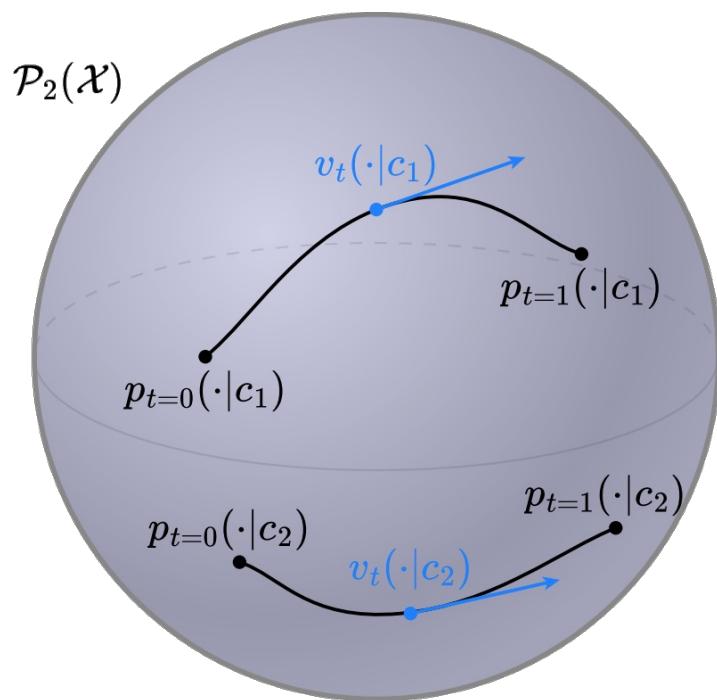


Transport and flows between distributions over distributions

Brandon Amos • Meta, NYC



slides



bamos.github.io/presentations

Generative models and media generation

Movie Gen: A Cast of Media Foundation Models. Meta, Oct 2024.



Prompt: A red-faced monkey with white fur is bathing in a natural hot spring. The monkey is playing in the water with a miniature sail ship in front of it, made of wood with a white sail and a small rudder. The hot spring is surrounded by lush greenery, with rocks and trees.

Flows: how we got here

(a non-exhaustive list)

(many extensions/applications)

- 
- 2022 • Building Normalizing Flows with Stochastic Interpolants
 - 2022 • Flow Straight and Fast: Learning to Generate and Transfer Data with Rectified Flow
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$$p_{Y \text{ (data)}}(y) = p_{X \text{ (base)}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$

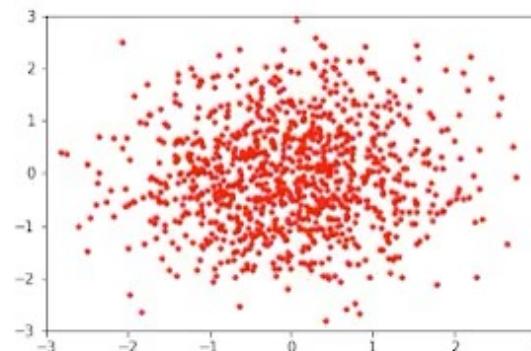
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$$p_{Y \text{ (data)}}(y) = p_{X \text{ (base)}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$



Source: Normalizing Flows in 100 Lines of JAX

parameterize with an invertible function
learn with likelihood

Flows: how we got here

(a non-exhaustive list)

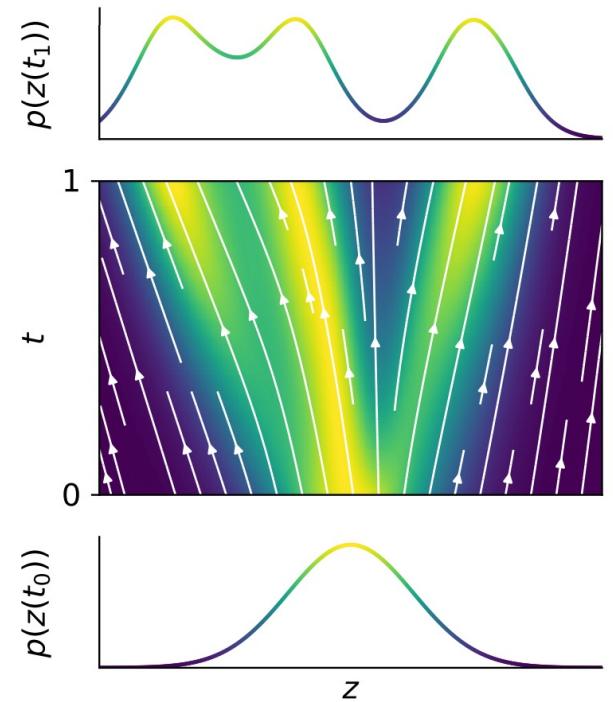
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$$p_{Y \text{ (data)}}(y) = p_{X \text{ (base)}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$

parameterize with an ODE
learn with likelihood

$$\dot{z}_t = g(z_t) \quad z_0 \sim p_X$$



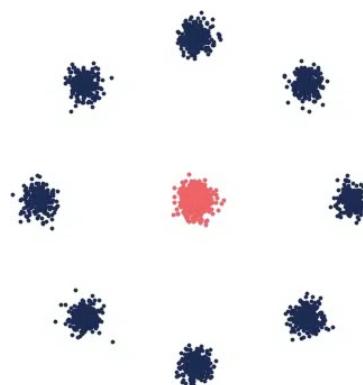
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DDPM



reference path SDE known
score decomposes nicely, learn via a decomposition

$$dX(t) = \nabla \log p(X(t)) dt + 2^{1/2} dB_t$$

$$X_{t+1} = X_t + \epsilon \nabla_x \log p(X_t) + \mathcal{N}(0, 2\epsilon)$$

Flows: how we got here

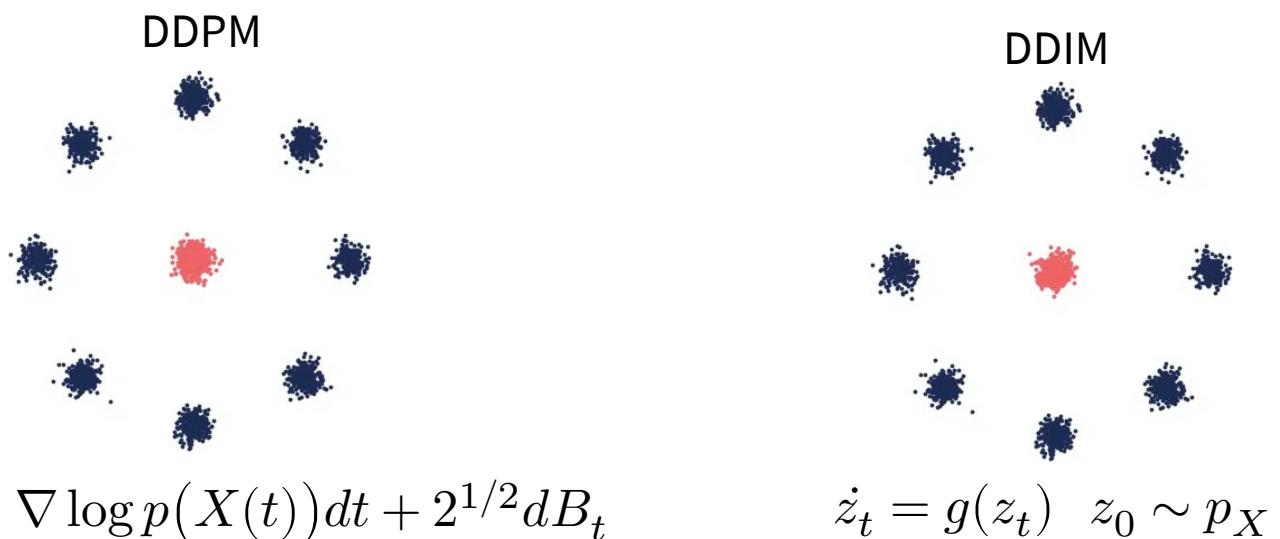
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$$p_{Y \text{ (data)}}(y) = p_{X \text{ (base)}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$

back to an ODE/flow with the same marginals!!
(probability flow ODE, implicit models)



Flows: how we got here

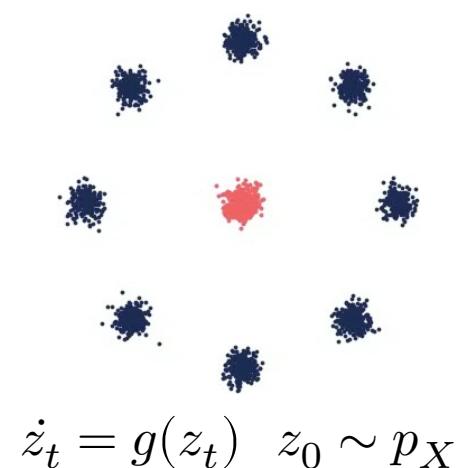
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$$p_Y(y) = p_{X_{(\text{data})}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$

Match the ODE directly, generalize diffusion path
Still use a ground-truth reference path (or interpolant)
Parameterize flow with an unconstrained neural network
(invertibility comes because the reference transport is invertible!!)



Flows and (optimal) transport

(a non-exhaustive list)

(many extensions/applications)

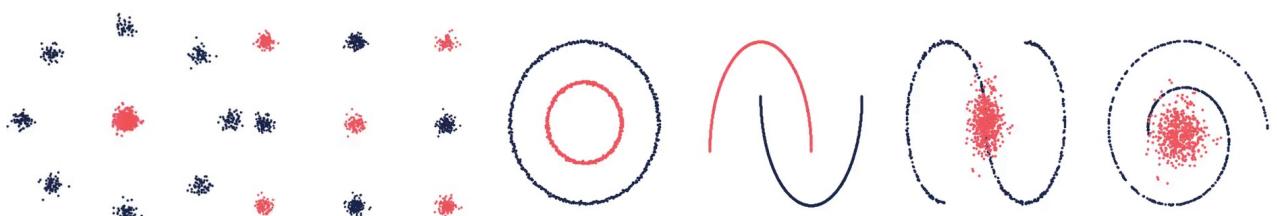
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- Optimal transport: old and new. Villani, 2009.
- Optimal Transport in Learning, Control, and Dynamical Systems. Bunne and Cuturi, ICML 2023 Tutorial.
- Computational Optimal Transport. Peyré and Cuturi, Foundations and Trends in Machine Learning, 2019.
- Optimal Transport for Applied Mathematicians. Santambrogio, Birkhäuser, 2015
- Optimal Transport in Systems and Control. Chen, Georgiou, and Pavon, 2021.
- Optimal mass transport: Signal processing and machine-learning applications. Kolouri et al., 2017.

Monge's problem (squared Euclidean)

$$\inf_{T \in \mathcal{T}(\alpha, \beta)} \int_{\mathcal{X}} \|T(x) - x\|_2^2 d\alpha(x)$$

find a map connecting α and β that minimally displaces mass



On amortizing convex conjugates for optimal transport. Amos, ICLR 2023.

Flows and (optimal) transport

(a non-exhaustive list)

(many extensions/applications)

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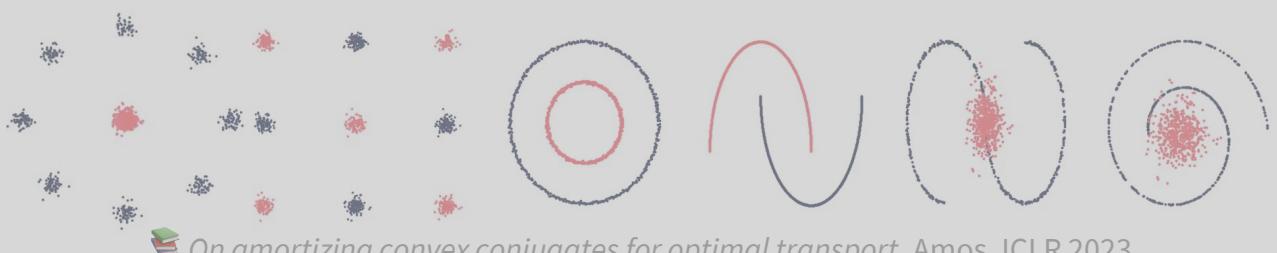
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Monge's problem (squared Euclidean)

all of this: single distribution to single distribution

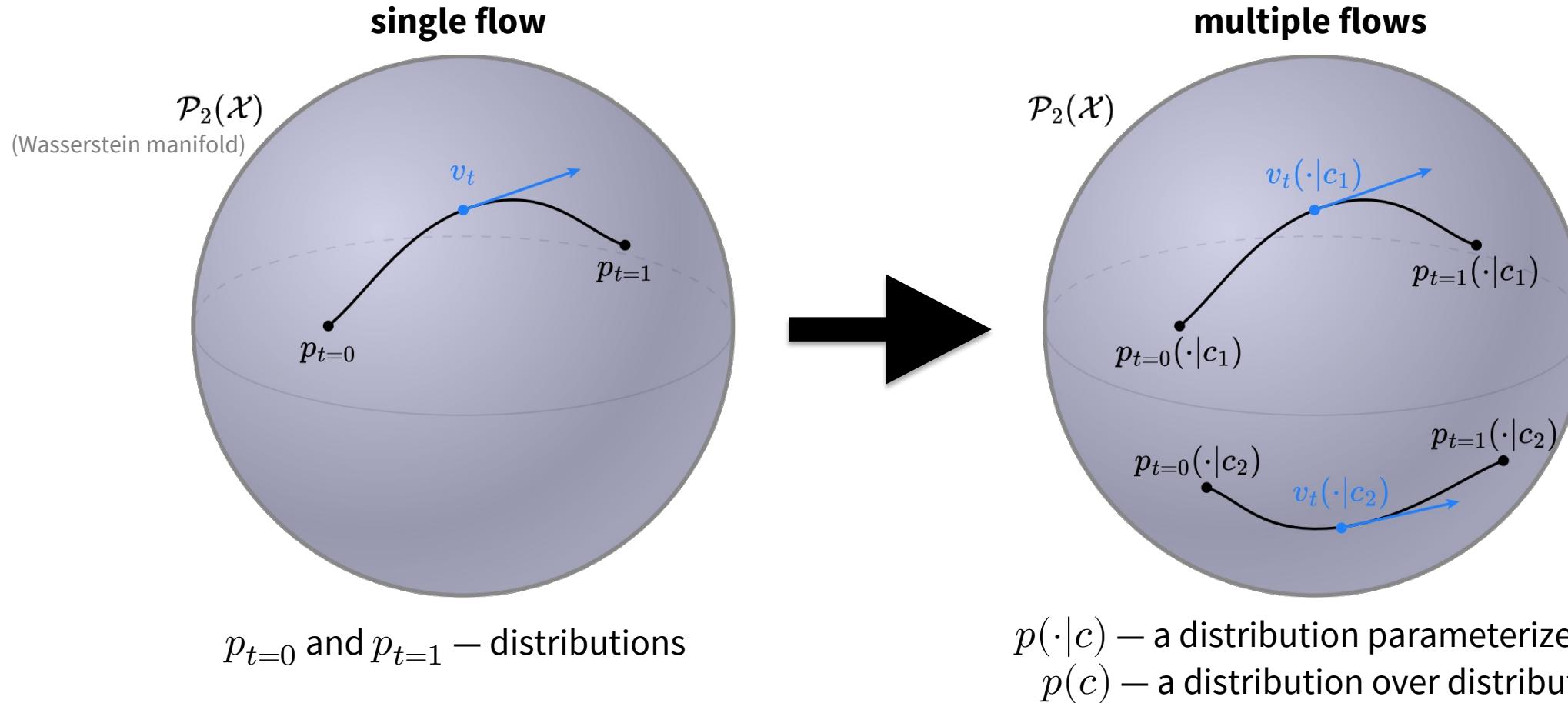
$\alpha, \beta \in \mathcal{P}(\mathcal{X})$

find a map connecting α and β that minimally displaces mass



• *On amortizing convex conjugates for optimal transport.* Amos, ICLR 2023.

