# A Distributed Algorithm for Wasserstein Proximal Operator Splitting

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# Topic of this talk

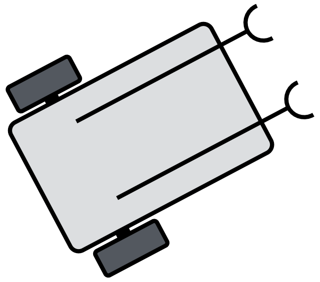
**Optimization over the space of measures a.k.a. distributions**

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

**measure a.k.a. distribution = mass**

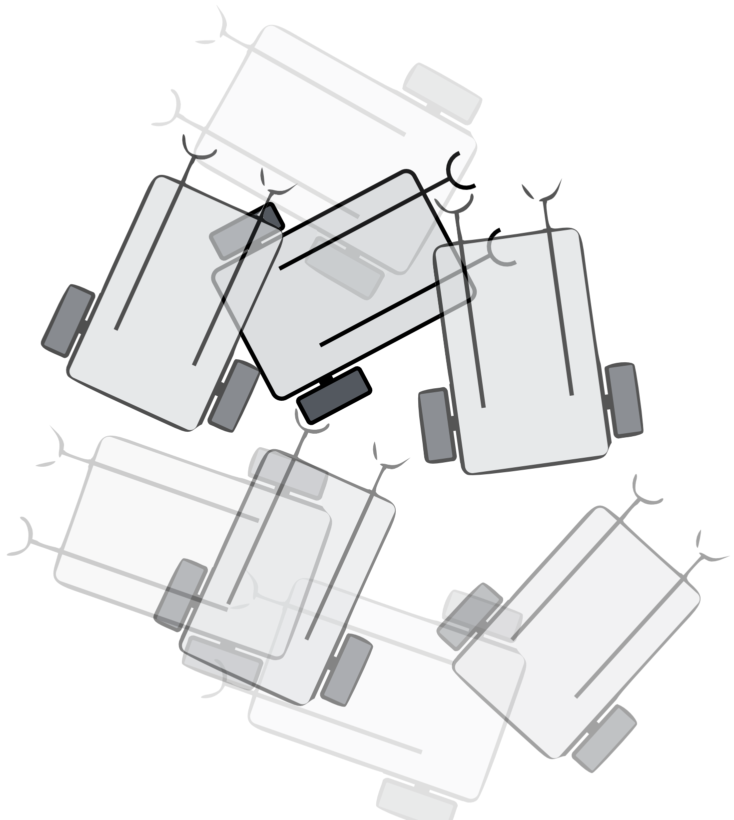
**mass = density $\times$ volume**

# 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



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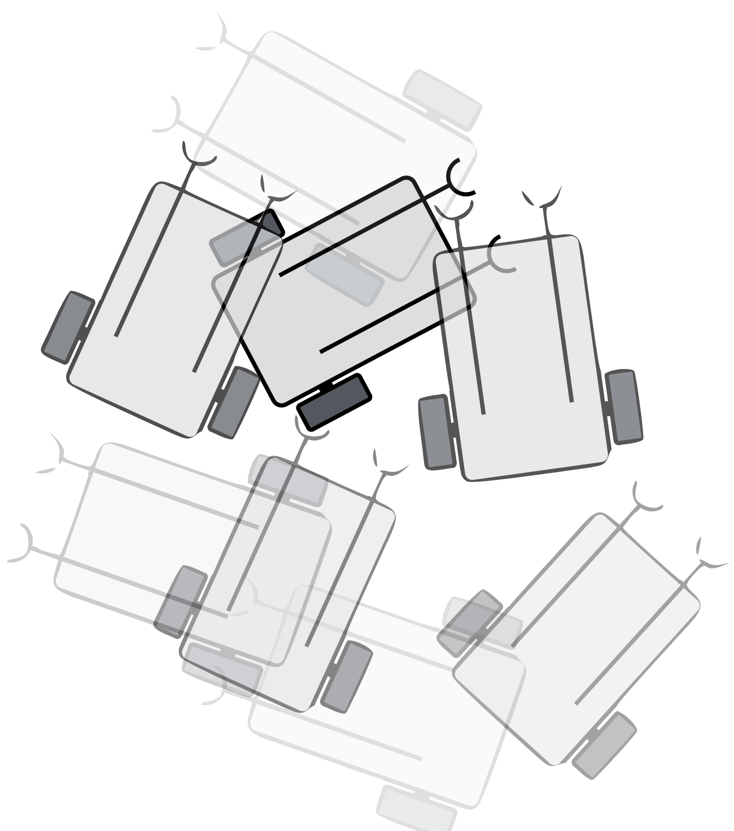
$$\rho\left(\boldsymbol{x}, t\right) : \mathcal{X} \times [0, \infty) \mapsto \mathbb{R}_{\geq 0}$$

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

# Probability Distribution



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probability measure probability density function

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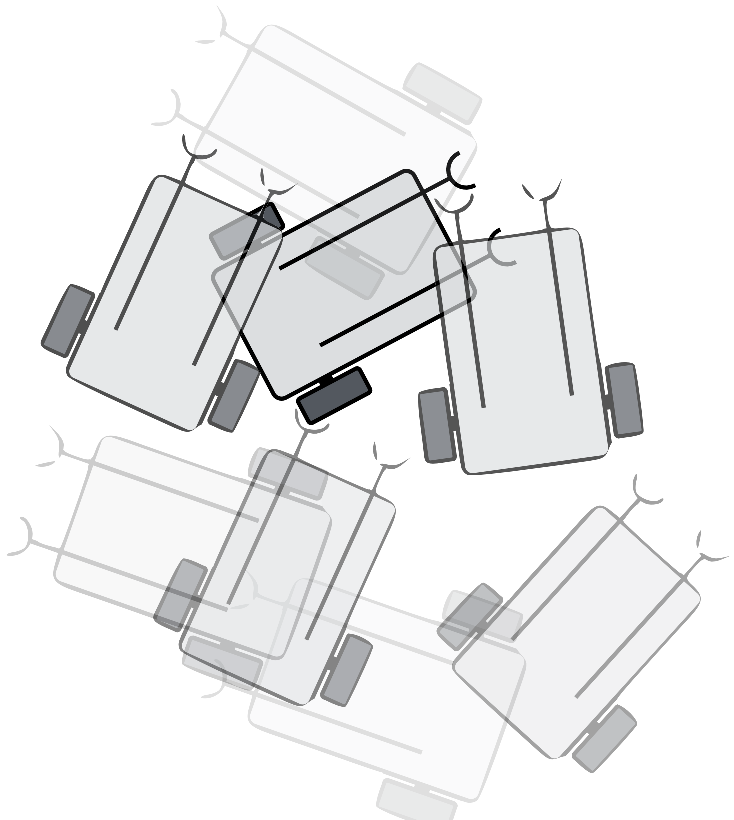
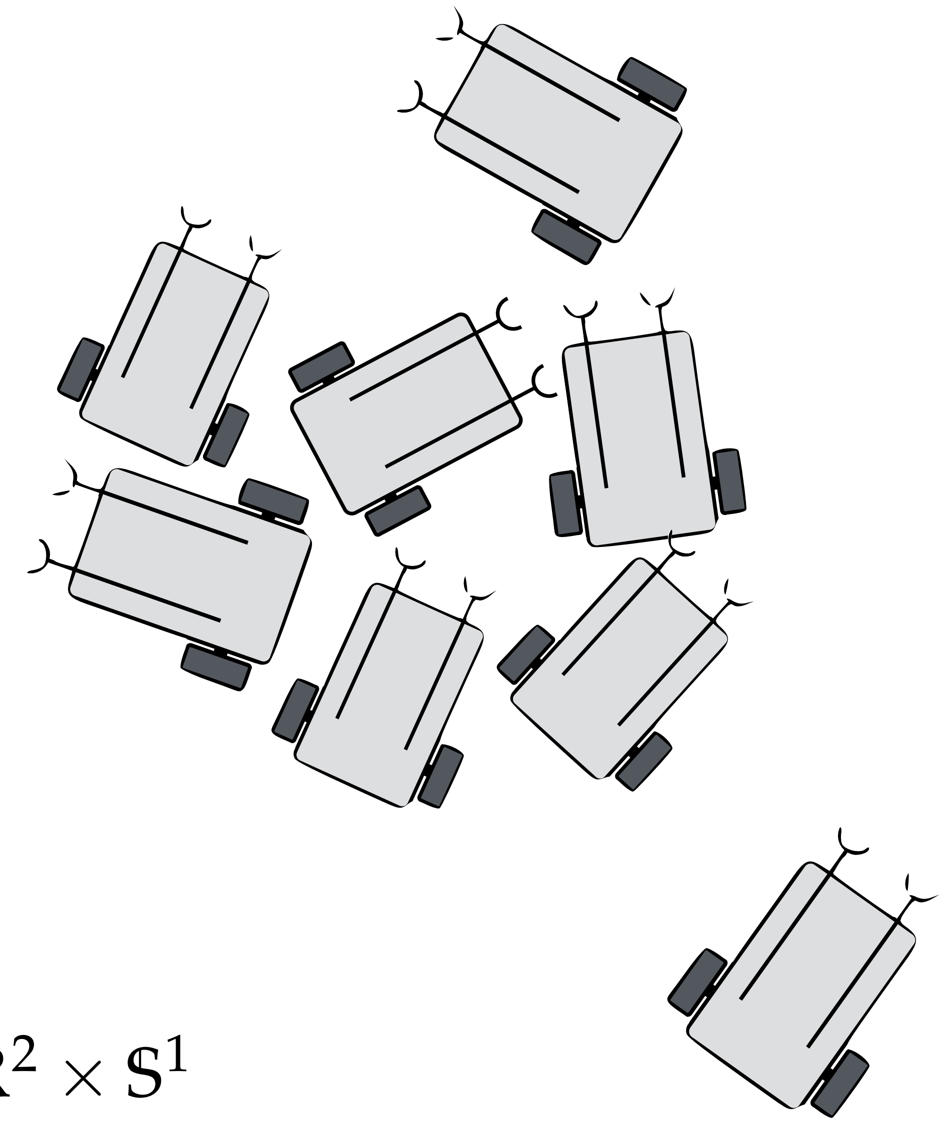
# Probability Distribution Population Distribution





