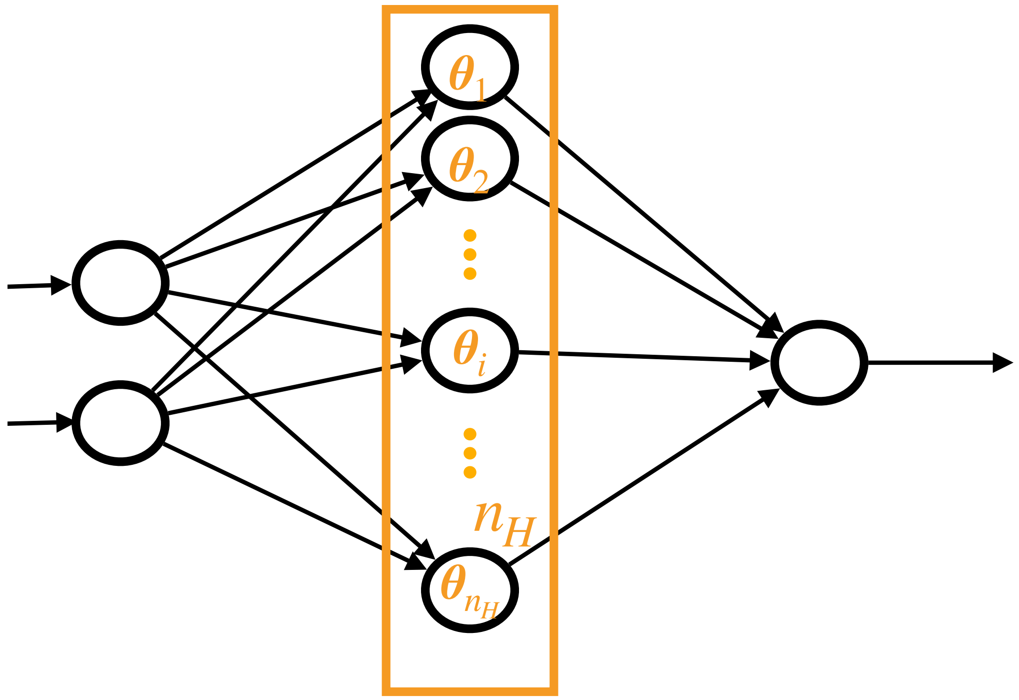
Chen, Georgiou and Pavon, *SIAM Journal on Applied Mathematics*, 2016

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

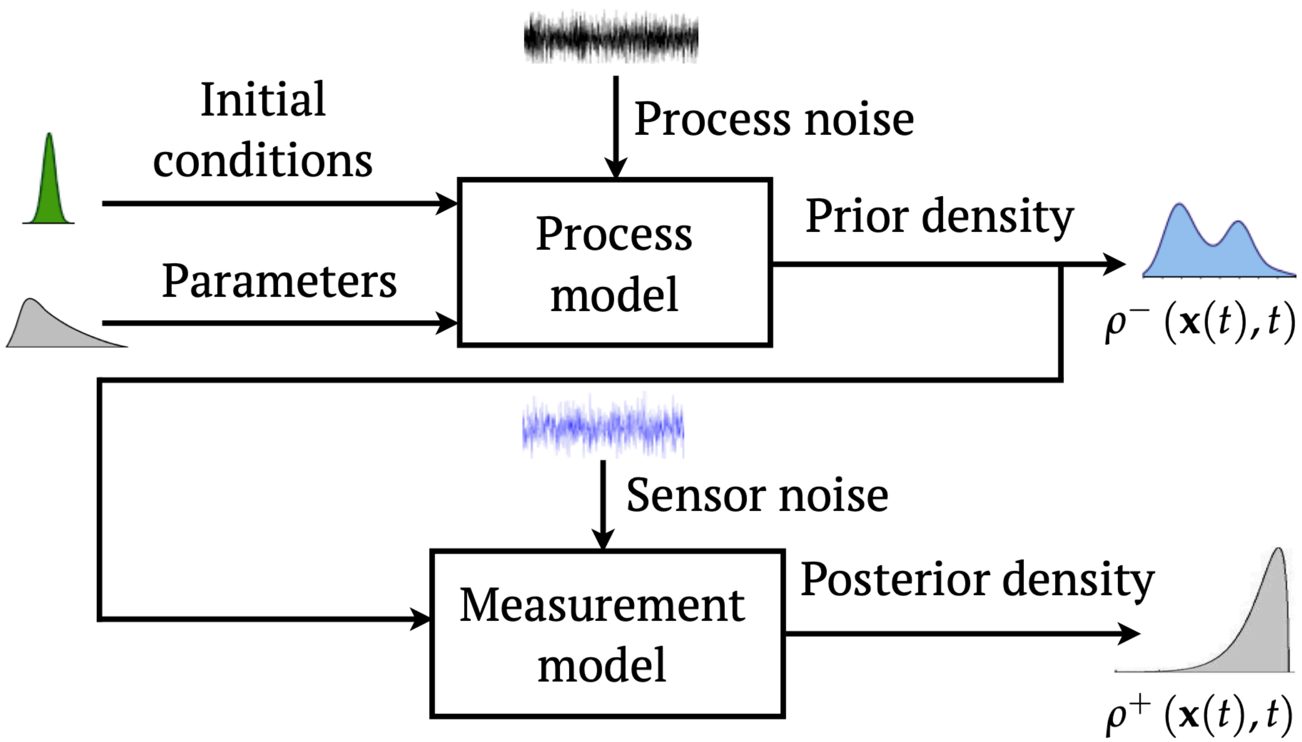
Caluya and Halder, *IEEE Transactions on Automatic Control*, 2021

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

Halder and Georgiou, ACC, 2018

Halder and Georgiou, *CDC*, 2017

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

Mokrov, Korotin, Li, Gnevay, Solomon, and Burnaev, *NeurIPS*, 2021

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

Wang, and Li, *Journal of Scientific Computing*, 2022

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

Mokrov, Korotin, Li, Gnevay, Solomon, and Burnaev, *NeurIPS*, 2021

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

Wang, and Li, *Journal of Scientific Computing*, 2022

But all require centralized computing

Our Present Work: Distributed Algorithm

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

Our Present Work: Distributed Algorithm

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

Main idea:

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

$$\underset{(\mu_1,\ldots,\mu_n,\zeta) \in \mathcal{P}_2^{n+1}(\mathbb{R}^d)}{\arg\inf} \quad F_1(\mu_1) + F_2(\mu_2) + \ldots + F_n(\mu_n)$$

$$\text{subject to} \quad \mu_i = \zeta \quad \text{for all } i \in [n]$$

Our Present Work: Distributed Algorithm

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

Main idea:

$\Big\Downarrow$ re-write

$$\underset{(\mu_1,\ldots,\mu_n,\zeta)\in\mathcal{P}_2^{n+1}(\mathbb{R}^d)}{\arg\inf} \quad F_1(\mu_1) + F_2(\mu_2) + \ldots + F_n(\mu_n)$$

$$\text{subject to} \quad \mu_i = \zeta \quad \text{for all } i \in [n]$$

Define Wasserstein augmented Lagrangian:

$$L_\alpha(\mu_1,\ldots,\mu_n,\zeta,\nu_1,\ldots,\nu_n) := \sum_{i=1}^{n}\left\{F_i(\mu_i) + \underbrace{\frac{\alpha}{2}}_{\text{regularization } > 0} W^2(\mu_i,\zeta) + \int_{\mathbb{R}^d} \underbrace{\nu_i(\boldsymbol{\theta})}_{\text{Lagrange multipliers}}(\mathrm{d}\mu_i - \mathrm{d}\zeta)\right\}$$

Proposed Consensus ADMM

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

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

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

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

Proposed Consensus ADMM

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

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

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

Proposed Consensus ADMM (contd.)

