

# A Distributed Algorithm for Wasserstein Proximal Operator Splitting

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



Decision and Control Seminar  
Coordinated Science Lab

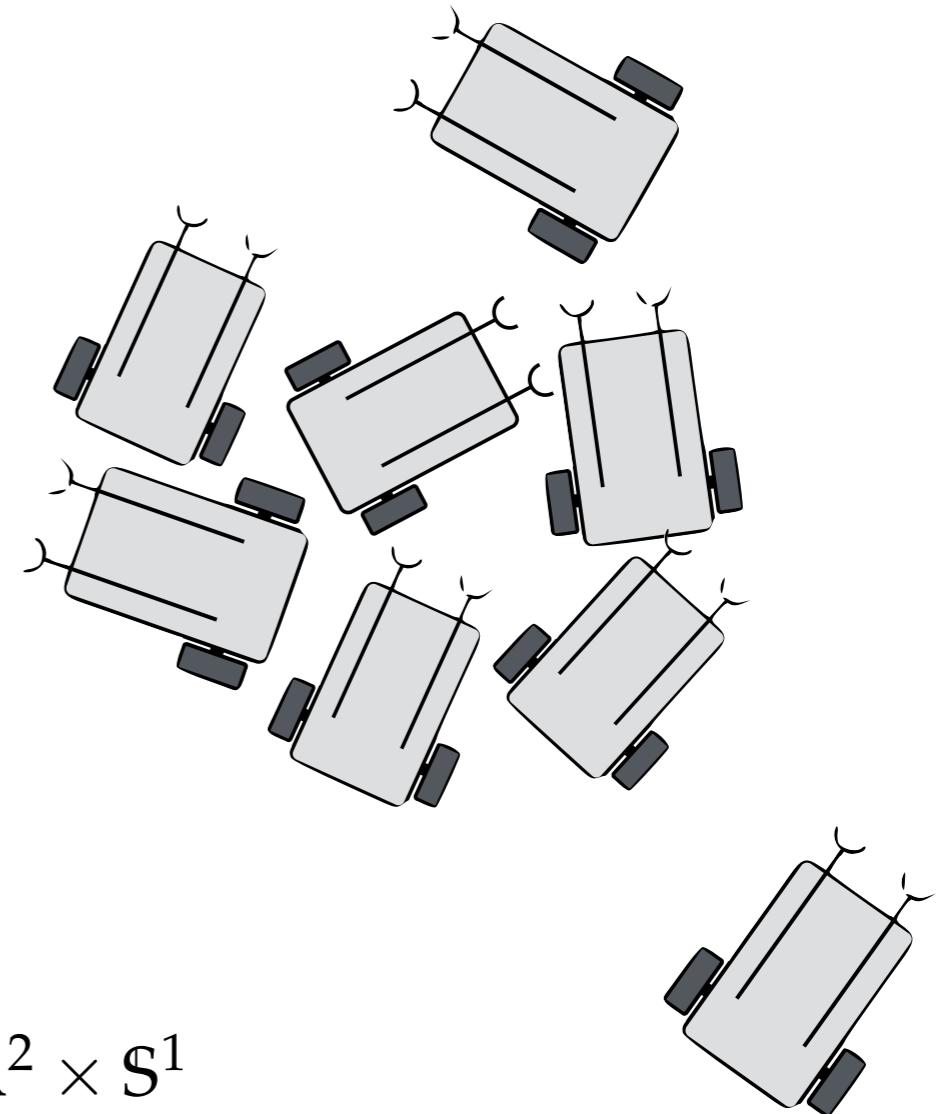
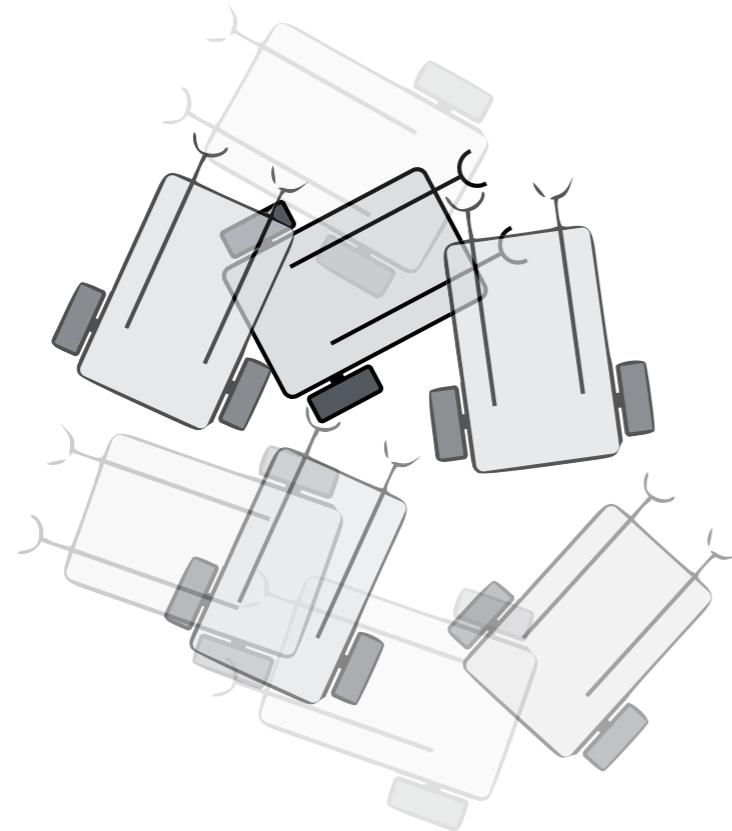
University of Illinois Urbana-Champaign, November 01, 2023



# Topic of this talk

Optimization over the space of  
measures or distributions

# Probability Distribution Population Distribution



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

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

measure = mass      density function

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

# Geometry on the Space of Prob. Measures

Numer. Math. (2000) 84: 375–393  
Digital Object Identifier (DOI) 10.1007/s002119900117

Numerische  
Mathematik  
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A computational fluid mechanics solution  
to the Monge-Kantorovich mass transfer problem

Jean-David Benamou<sup>1</sup>, Yann Brenier<sup>2</sup>



2-Wasserstein distance metric

$$W(\mu_0, \mu_1) := \left( \inf_{\mu, \mathbf{v}} \left\{ \frac{1}{2} \int_0^1 \int_{\mathcal{X}} \|\mathbf{v}\|^2 d\mu dt \right\} \right)^{1/2}$$

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

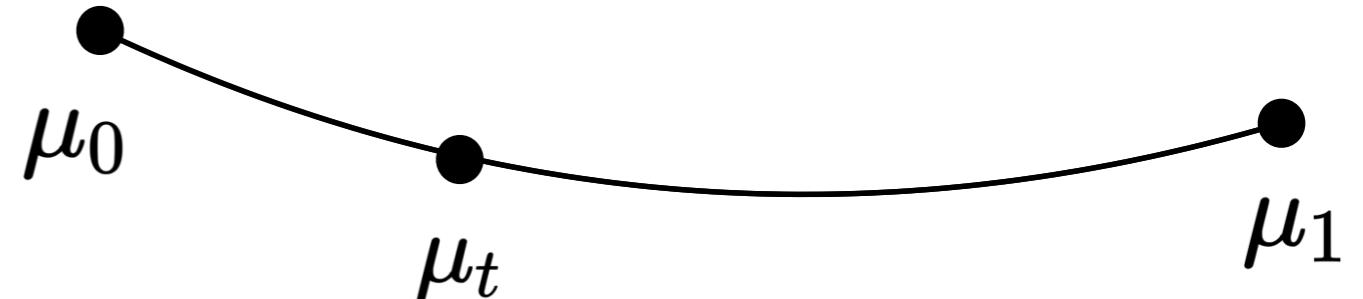
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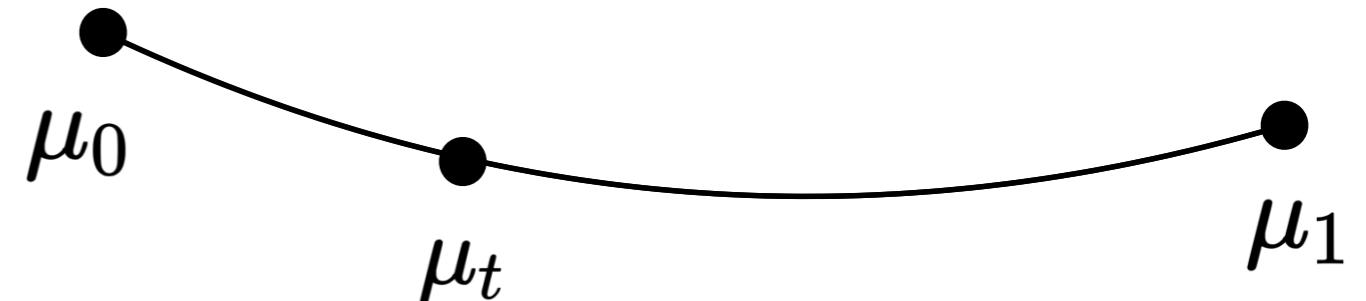
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Measure-valued **geodesic path** for any  $t \in [0,1]$

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

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

# Geometry on the Space of Prob. Measures



2-Wasserstein distance **metric**

$$W(\mu_0, \mu_1) := \left( \inf_{\mu, \mathbf{v}} \left\{ \frac{1}{2} \int_0^1 \int_{\mathcal{X}} \|\mathbf{v}\|^2 d\mu dt \right\} \right)^{1/2}$$

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

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

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

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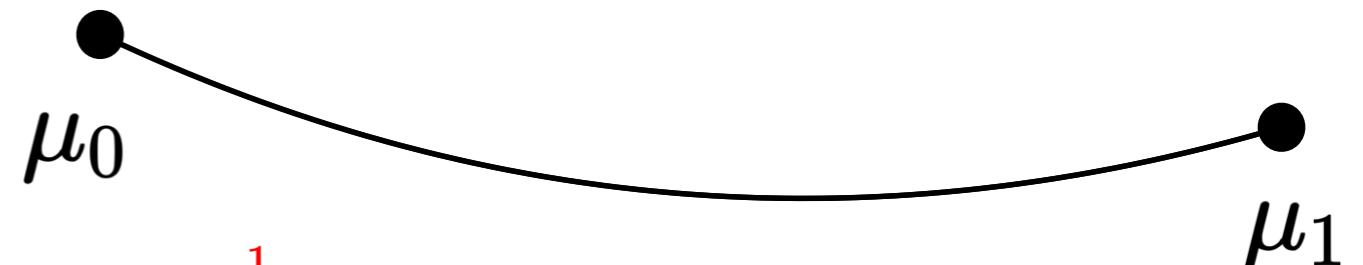
# Geometry on the Space of Prob. Measures

Optimal coupling formulation:

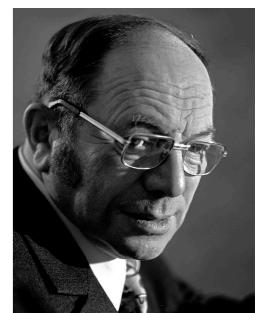
$$W(\mu_0, \mu_1) := \left( \inf_m \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) dm(\mathbf{x}, \mathbf{y}) \right)^{1/2}$$

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

subject to  $\int_{\mathcal{Y}} dm = \mu_0(d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(d\mathbf{y})$