To distributions over distributions



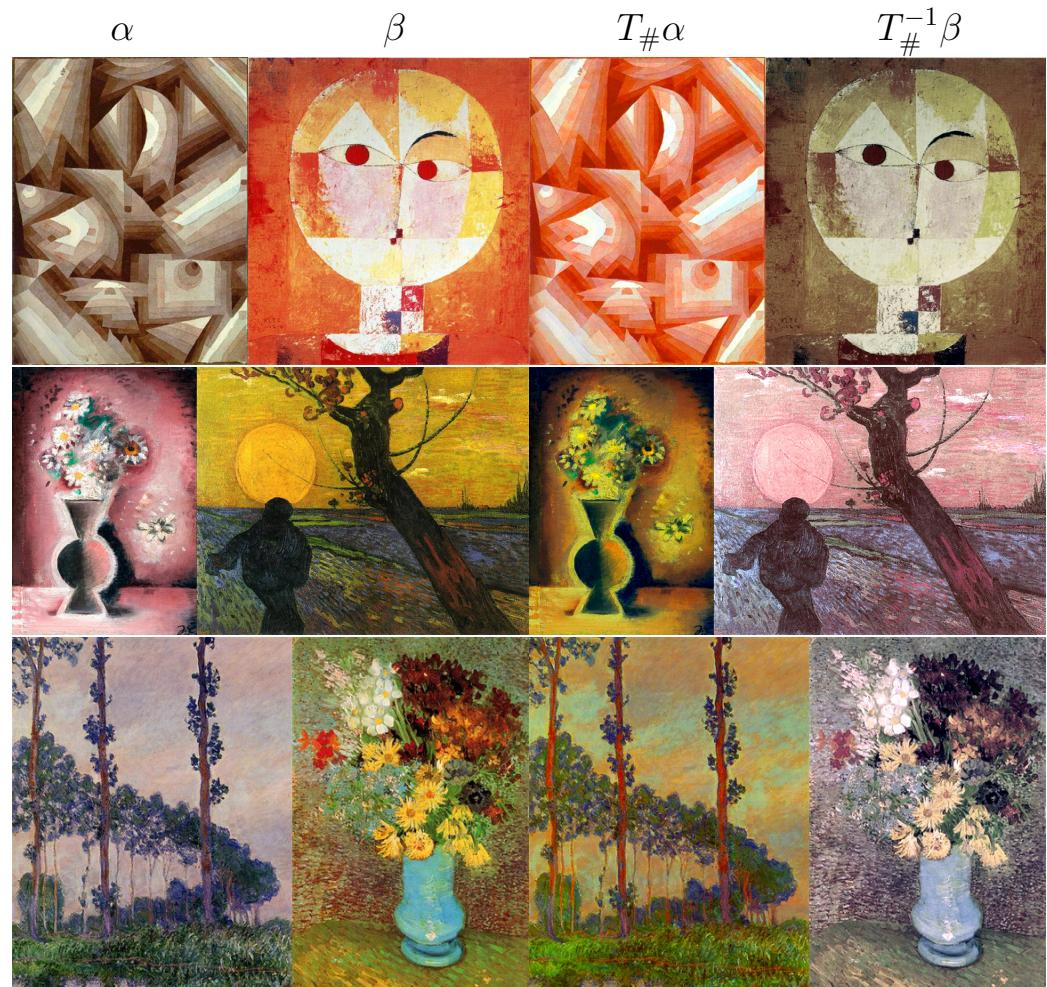
Why distributions over distributions?

1. **Text to image, video, or other media**

between many text prompts

Why distributions over distributions?

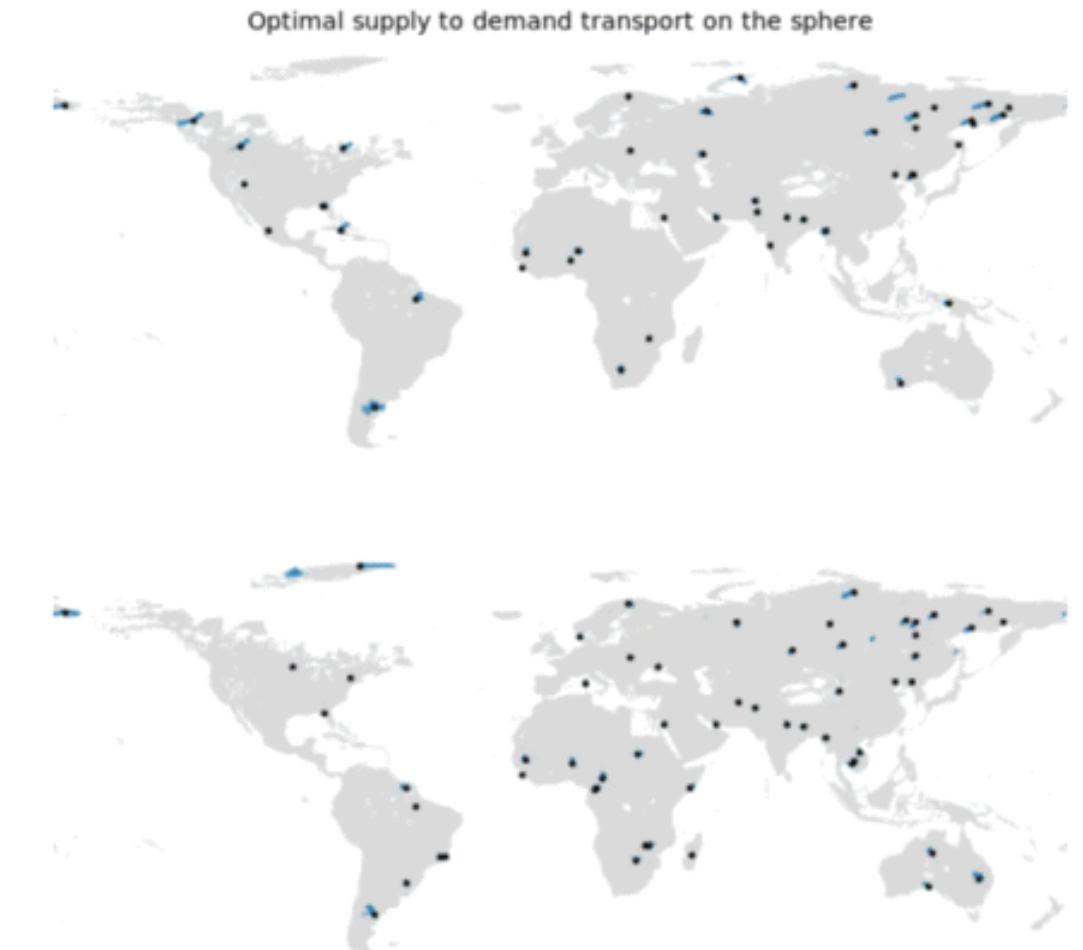
1. **Text to image, video, or other media**
between many text prompts
2. **Image editing**
between many pairs of images



 Meta Optimal Transport. Amos et al., ICML 2023.

Why distributions over distributions?

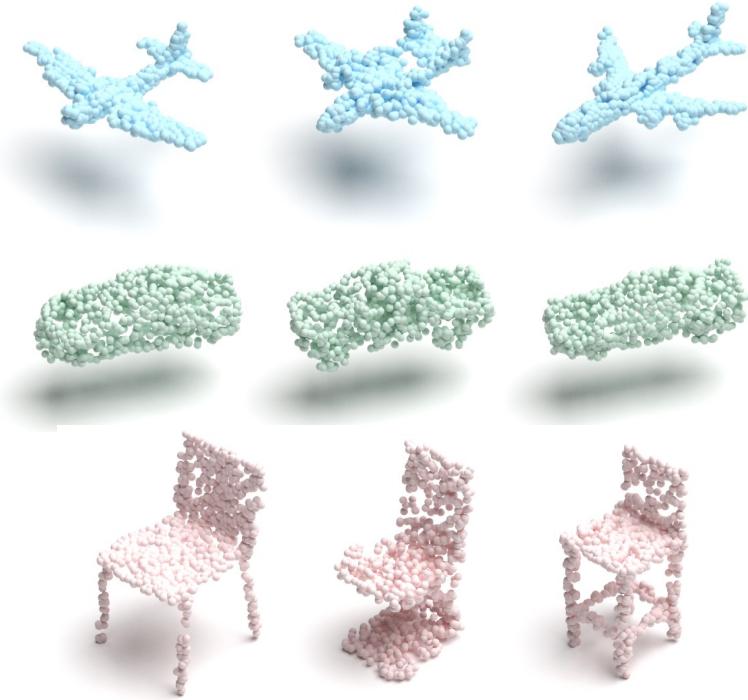
1. **Text to image, video, or other media**
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2. **Image editing**
between many pairs of images
3. **Scheduling and supply-demand allocations**
between many initial conditions



Meta Optimal Transport. Amos et al., ICML 2023.

Why distributions over distributions?

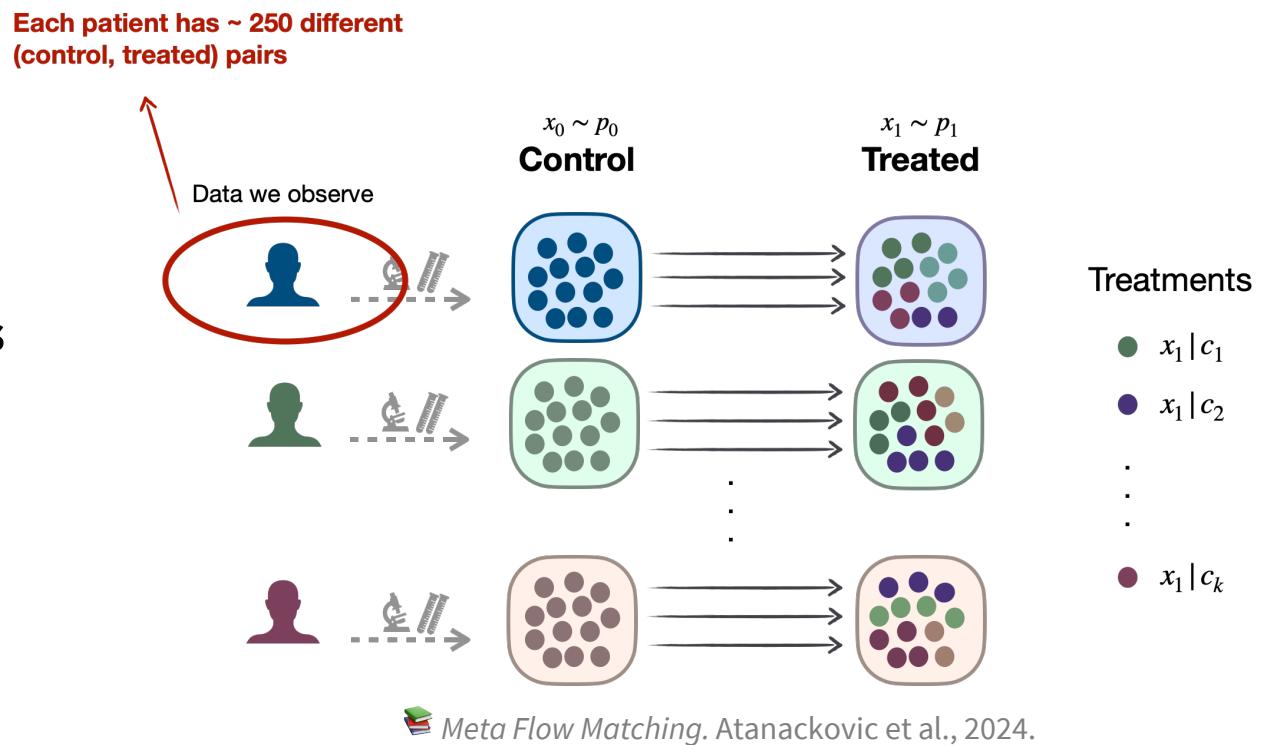
1. **Text to image, video, or other media**
between many text prompts
2. **Image editing**
between many pairs of images
3. **Scheduling and supply-demand allocations**
between many initial conditions
4. **Point cloud generation**
each point cloud is an empirical distribution



📚 *Wasserstein Flow Matching*. Haviv*, Pooladian*, Pe'er, Amos. 2024.

Why distributions over distributions?

1. **Text to image, video, or other media**
between many text prompts
2. **Image editing**
between many pairs of images
3. **Scheduling and supply-demand allocations**
between many initial conditions
4. **Point cloud generation**
each point cloud is an empirical distribution
5. **Cellular transport**
many pairs of untreated to treated populations



Talk overview

📚 **Meta Optimal Transport** [ICML 2023]



📚 **Meta Flow Matching** [2024]



📚 **Wasserstein Flow Matching** [2024]



Challenge: computing OT maps



Meta Optimal Transport. Amos et al., ICML 2023.