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

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

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

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.)

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

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

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

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 $\dfrac{\partial\tilde{\mu}_i}{\partial t} = -\nabla^W\Phi_i(\tilde{\mu}_i)$

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

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

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

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

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

where N is the number of samples

Discrete Version of the Proposed ADMM

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

With Sinkhorn regularization:

Discrete Sinkhorn divergence

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

Discrete Version of the Proposed ADMM

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

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

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

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

With Sinkhorn regularization:

Discrete Sinkhorn divergence

Outer layer ADMM

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

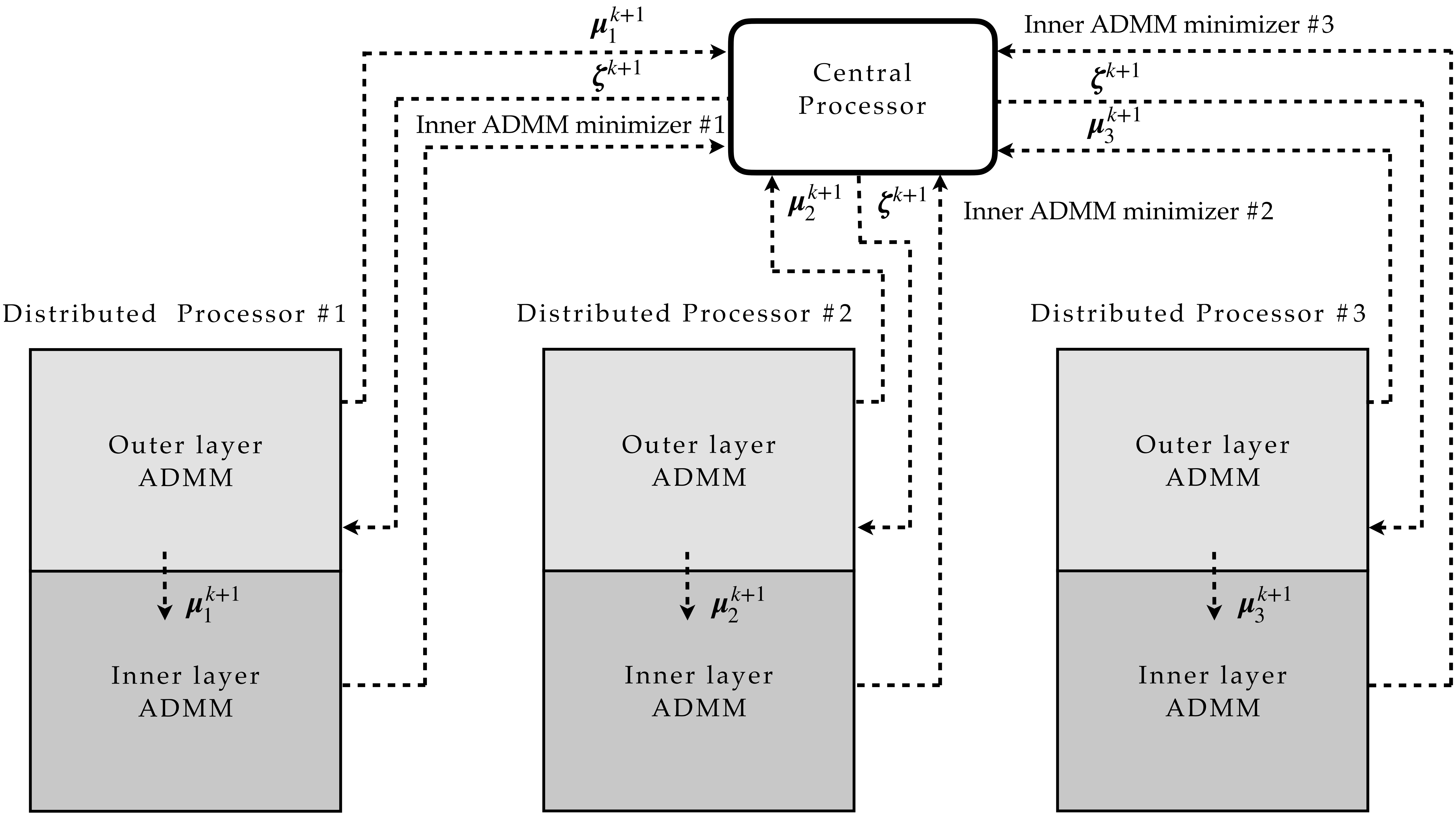
$$= \operatorname*{arg\,inf}_{\boldsymbol{\mu}_i\in\Delta^{N-1}} \left\{ \min_{M\in\Pi_N(\boldsymbol{\mu}_i,\zeta^k)} \left\langle \frac{1}{2}\boldsymbol{C} + \varepsilon\log \boldsymbol{M},\boldsymbol{M}\right\rangle + \frac{1}{\alpha}\big(F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k,\boldsymbol{\mu}_i\rangle\big)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

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

Inner layer ADMM

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

Overall Schematic



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

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

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

Convex

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

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

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

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

ζ update $\rightsquigarrow$ Inner (Euclidean) ADMM

Theorem.

Consider the convex problem

$$\begin{aligned}\left(\boldsymbol{u}_1^{\text{opt}},\ldots,\boldsymbol{u}_n^{\text{opt}}\right) = &\underset{(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n)\in\mathbb{R}^{nN}}{\arg\min} \sum_{i=1}^{n}\left\langle \boldsymbol{\mu}_i^{k+1}, \log\left(\boldsymbol{\Gamma}\exp\left(\boldsymbol{u}_i/\varepsilon\right)\right)\right\rangle \\ &\text{subject to} \quad \sum_{i=1}^{n}\boldsymbol{u}_i = \frac{2}{\alpha}\boldsymbol{\nu}_{\text{sum}}^{k}.\end{aligned} \qquad (\blacktriangledown)$$

Then

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

ζ update $\rightsquigarrow$ Inner (Euclidean) ADMM

Theorem.

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

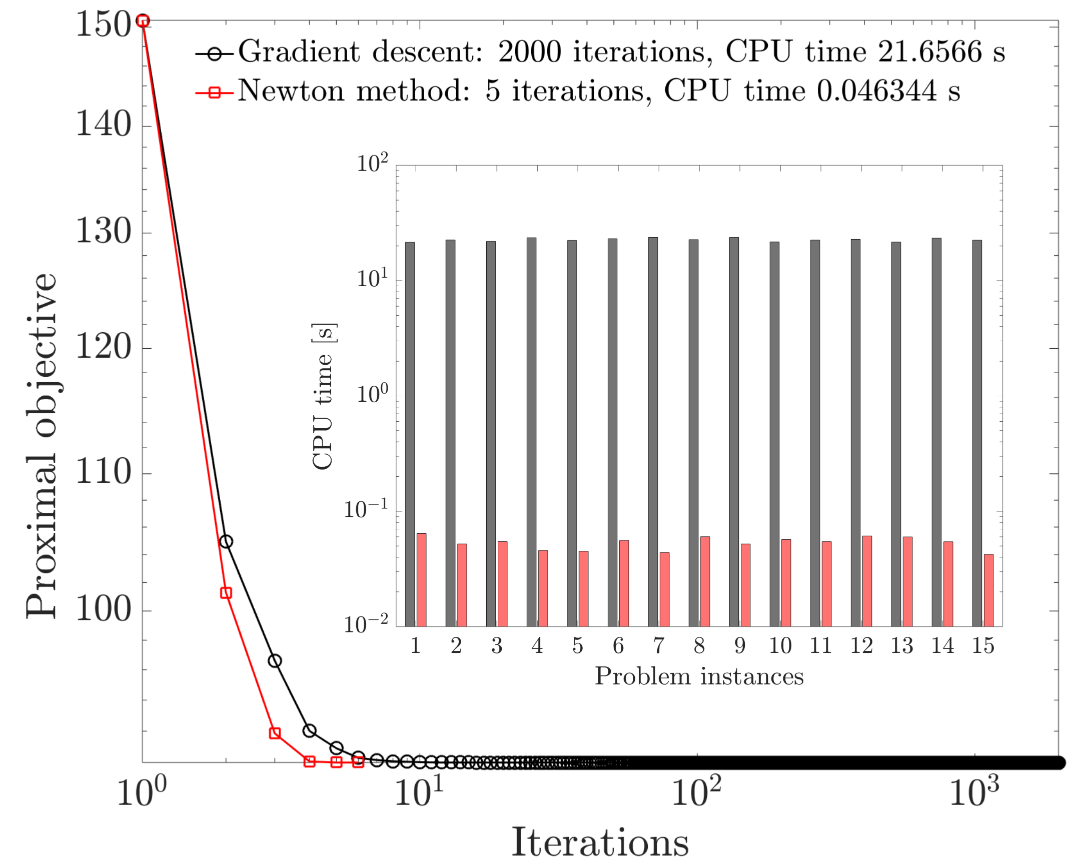
Then the following Euclidean ADMM solves (♥)

