

# A Machine Learning Framework for High-Dimensional Optimal Transport

Deep Learning and Medical Applications, IPAM January 2020

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<sup>1</sup>Departments of Mathematics and Computer Science, Emory University

<sup>2</sup>Department of Mathematics, University of California Los Angeles

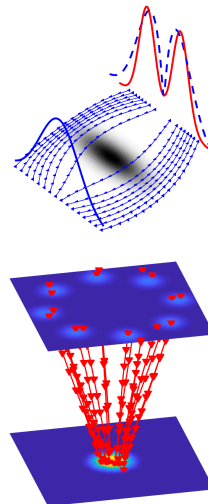
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 [@lruthotto](https://twitter.com/lruthotto)



# Agenda: Machine Learning for Optimal Transport

- ▶ **Background: Low-Dimensional OT**
  - ▶ (Mass-Preserving) Image Registration
- ▶ **Motivation: High-Dimensional OT**
  - ▶ Generative modeling
  - ▶ Challenge: curse of dimensionality
- ▶ **Three Options for OT as Mean Field Game**
  - ▶ macroscopic view: variational problem
  - ▶ microscopic view: coupled optimization problem
  - ▶ Hamilton-Jacobi-Bellman (HJB) equation
- ▶ **Our Framework: Variational approach with**
  - ▶ Lagrangian solver for continuity equation
  - ▶ Neural Network Parameterization
  - ▶ Penalize violations of HJB
- ▶ **Numerical Experiments**



LR, S Osher, W Li, L Nurbekyan, S Wu Fung  
A Machine Learning Framework for Solving  
High-Dimensional Mean Field Game and  
Mean Field Control Problems, arXiv, 2019.

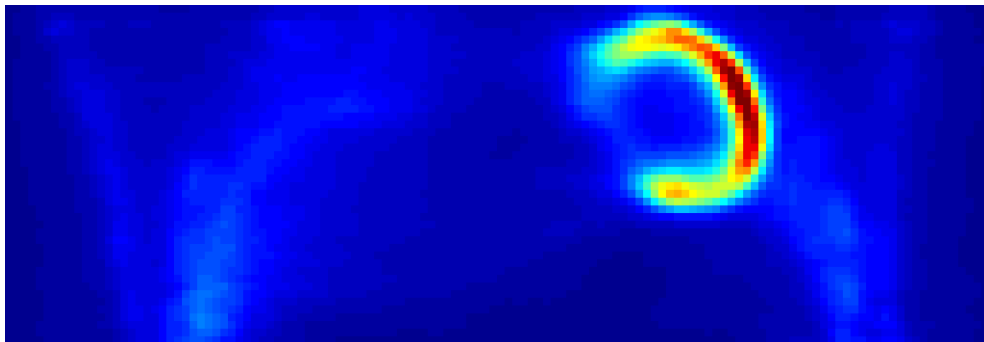


A Mang, LR.  
A Lagrangian Gauss–Newton–Krylov Solver  
for Mass- and Intensity-Preserving  
Diffeomorphic Image Registration. *SIAM  
SISC*,39(5), B5860–B5885 2017.

# Background: Mass-Preserving Image Registration

# Motion Correction of Cardiac PET

- ▶ Fabian Gigengack, Martin Burger, European Institute of Molecular Imaging, University of Münster
- ▶ Otmar Schober, Department of Nuclear Medicine, University of Münster



Thoracic FDG<sup>18</sup> PET, acquisition time  $\approx$  20 min



F. Gigengack, LR, M. Burger, C.H. Wolters,  
X. Jiang, K.P. Schäfers  
*Motion correction in dual gated cardiac PET  
using mass-preserving image registration.*  
IEEE Trans. Med. Imag.; 31(3):698–712, 2012.



LR, F. Gigengack, M. Burger, C.H. Wolters,  
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*A Simplified Pipeline for Motion Correction in  
Dual Gated Cardiac PET.*  
Bildverarbeitung f.d. Medizin: 51–56, 2012.

# Optimal Control Formulation of Image Registration

reference  $\mathcal{R}$ template  $\mathcal{T}$ 

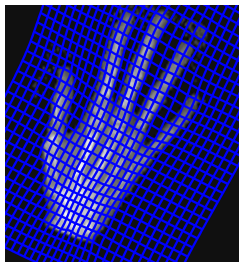
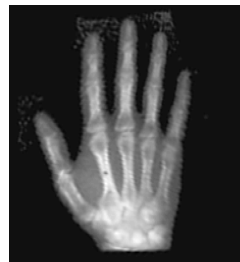
## Optimal Control Problem

Given a template image  $\mathcal{T}$  and a reference image  $\mathcal{R}$  find a **smooth velocity field**  $\mathbf{v}$ , such that the final state  $u(\cdot, 1)$  is **similar** to  $\mathcal{R}$ , i.e., solve

$$\text{minimize}_{\mathbf{v}, u} \quad \text{distance}[u(\cdot, 1), \mathcal{R}] + \text{regularizer}[\mathbf{v}]$$

$$\text{subject to} \quad u(\cdot, 0) = \mathcal{T} \text{ and } \begin{cases} \partial_t u + \mathbf{v} \cdot \nabla u = 0, & \text{intensity preservation} \\ \partial_t u + \nabla \cdot (u\mathbf{v}) = 0, & \text{mass-preservation.} \end{cases}$$

# Optimal Control Formulation of Image Registration

reference  $\mathcal{R}$ template  $\mathcal{T} + y(v)$  $u(\cdot, 1)$ 

## Optimal Control Problem

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# Numerical Methods for Forward Problem

Notation:  $\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N$  states,  $\mathbf{y}_0$  regular grid,  $\Delta t = 1/N$

**Eulerian methods** approximate states on fixed grid for all times

- ▶ Example (Lax-Friedrichs): for all cells,  $i = 1, \dots, n$  do

$$(\mathbf{u}_{k+1})_i = \frac{1}{2} ((\mathbf{u}_k)_{i+1} + (\mathbf{u}_k)_{i-1}) + \frac{\Delta t}{2\Delta x} ((\mathbf{v}_k \odot \mathbf{u}_k)_{i+1} - (\mathbf{v}_k \odot \mathbf{u}_k)_{i-1}).$$

- ▶ Others: Upwind, Lax-Wendroff, ENO (non-differentiable) / WENO (nonlinear in initial condition),...