Monge (primal, Wasserstein-2)

$$T^*(\alpha, \beta) \in \operatorname{argmin}_{T \in \mathcal{T}(\alpha, \beta)} \mathbb{E}_{x \sim \alpha} \|x - T(x)\|_2^2$$

we also consider other/discrete OT formulations

Many OT problems are **numerically solved**

Improving OT solvers is active research

Solving multiple OT problems: even harder

Standard solution: independently solve

Optimally transport between MNIST digits



Meta Optimal Transport

Idea: predict the solution to OT problems with amortized optimization
Simultaneously solve many OT problems, sharing info between instances

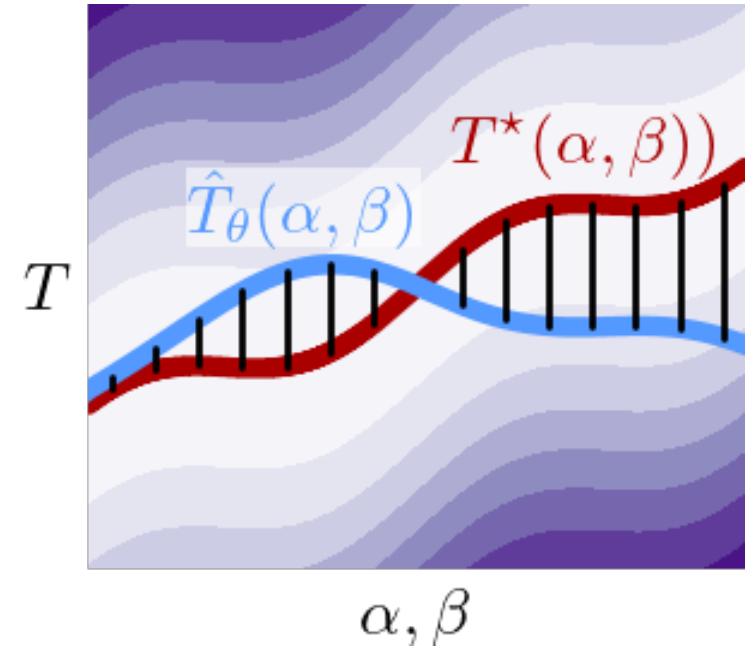
Why call it “meta”? Instead of solving a single OT problem, learn how to solve many (via amortization)

Monge (primal, Wasserstein-2)

$$T^*(\alpha, \beta) \in \underset{\substack{T \in \mathcal{T}(\alpha, \beta)}}{\operatorname{argmin}} \mathbb{E}_{x \sim \alpha} \|x - T(x)\|_2^2$$

$\hat{T}_\theta(\alpha, \beta)$ (parameterize dual potential via an MLP)

we also consider other/discrete OT formulations



Meta OT for Discrete OT (Sinkhorn)

 *Sinkhorn Distances: Lightspeed Computation of Optimal Transport.* Marco Cuturi, NeurIPS 2013.

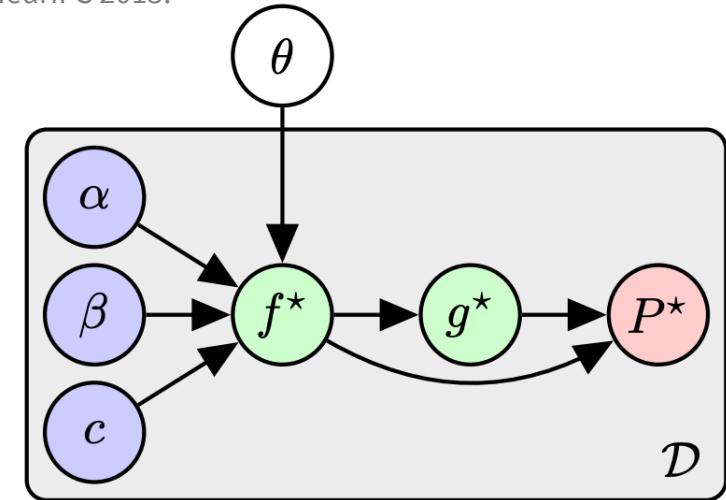
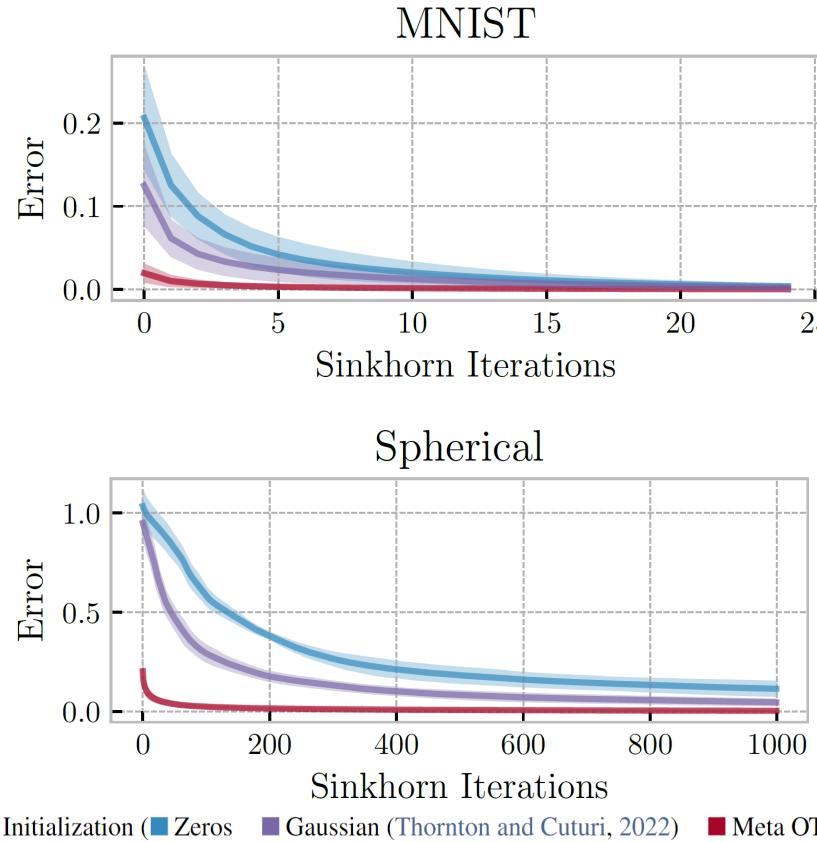
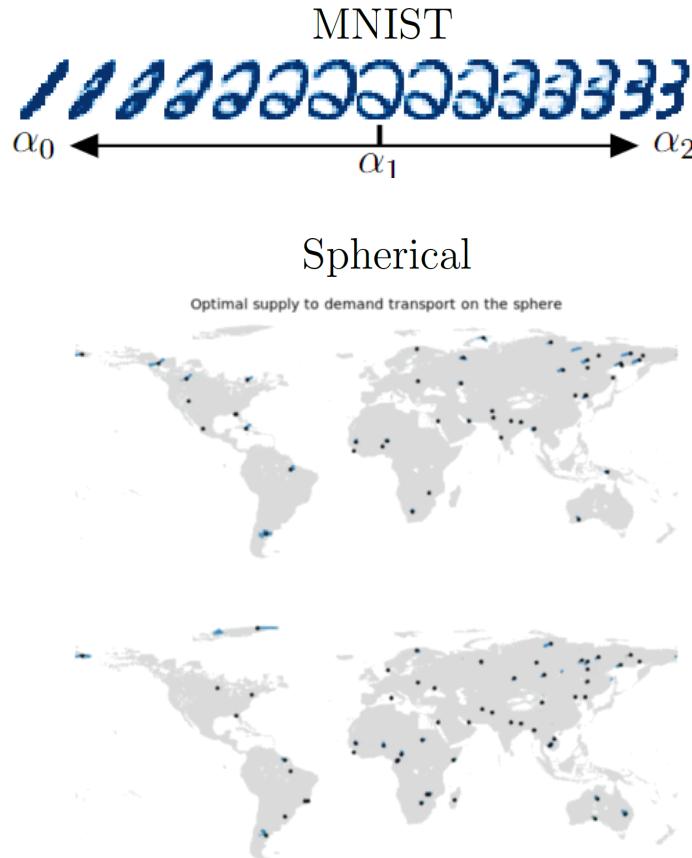


Table 1. Sinkhorn runtime (seconds) to reach a marginal error of 10^{-2} . Meta OT's initial prediction takes $\approx 5 \cdot 10^{-5}$ seconds. We report the mean and std across 10 test instances.

Initialization	MNIST	Spherical
Zeros (t_{zeros})	$4.5 \cdot 10^{-3} \pm 1.5 \cdot 10^{-3}$	0.88 ± 0.13
Gaussian	$4.1 \cdot 10^{-3} \pm 1.2 \cdot 10^{-3}$	$0.56 \pm 9.9 \cdot 10^{-2}$
Meta OT (t_{Meta})	$2.3 \cdot 10^{-3} \pm 9.2 \cdot 10^{-6}$	$7.8 \cdot 10^{-2} \pm 3.4 \cdot 10^{-2}$
Improvement ($t_{\text{zeros}}/t_{\text{Meta}}$)	1.96	11.3

Wasserstein adversarial regularization



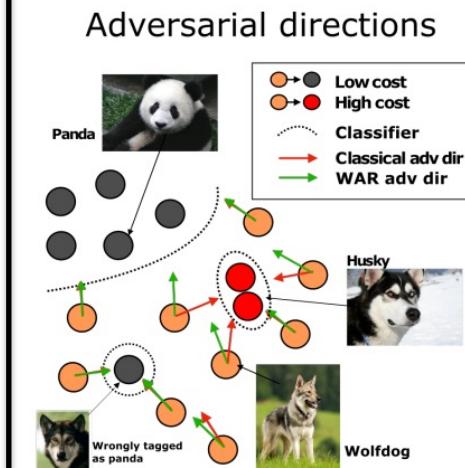
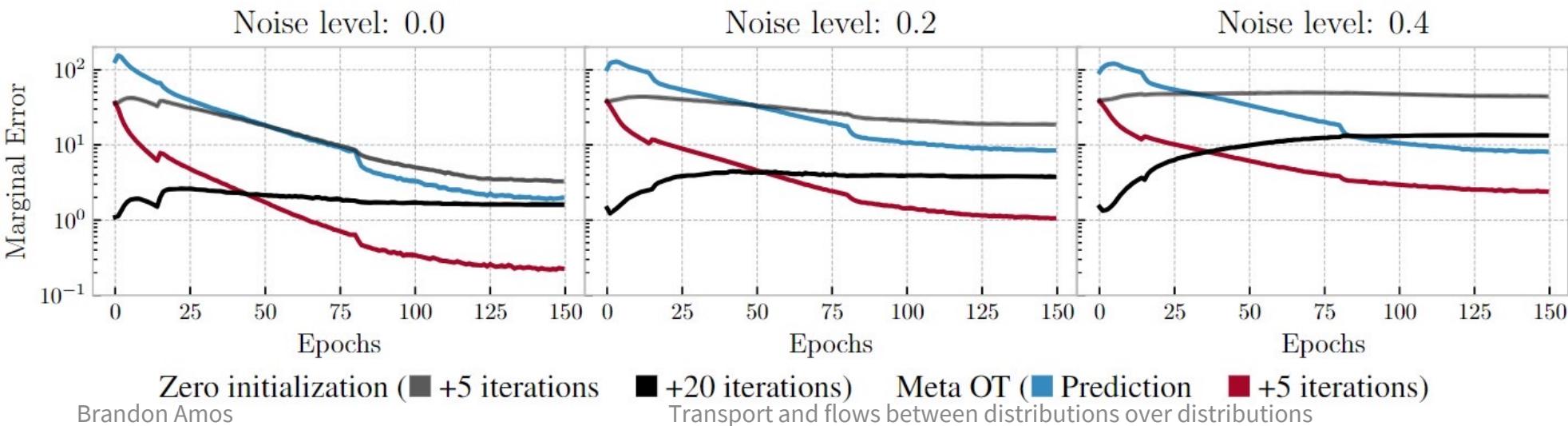
Wasserstein adversarial regularization for learning with label noise. Kilian Fatras et al., TPAMI 2021.

Setting: discrete OT for classification with label noise

OT is **repeatedly solved** across minibatches

Use Meta OT to **learn better solutions**

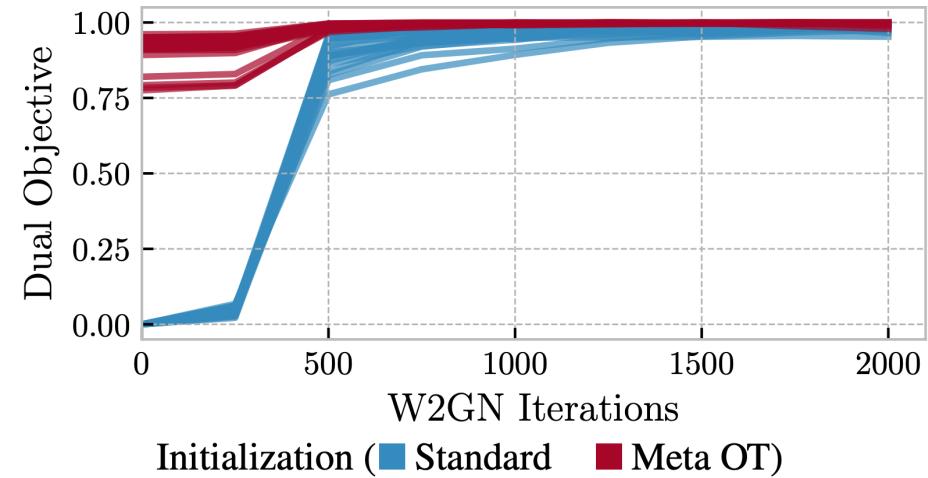
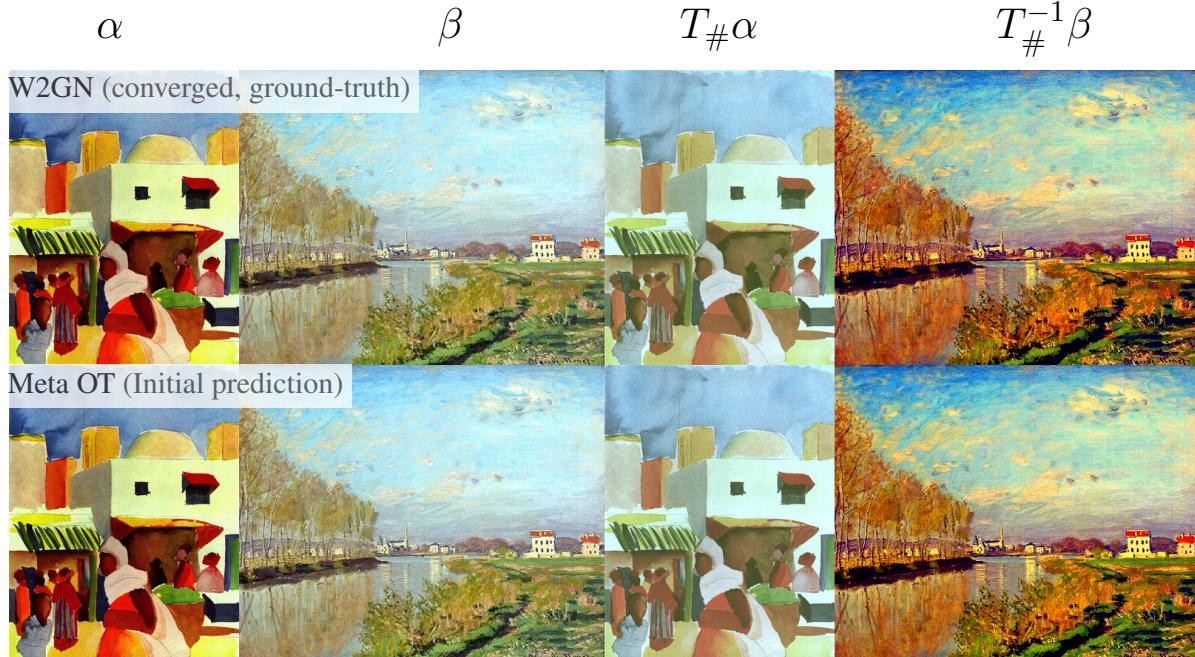
Fig. 1: AR vs. WAR. Given a number of samples, both methods regularize along adversarial directions (arrows in the left panel), leading to updated decision functions (right panel). While both regularizations prevent the classifier to overfit on the noisy labelled sample, AR also tends to oversmooth between similar classes (*wolfdog* and *husky*), while WAR preserves them by changing the adversarial direction.