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population measure population density function

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

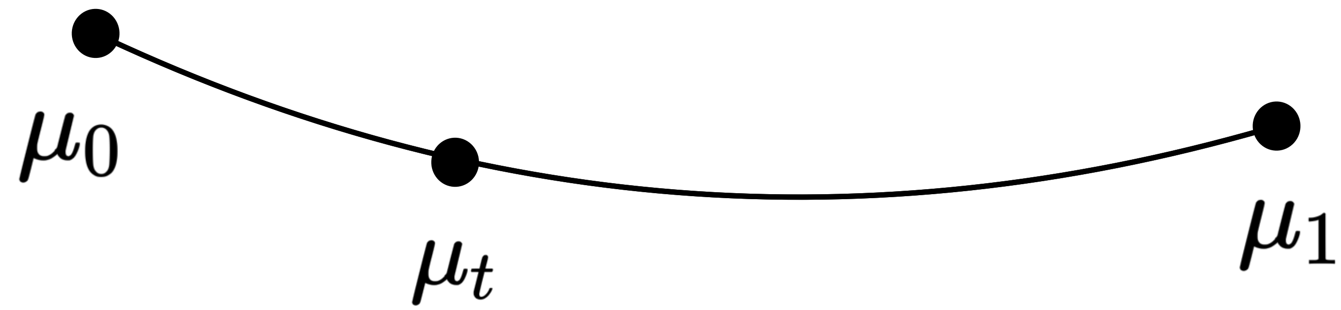
# Geometry on the Space of Prob. Measures


2-Wasserstein distance metric

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

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

# Geometry on the Space of Prob. Measures




2-Wasserstein distance metric

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

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

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

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

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

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

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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:**

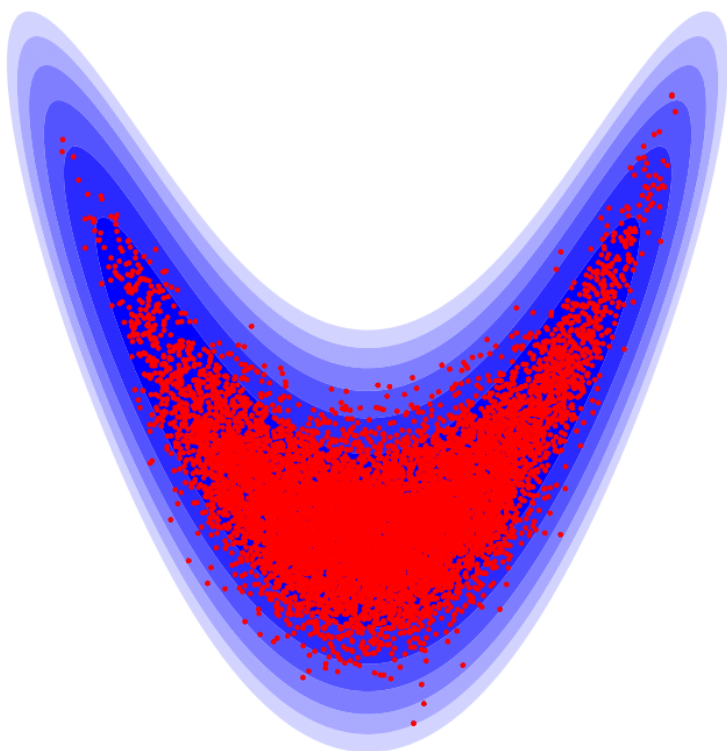
$$\mu_k \to \mu(\cdot, t = kh) \quad \text{as} \quad h \downarrow 0$$

**$F$ as Lyapunov functional:**

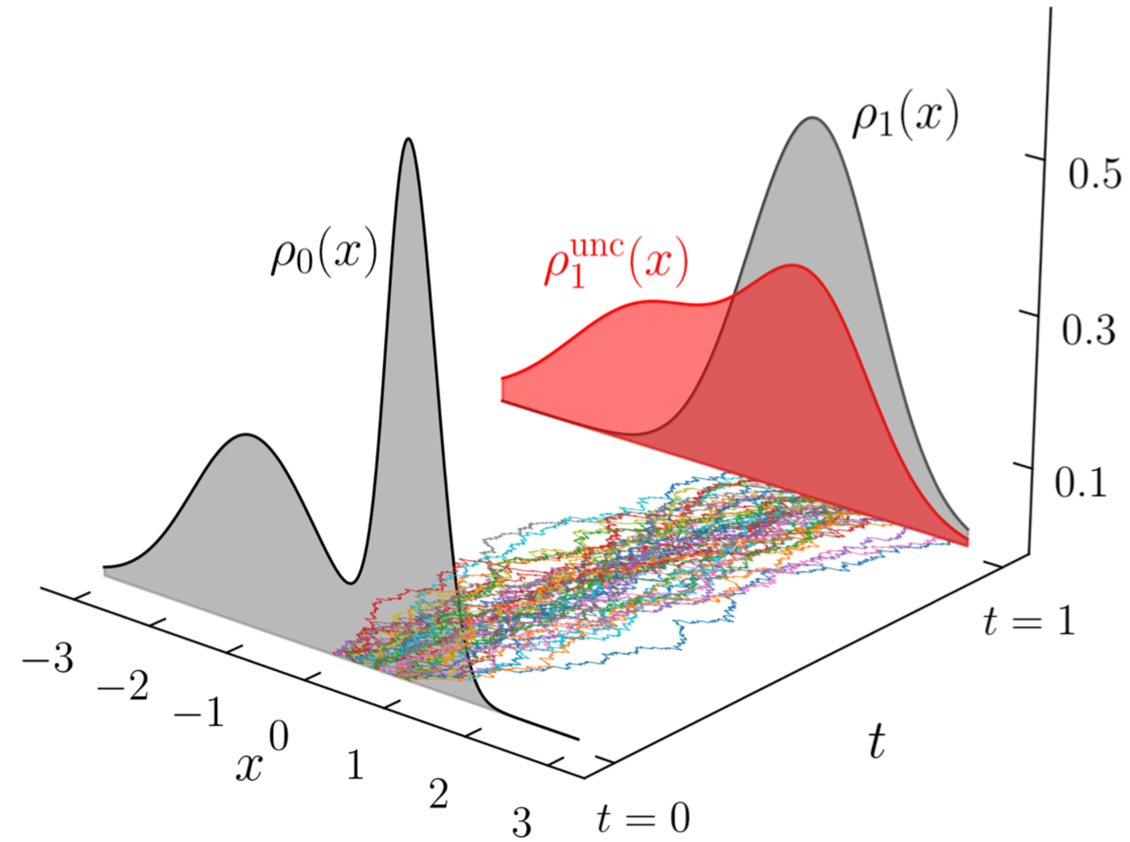
$$\frac{\mathrm{d}}{\mathrm{d}t} F = -\mathbb{E}_\mu\left[\left\|\nabla\frac{\delta F}{\delta \mu}\right\|_2^2\right] \leq 0$$