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**Lagrangian Methods** follow characteristics. Let  $\mathbf{I}$  be an interpolation matrix (sparse,  $\mathbf{I} \geq 0$ , row-sums of 1)

$$\mathbf{u}_N = \mathbf{I}(\mathbf{y}(v, \mathbf{y}_1, 1, 0)) \mathbf{u}_0 \quad \text{or} \quad \mathbf{u}_N = \mathbf{I}(\mathbf{y}(v, \mathbf{y}_0, 0, 1))^T \mathbf{u}_0$$

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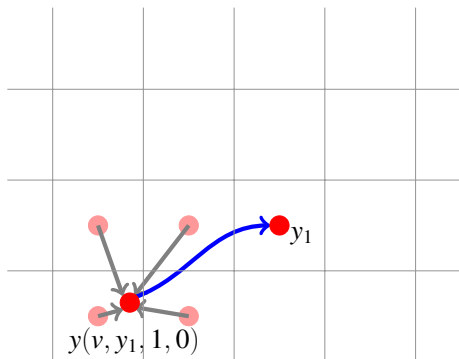
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**Semi-Lagrangian** follow characteristics for short time, interpolate/push, repeat

$$\mathbf{u}_N = \mathbf{I}(\mathbf{y}(v, \mathbf{y}_1, \Delta t, 0))^N \mathbf{u}_0 \quad \text{or} \quad \mathbf{u}_N = (\mathbf{I}(\mathbf{y}(v, \mathbf{y}_0, 0, \Delta t)))^\top)^N \mathbf{u}_0.$$

## Illustration: Lagrangian Methods

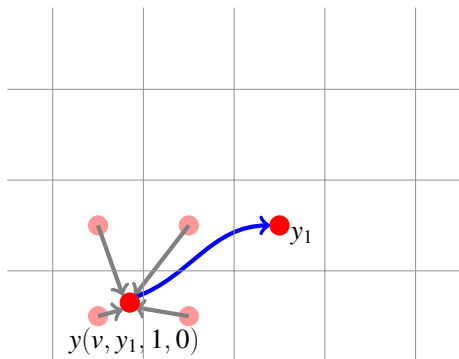
Let  $\mathbf{I}(\cdot) \in \mathbb{R}^{m \times n}$  be an interpolation matrix ( $\mathbf{I} \geq 0$ , sparse, rows sum to one),  
 $\mathbf{y}_0$  be fixed(!) grid point,  $v : \Omega \times [0, 1] \rightarrow \mathbb{R}^d$  velocity



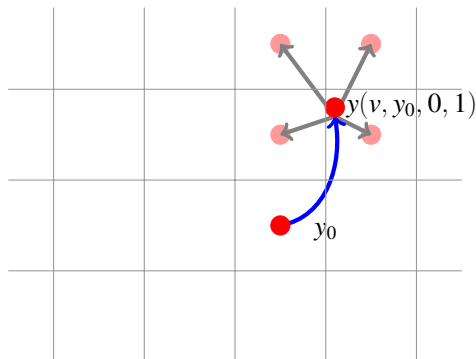
advection,  $u(\mathbf{y}_1, 1) = \mathbf{I}(y(v, \mathbf{y}_1, 1, 0))u_0$

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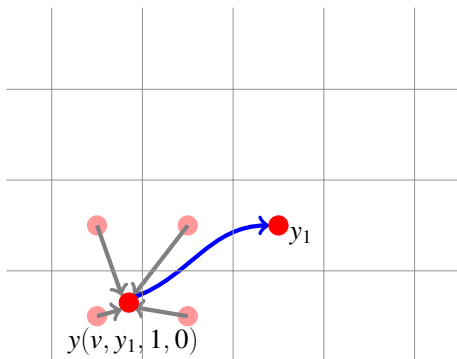
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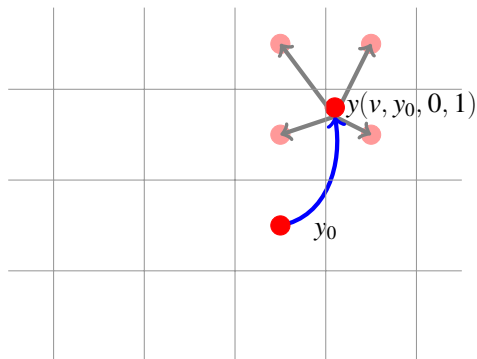
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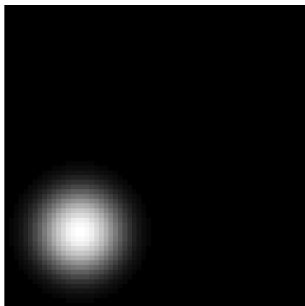


J. Fohring, E. Haber, LR.

Geophysical Imaging of Fluid Flow in Porous Media.

SIAM SISC, 36 (5): S218–S236, Oct. 2014.

# Particle Methods: A 2D Example



$\rho_0$

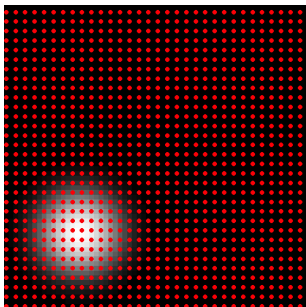
Example: Advection in incompressible flow, Chertock and Kurganov (2006)

$$\rho_t + \nabla \cdot (\vec{u}\rho) = 0, \quad \text{on } \Omega = [0, 1]^2$$

with  $\vec{u}_1(x, t) = (\sin(\pi x_1))^2 \cdot \sin(2\pi x_2) \cdot \cos(\pi t/5).$

$$\vec{u}_2(x, t) = (\sin(\pi x_2))^2 \cdot \sin(2\pi x_1) \cdot \cos(\pi t/5)$$

# Particle Methods: A 2D Example



$\rho_0$  + cell-centred grid

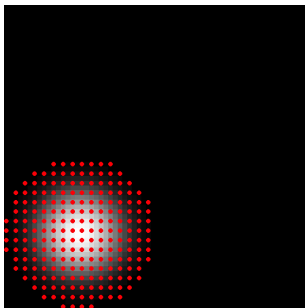
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# Particle Methods: A 2D Example



$\rho_0 + \text{particles}$

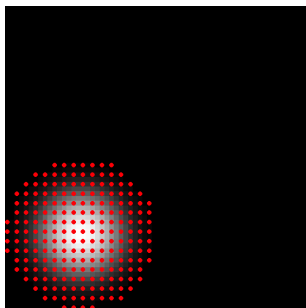
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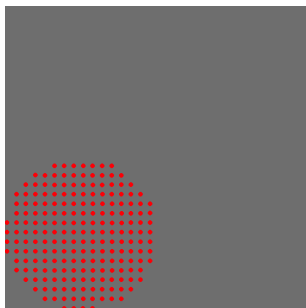
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# Particle Methods: A 2D Example



$\rho_0 + \text{particles}$



particle simulation

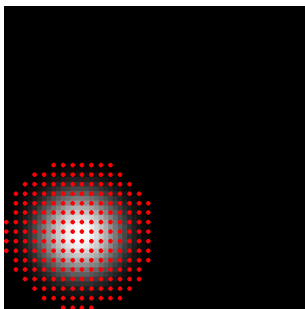
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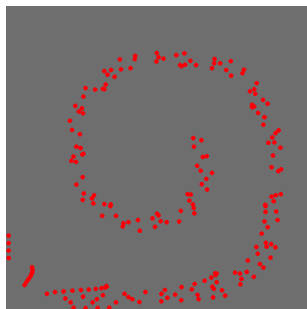
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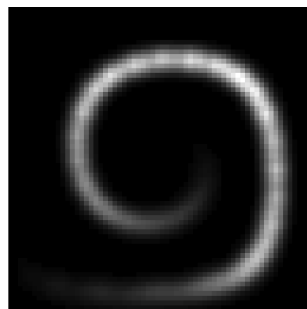
# Particle Methods: A 2D Example