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

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

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

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



ξ update $\rightsquigarrow$ Inner (Euclidean) ADMM

Theorem.

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

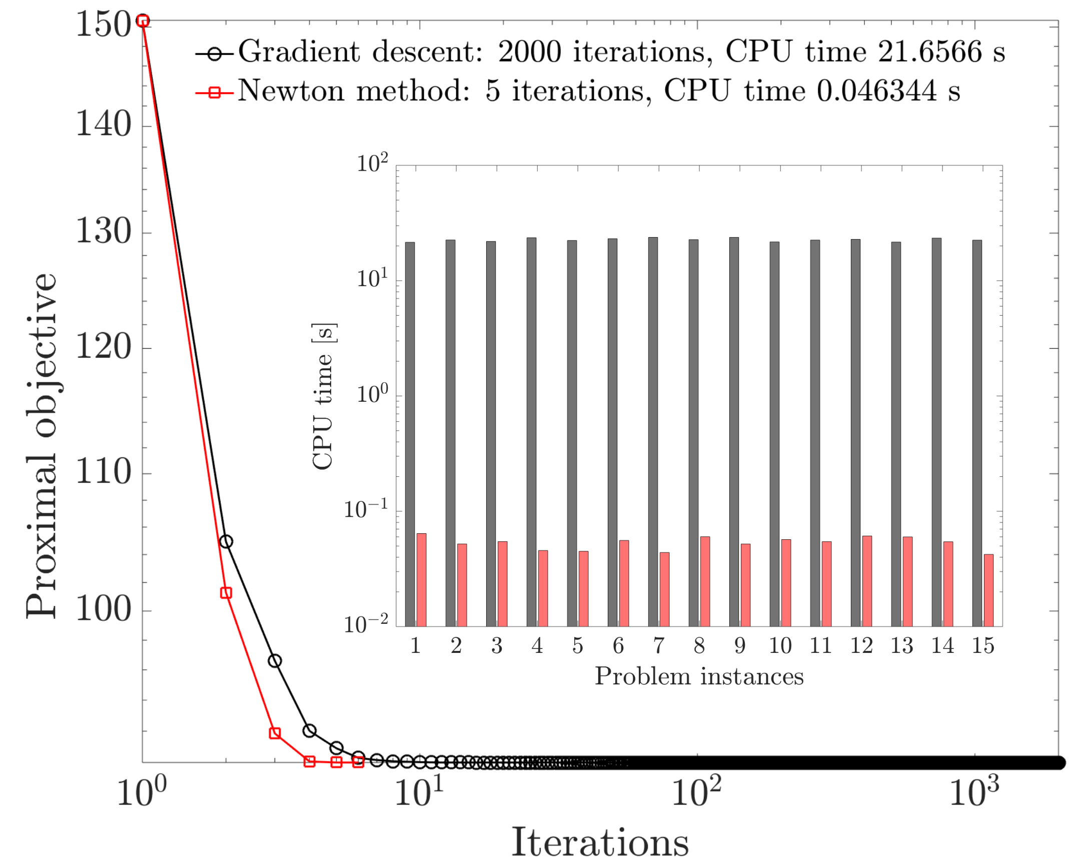
Then the following Euclidean ADMM solves (♥)

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

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

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

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

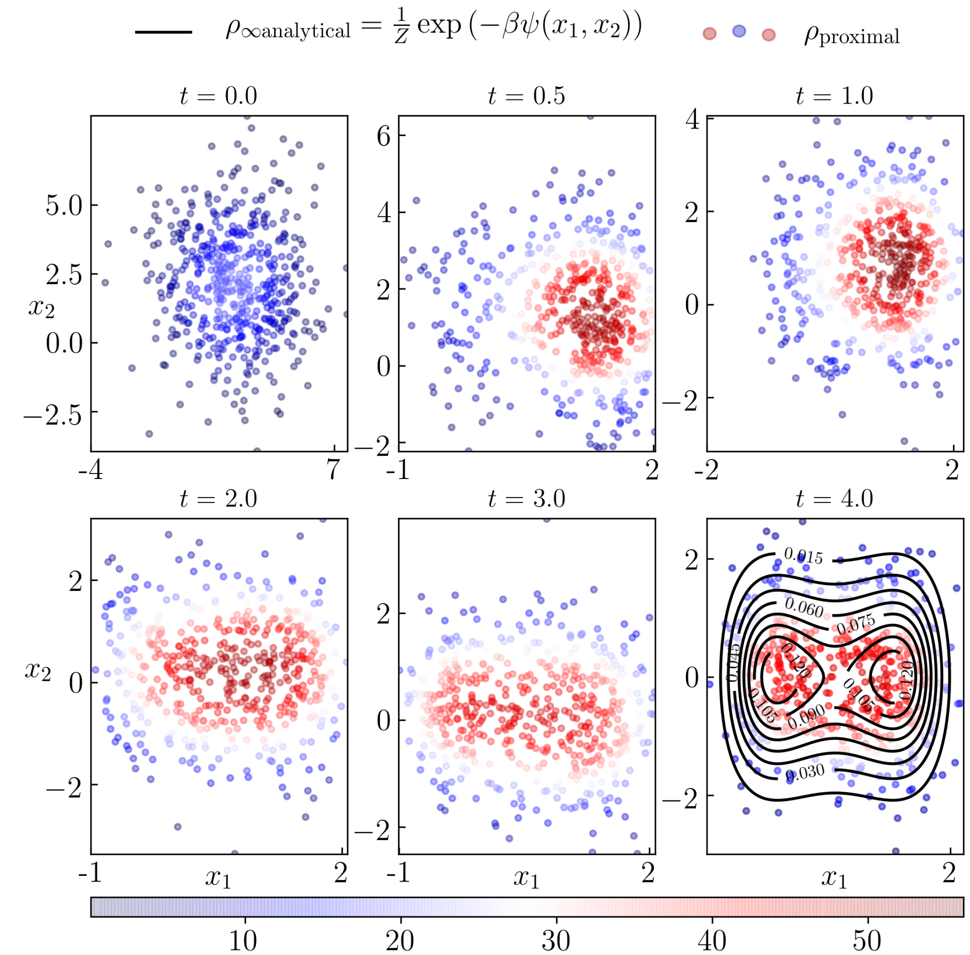


Theorem (informal).
Guaranteed convergence for inner layer ADMM under some constraints on hyper-parameters

Experiment #1

Centralized computation:

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



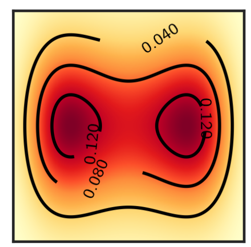
Runtime 99.89 s on Macbook Air 1.1 GHz intel i5 8GB RAM