# Motivating Applications

Langevin sampling from an unnormalized prior



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





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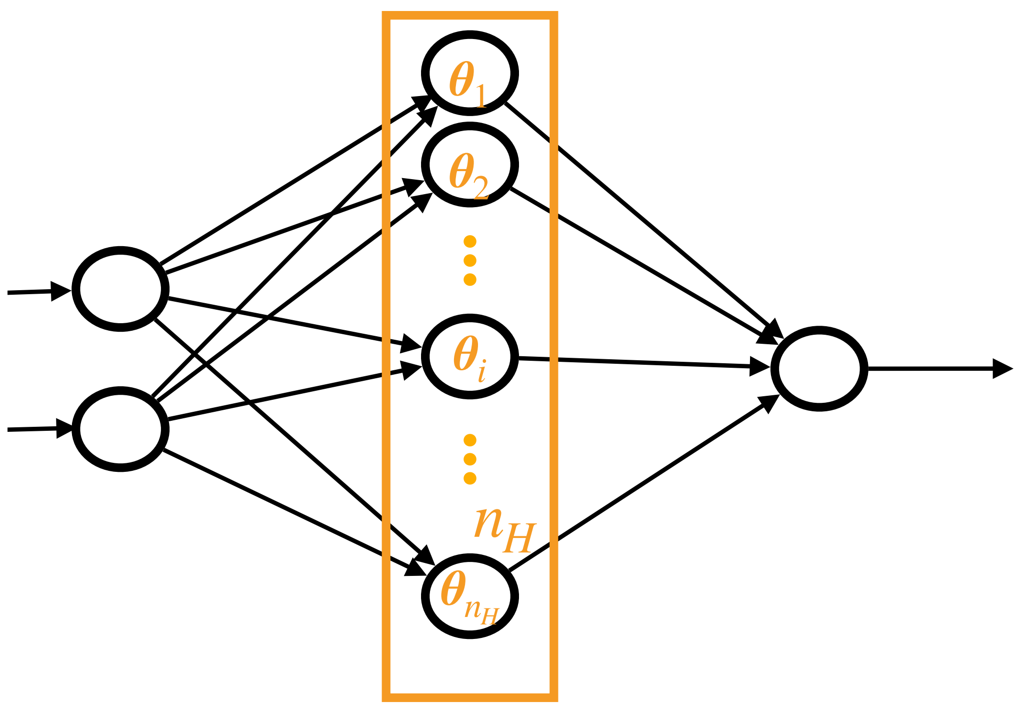
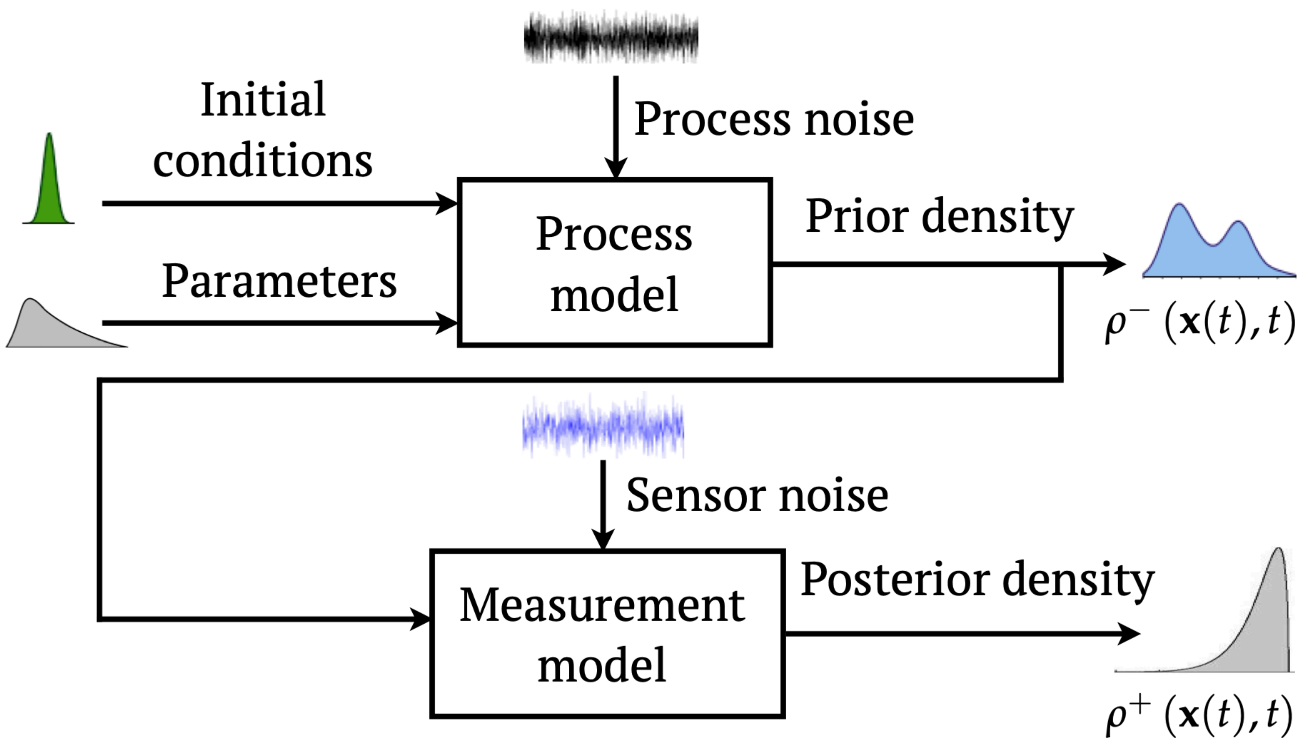
# Motivating Applications (contd.)

Mean field learning dynamics in neural networks




Prediction and estimation of time-varying joint state probability densities

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

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But all require centralized computing

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

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

For quadratic loss:

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

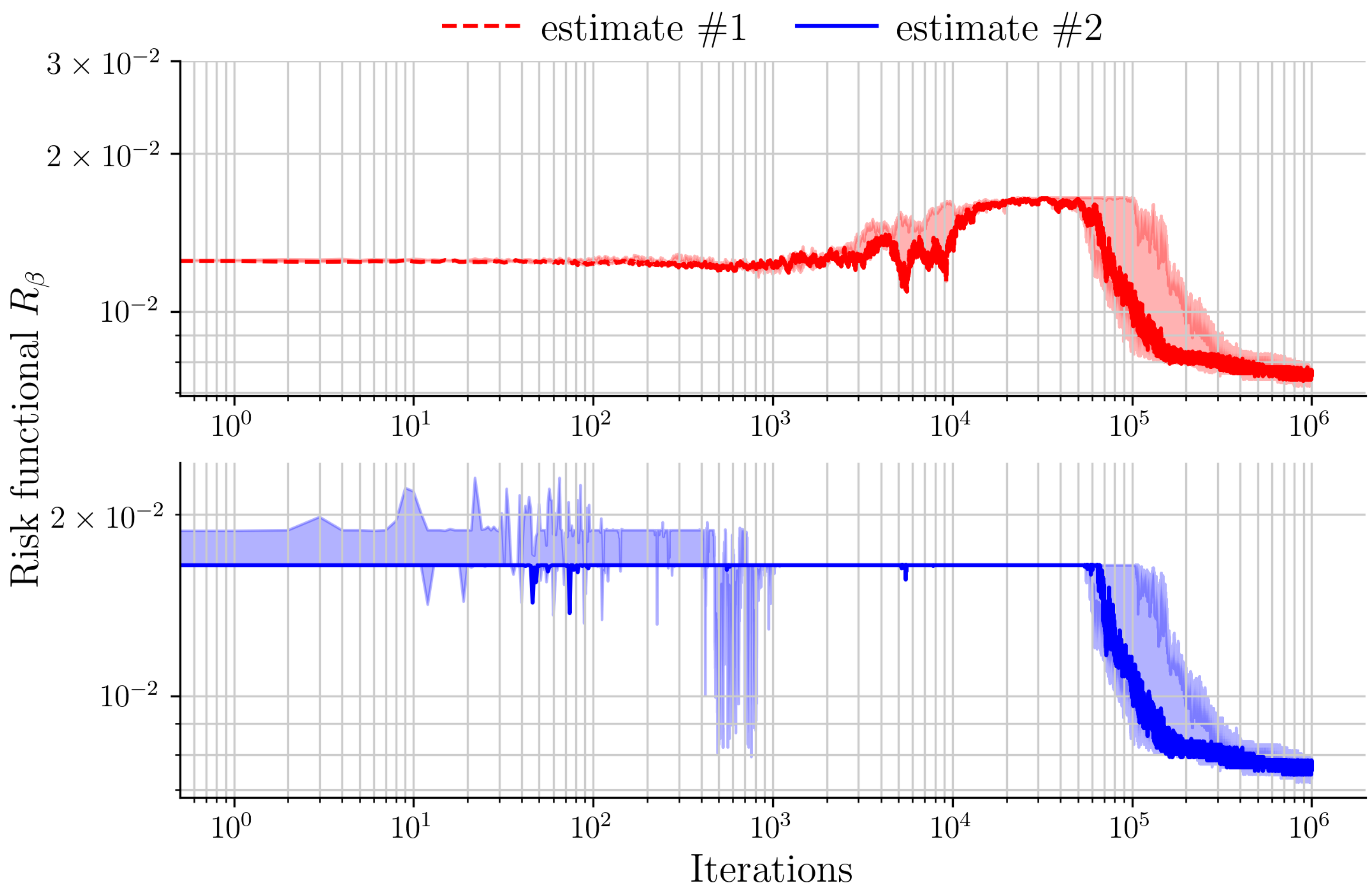
depend on activation functions of the NN