Gaspard Monge



Leonid Kantorovich

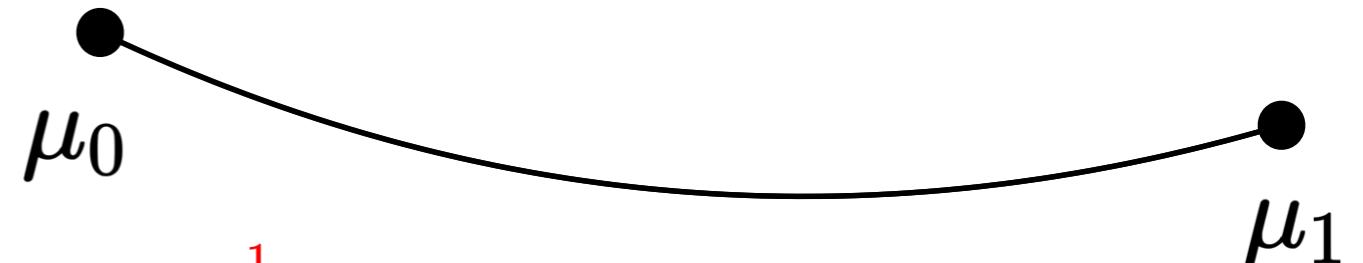
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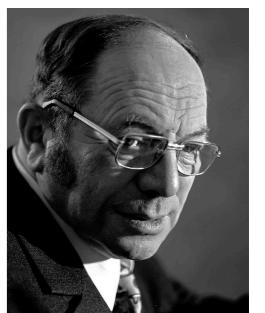
$$W(\mu_0, \mu_1) := \left( \inf_m \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) dm(\mathbf{x}, \mathbf{y}) \right)^{1/2}$$

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

subject to  $\int_{\mathcal{Y}} dm = \mu_0(d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(d\mathbf{y})$



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Entropic/Sinkhorn regularization:

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

subject to  $\int_{\mathcal{Y}} dm = \mu_0(d\mathbf{x}), \quad \int_{\mathcal{X}} dm = \mu_1(d\mathbf{y})$

# Measure-valued Optimization Problems

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

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:

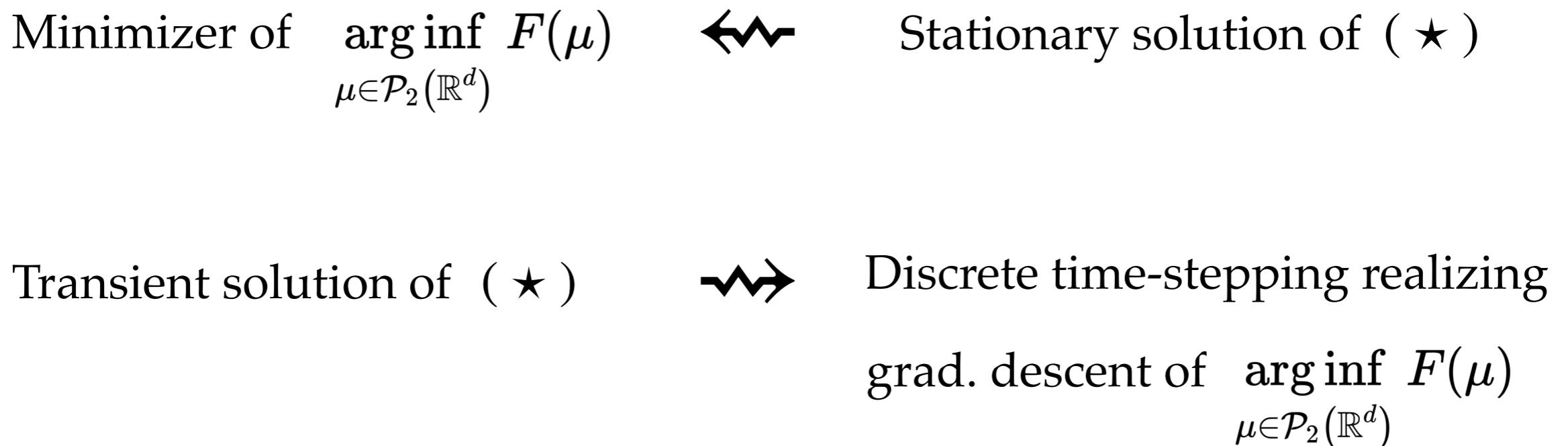
$$F(\mu) = F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

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

# Connection with Wasserstein Gradient Flows

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

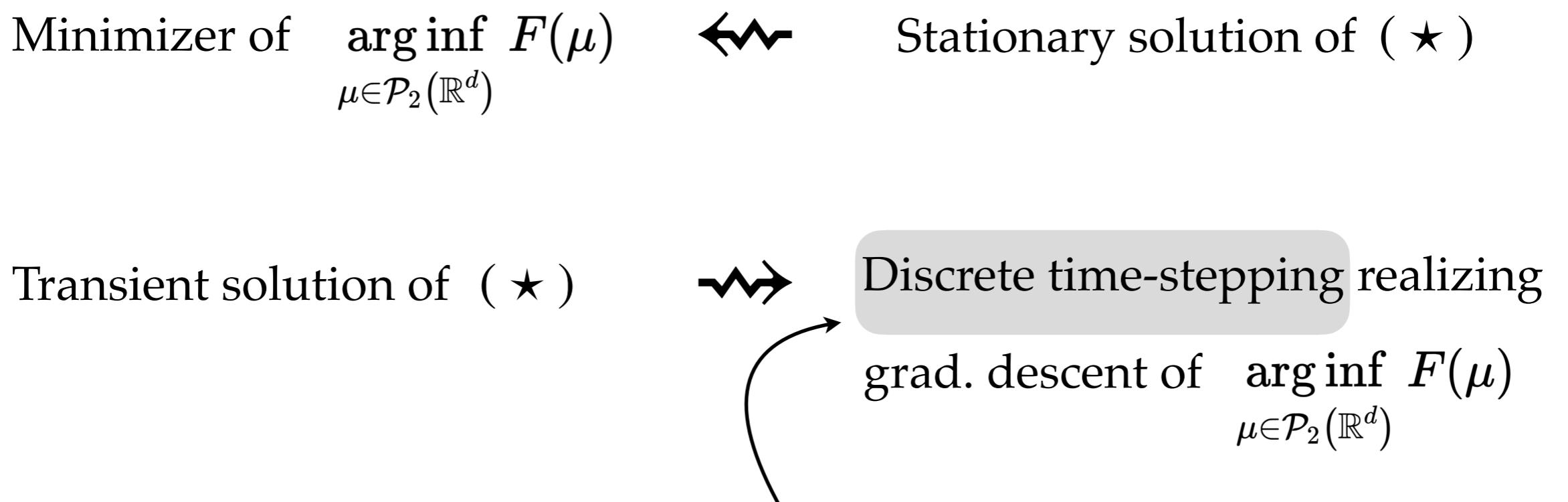
Wasserstein gradient



# Connection with Wasserstein Gradient Flows

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

Wasserstein gradient



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

# Gradient Flows

## Gradient Flow in $\mathcal{X}$

$$\frac{d\mathbf{x}}{dt} = -\nabla f(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0$$

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

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

### Recursion:

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

### Recursion:

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

### Convergence:

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

### Convergence:

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

### $f$ as Lyapunov function:

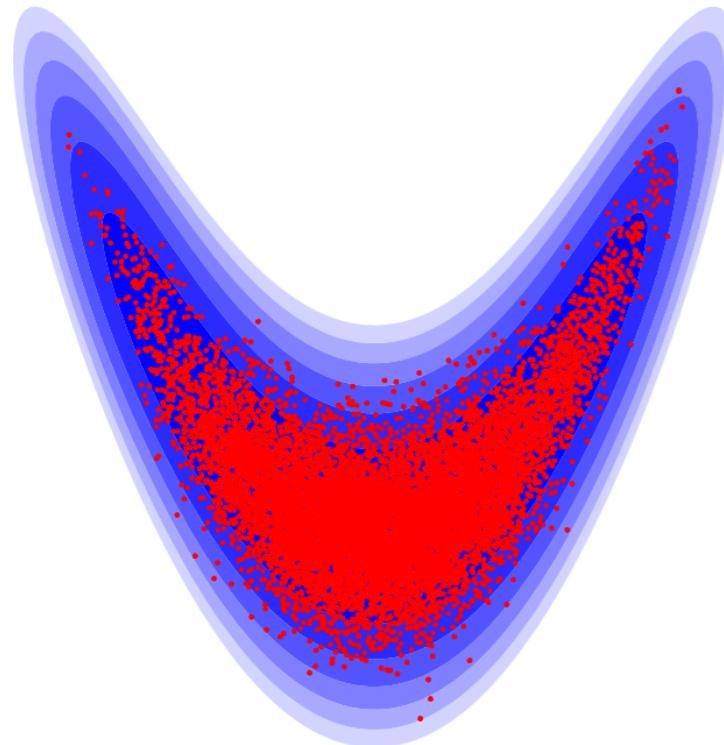
$$\frac{d}{dt} f = - \|\nabla f\|_2^2 \leq 0$$

### $F$ as Lyapunov functional:

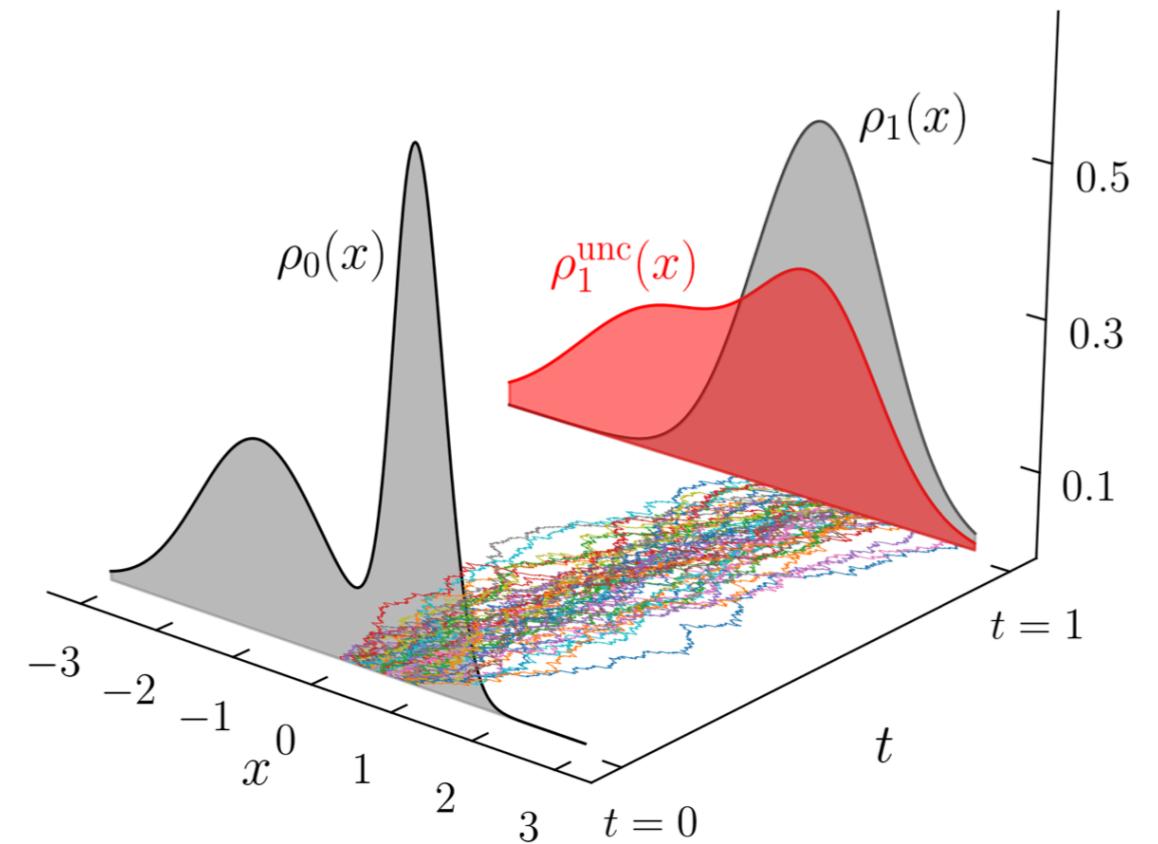
$$\frac{d}{dt} F = -\mathbb{E}_\mu \left[ \left\| \nabla \frac{\delta F}{\delta \mu} \right\|_2^2 \right] \leq 0$$