$\rho_0 + \text{particles}$



particles,  $t = 2.5$



$\rho(\cdot, 2.5)$

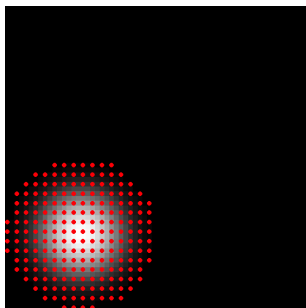
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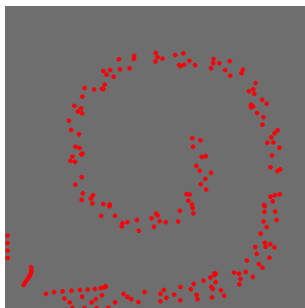
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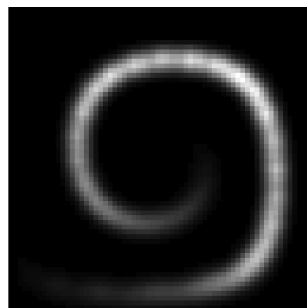
# Particle Methods: A 2D Example



$\rho_0 + \text{particles}$



particle simulation



$\rho(\cdot, 2.5)$

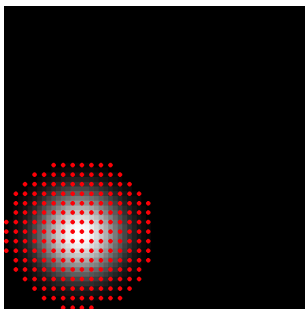
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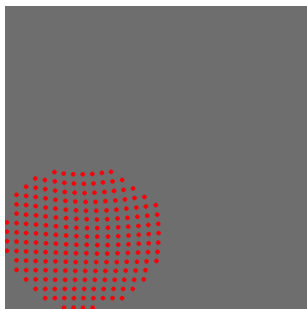
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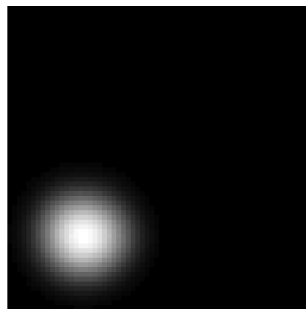
# Particle Methods: A 2D Example



$\rho_0 + \text{particles}$



particles,  $t = 5$



$\rho(\cdot, 5)$

Example: Advection in incompressible flow, Chertock and Kurganov (2006)

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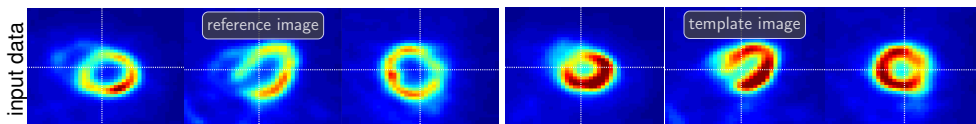
$$\vec{u}_2(x, t) = (\sin(\pi x_2))^2 \cdot \sin(2\pi x_1) \cdot \cos(\pi t/5)$$

# Example: 3D Mass-preserving Registration

levels:  $10^3$ ,  $20^3$ ,  $40^3$

VAMPIRE:  $\alpha_{\text{length}} = 1000$ ,  $\alpha_{\text{vol}} = 10$ , Jacobi-PCG (matrix-free)

MP-LDDMM: non-stationary diffusion,  $n_t = 1$ ,  $\alpha = 100$ , Spectral-PCG, RK4  $N = 2$

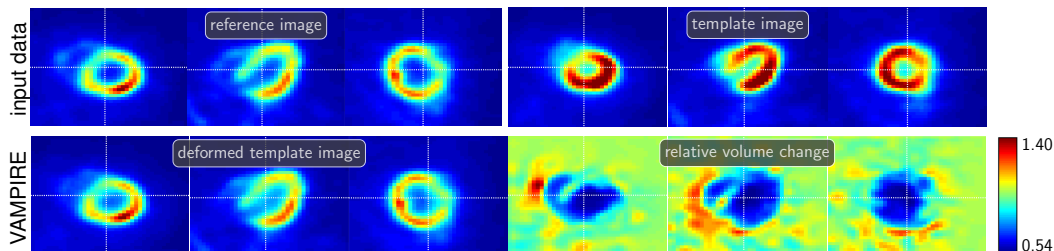


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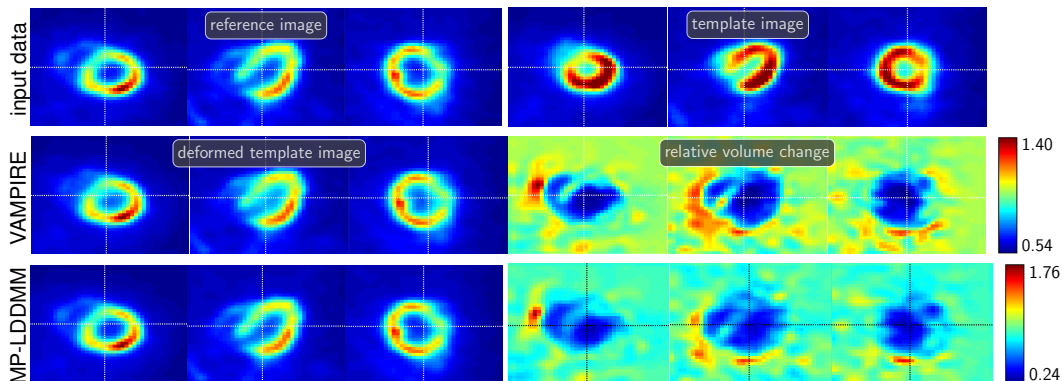


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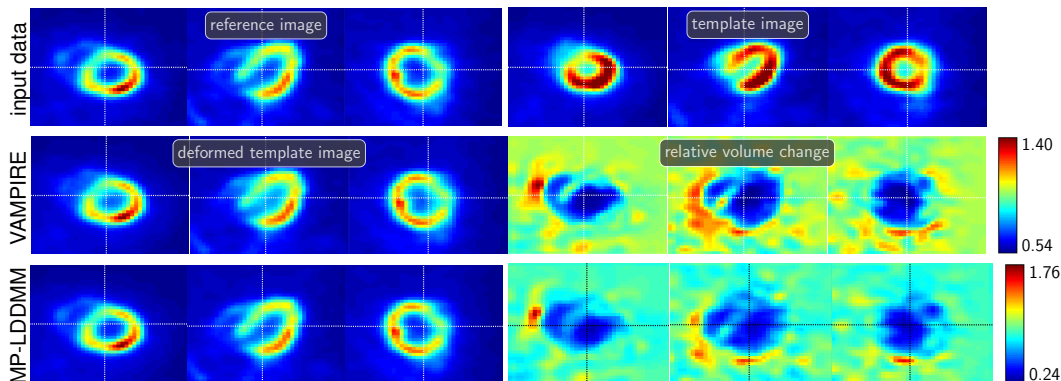