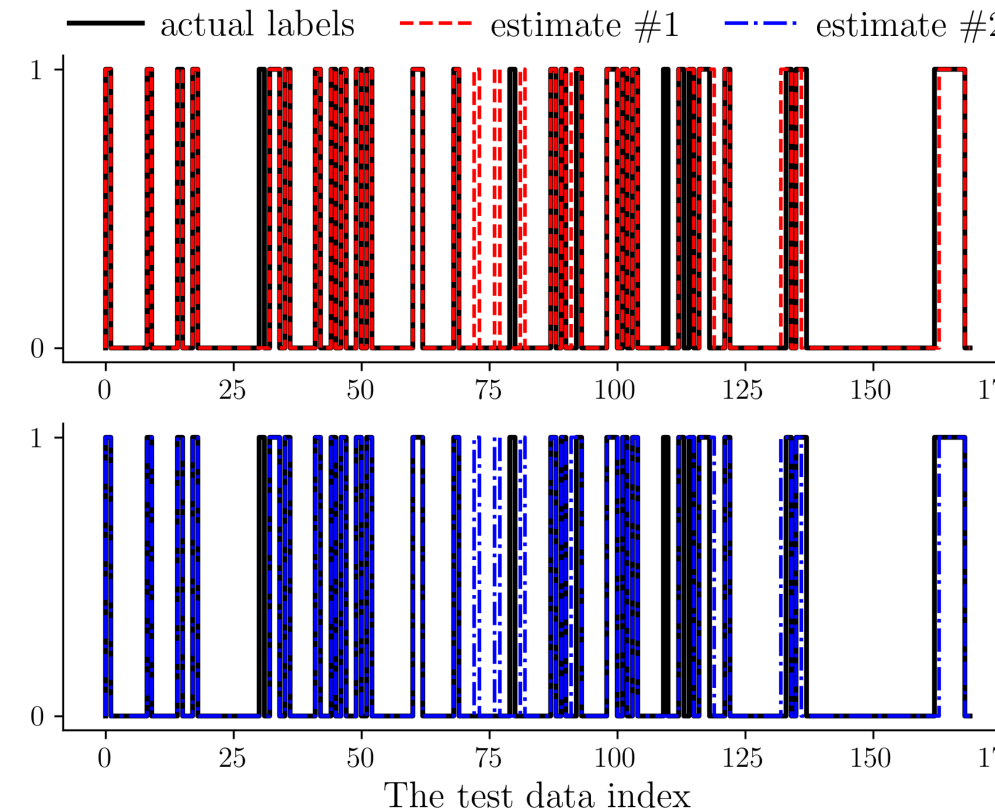
Neuronal population measure dynamics: $\dfrac{\partial \mu}{\partial t} = \nabla \cdot \left(\mu \nabla \dfrac{\delta F}{\delta \mu}\right) =: -\nabla^{W_2} F(\mu)$

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

| $\beta$ | 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)

# Present Work: Distributed Algorithm

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

# Present Work: Distributed Algorithm

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

**Main idea:** re-write

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

# 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:**

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

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

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

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

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

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

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

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

# Proposed Consensus ADMM

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

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

$$\nu_i^{k+1} = \nu_i^k + \alpha\left(\mu_i^{k+1} - \zeta^{k+1}\right) \qquad \text{where } i \in [n],\ k \in \mathbb{N}_0$$

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

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

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

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

# Proposed Consensus ADMM (contd.)

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

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

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

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.)