# Motivating Applications

Langevin sampling from  
an unnormalized prior



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



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

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

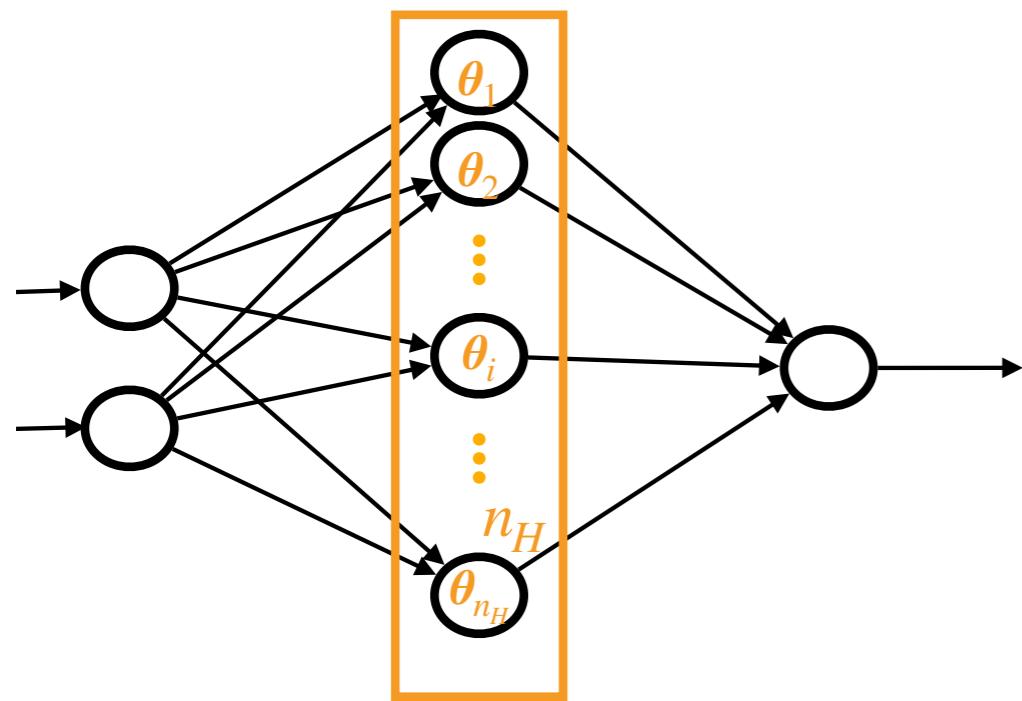
Chen, Georgiou and Pavon, *SIAM Journal on Applied Mathematics*, 2016

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

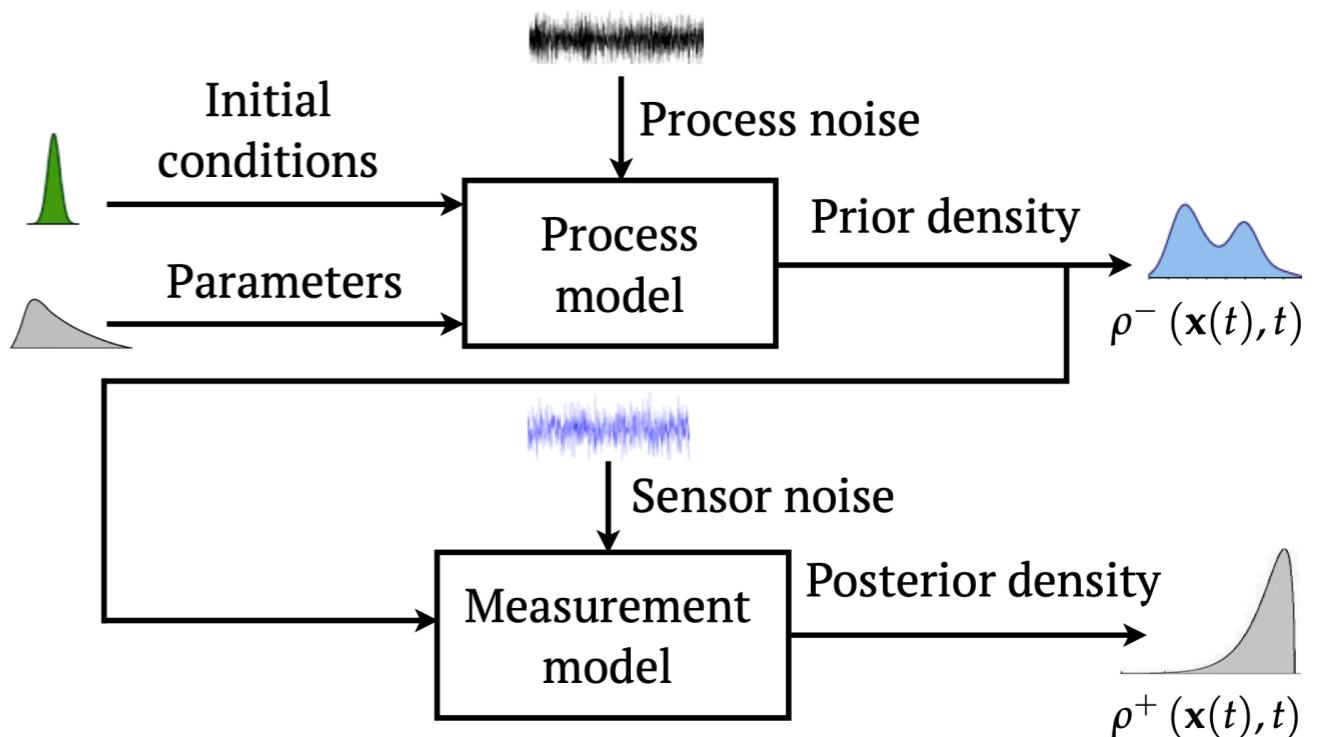
Caluya and Halder, *IEEE Transactions on Automatic Control*, 2021

# 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

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But all require centralized computing

# Centralized Computing Can Become Intensive: Mean Field SGD Dynamics in NN Classification

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

For quadratic loss:

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

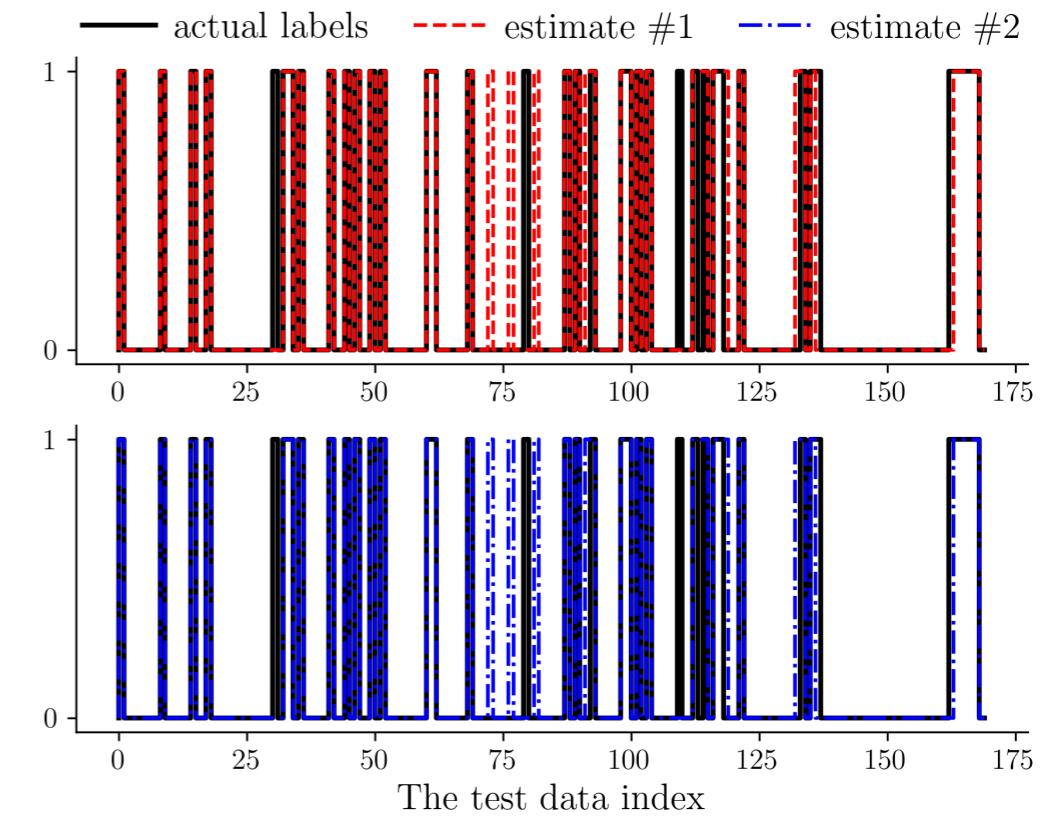
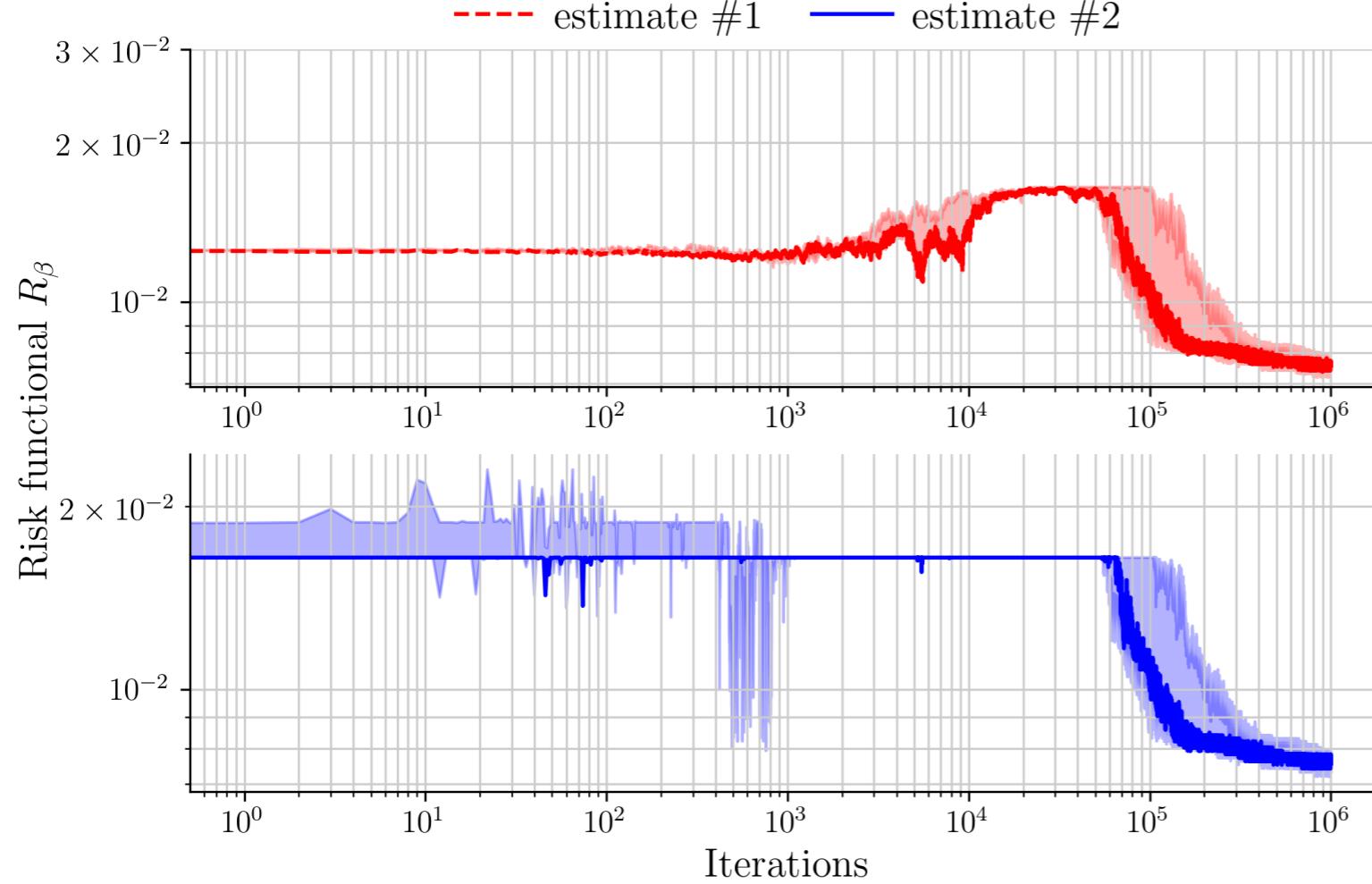
depend on activation functions of the NN