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time-to-solution: VAMPIRE  $\approx 74$  sec, MP-LDDMM  $\approx 36$  sec

# Motivation: High-Dimensional Optimal Transport

# Generative Modeling with Normalizing Flows

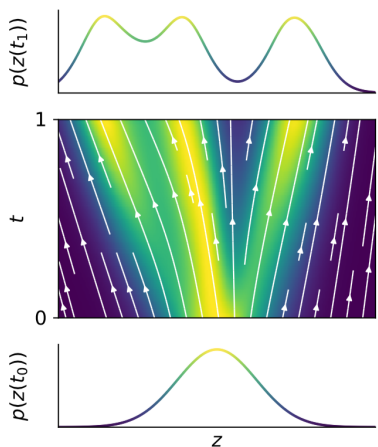







image: Grathwohl et al. 2019

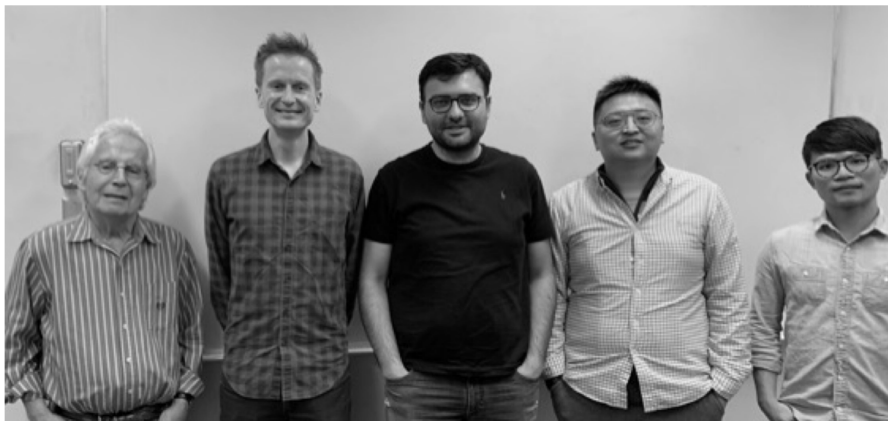
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 Variational Inference with Normalizing Flows.  
*SIAM SISC*,39(5), arXiv, 2015.
- 
 W Grathwohl et al.  
 FFJORD: Free-form Continuous Dynamics for  
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 L Yang, GE Karniadakis  
 Potential Flow Generator with  $L_2$  OT Regularity  
 for Generative Models. *arXiv:1908.11462v1*,  
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 Monge-Ampère Flow for Generative Modeling,  
*arXiv:1809.10188v1*, 2018.
- 
 J Lin, K Lensink, E Haber  
 Fluid Flow Mass Transport for Generative  
 Networks, *arXiv:1910.01694v2*, 2019.



Potential for medical imaging: data-driven priors and regularizers

**Problem: curse of dimensionality!**

Theory: OT as MFG  $\rightsquigarrow$  HJB

# Team and Acknowledgements

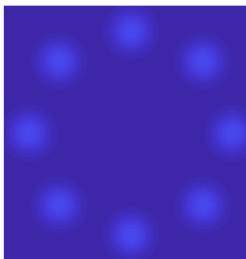


Emory Funding:  DMS 1751636  US-Israel BSF 2018209

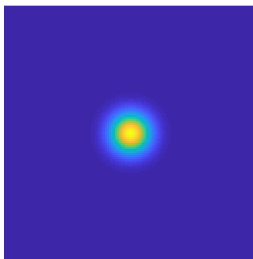
UCLA Funding: AFOSR MURI FA9550-18-1-0502, AFOSR  
FA9550-18-1-0167, ONR N00014-18-1-2527

Special thanks: Organizers and staff of IPAM Long Program MLP 2019.

# Optimal Mass Transport



initial density,  $\rho_0$



target density,  $\rho_1$

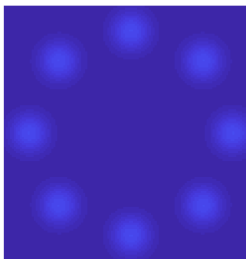
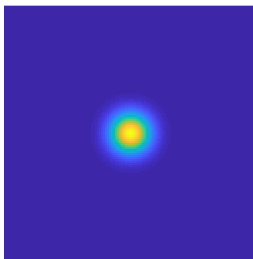
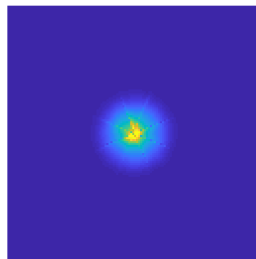
## Optimal Mass Transport

Given an initial density,  $\rho_0$ , and a target density,  $\rho_1$ , find the **velocity field  $v$**  that renders the push-forward of  $\rho_0$  equal to  $\rho_1$  and minimizes the transport costs, i.e., solve

$$\text{minimize}_{v, \rho} \int_0^1 \int_{\Omega} \|v(x, t)\|^2 \rho(x, t) dx dt$$

$$\text{subject to } \partial_t \rho + \nabla \cdot (\rho v) = 0, \quad \rho(\cdot, 0) = \rho_0(\cdot), \quad \rho(\cdot, 1) = \rho_1(\cdot)$$

# Optimal Mass Transport

initial density,  $\rho_0$ target density,  $\rho_1$ push-fwd of  $\rho_0$ 

## Optimal Mass Transport

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# Mean Field Games / Mean Field Control

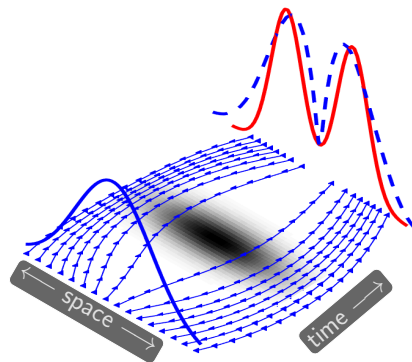
MFGs model large populations of rational agents playing non-cooperative differential game.