Linear Fokker-Planck-Kolmogorov PDE

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

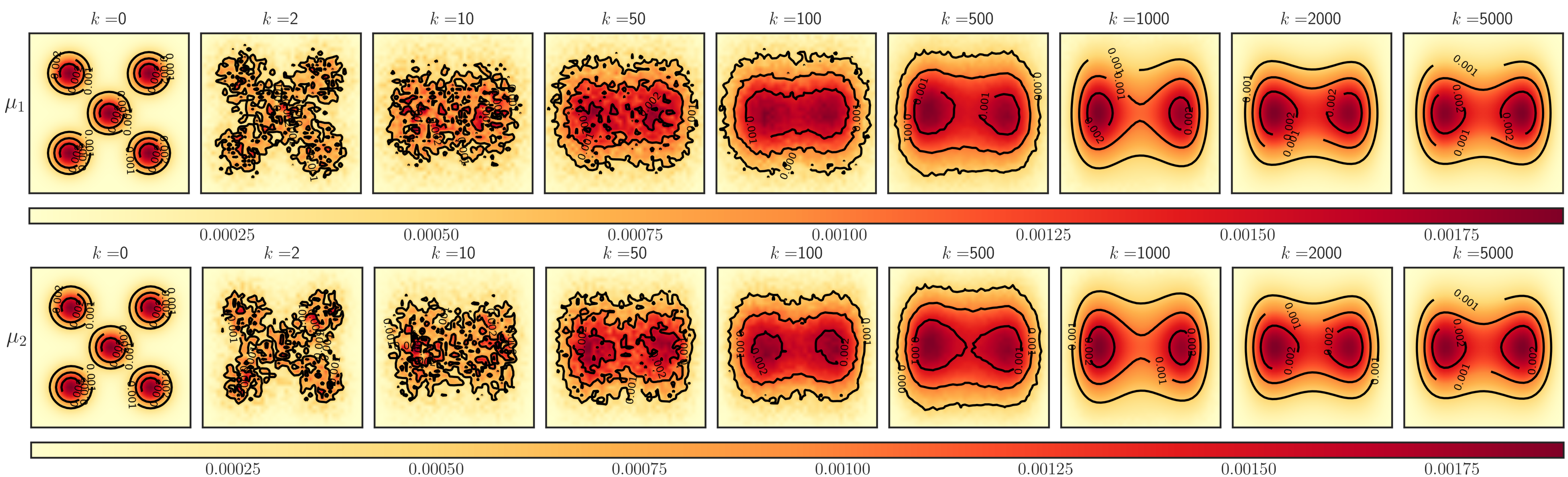
$$V(x_1, x_2) = \frac{1}{4}\left(1 + x_1^4\right) + \frac{1}{2}\left(x_2^2 - x_1^2\right)$$

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



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

Aggregation-drift-diffusion nonlinear PDE

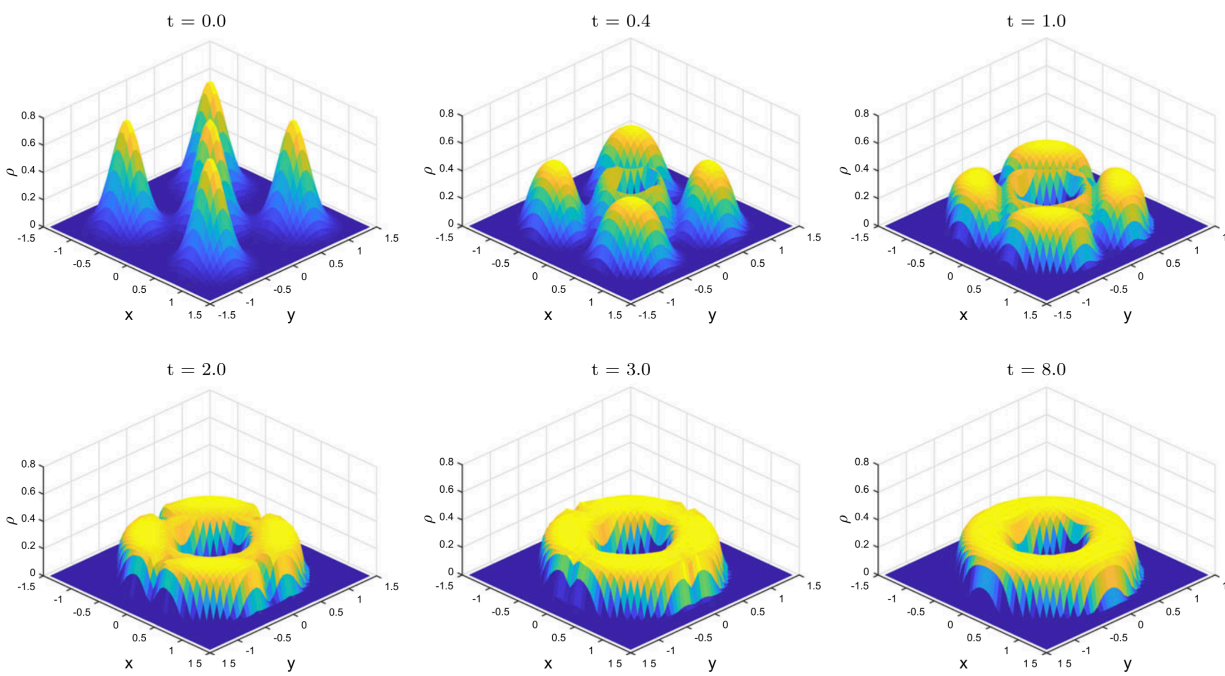
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

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

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

Centralized computation:

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

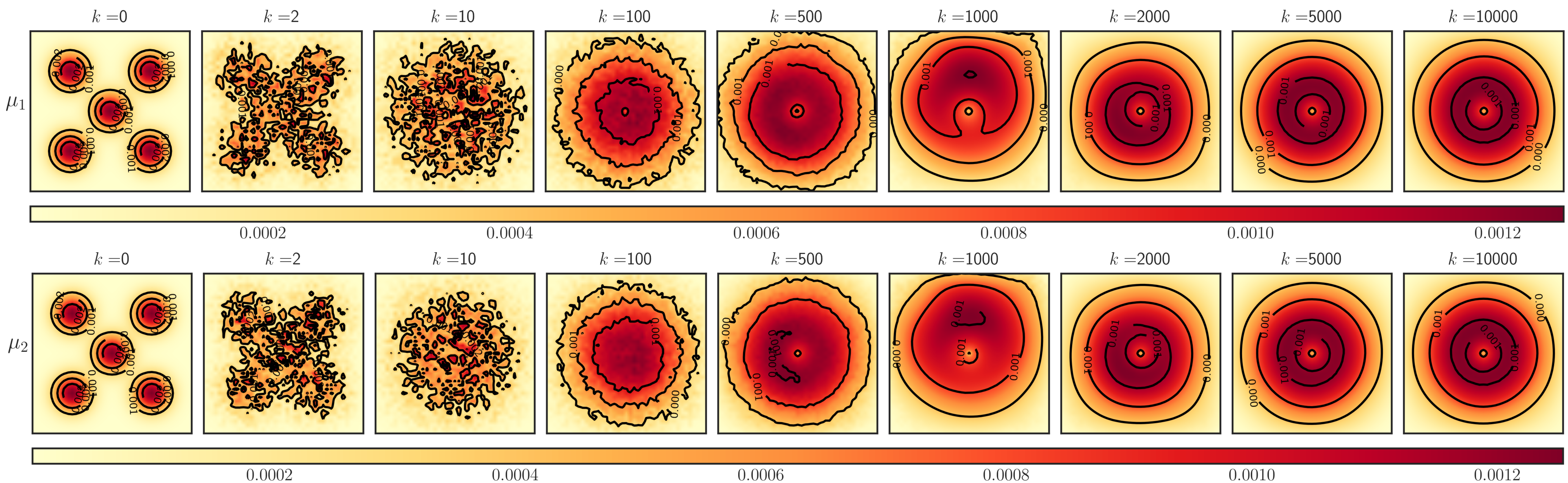


$$\lim_{\beta^{-1} \downarrow 0} \mu_\infty = \mathrm{Unif}\,(\mathscr{A})$$

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.)