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

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

# Centralized Computing can become intensive: 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 ( $\approx 33$  hrs runtime)

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

# Specific Instances of Additive Objective

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

## Maximum likelihood deconvolution

$Y_i = X_i + Z_i, \quad X \sim \mu$  (unknown), PDF of  $Z$  is  $\rho_Z$  (known)

$$F_i(\mu) = -\log \left( \int \rho_Z(Y_i - x) d\mu(x) \right)$$

If  $\rho_Z = \mathcal{N}(0, \varepsilon^2)$

then the optimizer is the projection:

$$\arg \inf_{\mu \in \mathcal{P}_2} W_\varepsilon^2 \left( \mu, \frac{1}{n} \sum_{i=1}^n \delta_{Y_i} \right)$$

C. R. Acad. Sci. Paris, Ser. I 356 (2018) 1228–1235



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C. R. Acad. Sci. Paris, Ser. I

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Statistics

Entropic optimal transport is maximum-likelihood deconvolution

*Le transport optimal entropique correspond à l'estimateur du maximum de vraisemblance en déconvolution*

Philippe Rigollet, Jonathan Weed

*Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA, USA*



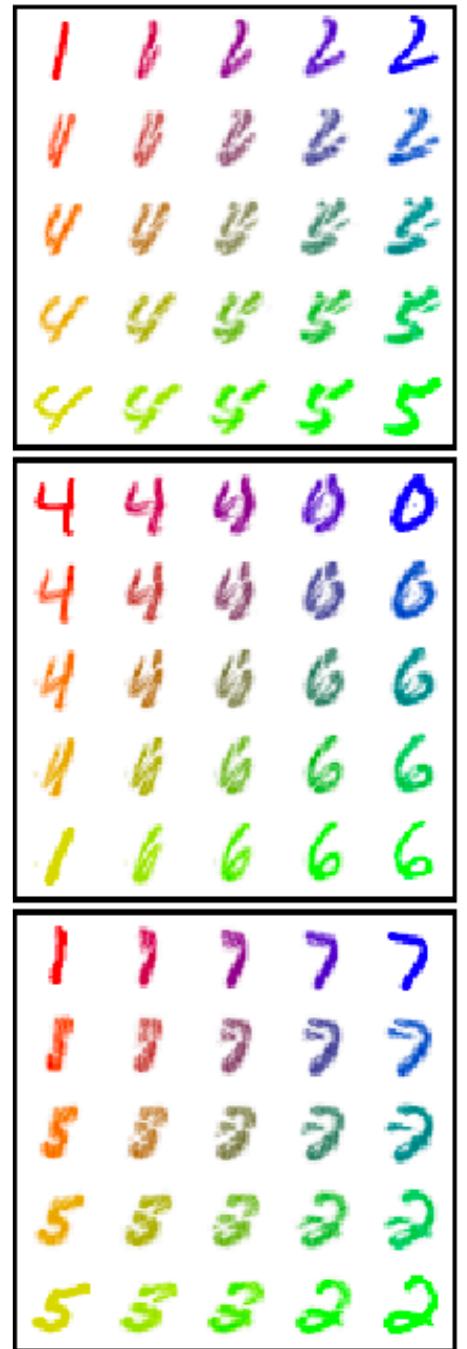
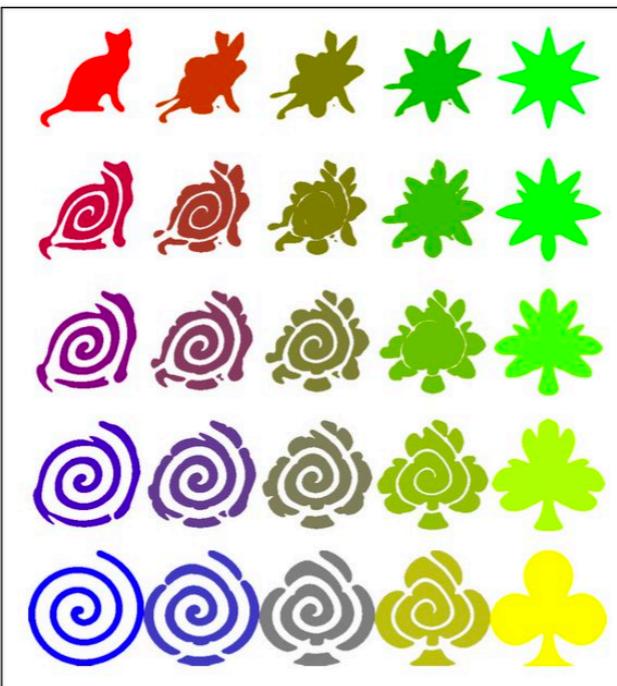
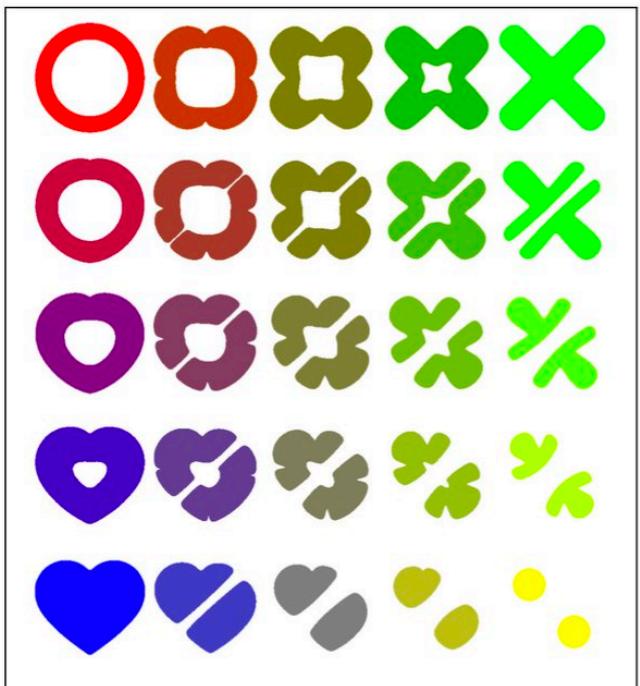
# Specific Instances of Additive Objective

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

Wasserstein Barycenter of measures

Unregularized:  $F_i(\mu) = w_i W^2(\mu, \mu_i), \quad w_i \geq 0$

Sinkhorn-regularized:  $F_i(\mu) = w_i W_\varepsilon^2(\mu, \mu_i), \quad w_i \geq 0$



# Our Present Work: Distributed Algorithm

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

# Our Present Work: Distributed Algorithm

Main idea:

$$\arg \inf_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} F_1(\mu) + F_2(\mu) + \dots + F_n(\mu)$$

 re-write

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

# Our Present Work: Distributed Algorithm

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Main idea:

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Define Wasserstein augmented Lagrangian:

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

↑ regularization > 0      ↑ ( Lagrange multipliers

# Proposed Consensus ADMM

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

# Proposed Consensus ADMM

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\nu_i^{k+1} &= \nu_i^k + \alpha(\mu_i^{k+1} - \zeta^{k+1})
\end{aligned}
\quad \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

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

# Proposed Consensus ADMM (contd.)

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\cdot) + \int \nu_i^k d(\cdot))}^W(\zeta^k)$$

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

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

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

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

# Proposed Consensus ADMM (contd.)

$$\mu_i^{k+1} = \text{prox}_{\frac{1}{\alpha}(F_i(\cdot) + \int \nu_i^k d(\cdot))}^W(\zeta^k)$$

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

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

**Examples:**

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

# Discrete Version of the Proposed ADMM

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

Euclidean distance matrix  
where  $N$  is the number of samples

# Discrete Version of the Proposed ADMM

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

With Sinkhorn regularization:

Discrete Sinkhorn divergence

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

# Discrete Version of the Proposed ADMM

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

With Sinkhorn regularization:

Outer layer ADMM

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

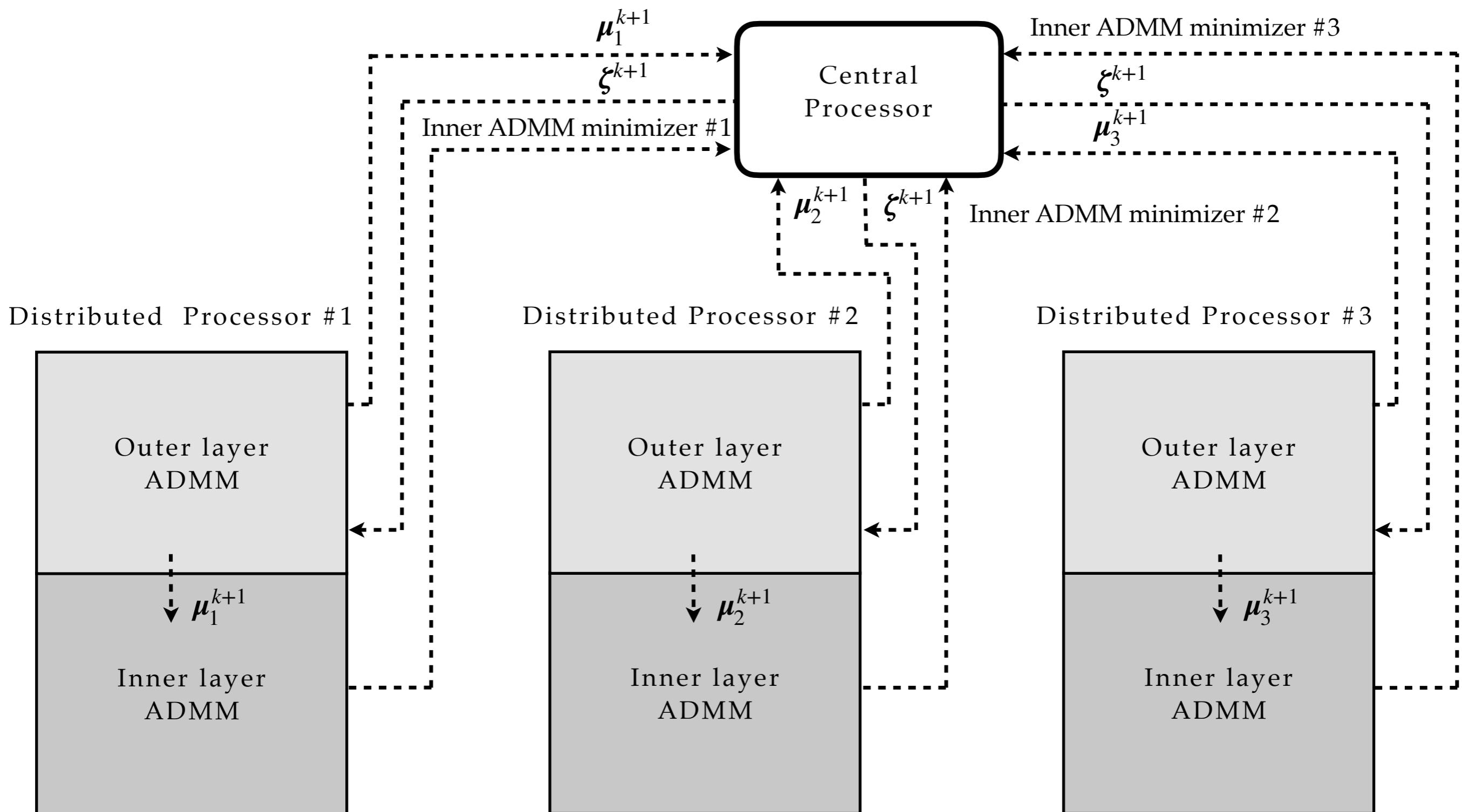
Discrete Sinkhorn divergence

$$\begin{aligned}
&= \arg \inf_{\boldsymbol{\mu}_i \in \Delta^{N-1}} \left\{ \min_{\boldsymbol{M} \in \Pi_N(\boldsymbol{\mu}_i, \boldsymbol{\zeta}^k)} \left\langle \frac{1}{2} \boldsymbol{C} + \varepsilon \log \boldsymbol{M}, \boldsymbol{M} \right\rangle + \frac{1}{\alpha} (F_i(\boldsymbol{\mu}_i) + \langle \boldsymbol{\nu}_i^k, \boldsymbol{\mu}_i \rangle) \right\}
\end{aligned}$$

Inner layer ADMM

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

# Overall Schematic



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

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

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

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

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

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

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

$\uparrow$   
 Convex

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

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

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

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

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

**Theorem.**

Consider the convex problem

$$(\mathbf{u}_1^{\text{opt}}, \dots, \mathbf{u}_n^{\text{opt}}) = \arg \min_{(\mathbf{u}_1, \dots, \mathbf{u}_n) \in \mathbb{R}^{nN}} \sum_{i=1}^n \langle \boldsymbol{\mu}_i^{k+1}, \log(\Gamma \exp(\mathbf{u}_i/\varepsilon)) \rangle$$

(♥)

subject to  $\sum_{i=1}^n \mathbf{u}_i = \frac{2}{\alpha} \boldsymbol{\nu}_{\text{sum}}^k$ .

Then

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

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

**Theorem.**

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

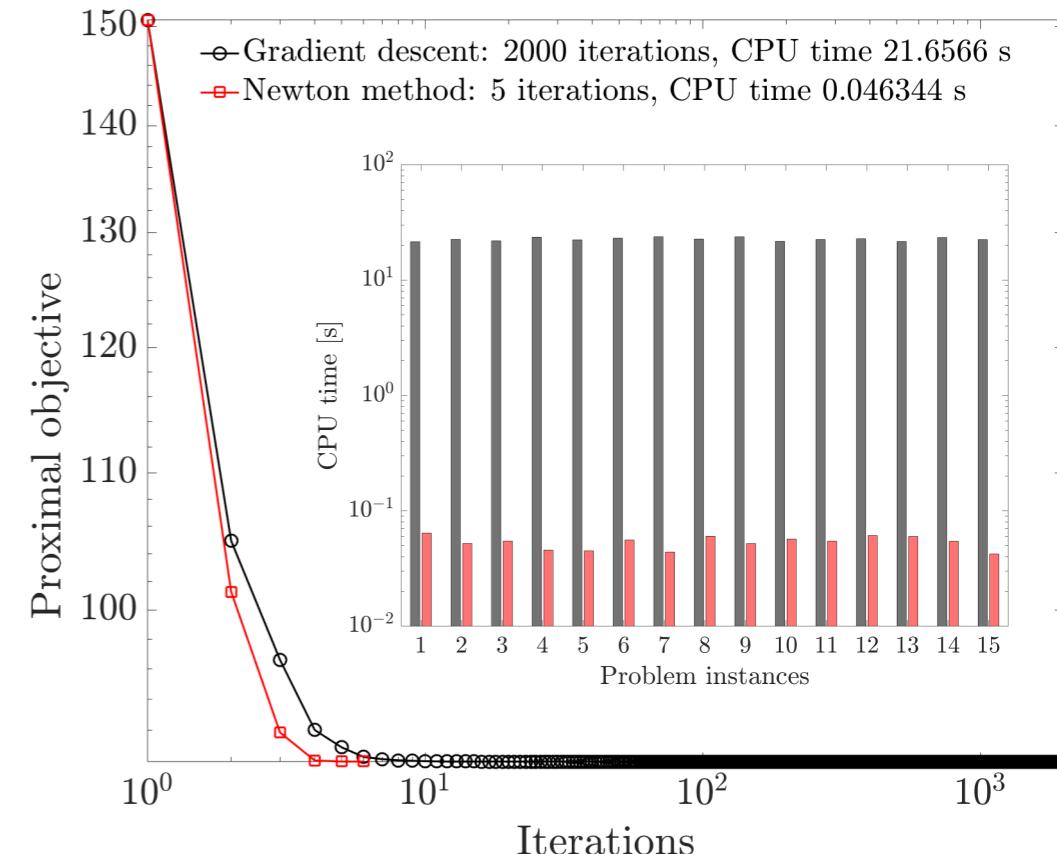
Then the following Euclidean ADMM solves (♥)

$$\mathbf{u}_i^{\ell+1} = \text{prox}_{\frac{1}{\tau} f_i}^{\|\cdot\|_2} (\mathbf{z}_i^\ell - \tilde{\boldsymbol{\nu}}_i^\ell)$$

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

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

$$\tilde{\boldsymbol{\nu}}_i^{\ell+1} = \tilde{\boldsymbol{\nu}}_i^\ell + (\mathbf{u}_i^{\ell+1} - \mathbf{z}_i^{\ell+1})$$



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

**Theorem.**

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

Then the following Euclidean ADMM solves (♥)

$$\mathbf{u}_i^{\ell+1} = \text{prox}_{\frac{1}{\tau} f_i}^{\|\cdot\|_2} (\mathbf{z}_i^\ell - \tilde{\boldsymbol{\nu}}_i^\ell)$$

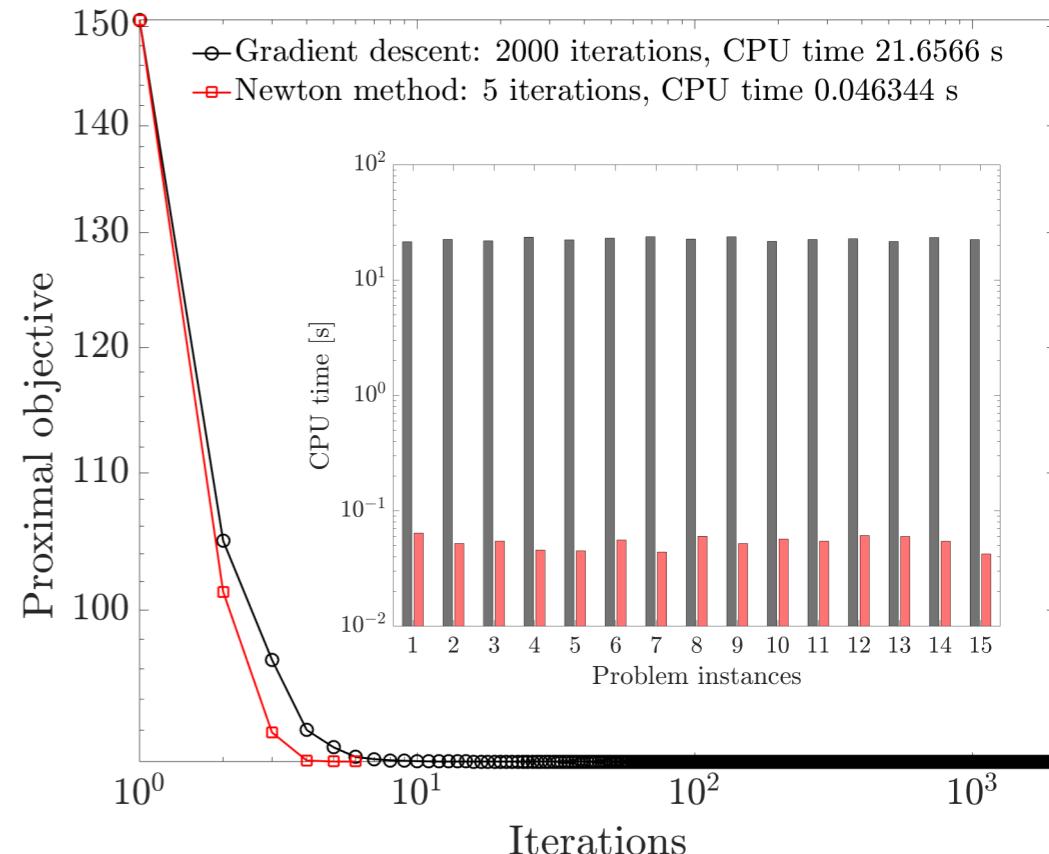
No analytical solution, use e.g.,  
Newton's method (has structured Hess)

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

$$\tilde{\boldsymbol{\nu}}_i^{\ell+1} = \tilde{\boldsymbol{\nu}}_i^\ell + (\mathbf{u}_i^{\ell+1} - \mathbf{z}_i^{\ell+1})$$

**Theorem (informal).**

Guaranteed convergence for inner layer ADMM  
under some constraints on hyper-parameters