# Mean Field Games / Mean Field Control

MFGs model large populations of rational agents playing non-cooperative differential game.

$$\begin{aligned} \text{minimize}_{v, \rho} \mathcal{J}_{\text{MFG}} := & \int_0^1 \int_{\mathbb{R}^d} L(x, v(x, t)) \rho(x, t) dx dt + \int_0^1 \mathcal{F}(\rho(\cdot, t)) dt + \mathcal{G}(\rho(\cdot, 1)) \\ \text{subject to} \quad & \partial_t \rho(x, t) + \nabla \cdot (\rho(x, t) v(x, t)) = 0, \quad \rho(x, 0) = \rho_0(x), \end{aligned}$$

- ▶  $\rho_0$ : initial density (given)
- ▶  $L$ : transport costs.  
Today:  $L(x, v) = \frac{1}{2} \|v\|^2$
- ▶  $\mathcal{F}$ : running costs.  
E.g., congestion, preference  
For OT:  $\mathcal{F} \equiv 0$
- ▶  $\mathcal{G}$ : terminal costs.  
E.g., cross entropy of  $\rho_1$  and  $\rho(\cdot, 1)$



# Agent-Based MFG Model

Let  $(x, t)$  be state of a single agent that aims at choosing  $v$  that minimizes

$$J_{x,t}(v) = \int_t^T \|v(s)\|^2 + F(z(s), \rho(z(s), s)) ds + G(z(T), \rho(z(T), T)),$$

where position changes as in

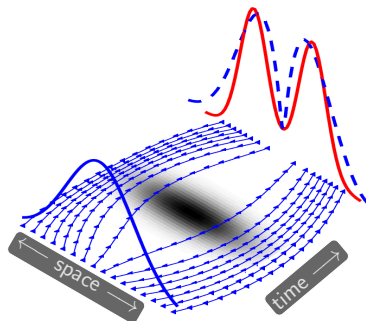
$$\partial_t z(t) = v(t), \quad 0 \leq t \leq T, \quad z(0) = x.$$

- ▶  $F$ : running costs (Ex: congestion, preference)
- ▶  $G$ : terminal costs (Ex: cross entropy)
- ▶ Define value function

$$\Phi(x, t) = \inf_v J_{x,t}(v)$$

- ▶ MFG is called potential MFG if

$$F(x, \rho) = \frac{\delta \mathcal{F}(\rho)}{\delta \rho}(x), \quad G(x, \rho) = \frac{\delta \mathcal{G}(\rho)}{\delta \rho}(x),$$



## Hamilton-Jacobi-Bellman (HJB) Equation

Lasry & Lions '06: First-order optimality conditions of potential MFG are

$$-\partial_t \Phi(x, t) + \frac{1}{2} \|\Phi(x, t)\|^2 = F(x, \rho(x, t)), \quad \Phi(x, 1) = G(x, \rho(x, 1)), \quad (\text{HJB})$$

and

$$\partial_t \rho(x, t) - \nabla \cdot (\rho(x, t) \nabla \Phi(x, t)) = 0, \quad \rho(x, 0) = \rho_0(x) \quad (\text{CE})$$

Three options for solving the problem

- ▶ minimize  $\mathcal{J}_{\text{MFG}}$  w.r.t.  $v$  or  $-\nabla \Phi$  (variational problem)
- ▶ minimize  $J_{x,t}$  w.r.t.  $v$  or  $-\nabla \Phi$  for all agents (microscopic view)
- ▶ solve (HJB) and (CE) (high-dimensional PDEs)

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**Today: Combine advantages of the above to tackle curse of dimensionality**

- ▶ formulate as variational problem. minimize  $\mathcal{J}_{\text{MFG}}(-\nabla \Phi)$
- ▶ eliminate (CE) with Lagrangian PDE solver  $\rightsquigarrow$  🍌 mesh-free, parallel
- ▶ parameterize  $\Phi$  with Neural Network  $\rightsquigarrow$  🍌 mesh-free, efficient(?)
- ▶ penalize violations of (HJB)  $\rightsquigarrow$  🍌 regularity, global convergence(?)

# Lagrangian Method

# Lagrangian Method for Continuity Equation

Assume  $\Phi$  given. Then, the solution to

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satisfies

$$\rho(z(x, t), t) \det \nabla z(x, t) = \rho_0(x)$$

along the characteristic curve given by

$$\partial_t z(x, t) = -\nabla \Phi(z(x, t)), \quad z(x, 0) = x.$$

Problem: Computing  $\det \nabla z(x, t)$  needs  $\mathcal{O}(d^3)$  flops.

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Problem: Computing  $\det \nabla z(x, t)$  needs  $\mathcal{O}(d^3)$  flops.

Idea: Use Jacobi's identity to compute  $l(x, t) = \log \det(\nabla z(x, t))$

$$\partial_t l(x, t) = \Delta \Phi(z(x, t), t), \quad l(x, 0) = 0.$$

**Note: Can combine the ODE solves for position and  $\log \det$  along  $z(x, \cdot)$**

# Lagrangian Method for Optimal Transport

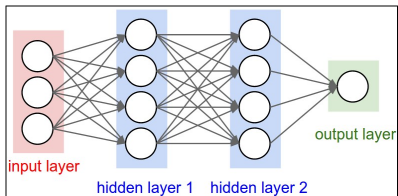
$$\begin{aligned} & \text{minimize}_{\Phi} \mathbb{E}_{\rho_0} (c_L(x, 1) + G(z(x, 1)) + \alpha_1 c_H(x, 1) + \alpha_2 \|\Phi(z(x, 1), 1) - G(z(x, 1))\|) \\ & \text{subject to } \partial_t \begin{pmatrix} z(x, t) \\ l(x, t) \\ c_L(x, t) \\ c_H(x, t) \end{pmatrix} = \begin{pmatrix} -\nabla \Phi(z(x, t), t) \\ -\Delta \Phi(z(x, t), t) \\ \frac{1}{2} \|\nabla \Phi(z(x, t), t)\|^2 \\ |\partial_t \Phi(z(x, t), t) - \frac{1}{2} \|\nabla \Phi(z(x, t), t)\|^2| \end{pmatrix}, \quad t \in (0, 1] \\ & z(x, 0) = 0, \quad l(x, 0) = c_L(x, 0) = c_H(x, 0) = 0 \end{aligned}$$

- ▶  $z$  and  $l = \log \det$  needed to solve continuity eq.
- ▶  $c_L$  and  $c_H$  accumulate cost along characteristic
- ▶  $\alpha_1, \alpha_2$ : penalty parameters for HJB violation
- ▶ discretize with Monte Carlo
- ▶ can use SA (SGD, ADAM, ...) or SAA (BFGS, Newton, ...) methods
- ▶ 🌟 no grid needed and 🌟 computation can be parallelized over  $x$

Next, parameterize  $\Phi$  with NN. Needed:  $\nabla \Phi$  and  $\Delta \Phi$

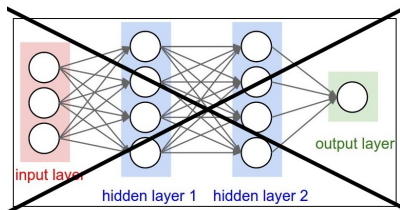
# Neural Network Model

# Deep Learning Revolution (?)



- ▶ deep learning: use neural networks (from  $\approx$  1950's) with many hidden layers
- ▶ able to "learn" complicated patterns from data
- ▶ applications: image classification, face recognition, segmentation, driverless cars, . . .
- ▶ recent success fueled by: massive data sets, computing power
- ▶ A few recent references:
  - ▶ **A radical new neural network design could overcome big challenges in AI**, MIT Tech Review '18
  - ▶ Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17