Meta OT in continuous settings (W2GN)

📚 Wasserstein-2 Generative Networks. Alexander Korotin et al., ICLR 2021.

RGB color palette transport



	Iter	Runtime (s)	Dual Value
Meta OT + W2GN	None	$3.5 \cdot 10^{-3} \pm 2.7 \cdot 10^{-4}$	$0.90 \pm 6.08 \cdot 10^{-2}$
	1k	$0.93 \pm 2.27 \cdot 10^{-2}$	$1.0 \pm 2.57 \cdot 10^{-3}$
	2k	$1.84 \pm 3.78 \cdot 10^{-2}$	$1.0 \pm 5.30 \cdot 10^{-3}$
W2GN	1k	$0.90 \pm 1.62 \cdot 10^{-2}$	$0.96 \pm 2.62 \cdot 10^{-2}$
	2k	$1.81 \pm 3.05 \cdot 10^{-2}$	$0.99 \pm 1.14 \cdot 10^{-2}$

More Meta OT color transfer predictions

 Meta Optimal Transport. Amos et al., ICML 2023.

α

β

$T_{\#}\alpha$

$T_{\#}^{-1}\beta$

α

β

$T_{\#}\alpha$

$T_{\#}^{-1}\beta$



Conditional Monge Maps

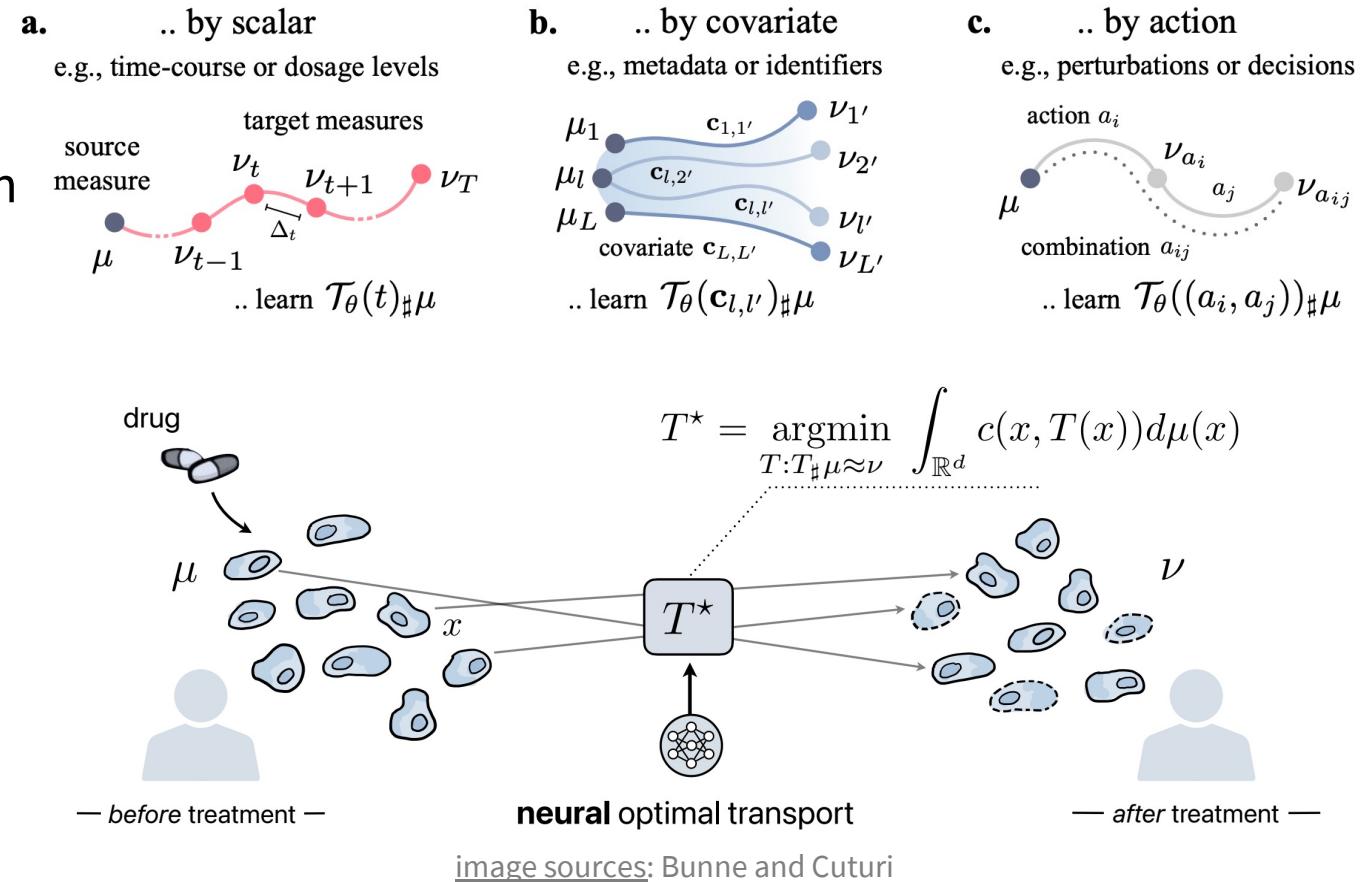
 Supervised Training of Conditional Monge Maps. Bunne, Krause, Cuturi, NeurIPS 2022.

Focus: predicting drug treatments with OT
Idea: condition OT map on patient information

Methodological differences

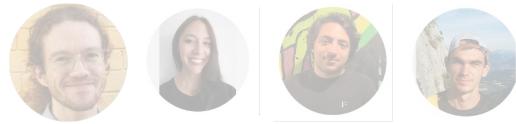
Conditional Monge Maps \approx Neural Processes
Predict conditioning inputs of the OT map

Meta OT \approx Hyper-Networks
Predict parameters of an OT map



Talk overview

📚 **Meta Optimal Transport** [ICML 2023]



📚 **Meta Flow Matching** [2024]



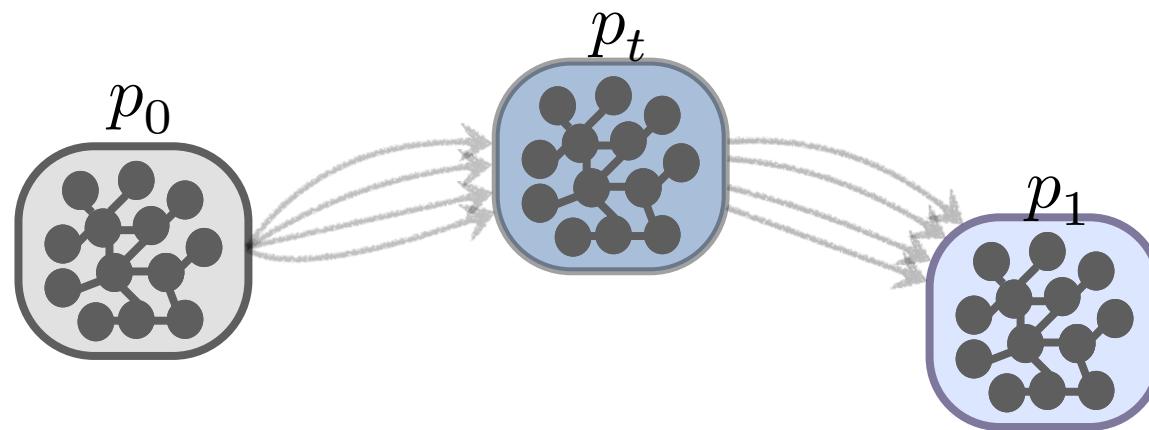
📚 **Wasserstein Flow Matching** [2024]



Background and Motivation

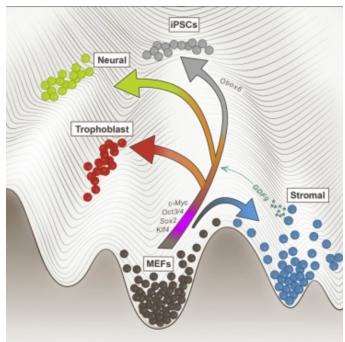
In many scientific problems, we want to understand the **dynamics of many-body problems** (the dynamic evolution of interacting particles)

E.g. the dynamic processes **cells** undergo w.r.t. their **environment** and **interactions** with each other

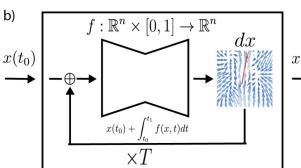
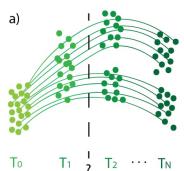


Background and Motivation

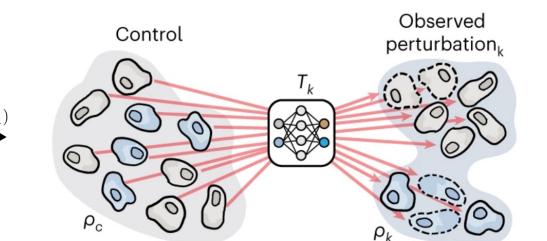
We want to model the dynamics of particles (or cells) at the **population level**. Many methods do this:



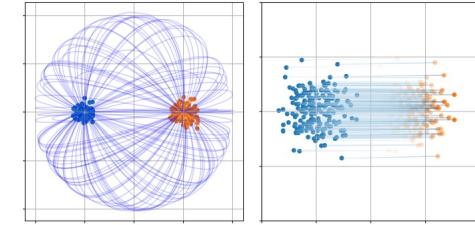
Schiebinger et al, *Cell*, 2019



Tong et al, *ICML*, 2020



Bunne et al, *Nature Methods*, 2023

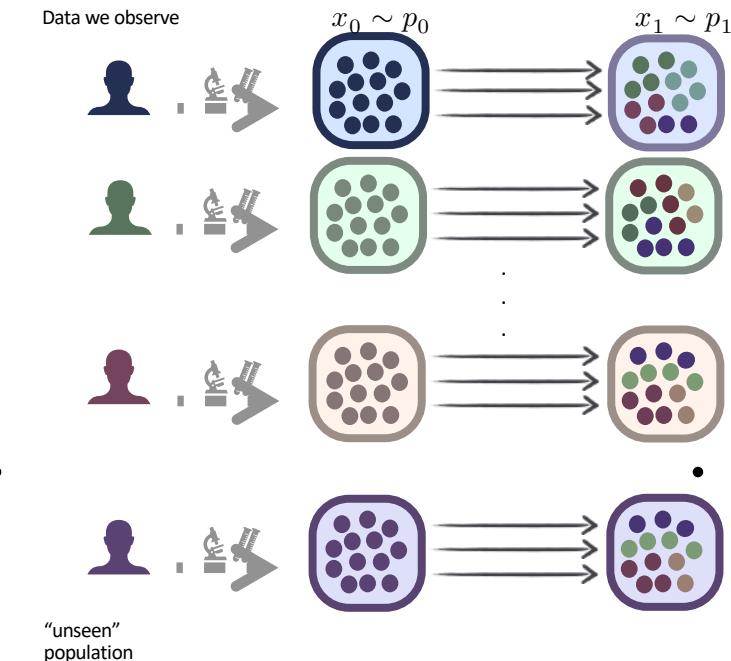


Neklydov et al, *ICML*, 2024

Existing methods typically only model the evolution of cells as independent particles.

Background and Motivation

We would also like a model that can **generalize across measures** (populations)

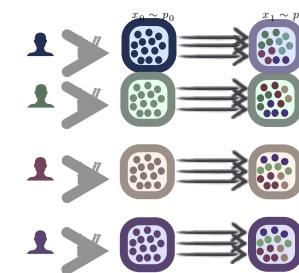


Existing methods are typically restricted to a single measure (population, patient). At best can condition on different dynamics.