Aggregation-drift-diffusion nonlinear PDE

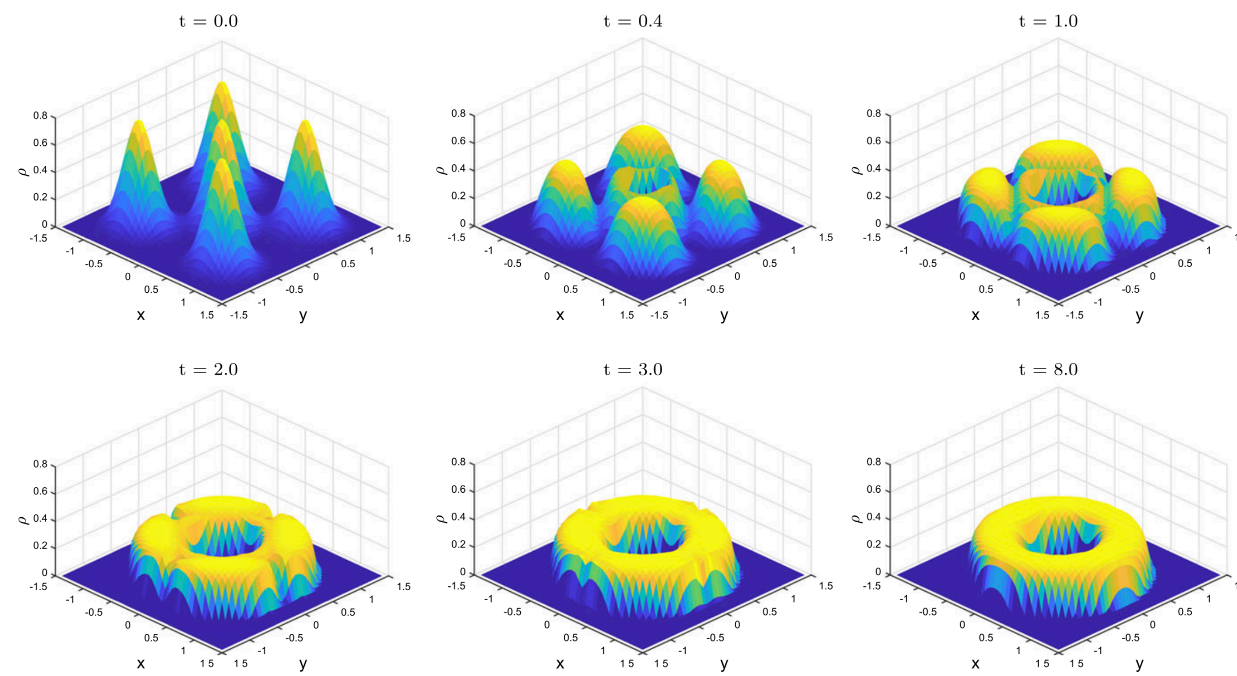
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

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

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

Centralized computation:

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

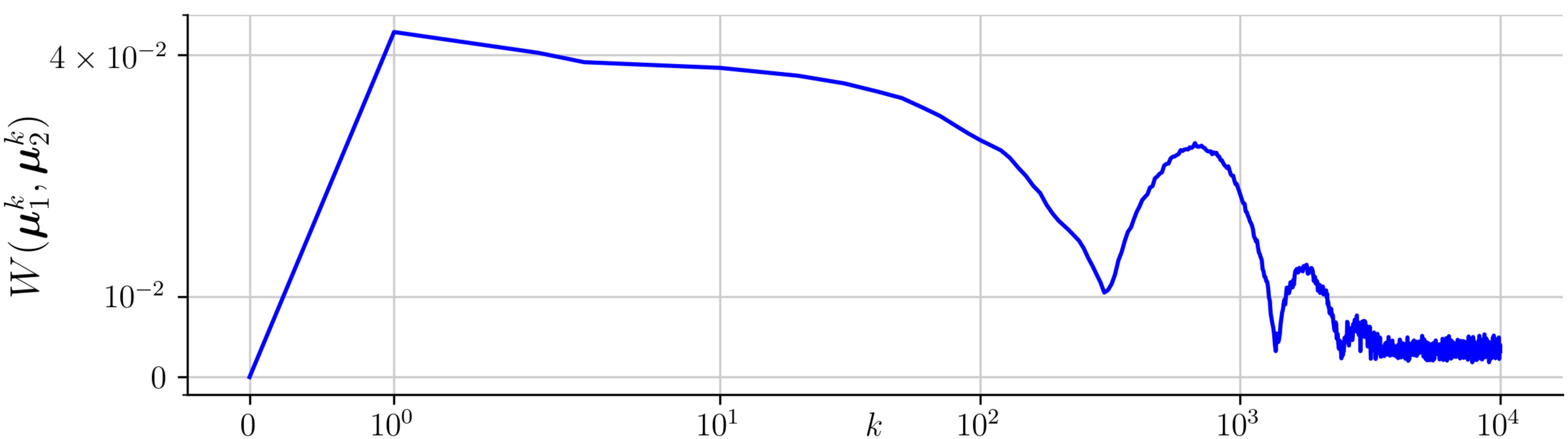


$$\lim_{\beta^{-1}\downarrow 0} \mu_\infty = \mathrm{Unif}\,(\mathscr{A})$$

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

Distributed computation:

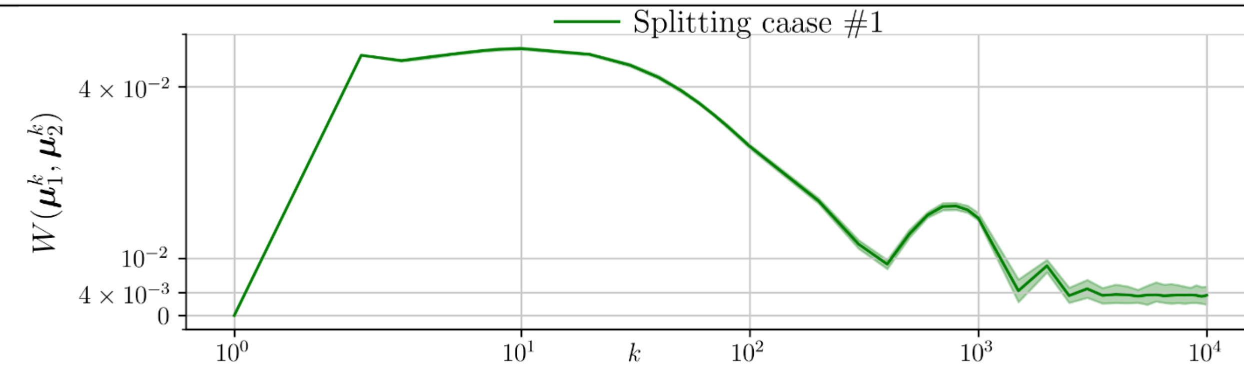
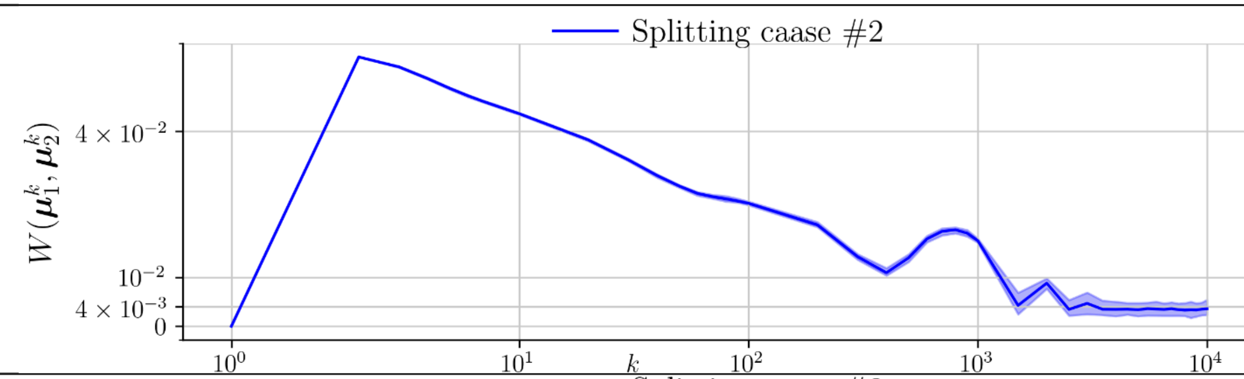
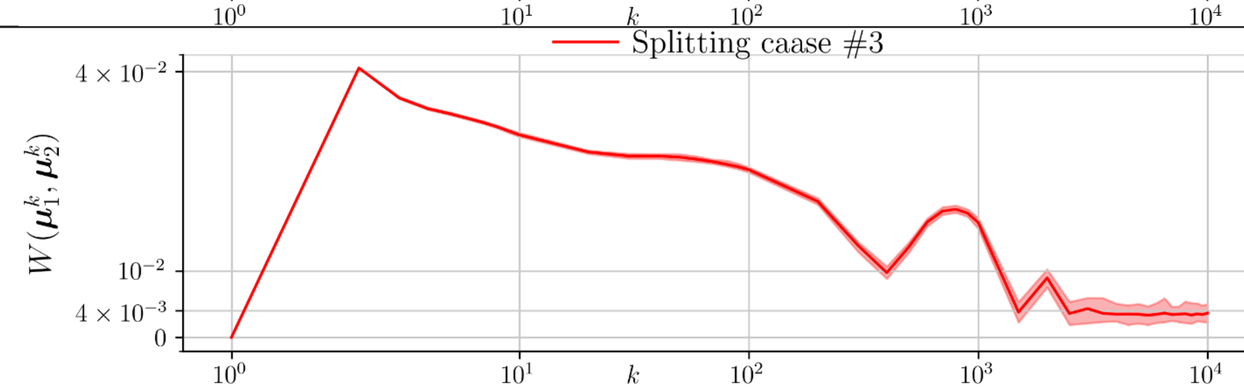
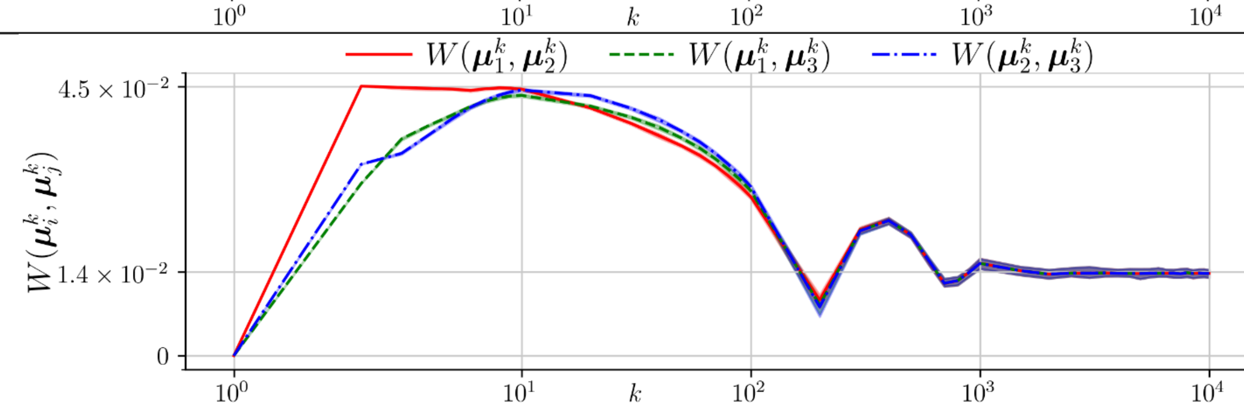
$$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{U}_k \boldsymbol{\mu}, \boldsymbol{\mu} \rangle \qquad F_2(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k + \beta^{-1} \log \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$$



Experiment # 2 (contd.)

B_n is nth Bell number, e.g.,
$B_2 = 2, B_3 = 5, B_4 = 15, B_5 = 52, \ldots$

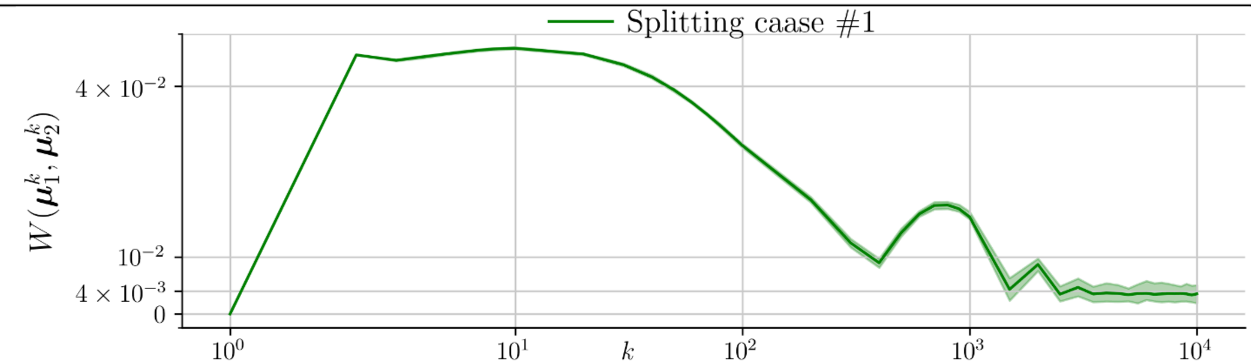
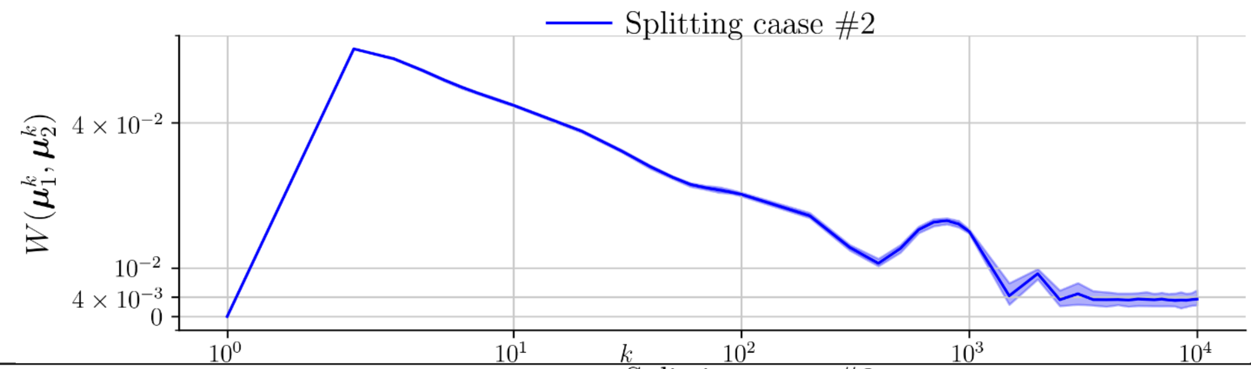
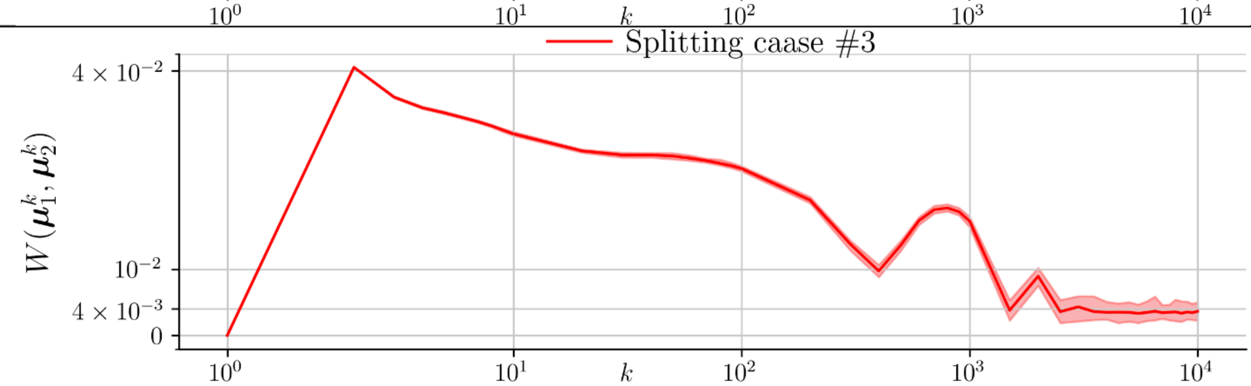
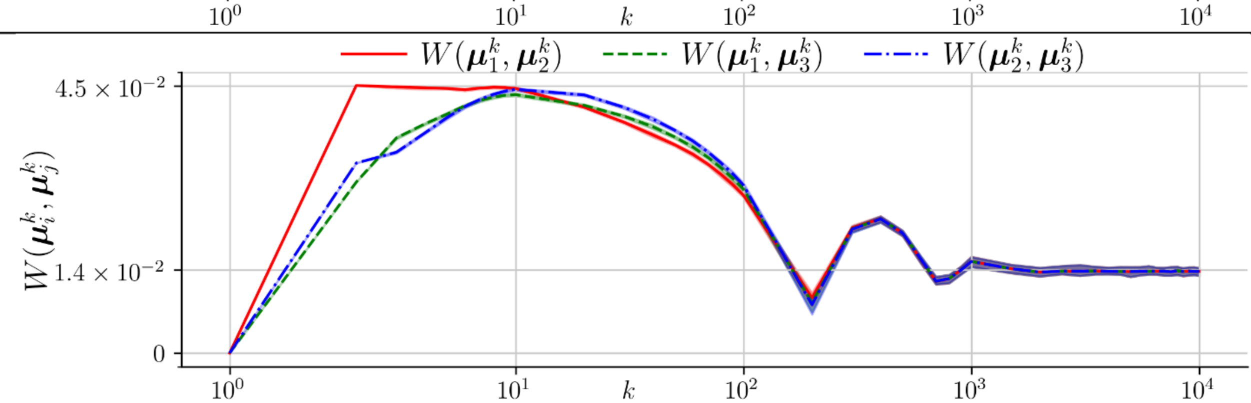
100 run statistics for each of the 4 ways of splitting: ($B_n - 1$ ways in general)