# Deep Learning Revolution (?)



$$\left\{ \begin{array}{l} \mathbf{Y}_{j+1} = \sigma(\mathbf{K}_j \mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} = \mathbf{Y}_j + \sigma(\mathbf{K}_j \mathbf{Y}_j + \mathbf{b}_j) \\ \mathbf{Y}_{j+1} = \mathbf{Y}_j + \sigma(\mathbf{K}_{j,2} \sigma(\mathbf{K}_{j,1} \mathbf{Y}_j + \mathbf{b}_{j,1}) + \mathbf{b}_{j,2}) \\ \vdots \end{array} \right.$$

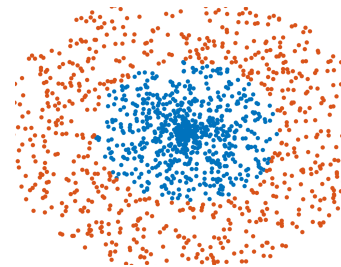
(Notation:  $\mathbf{Y}_j$  : features,  $\mathbf{K}_j, \mathbf{b}_j$ : weights,  $\sigma$  : activation)

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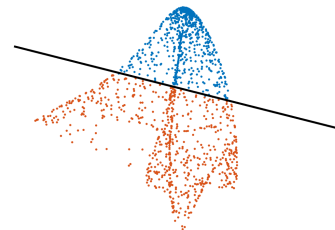
# Deep Residual Neural Networks (simplified)

Award-winning forward propagation

$$\mathbf{Y}_{j+1} = \mathbf{Y}_j + \mathbf{K}_{j,2}\sigma(\mathbf{K}_{j,1}\mathbf{Y}_j + \mathbf{b}_j), \quad \forall j = 0, 1, \dots, N-1.$$



input features,  $\mathbf{Y}_0$



propagated features,  $\mathbf{Y}_N$

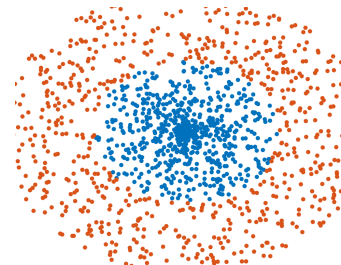


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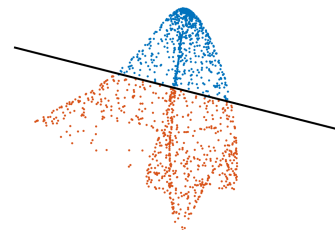
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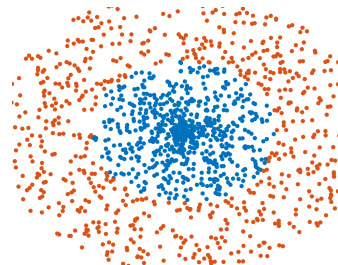
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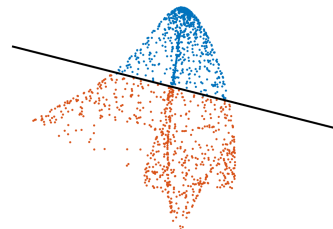
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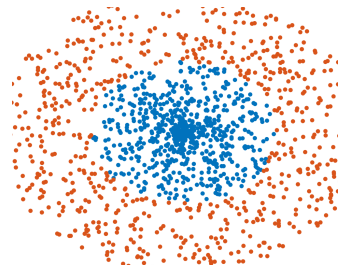
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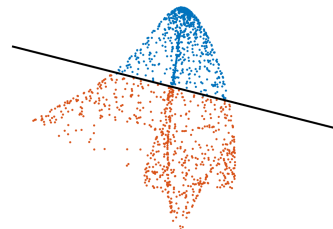
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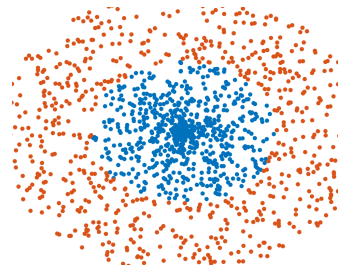
Notation:  $\theta(t) = (\mathbf{K}_1(t), \mathbf{K}_2(t), \mathbf{b}(t))$  and

$$\partial_t \mathbf{y}(t) = f(\mathbf{y}, \theta(t)), \quad \mathbf{y}(0) = \mathbf{y}_0$$

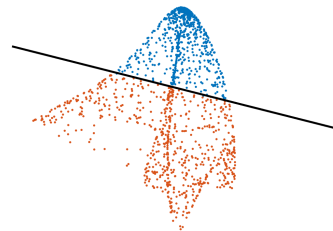
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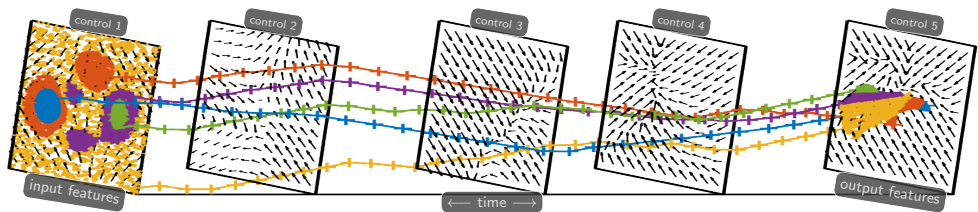


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# Optimal Control Approaches to Deep Learning



Deep Learning meets optimal control / parameter estimation.

- ▶ new ways to analyze and design neural networks
- ▶ expose similarities to trajectory problem, optimal transport, image registration, ...
- ▶ training algorithms motivated by (robust) optimal control
- ▶ discrete ResNet  $\rightsquigarrow$  continuous problem  $\rightsquigarrow$  discrete architecture

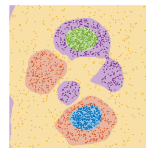
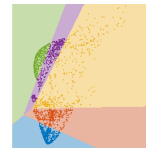
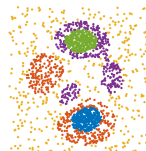
# Overview: Deep Neural Networks motivated by PDEs

## Optimal control formulation

- ▶ new insights, theory, algorithms
- ▶ stability and impact on convergence/generalization

## Stability and well-posedness

- ▶ stability: continuous (constraints/design) vs. discrete
- ▶ Verlet: reversible and stable networks (memory-free)



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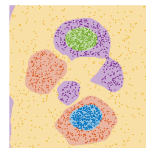
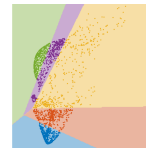
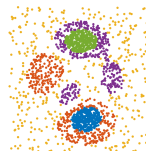
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- ▶ parabolic: numerical stability, multiscale, . . .
- ▶ hyperbolic: reversible, preserve high-frequency features, . . .
- ▶ IMEX: stability, global coupling in feature space
- ▶ Lean: drastical reduction in #weights and flops