Problem setup

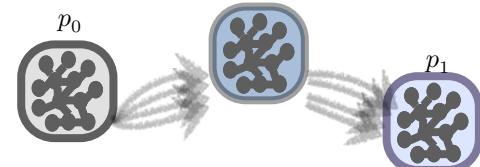
We want a model that can:

1. model the **evolution of particles** while taking into account their **interactions**
2. **generalize** across **unseen populations**



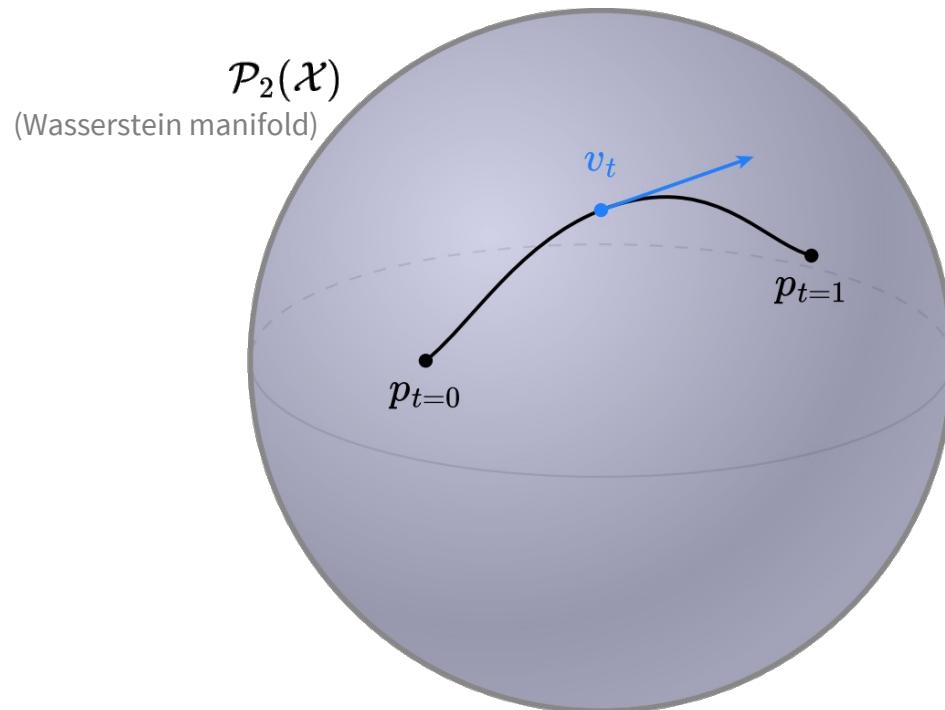
Main assumptions:

1. **Coupled distribution**/population pairs $\{(p_0(x_0|i), p_1(x_1|i))\}_{i=1}^N$
2. The collected data undergoes a **universal developmental process**
depends only on the population itself (e.g., interacting particles or communicating cells)



From Flow Matching

$$\frac{\partial p_t(x)}{\partial t} = -\langle \nabla_x, p_t(x) v_t^*(x) \rangle$$

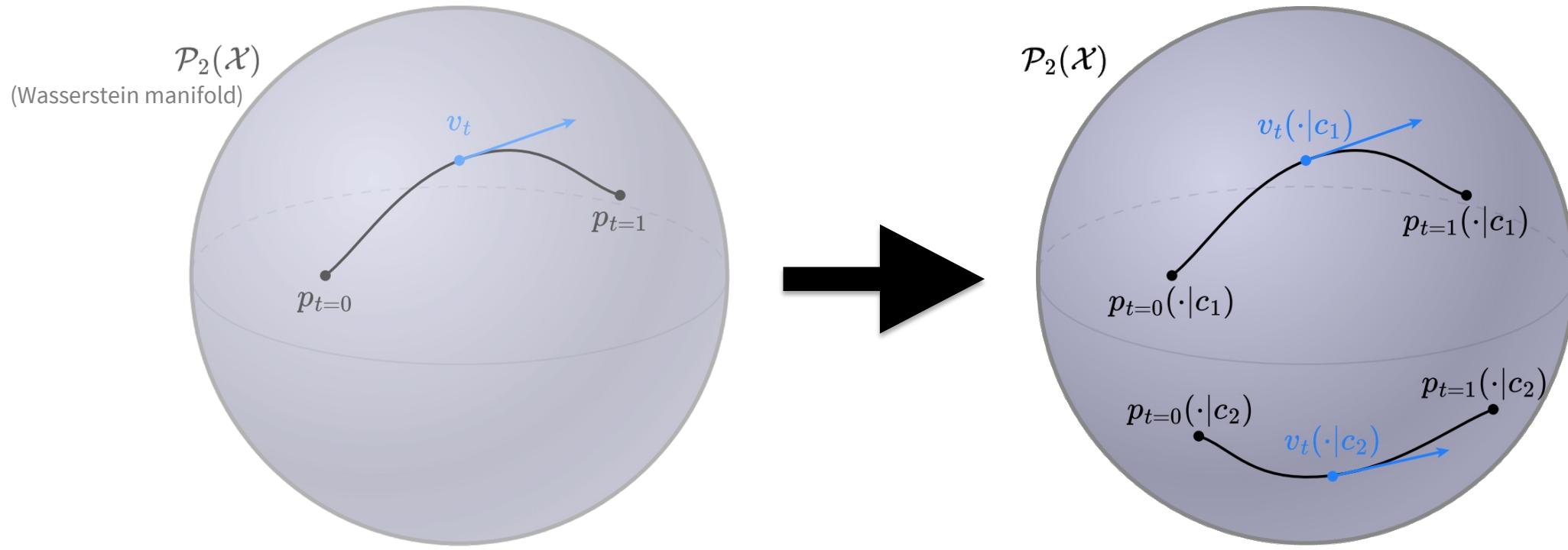


From Flow Matching to Meta Flow Matching

$$\frac{\partial p_t(x)}{\partial t} = -\langle \nabla_x, p_t(x) v_t^*(x) \rangle$$

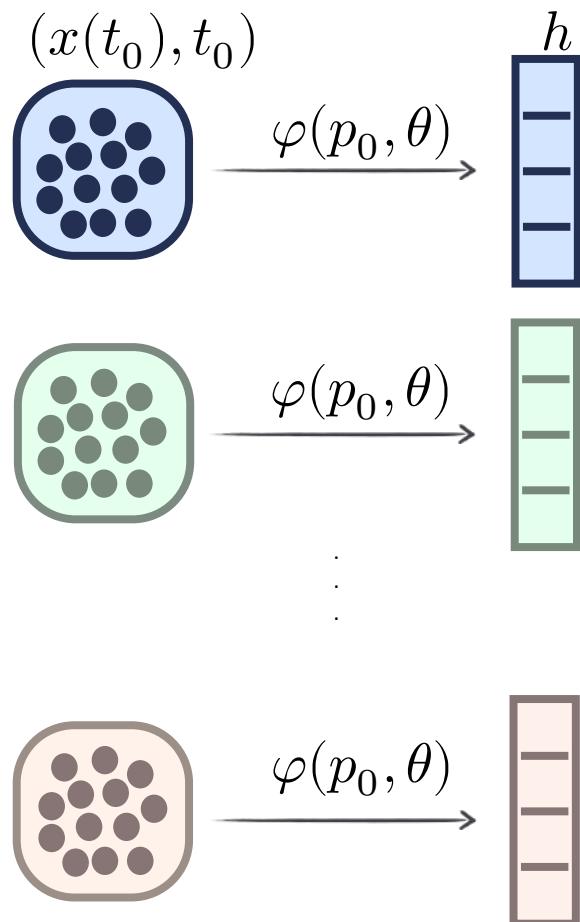
$$\frac{\partial p_t(x)}{\partial t} = -\langle \nabla_x, p_t(x) v_t^*(x, p_t) \rangle$$

(from assumptions: end up just conditioning on p_0)



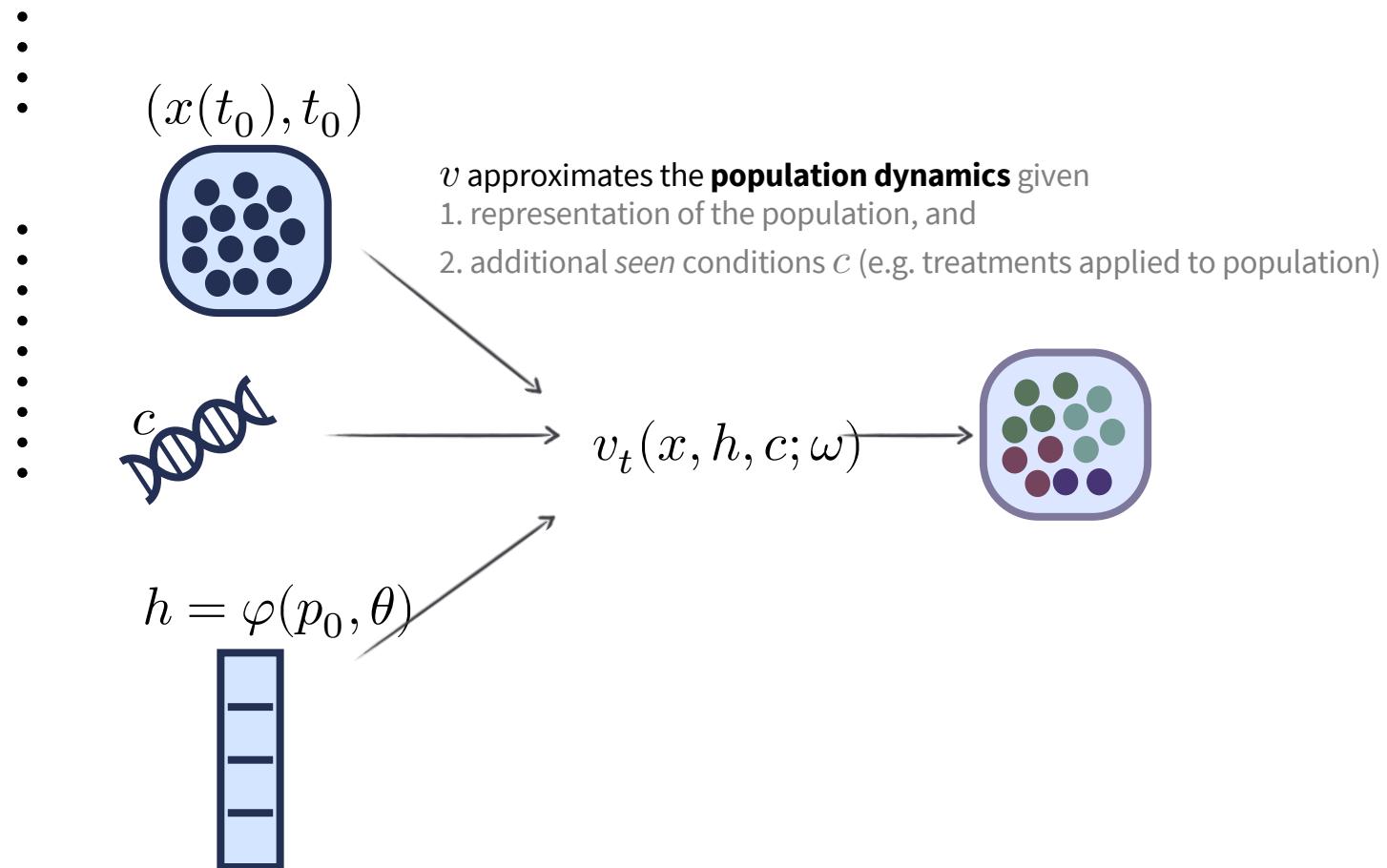
Meta Flow Matching

A **model** to learn to represent the population (GCN w/ *knn* edge pooling)



$\varphi(p_0, \theta)$ (GCN) captures **interactions** between particles

Brandon Amos



Transport and flows between distributions over distributions

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Algorithm 1: Meta Flow Matching (training)

Input : dataset of populations $\{(\pi(x_0, x_1 | i), c^i)\}_{i=1}^N$ and treatments c^i , and parametric models for the velocity, $v_t(\cdot; \omega)$, and population embedding $\varphi(\cdot; \theta)$.

for *training iterations* **do**

```
i ~  $\mathcal{U}_{\{1, N\}}(i)$  // sample batch of  $n$  populations ids  
 $(x_0^j, x_1^j, t^j) \sim \pi(x_0, x_1 | i) \mathcal{U}_{[0, 1]}(t)$  // sample  $N_i$  particles for every population  $i$   
 $f_t(x_0^j, x_1^j) \leftarrow (1 - t^j)x_0^j + t^j x_1^j$   
 $h^i(\theta) \leftarrow \varphi\left(\{x_0^j\}_{j=1}^{N_i}; \theta\right)$  // embed population  $\{x_0^j\}_{j=1}^{N_i}$ . For CGFM  $h \leftarrow i$ , FM  $h \leftarrow \emptyset$ .  
 $\mathcal{L}_{\text{MFM}}(\omega, \theta) \leftarrow \frac{1}{n} \sum_i \frac{1}{n_i} \sum_j \left\| \frac{d}{dt} f_t(x_0^j, x_1^j) - v_{t^j}(f_t(x_0^j, x_1^j) | h^i(\theta), c^i; \omega) \right\|^2$   
 $\omega' \leftarrow \text{Update}(\omega, \nabla_\omega \mathcal{L}_{\text{MFM}}(\omega, \theta))$  // evaluate new parameters of the flow model  
 $\theta' \leftarrow \text{Update}(\theta, \nabla_\theta \mathcal{L}_{\text{MFM}}(\omega, \theta))$  // evaluate new parameters of the embedding model  
 $\omega \leftarrow \omega'$ ,  $\theta \leftarrow \theta'$  // update both models
```

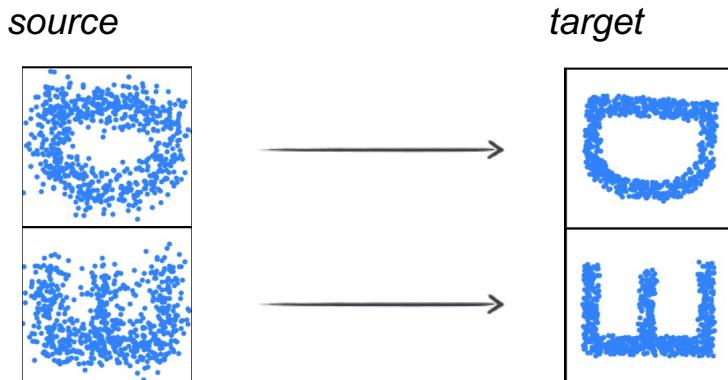
return $v_t(\cdot; \omega^*), \varphi(\cdot; \theta^*)$

Synthetic Example

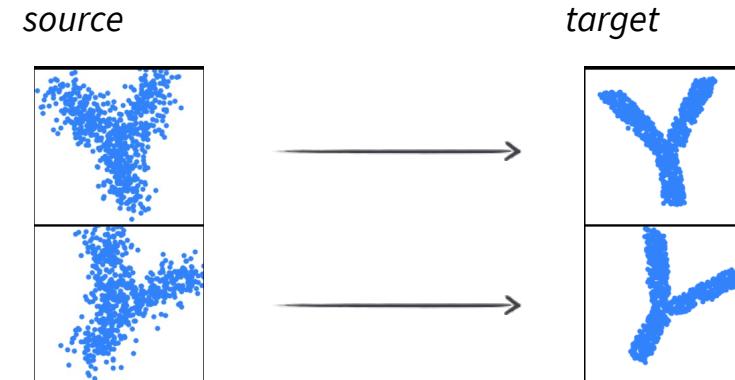
We create a **synthetic dataset** of paired joint distributions $\{(p_0(x_0|i), p_1(x_1|i))\}_{i=1}^N$

- We define a set of pre-defined **target** distributions $p_1(x_1|i)$ for $i = 1, \dots, N$ (letter silhouettes)
- To get paired $p_0(x_0|i)$ we **simulate the forward diffusion process** without drift $x_0 \sim \mathcal{N}(x_1, \sigma)$
- We **reverse** the diffusion process and learn the push-forward map from $p_0(x_0|i)$ (**source**) to $p_1(x_1|i)$ (**target**) for every index i