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

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

# Discrete Version of the Proposed ADMM

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

Euclidean distance matrix

where $N$ is the number of samples

# Discrete Version of the Proposed ADMM

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

**With Sinkhorn regularization:**

Discrete Sinkhorn divergence

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

# Discrete Version of the Proposed ADMM

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

**With Sinkhorn regularization:**

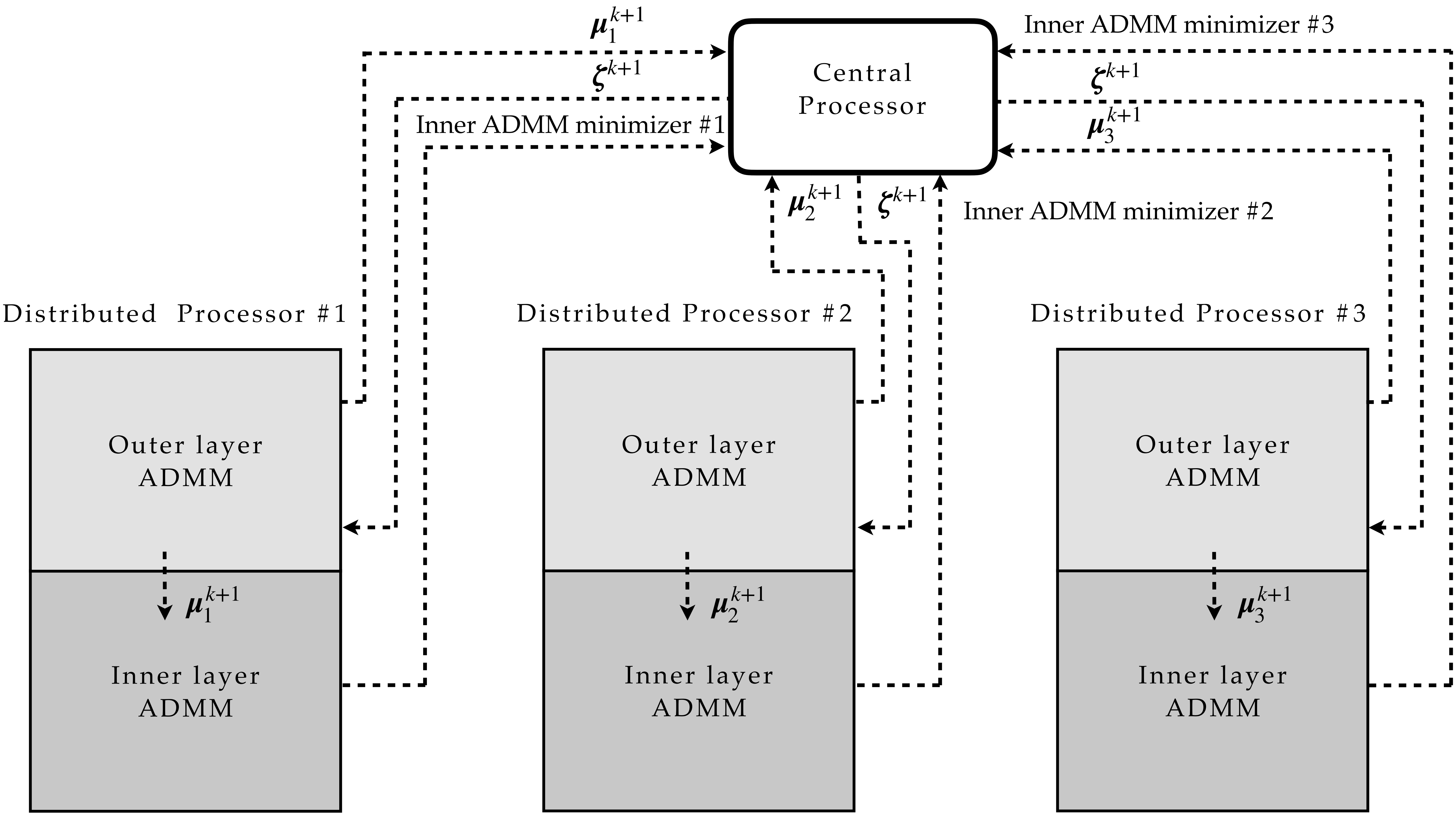
Discrete Sinkhorn divergence

Outer layer ADMM

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

Inner layer ADMM

# Overall Schematic



# $\mu_i$ update $\rightsquigarrow$ Outer Consensus (Sinkhorn) ADMM

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

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

# $\mu_i$ update ⇝ Outer Consensus (Sinkhorn) ADMM

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

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

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

Convex

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

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

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

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

# $\zeta$ update $\rightsquigarrow$ Inner (Euclidean) ADMM

**Theorem.**

Consider the convex problem

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

Then

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

# $\zeta$ 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 $i \in [n]$,

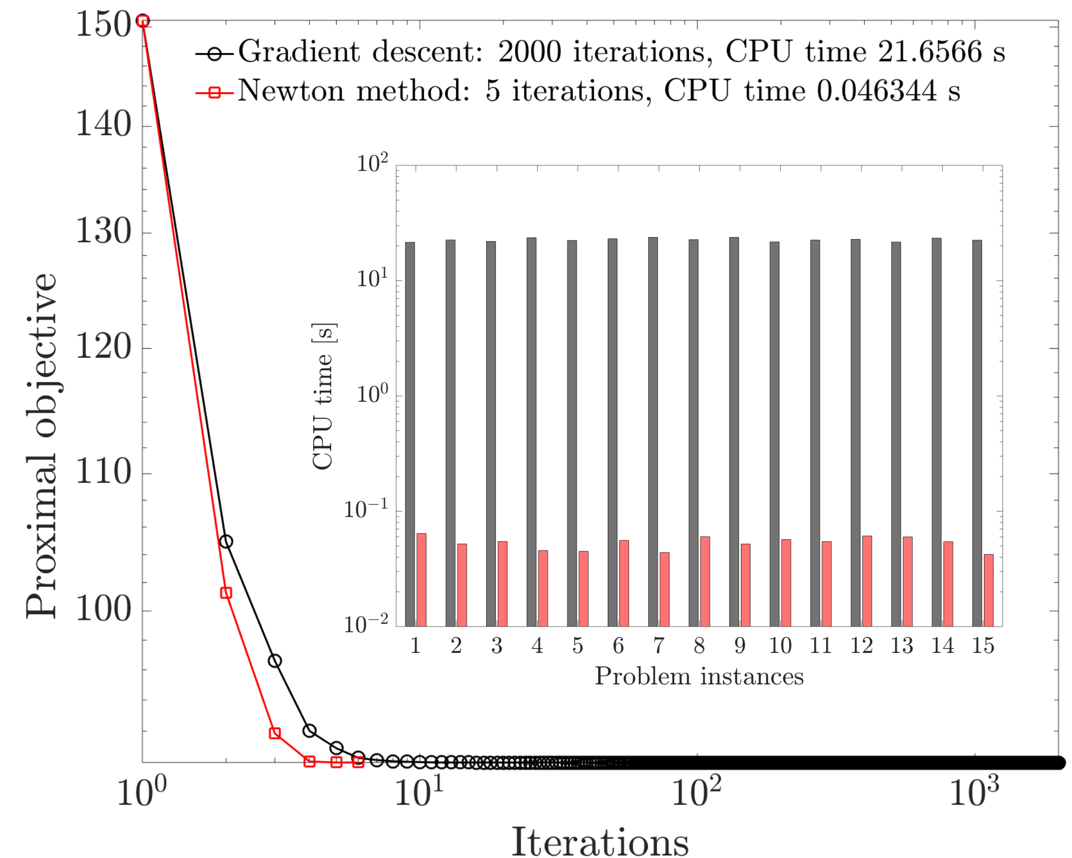
Then the following Euclidean ADMM solves ( ♥ )

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

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

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

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



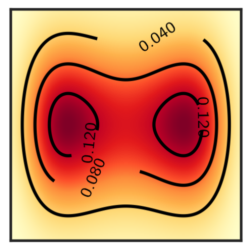
# Experiment #1

Linear Fokker-Planck-Kolmogorov PDE

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

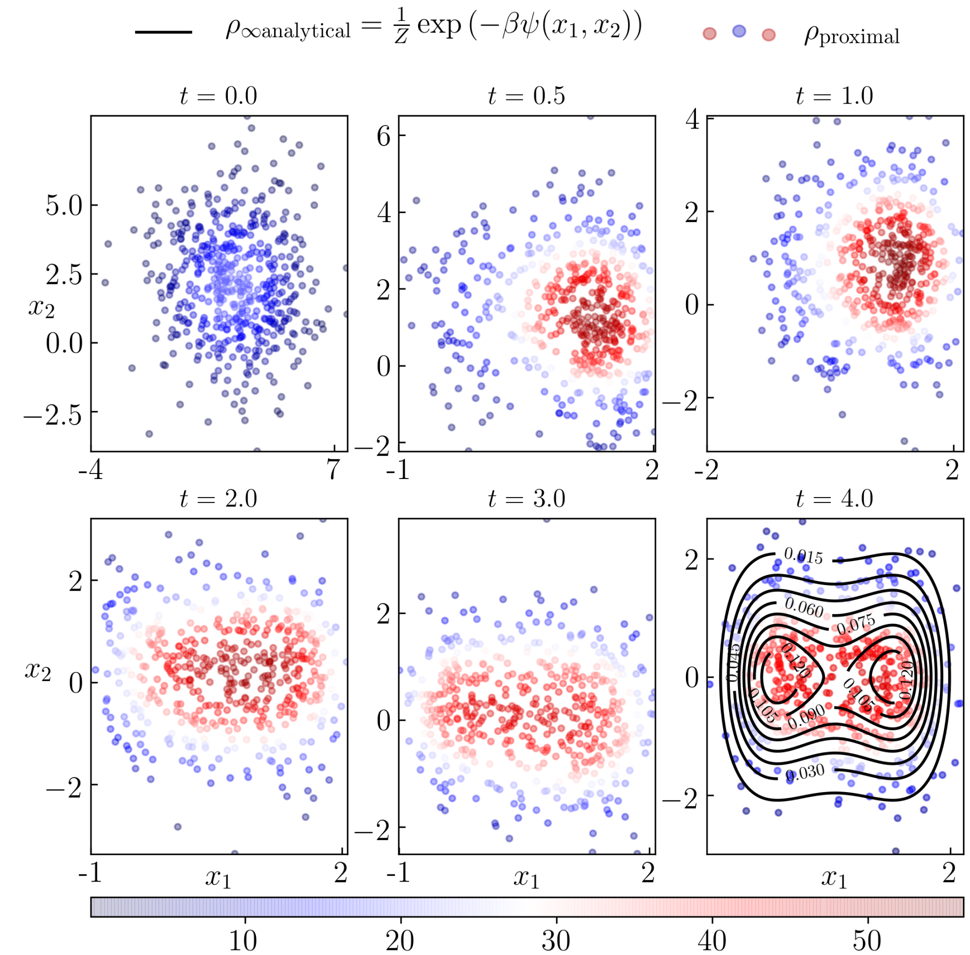
$$V(x_1, x_2) = \frac{1}{4}\left(1 + x_1^4\right) + \frac{1}{2}\left(x_2^2 - x_1^2\right)$$

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




## Centralized computation:

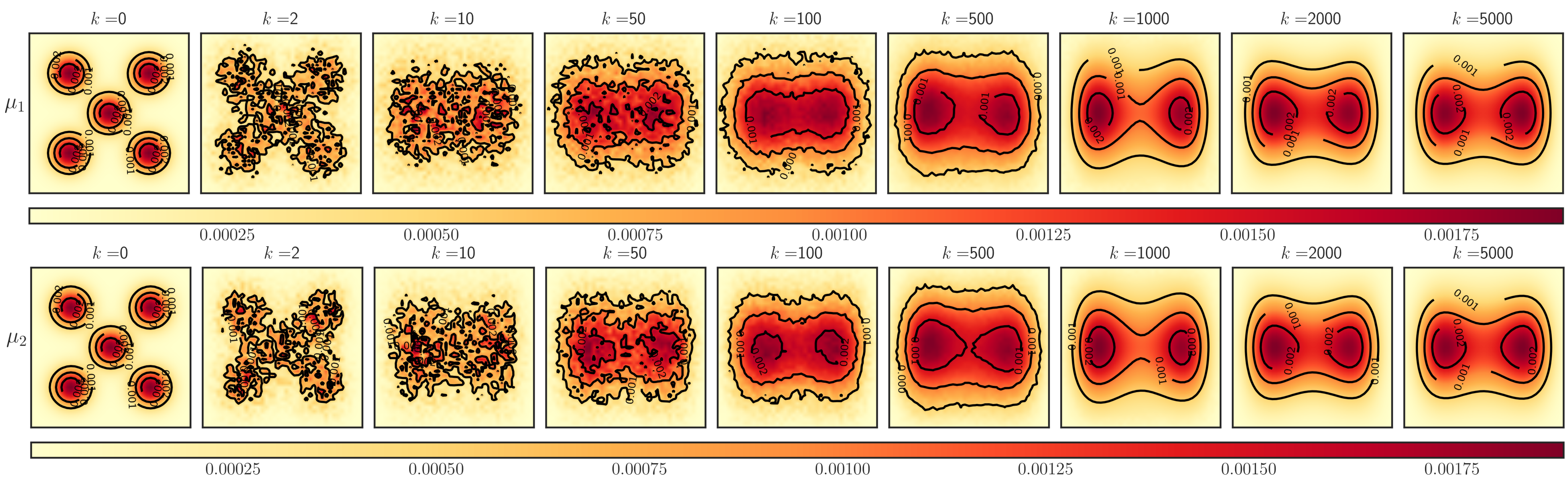
Caluya and Halder, *IEEE Trans. Automatic Control*, 2019