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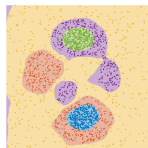
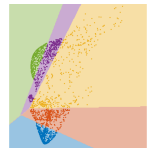
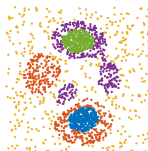
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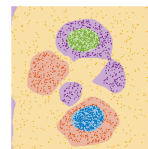
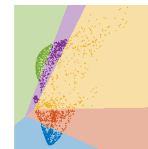
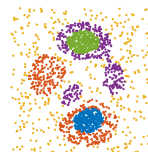
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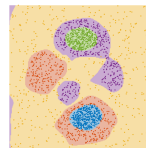
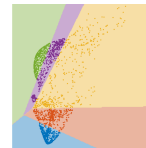
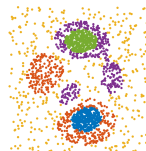
- ▶ new insights, theory, algorithms
- ▶ stability and impact on convergence/generalization

## Stability and well-posedness

- ▶ stability: continuous (constraints/design) vs. discrete
- ▶ Verlet: reversible and stable networks (memory-free)

## Properties of PDE-inspired CNNs

- ▶ parabolic: numerical stability, multiscale, ...
- ▶ hyperbolic: reversible, preserve high-frequency features, ...
- ▶ IMEX: stability, global coupling in feature space
- ▶ Lean: drastical reduction in #weights and flops



## See also recorded talks in IPAM Long Program MLP 2019



E Haber, LR  
*Stable Architectures  
for DNNs.*  
Inverse Problems,  
2017.



E Holtham et al.  
*Learning Across  
Scales.*  
AAAI, 2018.



B Chang et al.,  
*Reversible  
Architectures for  
Deep ResNNs.*  
AAAI, 2018.



LR, E Haber  
*Deep Neural  
Networks motivated  
by PDEs.*  
arXiv, 2018.

# Neural Network Model for Mean Field Games

Estimate mapping from  $s = (x, t) \in \mathbb{R}^{d+1}$  to  $\Phi(x, t) \in \mathbb{R}$  via (NN + quadratic)

$$\Phi(s, \theta) = w^\top N(s, \theta_N) + \frac{1}{2} s^\top A s + c^\top s + b, \quad \theta = (w, \theta_N, \text{vec}(A), c, b)$$

We use  $M$ -layer ResNet with weights  $\theta_N = (\text{vec}(K_0), \dots, \text{vec}(K_M), b_0, \dots, b_M)$ .

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forward propagation:

$$w^\top N(s, t) = w^\top u_M$$

$$u_0 = \sigma(K_0 s + b_0)$$

$$u_1 = u_0 + h\sigma(K_1 u_0 + b_1)$$

$$\vdots \quad \quad \quad \vdots$$

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backward propagation:  $\nabla_s(w^\top N(s, t))$

$$z_M = w + hK_M^\top \text{diag}(\sigma'(K_M u_{M-1} + b_M))w,$$

$$\vdots \quad \quad \quad \vdots$$

$$z_1 = z_2 + hK_1^\top \text{diag}(\sigma'(K_1 u_0 + b_1))z_2,$$

$$z_0 = K_0^\top \text{diag}(\sigma'(K_0 s + b_0))z_1,$$

Next: Compute  $\Delta\Phi(s, \theta) = \text{tr}(E^\top (\nabla_s^2(N(s, \theta_N)w) + A)E)$ ,

💡 If  $E \in \mathbb{R}^{m \times d}$  this can be done in  $\mathcal{O}(m^2 \cdot d \cdot M)$  FLOPS 💡

# Numerical Experiments

# Optimal Transport Experiment - Setup

## ► initial density

$$\rho_0(x) = \frac{1}{8} \sum_{j=1}^8 \rho_G(x, \mathbf{m}_j, 0.3 \cdot \mathbf{I}),$$

$$\mathbf{m}_j = 4 \cdot \cos\left(\frac{2\pi j}{9}\right) \mathbf{e}_1 + 4 \cdot \sin\left(\frac{2\pi j}{9}\right) \mathbf{e}_2$$

## ► target density

$$\rho_1(x) = \rho_G(x, \mathbf{0}, 0.3 \cdot \mathbf{I}).$$

# Optimal Transport Experiment - Setup

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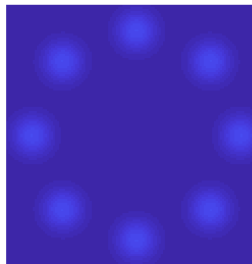
$$\rho_1(x) = \rho_G(x, \mathbf{0}, 0.3 \cdot \mathbf{I}).$$

## ▶ small ResNet (two layers, width 16)

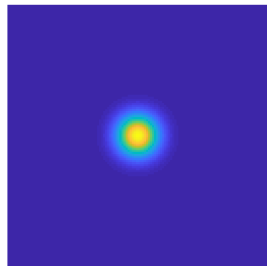
## ▶ optimization strategy

- ▶ SAA approach with BFGS
- ▶ 500 iter / resample every 25 iter
- ▶ simple Armijo Backtracking