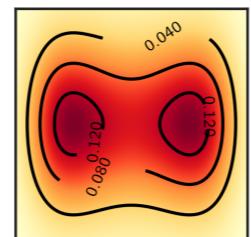
# Experiment #1

## Linear Fokker-Planck-Kolmogorov PDE

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

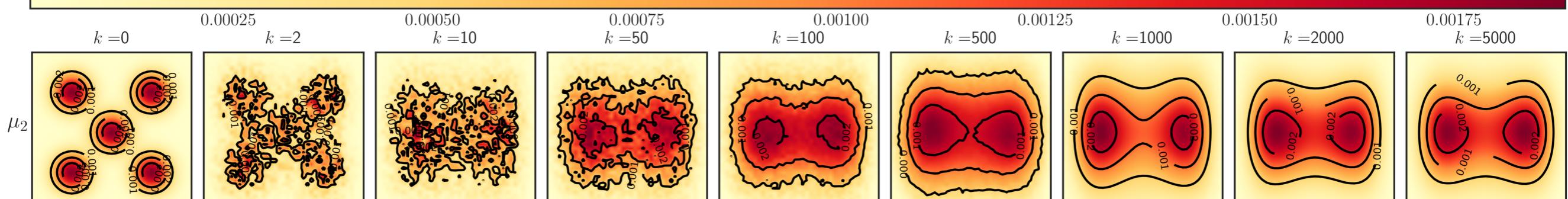
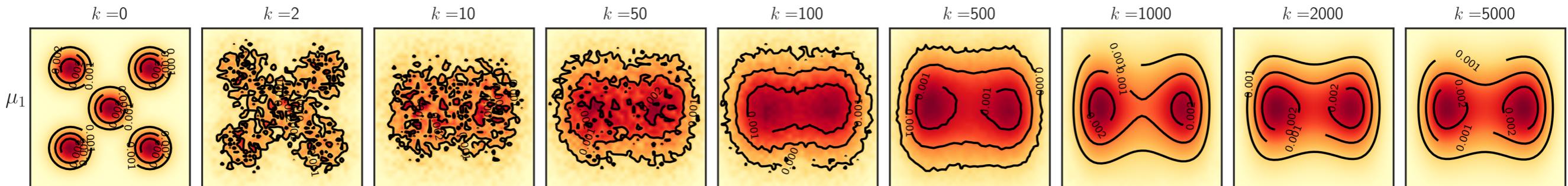
$$V(x_1, x_2) = \frac{1}{4} (1 + x_1^4) + \frac{1}{2} (x_2^2 - x_1^2)$$

$$\mu_\infty \propto \exp(-\beta V(x_1, x_2)) dx_1 dx_2$$



## Distributed computation:

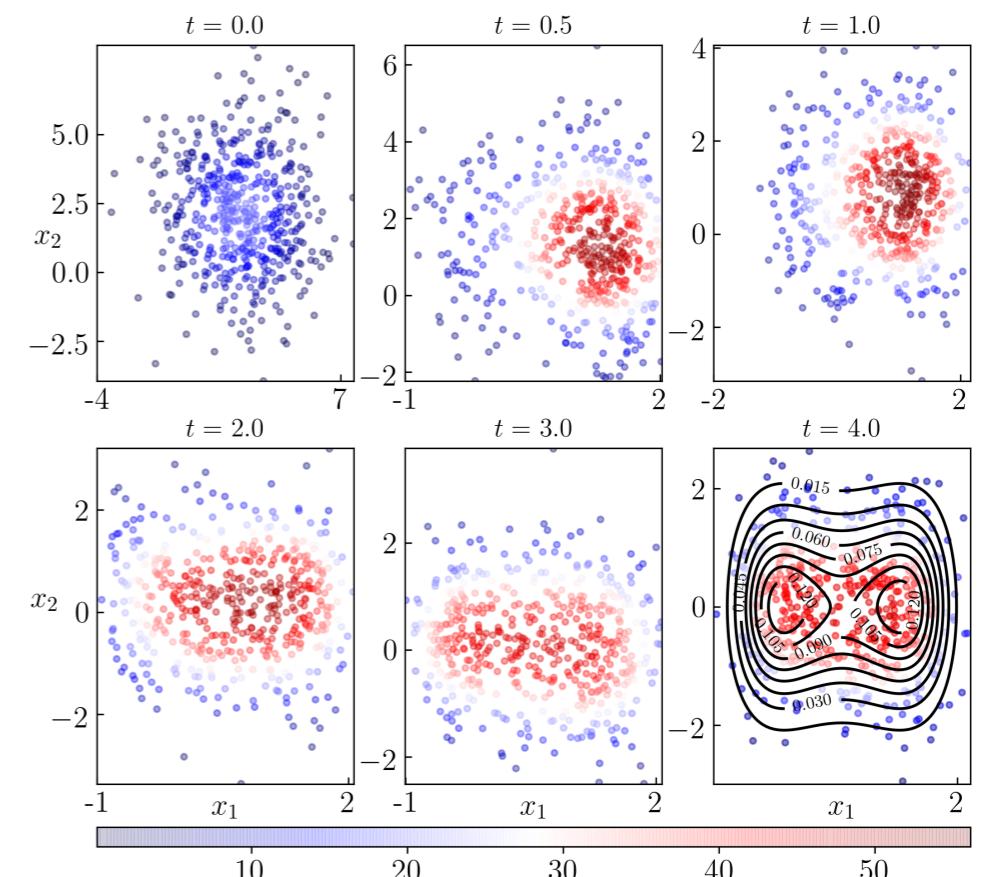
$$F_1(\mu) = \langle V_k, \mu \rangle \quad F_2(\mu) = \langle \beta^{-1} \log \mu, \mu \rangle$$



## Centralized computation:

Caluya and Halder, IEEE Trans. Automatic Control, 2019

—  $\rho_{\infty \text{analytical}} = \frac{1}{Z} \exp(-\beta \psi(x_1, x_2))$  ●  $\rho_{\text{proximal}}$



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

# Experiment #2

Aggregation-drift-diffusion nonlinear PDE

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

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

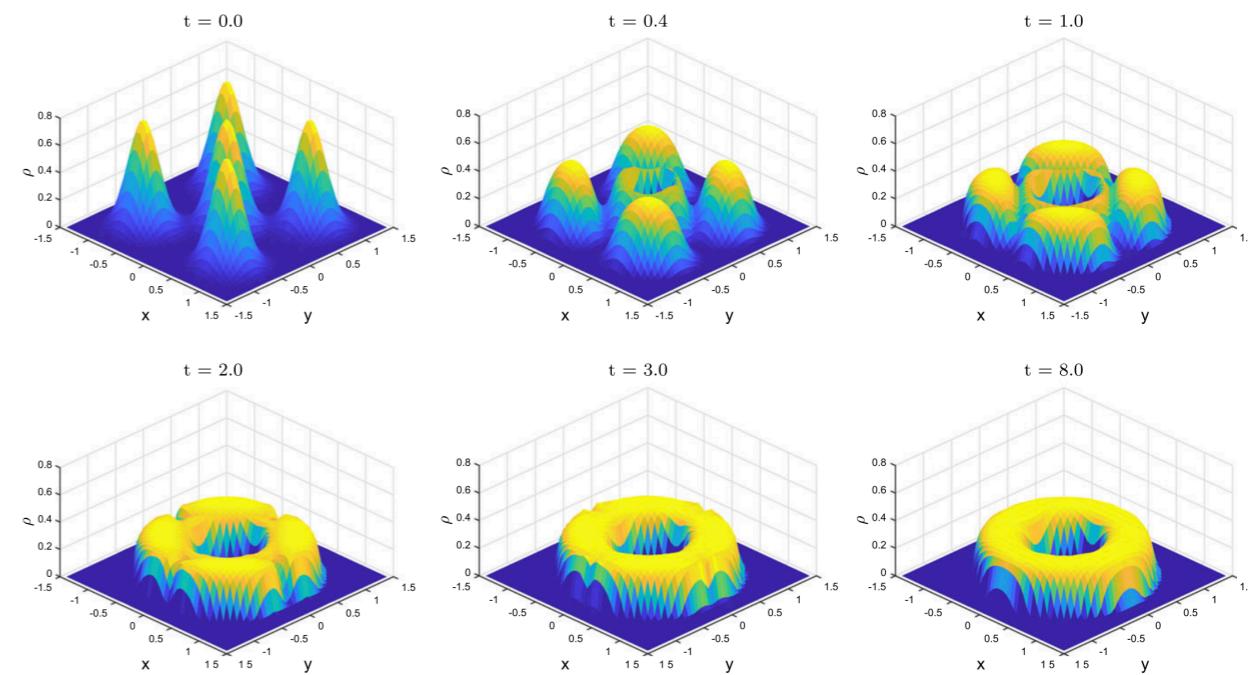
$$V(\mathbf{x}) = -\frac{1}{4} \ln \|\mathbf{x}\|_2$$

Distributed computation:

$$F_1(\mu) = \langle U_k \mu, \mu \rangle \quad F_2(\mu) = \langle V_k + \beta^{-1} \log \mu, \mu \rangle$$

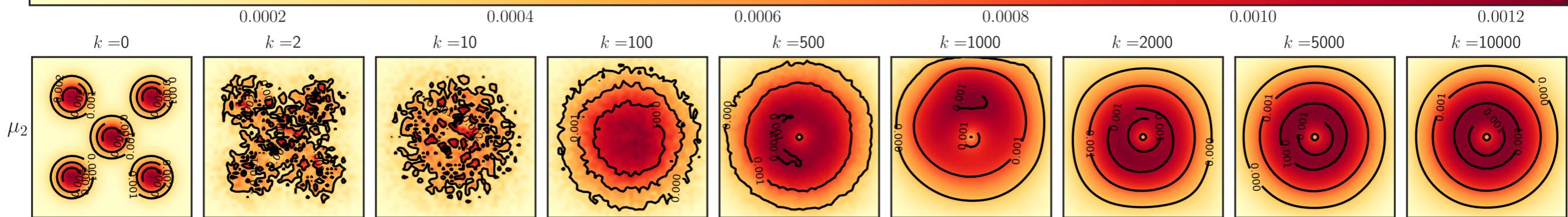
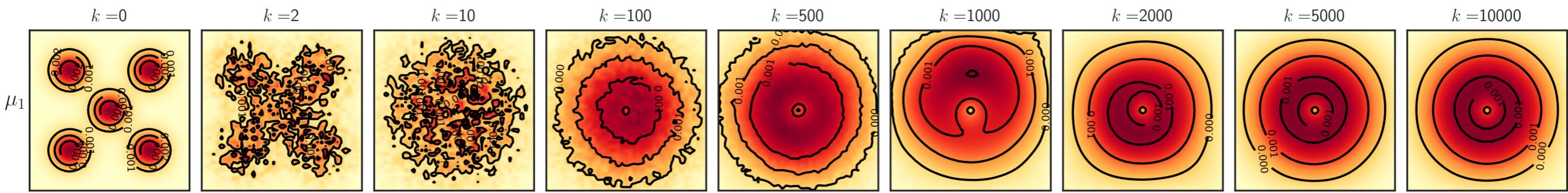
Centralized computation:

Carrillo, Craig, Wang and Wei, FOCM, 2021



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

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



# Experiment #2 (contd.)

Aggregation-drift-diffusion nonlinear PDE

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

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

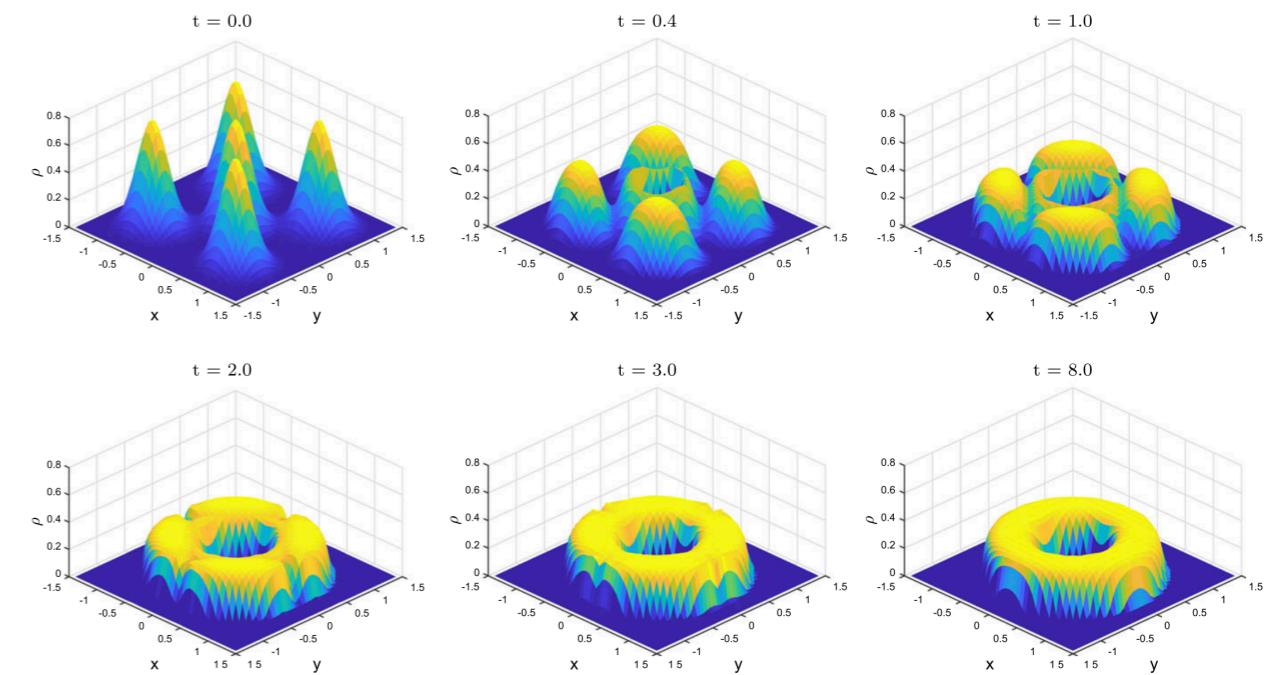
$$V(\mathbf{x}) = -\frac{1}{4} \ln \|\mathbf{x}\|_2$$

Distributed computation:

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

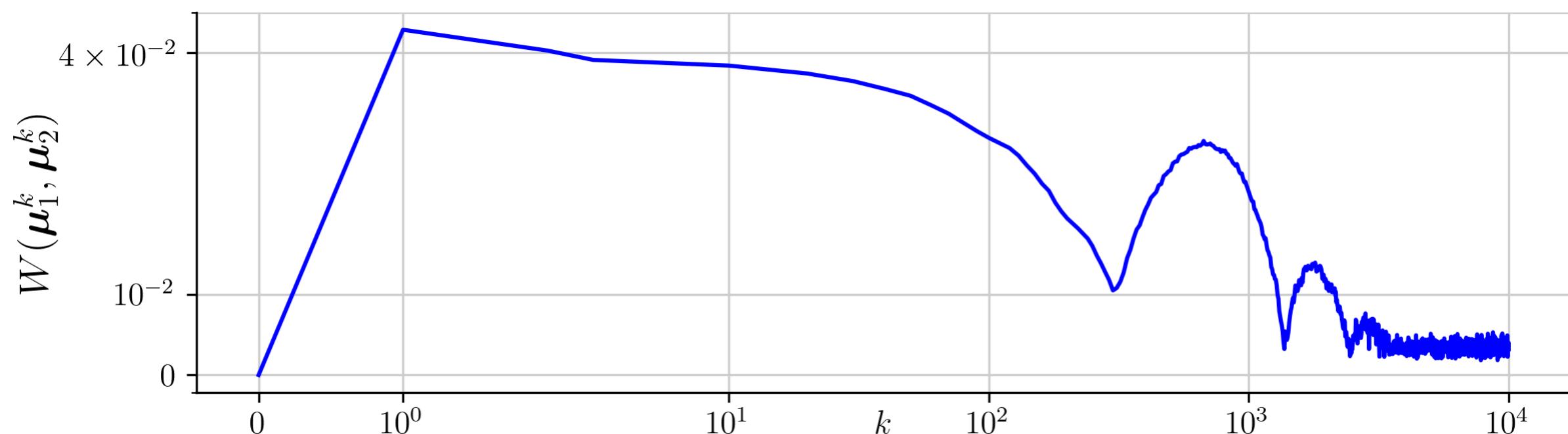
Centralized computation:

Carrillo, Craig, Wang and Wei, FOCM, 2021



$$\lim_{\beta^{-1} \downarrow 0} \boldsymbol{\mu}_\infty = \text{Unif}(\mathcal{A})$$

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



# Experiment #2 (contd.)

$B_n$  is  $n$ th Bell number, e.g.,  
 $B_2 = 2, B_3 = 5, B_4 = 15, B_5 = 52, \dots$

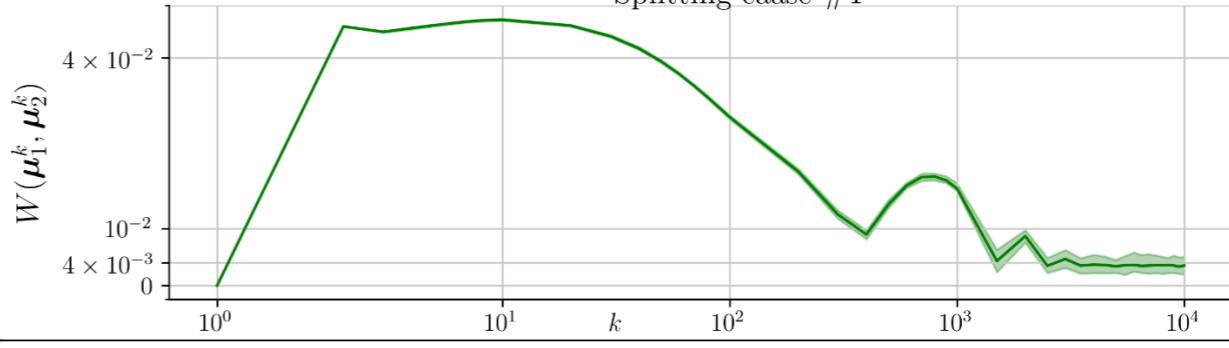
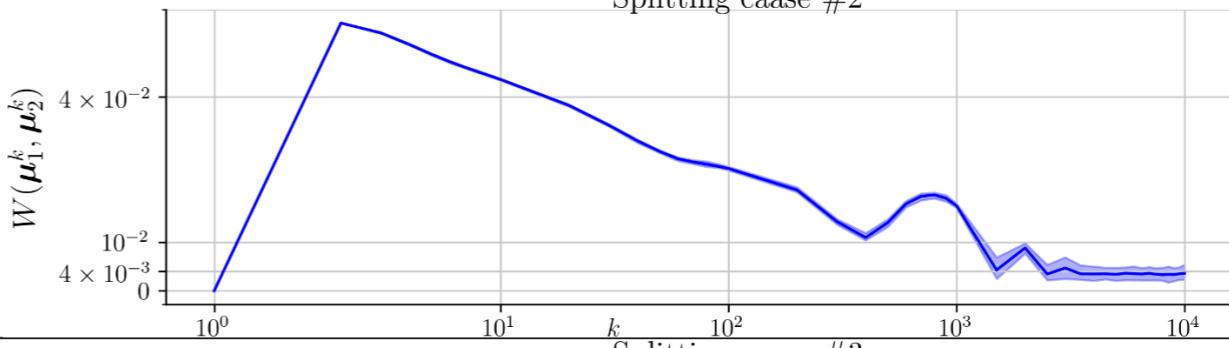
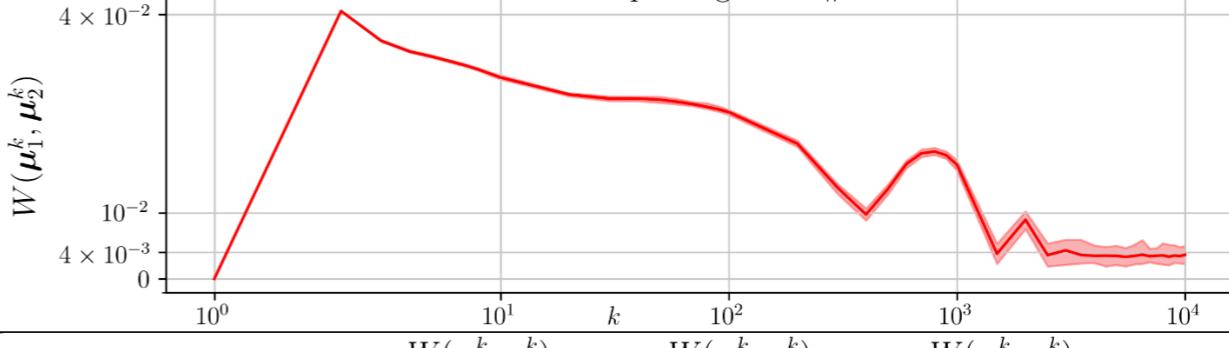
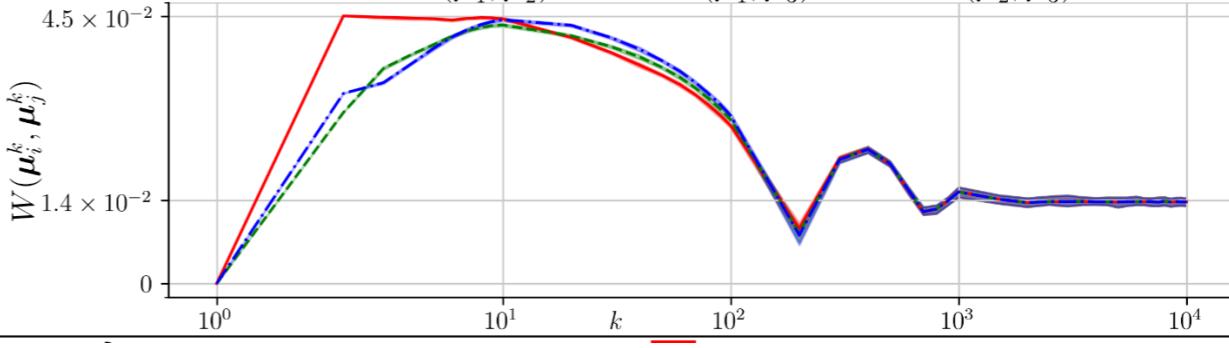
100 run statistics for each of the 4 ways of splitting: ( $B_n - 1$  ways in general)