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

## Distributed computation:

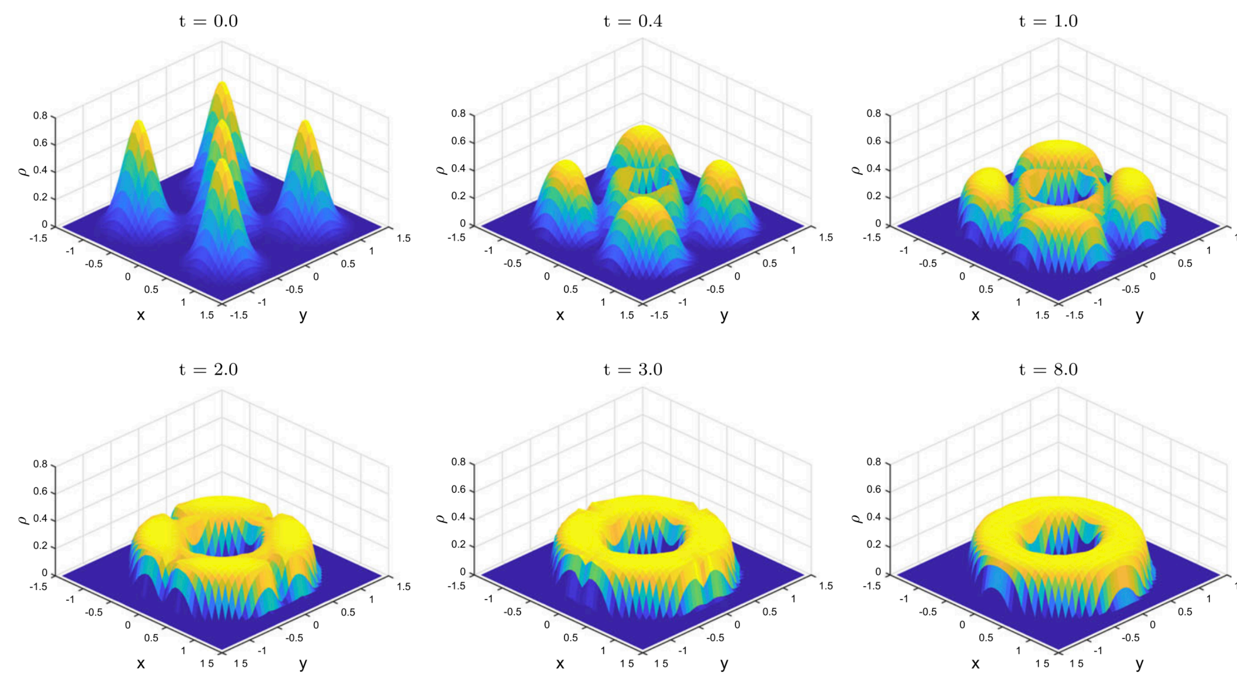
$$F_1(\boldsymbol{\mu}) = \langle \boldsymbol{V}_k, \boldsymbol{\mu} \rangle \qquad F_2(\boldsymbol{\mu}) = \langle \beta^{-1} \log \boldsymbol{\mu}, \boldsymbol{\mu} \rangle$$



# Experiment #2

## Centralized computation:

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




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

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

Aggregation-drift-diffusion nonlinear PDE

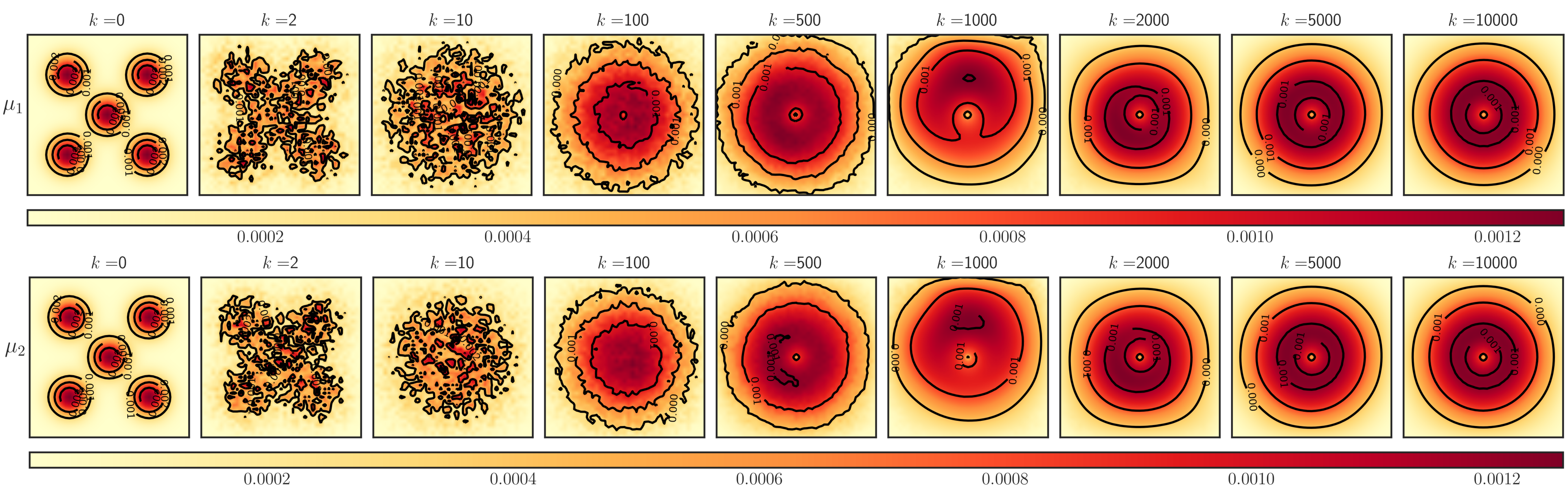
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

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

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

## 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

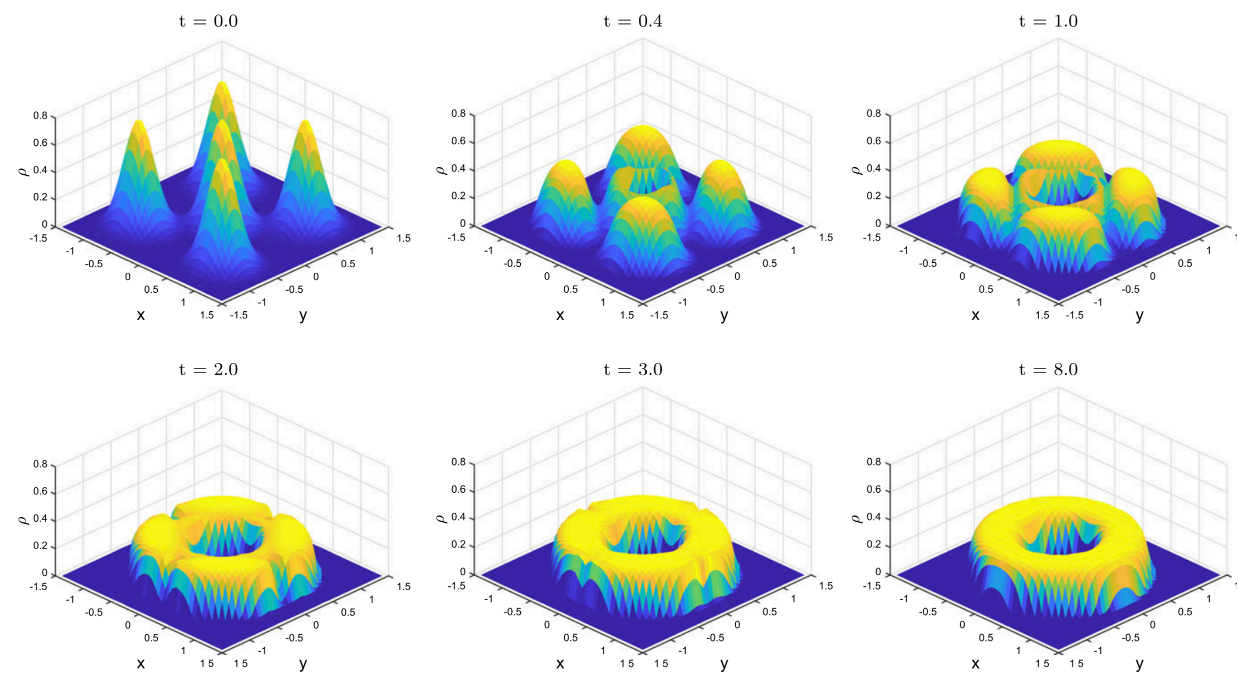
$$\frac{\partial \mu}{\partial t} = \underbrace{\nabla \cdot (\mu \nabla (U * \mu))}_{i=1} + \underbrace{\nabla \cdot (\mu \nabla V) + \beta^{-1} \Delta \mu^2}_{i=2}$$