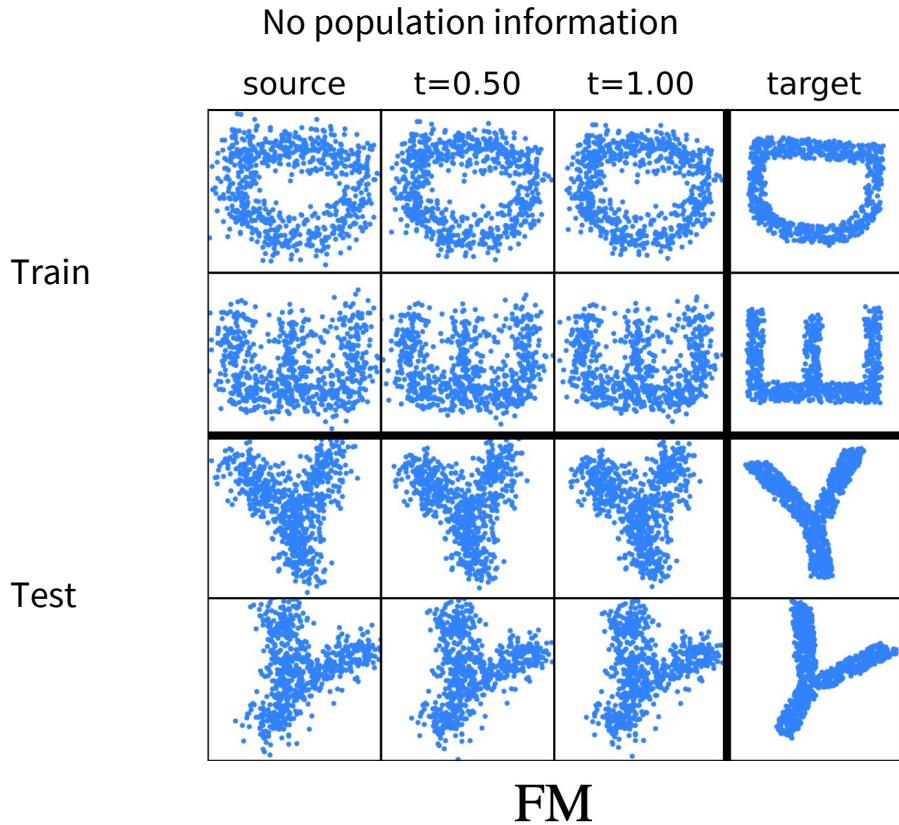
Train: 24 letters (excluding 'Y' and 'X'), each in 10 orientations



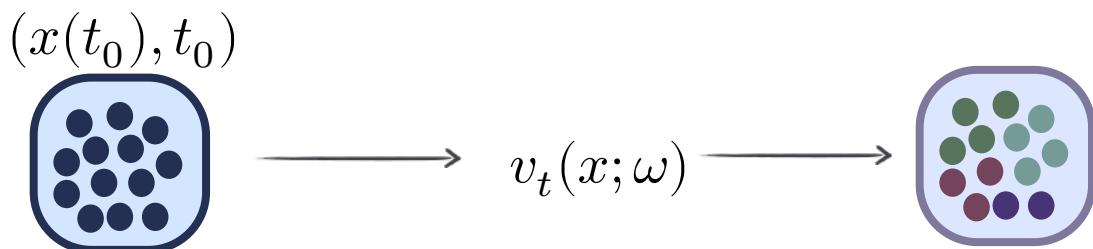
Test: 'Y' and 'X', each in 10 orientations



Synthetic Example (FM baseline)



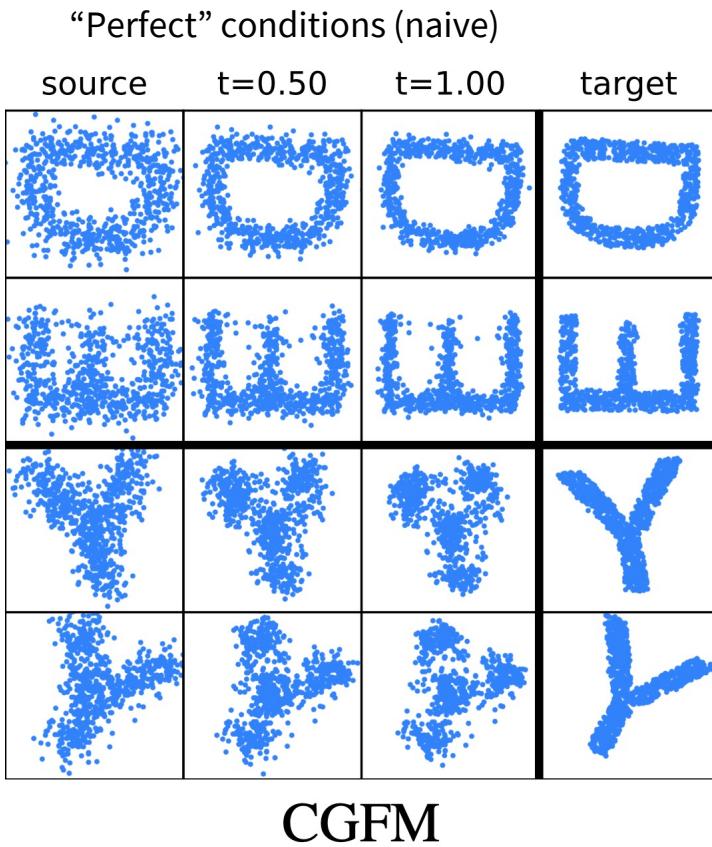
Predicts aggregate response over populations



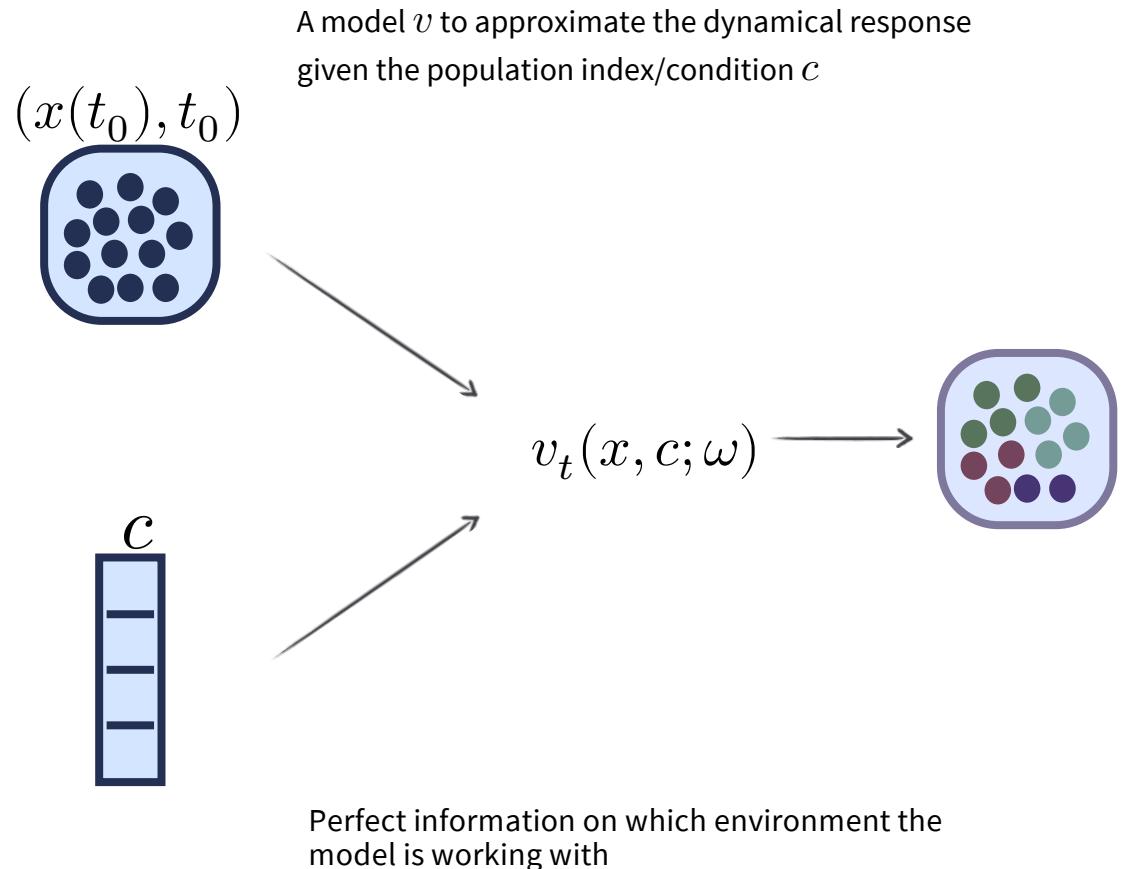
Synthetic Example (CGFM baseline)

Train

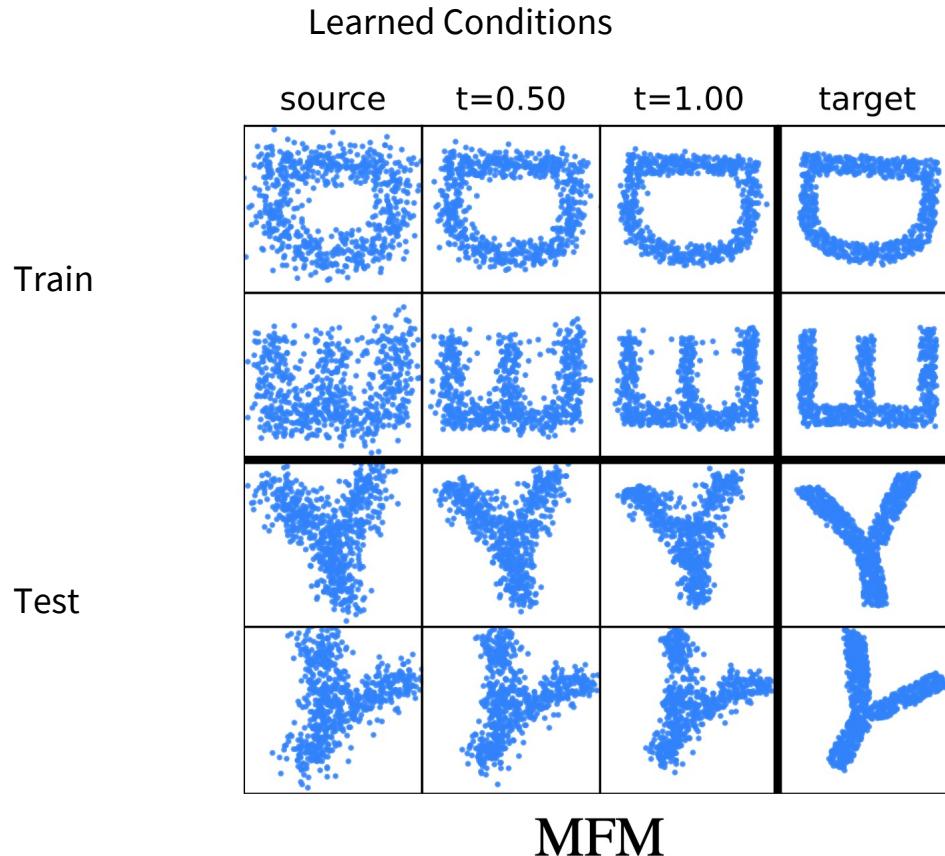
Test



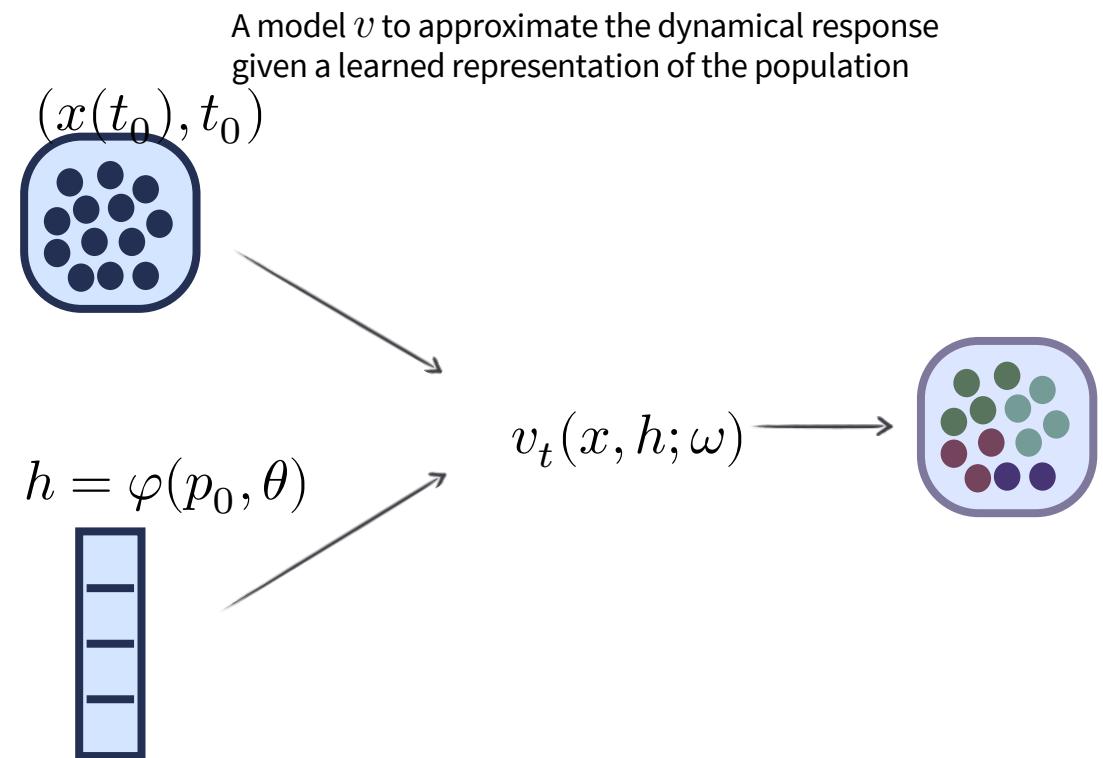
CGFM cannot generalize to the conditions
of *unseen* populations



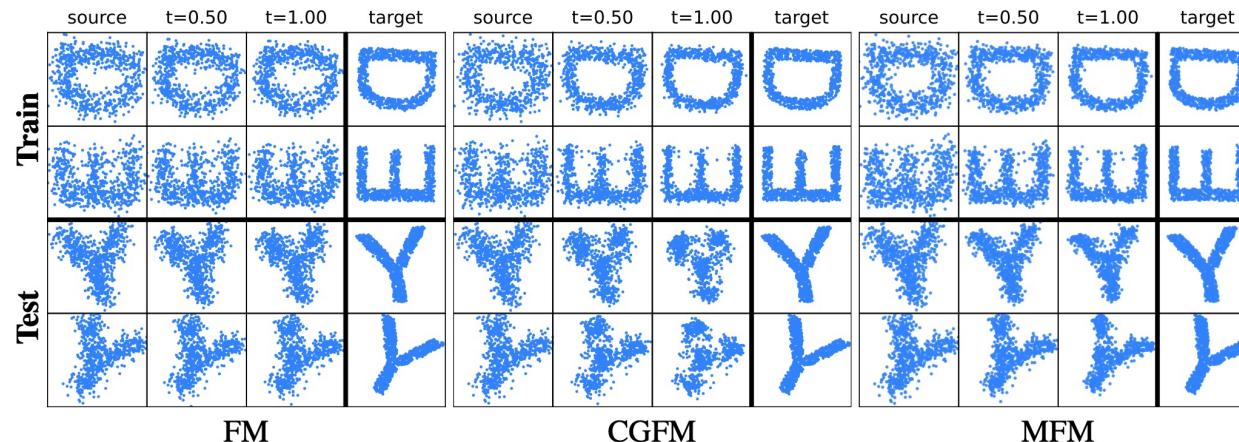
Synthetic Example (MFM)