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.)

Centralized av. runtime = 310.21 s

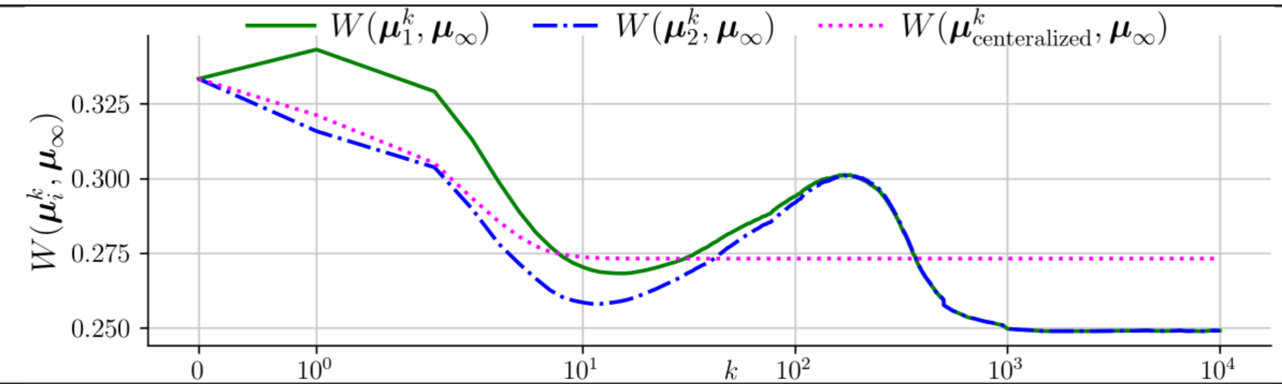
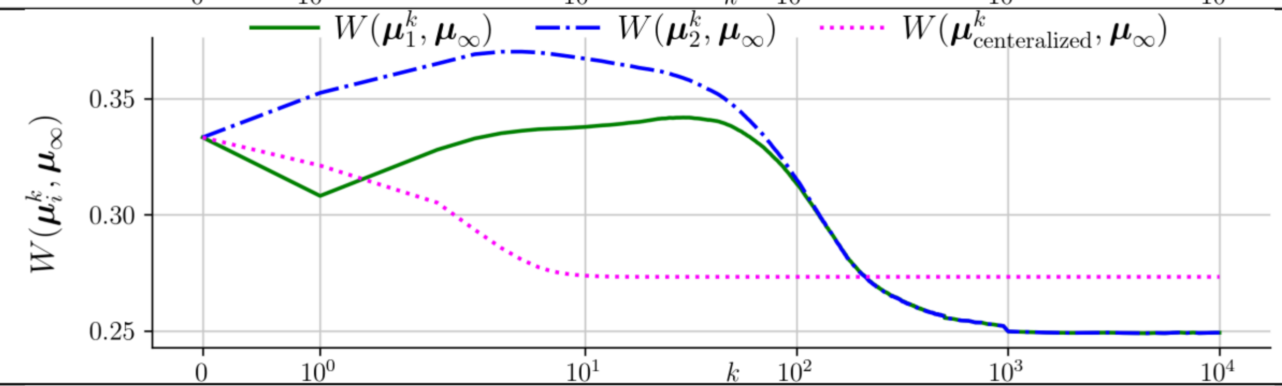
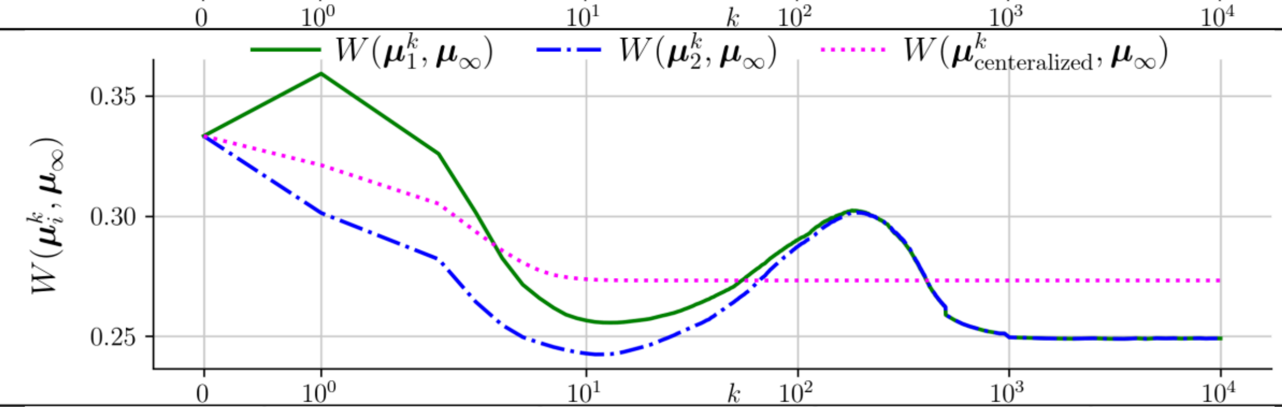
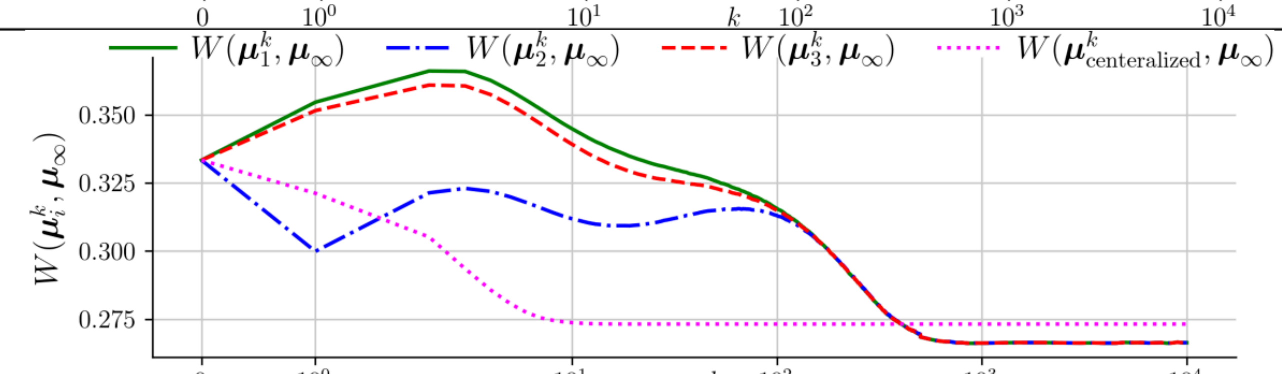
100 run statistics for each of the 4 ways of splitting: ($B_n - 1$ ways in general)