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

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

## Centralized computation:

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

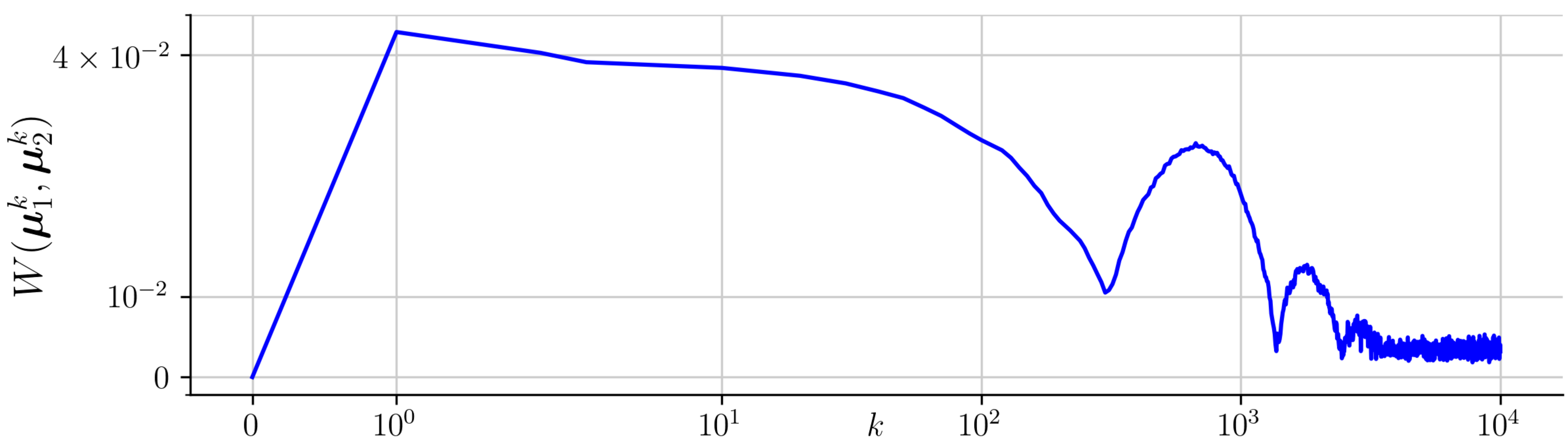



$$\lim_{\beta^{-1} \downarrow 0} \mu_\infty = \mathrm{Unif}\,(\mathscr{A})$$

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

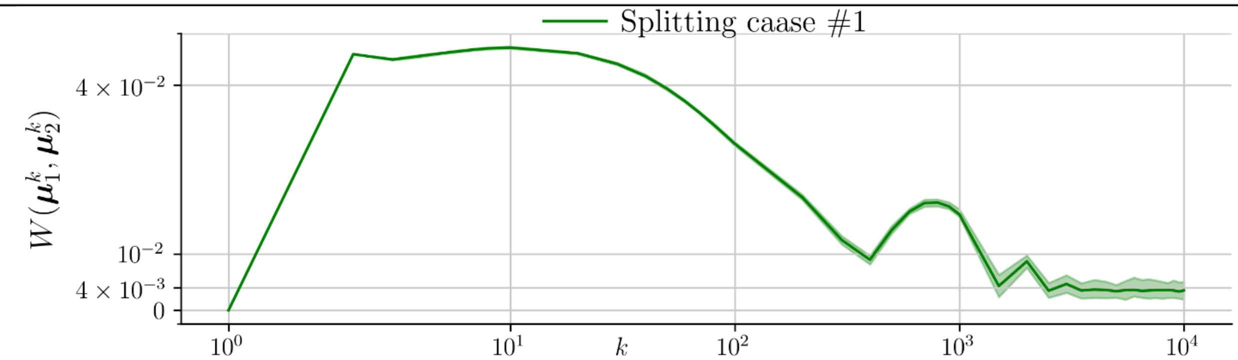
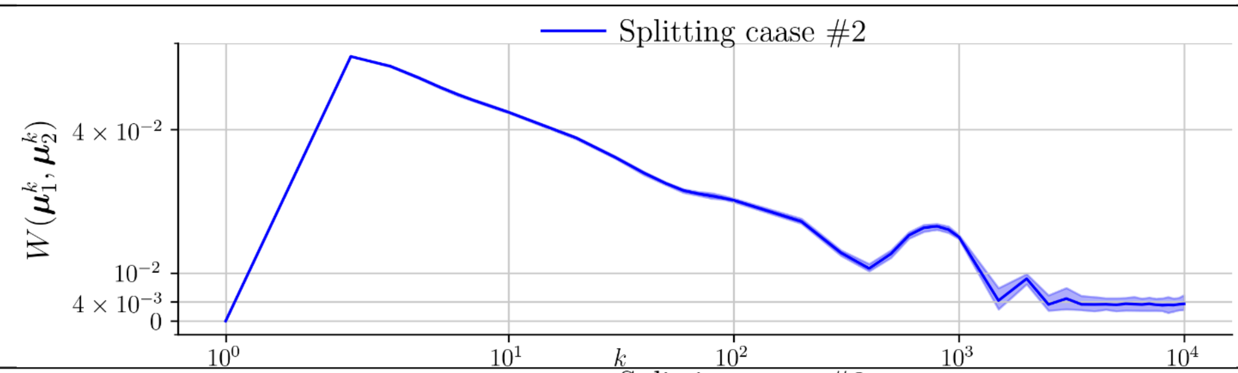
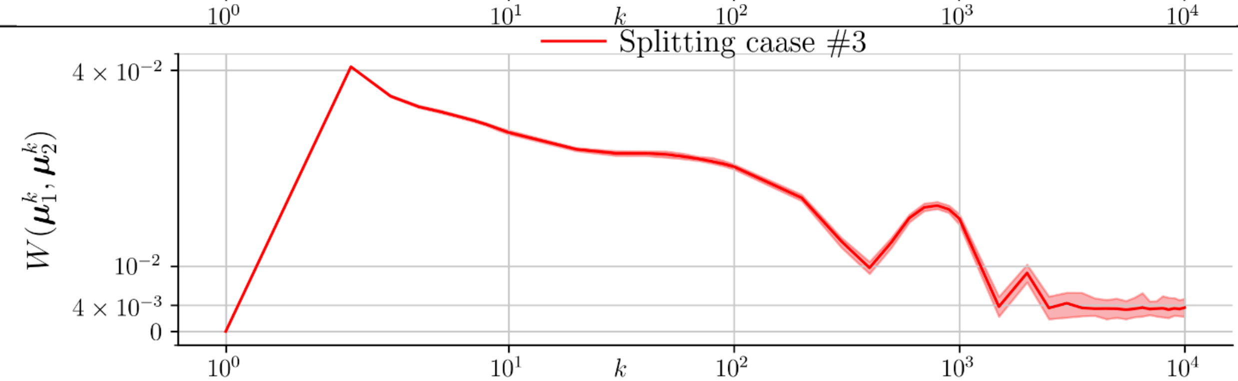
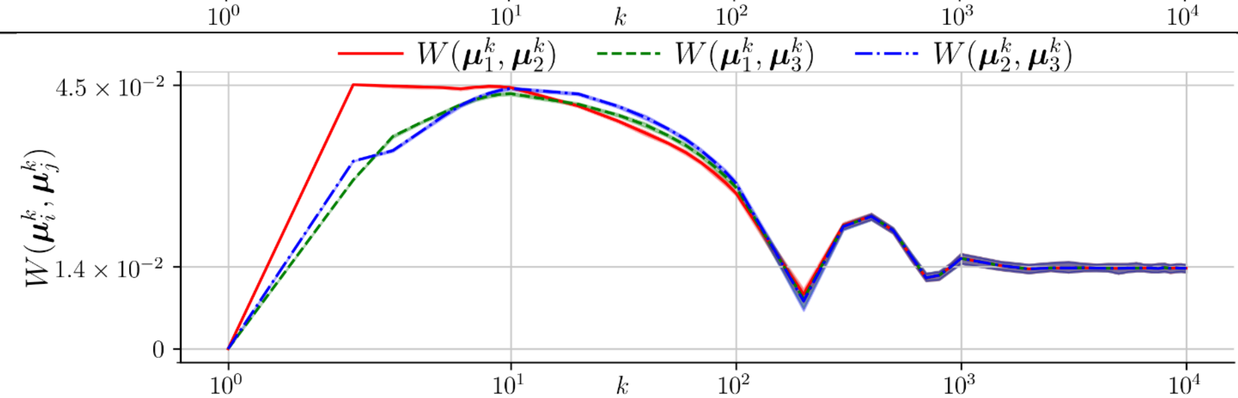
## Distributed computation:

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



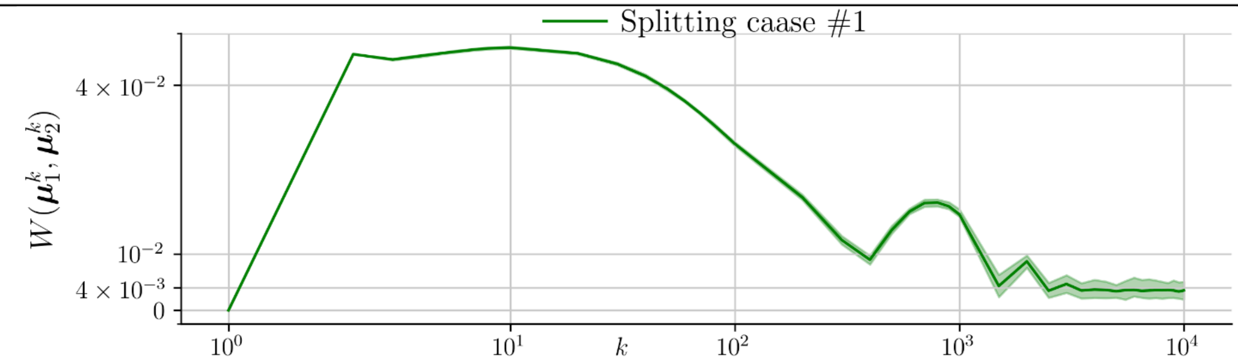
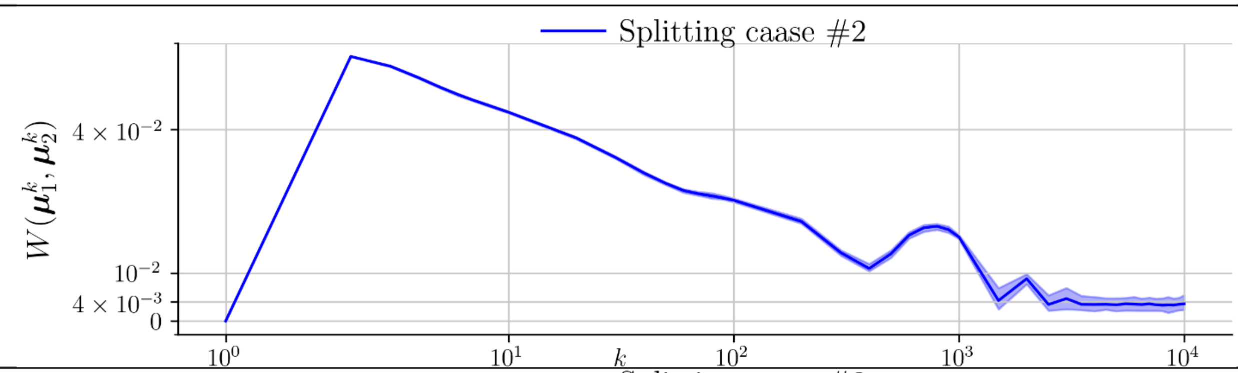
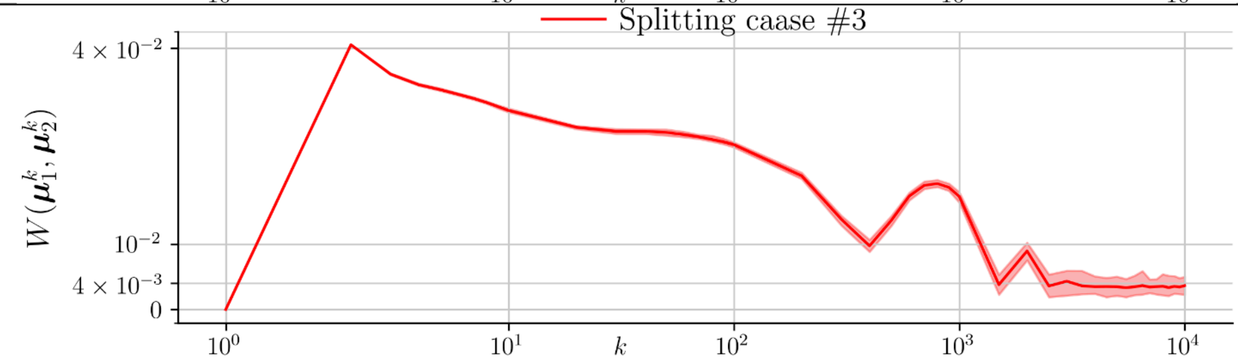
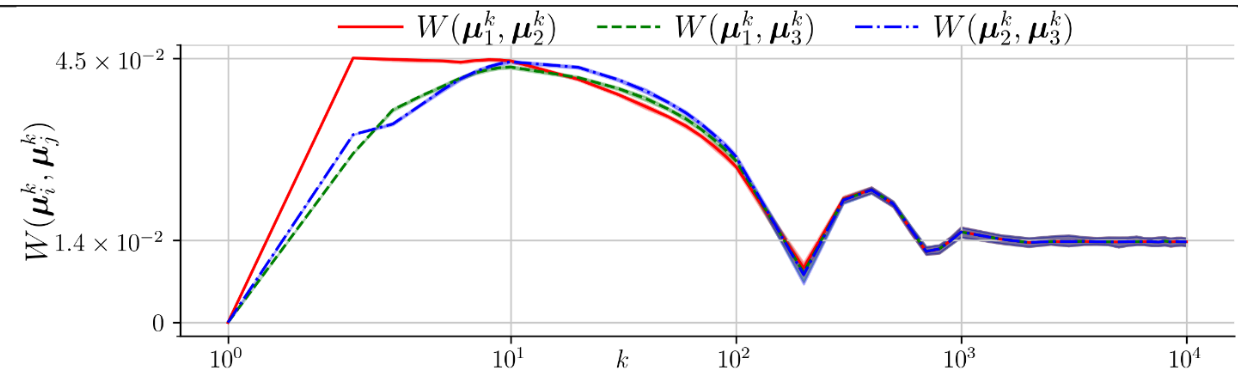
# Experiment # 2 (contd.)

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

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

# Experiment # 2 (contd.)

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

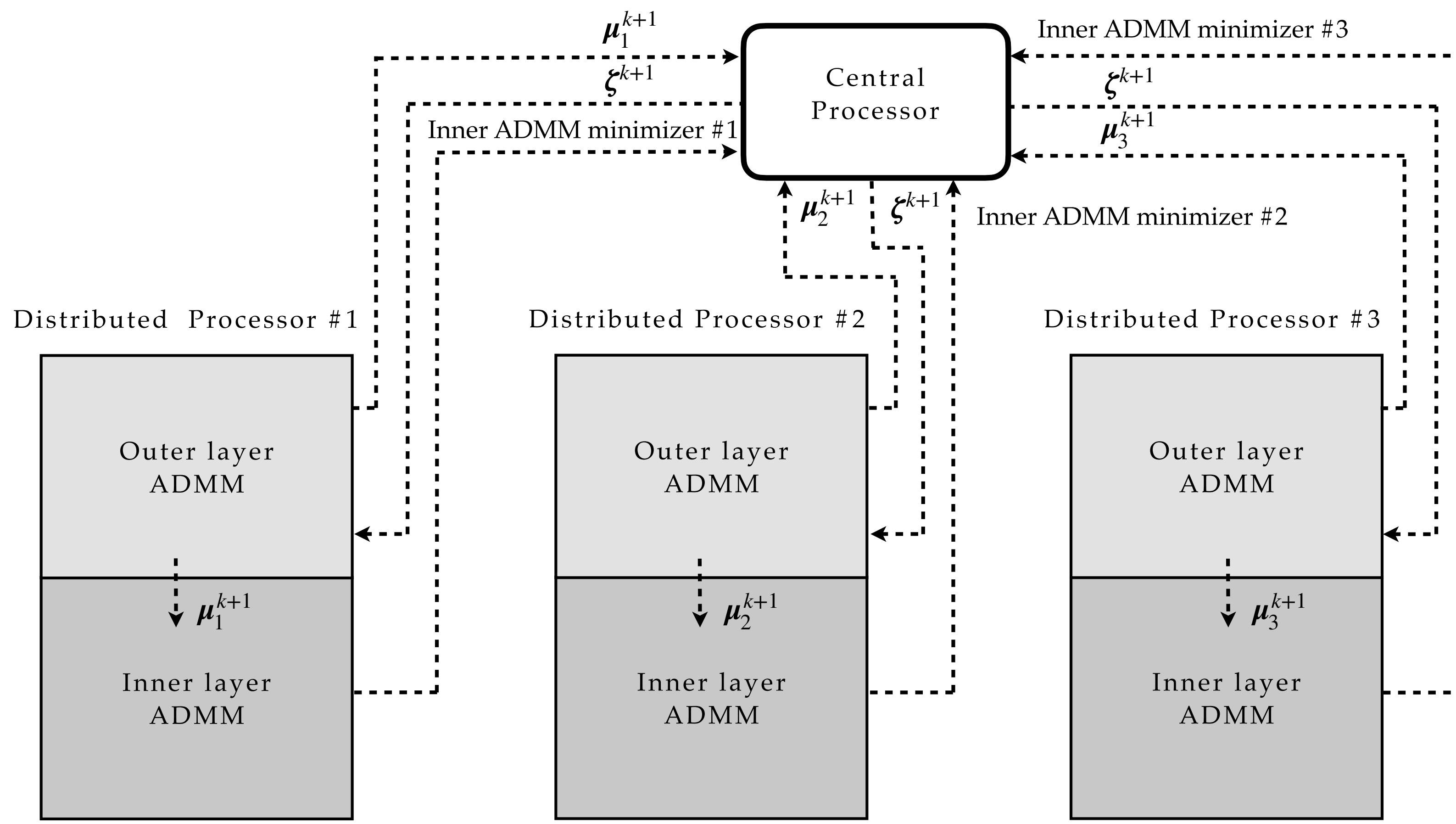
| Splitting case | Functionals | Wasserstein distance |
|---|---|---|
| #1 | $F_1(\boldsymbol{\mu}) = \left\langle \boldsymbol{V}_k + \beta^{-1}\boldsymbol{\mu}, \boldsymbol{\mu} \right\rangle,$ <br> $F_2(\boldsymbol{\mu}) = \left\langle \boldsymbol{U}_k \boldsymbol{\mu}^k, \boldsymbol{\mu} \right\rangle$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