MFM learns to represent entire populations, hence generalizes across *unseen* populations



Synthetic Example

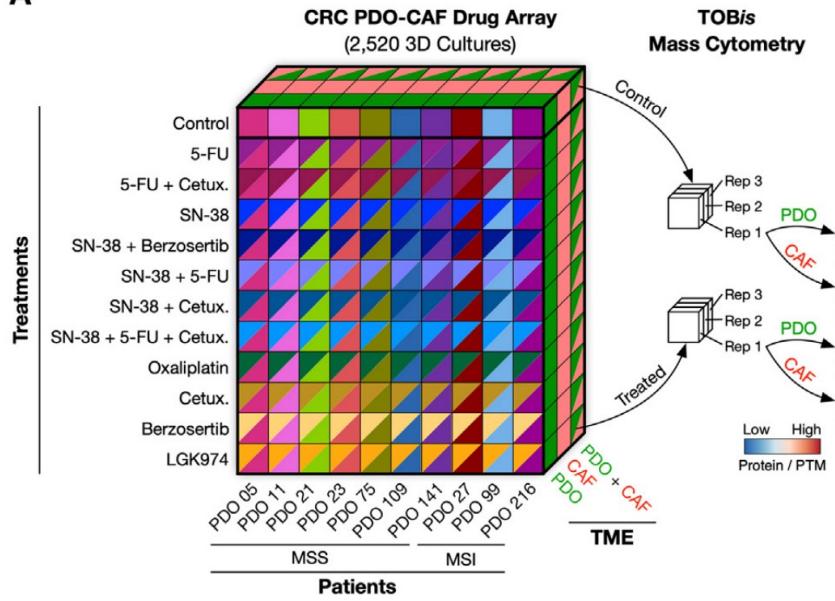


	Train			Test (X's)			Test (Y's)		
	\mathcal{W}_1	\mathcal{W}_2	MMD ($\times 10^{-3}$)	\mathcal{W}_1	\mathcal{W}_2	MMD ($\times 10^{-3}$)	\mathcal{W}_1	\mathcal{W}_2	MMD ($\times 10^{-3}$)
FM	0.209 ± 0.000	0.277 ± 0.000	2.54 ± 0.00	0.234 ± 0.000	0.309 ± 0.000	2.45 ± 0.00	0.238 ± 0.000	0.316 ± 0.000	3.32 ± 0.01
FM ^{w/N}	0.806 ± 0.000	0.960 ± 0.000	31.68 ± 0.00	0.764 ± 0.000	0.931 ± 0.000	25.04 ± 0.00	1.030 ± 0.000	1.228 ± 0.000	45.36 ± 0.00
CGFM	0.090 ± 0.000	0.113 ± 0.000	0.25 ± 0.00	0.334 ± 0.000	0.407 ± 0.000	5.55 ± 0.00	0.327 ± 0.000	0.405 ± 0.000	6.85 ± 0.00
CGFM ^{w/N}	0.156 ± 0.025	0.201 ± 0.027	1.02 ± 0.39	0.849 ± 0.004	0.993 ± 0.003	35.08 ± 0.75	1.062 ± 0.011	1.229 ± 0.010	55.66 ± 0.76
MFM ^{w/N} ($k = 0$)	0.148 ± 0.003	0.195 ± 0.010	0.94 ± 0.11	0.347 ± 0.011	0.431 ± 0.012	6.47 ± 0.44	0.402 ± 0.011	0.485 ± 0.010	10.92 ± 0.18
MFM ^{w/N} ($k = 1$)	0.154 ± 0.004	0.208 ± 0.010	0.91 ± 0.01	0.349 ± 0.023	0.433 ± 0.023	6.53 ± 0.52	0.391 ± 0.035	0.477 ± 0.041	10.71 ± 1.86
MFM ^{w/N} ($k = 10$)	0.151 ± 0.013	0.197 ± 0.015	0.94 ± 0.15	0.343 ± 0.020	0.427 ± 0.019	6.38 ± 0.67	0.413 ± 0.018	0.502 ± 0.024	11.93 ± 1.14
MFM ^{w/N} ($k = 50$)	0.174 ± 0.005	0.232 ± 0.006	1.40 ± 0.13	0.363 ± 0.010	0.449 ± 0.013	7.46 ± 0.44	0.446 ± 0.021	0.536 ± 0.028	13.40 ± 0.23
MFM ($k = 0$)	0.081 ± 0.003	0.100 ± 0.004	0.16 ± 0.06	0.202 ± 0.002	0.249 ± 0.003	2.29 ± 0.05	0.218 ± 0.001	0.262 ± 0.002	3.79 ± 0.11
MFM ($k = 1$)	0.082 ± 0.001	0.101 ± 0.002	0.16 ± 0.01	0.205 ± 0.008	0.251 ± 0.008	2.38 ± 0.22	0.215 ± 0.006	0.258 ± 0.007	3.78 ± 0.25
MFM ($k = 10$)	0.088 ± 0.002	0.109 ± 0.003	0.21 ± 0.01	0.201 ± 0.006	0.248 ± 0.006	2.20 ± 0.15	0.208 ± 0.003	0.252 ± 0.002	3.55 ± 0.06
MFM ($k = 50$)	0.092 ± 0.004	0.116 ± 0.004	0.25 ± 0.06	0.206 ± 0.008	0.257 ± 0.008	2.18 ± 0.25	0.204 ± 0.005	0.249 ± 0.006	3.14 ± 0.18

Biological data – patient-specific organoid drug screen dataset

Mass Cytometry

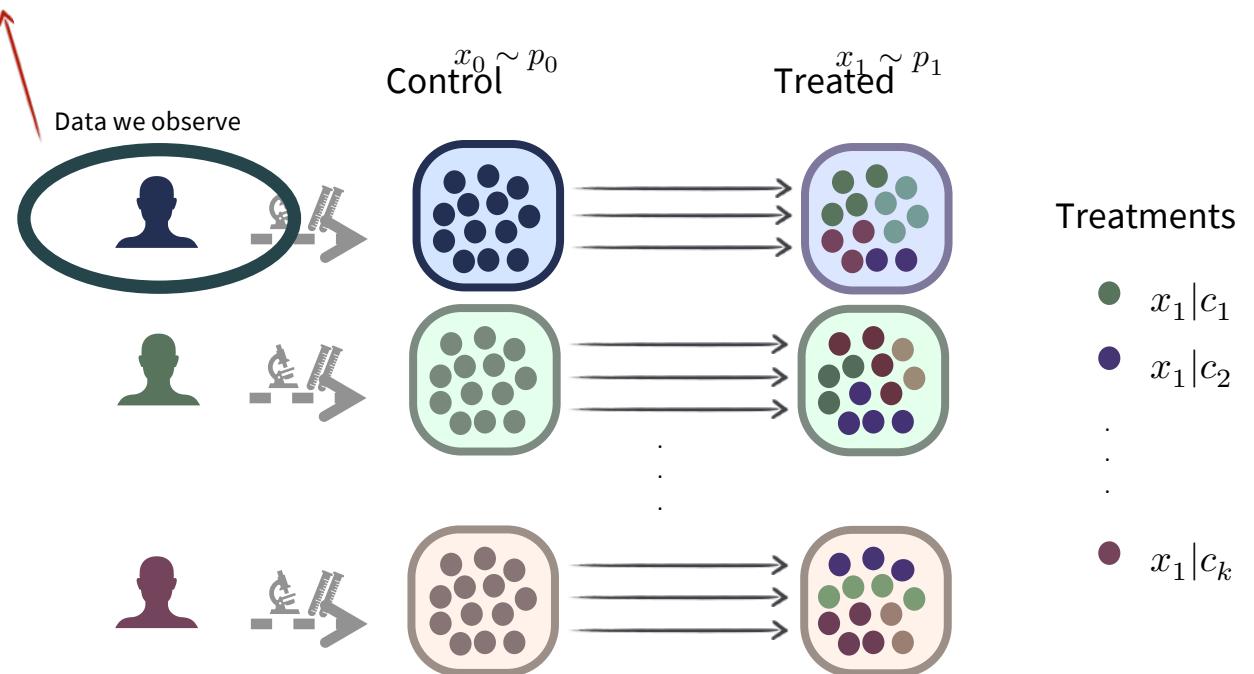
A



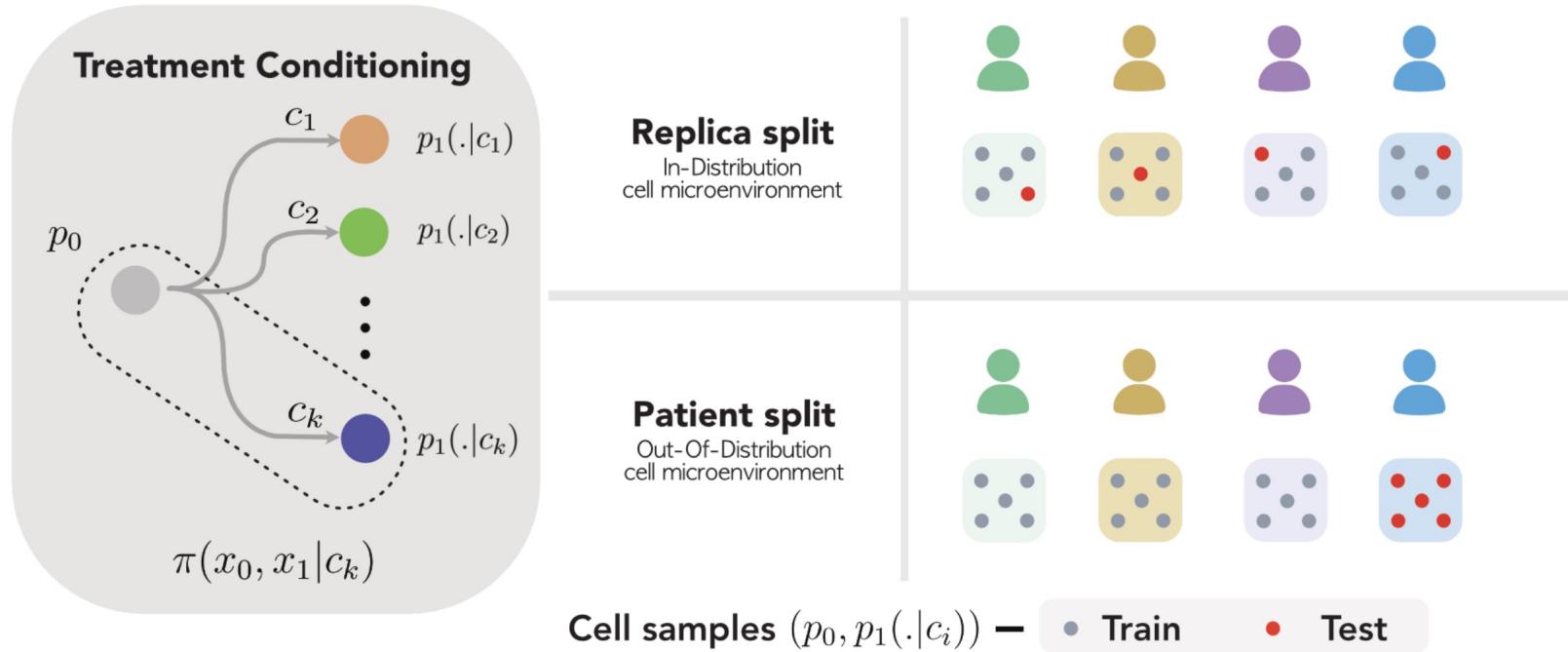
(Zapatero et al, Cell, 2023)

10 patients, 11 treatments, varying doses, 3 different cell cultures ... ***up to 2500 different environmental conditions!***
(we use ~ 1000)

Each patient has ~ 250 different (control, treated) pairs



Organoid Drug Screen Data



“Replica” Split

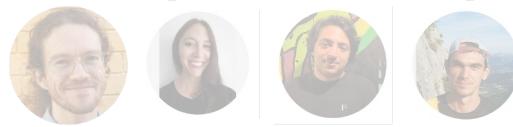
	Train				Test			
	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) (\downarrow)	$r^2(\uparrow)$	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) (\downarrow)	$r^2(\uparrow)$
FM	3.925 ± 0.019	4.041 ± 0.023	3.76 ± 0.26	0.952 ± 0.007	3.961 ± 0.036	4.089 ± 0.042	5.90 ± 0.25	0.941 ± 0.010
$FM^{w/\mathcal{N}}$	6.908 ± 0.037	7.181 ± 0.033	57.70 ± 0.75	0.639 ± 0.005	6.972 ± 0.022	7.244 ± 0.022	60.39 ± 0.98	0.642 ± 0.007
CGFM	3.864 ± 0.064	3.975 ± 0.069	3.16 ± 0.89	0.964 ± 0.006	4.087 ± 0.063	4.211 ± 0.066	8.84 ± 0.75	0.938 ± 0.006
$CGFM^{w/\mathcal{N}}$	4.187 ± 0.008	4.340 ± 0.009	8.69 ± 0.50	0.936 ± 0.002	6.852 ± 0.045	7.114 ± 0.044	71.24 ± 3.71	0.666 ± 0.016
ICNN	4.286 ± 0.018	4.313 ± 0.112	38.6 ± 0.212	0.897 ± 0.031	4.194 ± 0.110	4.313 ± 0.112	37.9 ± 2.84	0.897 ± 0.008
$MFM^{w/\mathcal{N}} (k=0)$	3.940 ± 0.022	4.047 ± 0.023	3.91 ± 0.18	0.959 ± 0.006	3.896 ± 0.026	4.002 ± 0.030	4.35 ± 0.18	0.950 ± 0.005
$MFM^{w/\mathcal{N}} (k=10)$	3.976 ± 0.044	4.086 ± 0.049	4.52 ± 0.42	0.961 ± 0.002	3.943 ± 0.032	4.051 ± 0.034	5.28 ± 0.25	0.952 ± 0.001
$MFM^{w/\mathcal{N}} (k=50)$	3.968 ± 0.013	4.075 ± 0.014	4.36 ± 0.44	0.961 ± 0.002	3.934 ± 0.007	4.041 ± 0.008	4.99 ± 0.35	0.954 ± 0.000
$MFM^{w/\mathcal{N}} (k=100)$	3.937 ± 0.014	4.040 ± 0.015	3.94 ± 0.00	0.963 ± 0.001	3.908 ± 0.030	4.011 ± 0.033	4.68 ± 0.52	0.953 ± 0.002
$MFM (k=0)$	3.874 ± 0.015	3.973 ± 0.020	3.37 ± 0.14	0.967 ± 0.003	3.880 ± 0.009	3.990 ± 0.011	4.68 ± 0.16	0.955 ± 0.002
$MFM (k=10)$	3.896 ± 0.021	4.000 ± 0.021	3.82 ± 0.12	0.964 ± 0.001	3.899 ± 0.013	4.012 ± 0.011	5.13 ± 0.48	0.955 ± 0.001
$MFM (k=50)$	3.888 ± 0.038	3.991 ± 0.030	3.59 ± 0.41	0.963 ± 0.001	3.900 ± 0.038	4.013 ± 0.034	5.06 ± 0.22	0.954 ± 0.003
$MFM (k=100)$	3.906 ± 0.010	4.008 ± 0.005	4.05 ± 0.38	0.964 ± 0.002	3.898 ± 0.008	4.009 ± 0.009	5.19 ± 0.05	0.957 ± 0.000