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	

Experiment #2 (contd.)

Centralized is pink dotted (repeated in subplots)

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

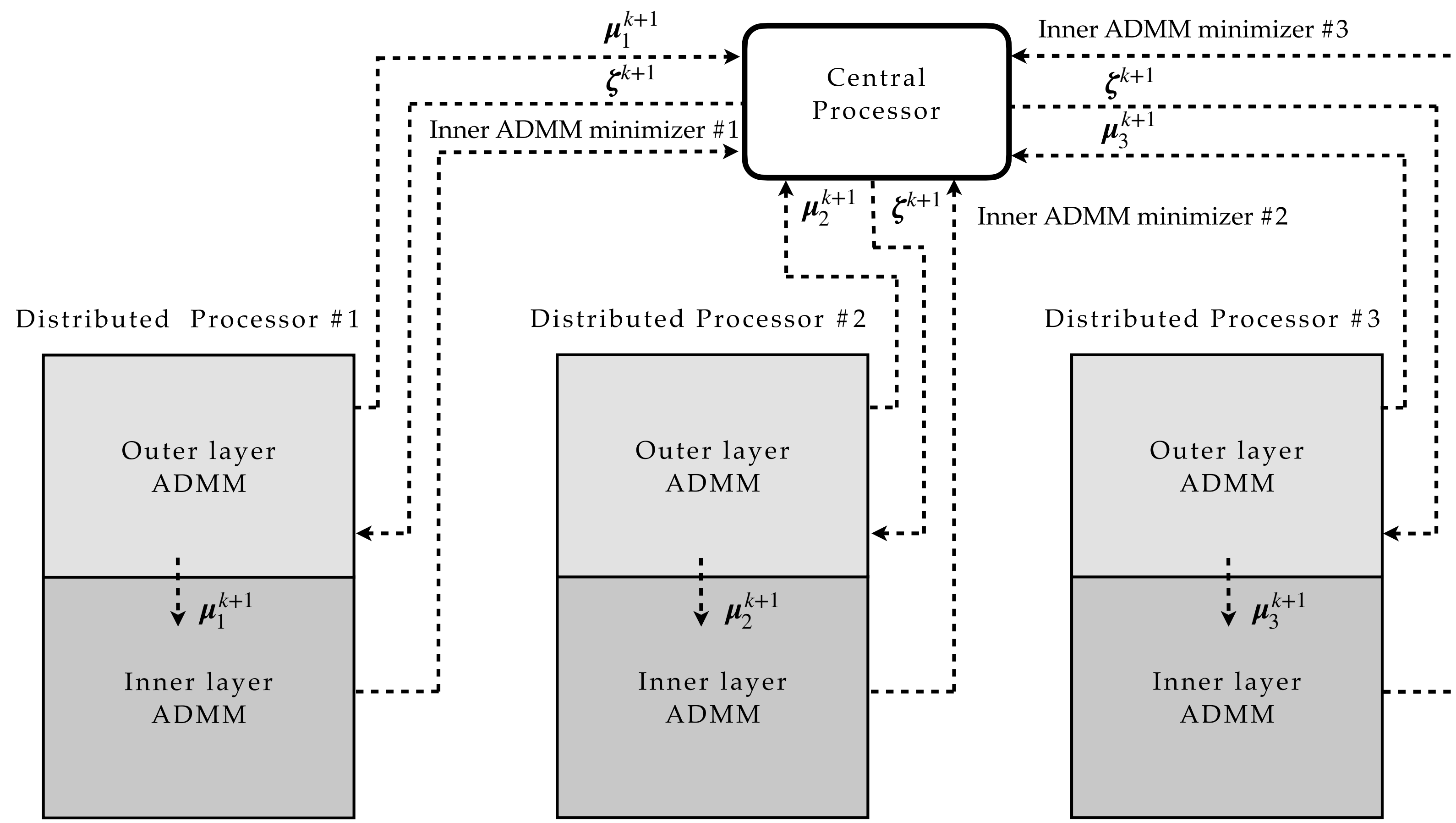
Case	Functionals	Wasserstein distances
#1	$F_1(\boldsymbol{\mu}) = \left\langle \boldsymbol{V}_k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle,$ $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \right\rangle$	
#2	$F_1(\boldsymbol{\mu}) = \langle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

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 outer layer ADMM (technically challenging)

High dimensional case studies

Thank You

Back up Slides

More Results for Experiment #2

Effect of Varying the Outer Layer ADMM Barrier Parameter α

α	10	10.5	11	11.5	12	12.5	13	13.5	14	14.5	15
F^{10000}, case #1	10.8945	10.9153	10.9058	10.9224	10.8978	10.9064	10.8922	10.9203	10.9124	10.9203	10.9139
F^{10000}, case #2	11.0544	11.0586	11.0624	11.0598	11.0618	11.0578	11.0694	11.0692	11.0591	11.0570	11.0561
F^{10000}, case #3	11.0282	11.0344	11.0296	11.0325	11.0275	11.0312	11.0338	11.0301	11.0395	11.0351	11.0305
F^{10000}, case #4	16.5034	16.5051	16.5087	16.5012	16.5106	16.5080	16.5049	16.5029	16.5030	16.5018	16.5057

Effect of Varying the Inner Layer ADMM Iteration Number

Inner layer ADMM iter. #	3	4	5	6	7	8	9	10
F^{10000}, case #1	10.9263	10.8981	10.9165	10.8997	10.9124	10.9157	10.8813	10.9009
F^{10000}, case #2	11.0638	11.0546	11.0643	11.0625	11.0632	11.0583	11.0701	11.0678
F^{10000}, case #3	11.0368	11.0457	11.0374	11.0381	11.0363	11.0359	11.0318	11.0322
F^{10000}, case #4	16.5072	16.5023	16.5046	16.5001	16.5123	16.5039	16.5045	16.5034