Splitting case	Functionals	Wasserstein distance
#1	$F_1(\mu) = \langle \mathbf{V}_k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{U}_k \mu^k, \mu \rangle$	<p>Plot of Wasserstein distance <math>W(\mu_1^k, \mu_2^k)</math> versus iteration <math>k</math> (log scale from <math>10^0</math> to <math>10^4</math>). The green curve shows an initial rise followed by oscillations around a value of approximately <math>10^{-2}</math>.</p>
#2	$F_1(\mu) = \langle \mathbf{U}_k \mu^k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{V}_k, \mu \rangle$	<p>Plot of Wasserstein distance <math>W(\mu_1^k, \mu_2^k)</math> versus iteration <math>k</math> (log scale from <math>10^0</math> to <math>10^4</math>). The blue curve shows an initial rise followed by oscillations around a value of approximately <math>10^{-2}</math>.</p>
#3	$F_1(\mu) = \langle \mathbf{U}_k \mu^k + \mathbf{V}_k, \mu \rangle,$ $F_2(\mu) = \langle \beta^{-1}\mu, \mu \rangle$	<p>Plot of Wasserstein distance <math>W(\mu_1^k, \mu_2^k)</math> versus iteration <math>k</math> (log scale from <math>10^0</math> to <math>10^4</math>). The red curve shows an initial rise followed by oscillations around a value of approximately <math>10^{-2}</math>.</p>
#4	$F_1(\mu) = \langle \mathbf{V}_k, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{U}_k \mu^k \rangle,$ $F_3(\mu) = \langle \beta^{-1}\mu, \mu \rangle$	<p>Plot of Wasserstein distances <math>W(\mu_i^k, \mu_j^k)</math> versus iteration <math>k</math> (log scale from <math>10^0</math> to <math>10^4</math>). Three curves are shown: red for <math>W(\mu_1^k, \mu_2^k)</math>, green for <math>W(\mu_1^k, \mu_3^k)</math>, and blue for <math>W(\mu_2^k, \mu_3^k)</math>. All three curves peak at <math>k=1</math> and then decay towards zero.</p>

# Experiment #2 (contd.)

Centralized av. runtime = 310.21 s

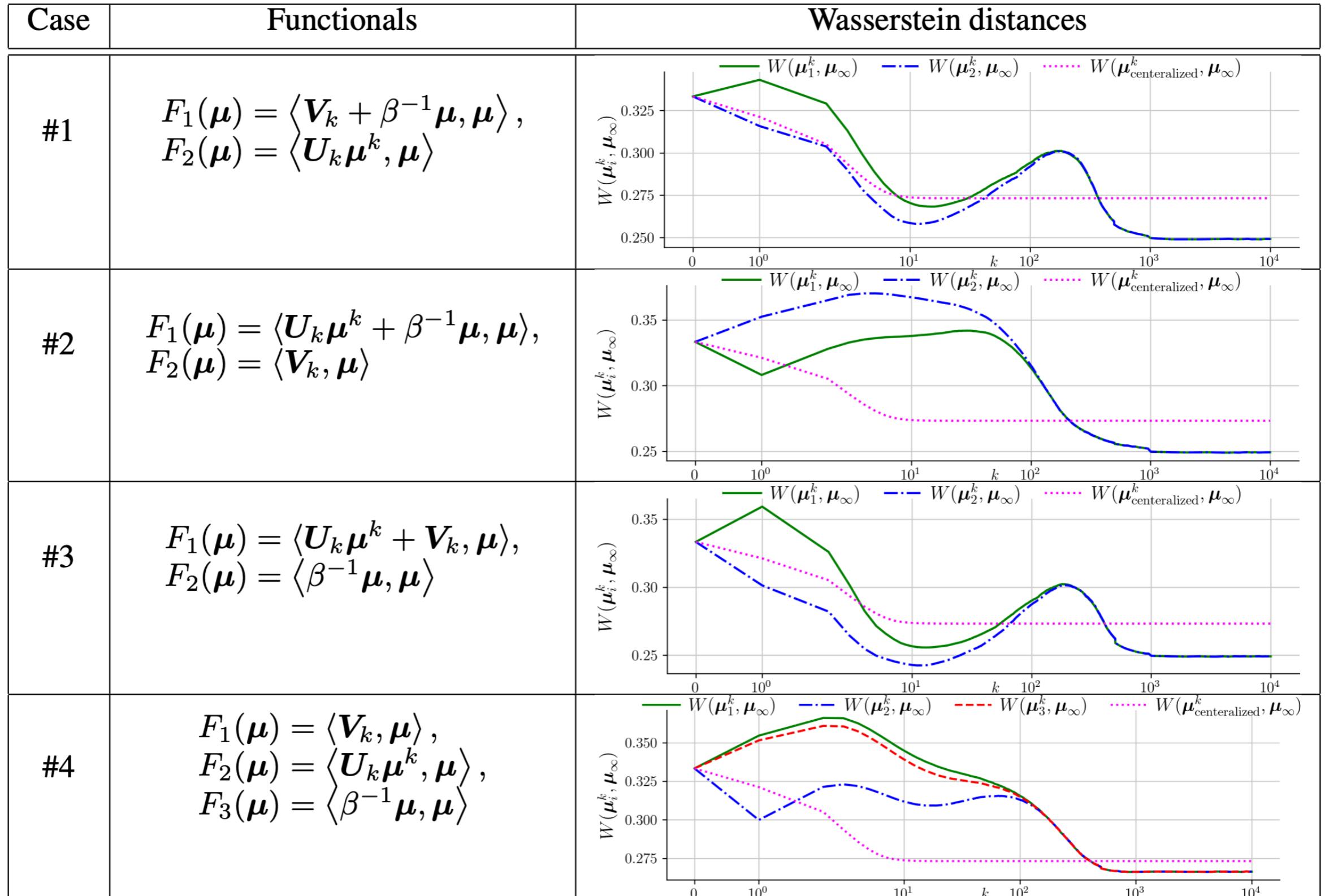
100 run statistics for each of the 4 ways of splitting: ( $B_n - 1$  ways in general)

Splitting case	Functionals	Wasserstein distance
#1	$F_1(\mu) = \langle \mathbf{V}_k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{U}_k \mu^k, \mu \rangle$  <span style="color: red;">av. runtime = 294.06 s</span>	 <p>Splitting caase #1</p>
#2	$F_1(\mu) = \langle \mathbf{U}_k \mu^k + \beta^{-1}\mu, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{V}_k, \mu \rangle$  <span style="color: red;">av. runtime = 285.32 s</span>	 <p>Splitting caase #2</p>
#3	$F_1(\mu) = \langle \mathbf{U}_k \mu^k + \mathbf{V}_k, \mu \rangle,$ $F_2(\mu) = \langle \beta^{-1}\mu, \mu \rangle$  <span style="color: red;">av. runtime = 289.87 s</span>	 <p>Splitting caase #3</p>
#4	$F_1(\mu) = \langle \mathbf{V}_k, \mu \rangle,$ $F_2(\mu) = \langle \mathbf{U}_k \mu^k \rangle,$ $F_3(\mu) = \langle \beta^{-1}\mu, \mu \rangle$  <span style="color: red;">av. runtime = 108.99 s</span>	 <p><math>W(\mu_1^k, \mu_2^k)</math> <math>W(\mu_1^k, \mu_3^k)</math> <math>W(\mu_2^k, \mu_3^k)</math></p>

# Experiment #2 (contd.)

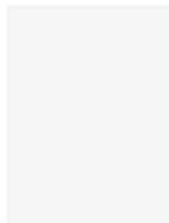
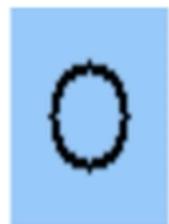
Centralized is pink dotted (repeated in subplots)

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

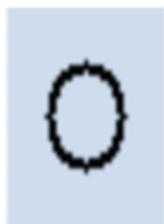


# Experiment #3

Sinkhorn regularized barycenter



Distributed Processor #1



Distributed Processor #2



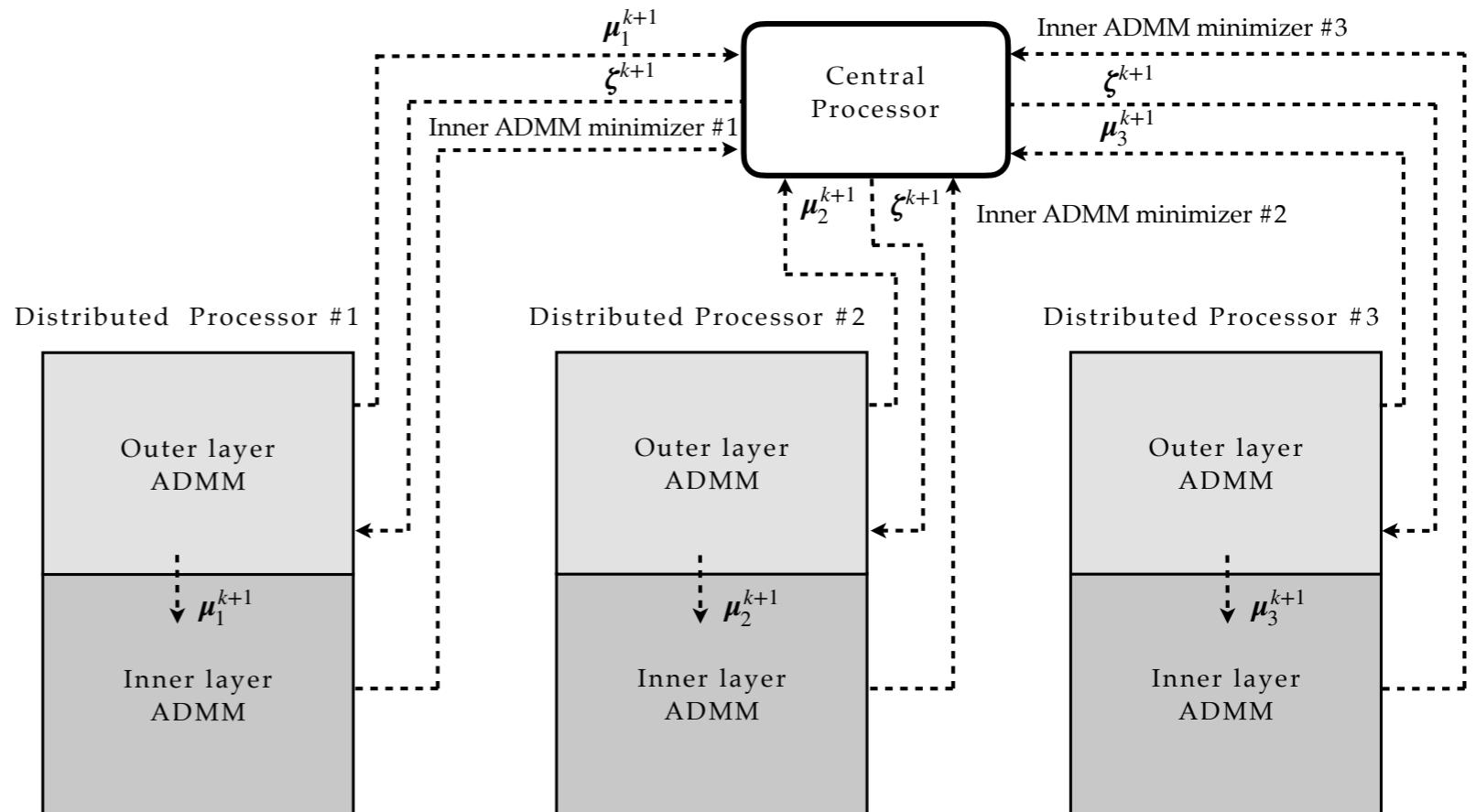
Distributed Processor #3

# Summary

Distributed computation for measure-valued optimization

Realizes measure-valued operator splitting

Takes advantage of the existing proximal and JKO type algorithms



preprint arXiv:2309.07351

# Ongoing

Convergence guarantees for the outer layer ADMM (technically challenging)

Is there an optimal way to split?

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# Thank You

**Support:**



1923278, 2112755, 2111688



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# More Results for Experiment #2

## Effect of Varying the Outer Layer ADMM Barrier Parameter $\alpha$

$\alpha$	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