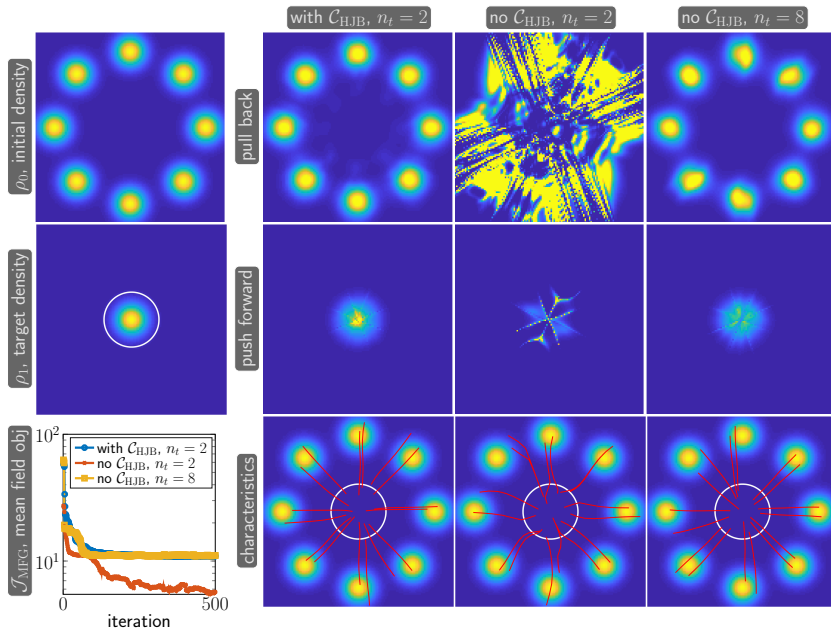
initial density



target density

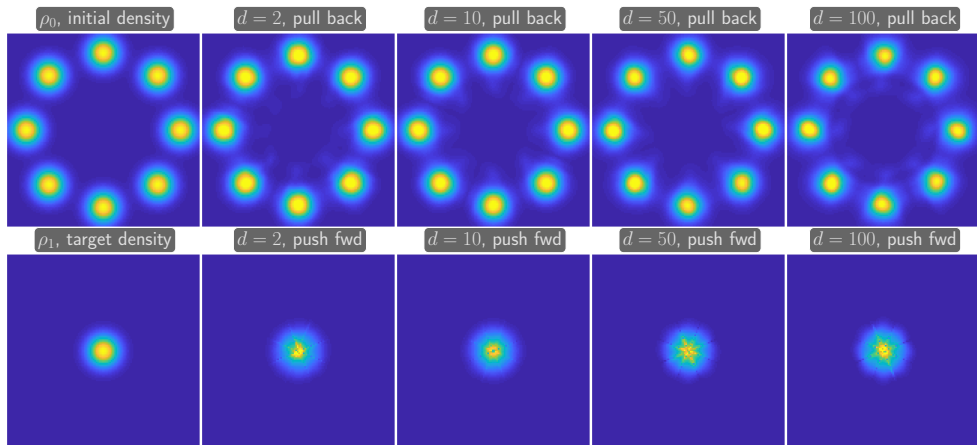


# Experiment 1: Benefit of HJB Penalty



HJB penalty improves accuracy and(!) lowers computational costs

## Experiment 2: Scalability to Higher Dimensions

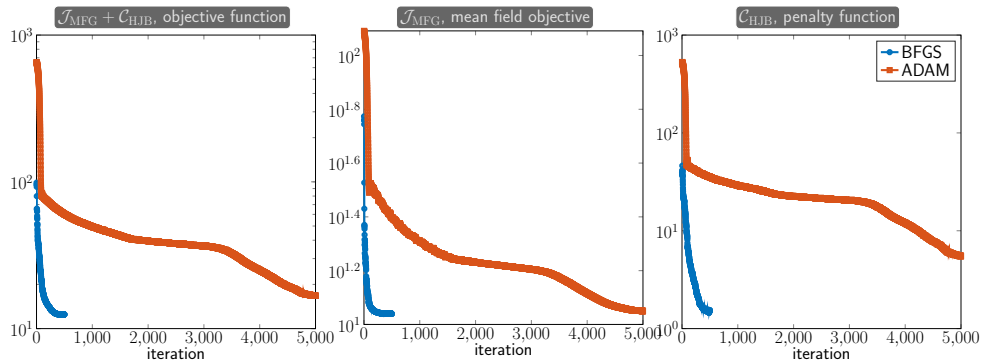


$d$	$N$	$\mathcal{L}$	$\mathcal{G}$	$\mathcal{C}_{\text{HJB}}$	time/iter (s)
2	1,024	1.08e+01	1.41e-01	1.53e+00	1.437
10	4,096	1.08e+01	1.85e-01	1.25e+00	8.408
50	16,384	1.10e+01	2.41e-01	4.85e+00	65.706
100	36,864	1.11e+01	3.22e-01	7.37e+00	283.259

qualitatively similar results in all dimensions / moderate growth of runtime

# Experiment 3: SAA vs. SA

Compare SAA method with BFGS to ADAM



objective function approximated using 1,024 validation samples.

**BFGS converges faster and reduces HJB penalty more substantially**

# Experiment: Comparison with Eulerian Solver

Eulerian scheme:

- ▶ dynamical OT formulation
- ▶ conservative finite volume
- ▶ leads to convex optimization
- ▶ solved to high accuracy with Newton's method



E Haber, R Horesh

A Multilevel Method for the Solution  
of Time Dependent Optimal  
Transport, NM-TMA 8(1), 2015.

# Experiment: Comparison with Eulerian Solver

Eulerian scheme:

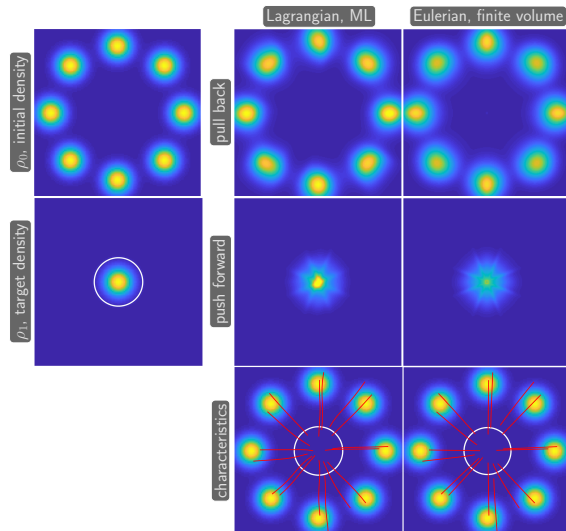
- ▶ dynamical OT formulation
- ▶ conservative finite volume
- ▶ leads to convex optimization
- ▶ solved to high accuracy with Newton's method

Comparison:

- ▶ no. of parameters:  
3,080,448 vs. 365
- ▶ suboptimality of NN  $\approx 0.5\%$



E Haber, R Horesh  
A Multilevel Method for the Solution  
of Time Dependent Optimal  
Transport, NM-TMA 8(1), 2015.



# Summary

# MFGnet.jl - Julia Package

EmoryMLIP / MFGnet.jl Unwatch 3 Star 4 Fork 1


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10 commits 1 branch 0 packages 0 releases 2 contributors MIT

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 lruthotto updated drivers and viewers Latest commit 9a9ef5c 8 days ago

examples/ROLNWF2019	updated drivers and viewers	8 days ago
src	pushing version of code used in the paper	2 months ago
test	pushing version of code used in the paper	2 months ago

<https://github.com/EmoryMLIP/MFGnet.jl>

# $\Sigma$ : Machine Learning for High-Dimensional OT

## ► Math: Lagrangian Method for MFG

- MFG theory: HJB, potential, and optimality conditions
- combine microscopic computation and macroscopic penalty
- mesh-free PDE solver and integration

## ► ML: Neural Network for Potential

- allows to monitor and enforce HJB
- direct computation of Laplacian (for now)
- ResNet: multilevel, stability

## ► Optimal Transport

- HJB penalty improves accuracy and efficiency
- Scalability to higher dimensions
- Open issue: optimization

more examples and generalizations at

[github.com/EmoryMLIP/MFGnet.jl](https://github.com/EmoryMLIP/MFGnet.jl) and in:



LR, S Osher, W Li, L Nurbekyan, S Wu Fung

A Machine Learning Framework for Solving High-Dimensional Mean Field Game and Mean Field Control Problems, arXiv, 2019.