Patient Split

	Train				Test			
	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) (\downarrow)	$r^2(\uparrow)$	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) (\downarrow)	$r^2(\uparrow)$
FM	3.985 ± 0.054	4.115 ± 0.067	4.64 ± 0.43	0.938 ± 0.014	4.340 ± 0.078	4.564 ± 0.111	13.00 ± 0.67	0.865 ± 0.034
$FM^{w/\mathcal{N}}$	6.892 ± 0.027	7.164 ± 0.033	57.03 ± 1.00	0.655 ± 0.003	7.114 ± 0.100	7.404 ± 0.086	64.97 ± 3.79	0.613 ± 0.008
CGFM	3.882 ± 0.019	3.999 ± 0.020	3.16 ± 0.59	0.952 ± 0.004	4.443 ± 0.033	4.621 ± 0.041	17.00 ± 1.03	0.899 ± 0.008
$CGFM^{w/\mathcal{N}}$	4.313 ± 0.077	4.480 ± 0.081	11.51 ± 1.96	0.918 ± 0.004	7.135 ± 0.045	7.390 ± 0.037	79.78 ± 4.67	0.637 ± 0.010
ICNN	4.289 ± 0.020	4.382 ± 0.021	37.0 ± 2.84	0.913 ± 0.003	4.525 ± 0.051	4.681 ± 0.054	74.00 ± 0.57	0.862 ± 0.127
$MFM^{w/\mathcal{N}}(k=0)$	3.982 ± 0.014	4.095 ± 0.015	5.04 ± 0.36	0.951 ± 0.002	4.177 ± 0.042	4.355 ± 0.048	10.53 ± 0.59	0.911 ± 0.001
$MFM^{w/\mathcal{N}}(k=10)$	4.006 ± 0.008	4.119 ± 0.012	5.13 ± 0.30	0.948 ± 0.001	4.156 ± 0.065	4.324 ± 0.067	9.58 ± 1.63	0.912 ± 0.003
$MFM^{w/\mathcal{N}}(k=50)$	3.982 ± 0.018	4.095 ± 0.016	4.74 ± 0.21	0.951 ± 0.002	4.153 ± 0.069	4.324 ± 0.070	9.63 ± 1.45	0.912 ± 0.002
$MFM^{w/\mathcal{N}}(k=100)$	4.004 ± 0.012	4.119 ± 0.014	5.19 ± 0.43	0.949 ± 0.002	4.166 ± 0.001	4.341 ± 0.003	9.52 ± 0.33	0.915 ± 0.005
$MFM(k=0)$	3.905 ± 0.005	4.012 ± 0.006	4.18 ± 0.25	0.958 ± 0.001	4.209 ± 0.007	4.380 ± 0.012	12.34 ± 0.50	0.918 ± 0.002
$MFM(k=10)$	3.896 ± 0.033	4.005 ± 0.036	3.89 ± 0.44	0.957 ± 0.005	4.216 ± 0.090	4.395 ± 0.098	11.99 ± 2.36	0.917 ± 0.005
$MFM(k=50)$	3.902 ± 0.018	4.008 ± 0.022	4.20 ± 0.17	0.958 ± 0.000	4.214 ± 0.017	4.396 ± 0.020	12.09 ± 0.75	0.916 ± 0.002
$MFM(k=100)$	3.884 ± 0.039	3.986 ± 0.044	3.77 ± 0.49	0.955 ± 0.001	4.100 ± 0.093	4.269 ± 0.104	8.96 ± 1.88	0.917 ± 0.004

Talk overview

📚 **Meta Optimal Transport [ICML 2023]**



📚 **Meta Flow Matching [2024]**

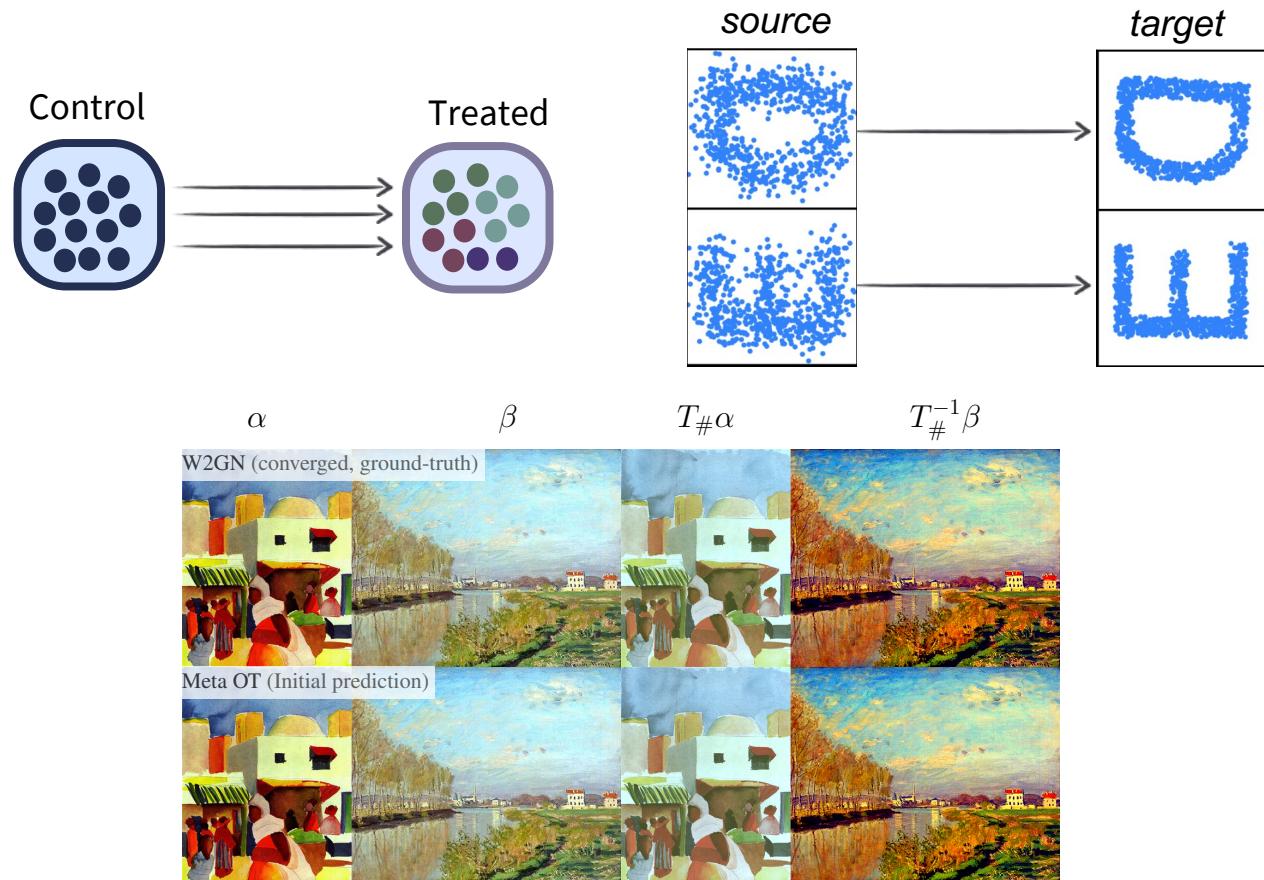
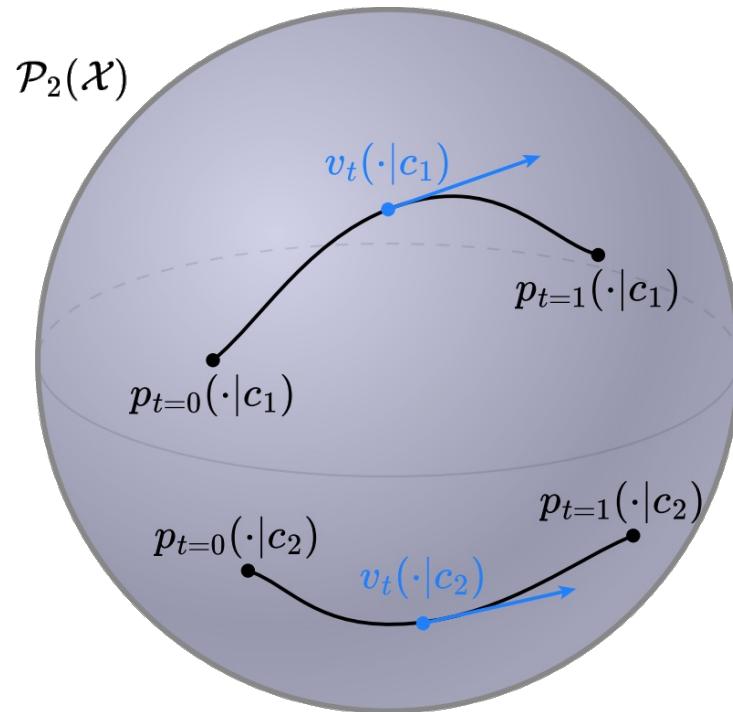


📚 **Wasserstein Flow Matching [2024]**



So far: distributions over pairs of distributions

Meta OT and Meta FM assume (coupled) **pairs of distributions**



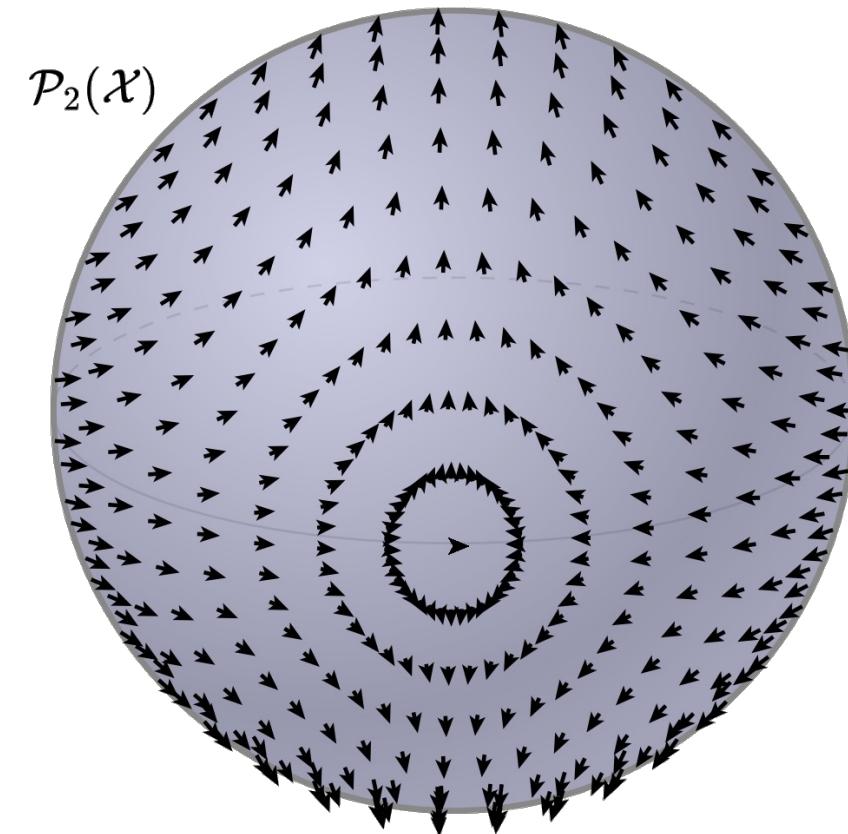
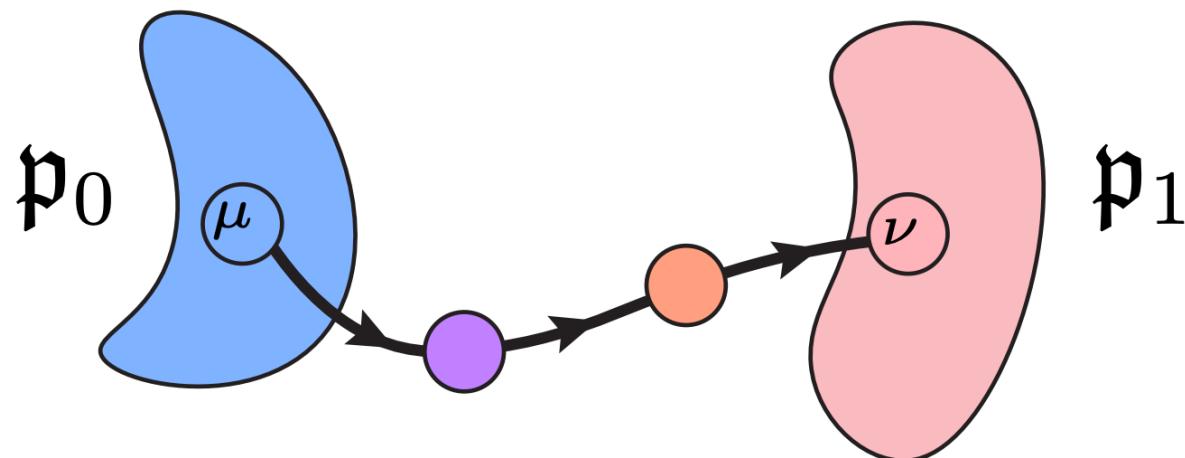
What if we have unpaired distributions?



Wasserstein Flow Matching. Haviv, Pooladian, Pe'er, Amos. 2024.

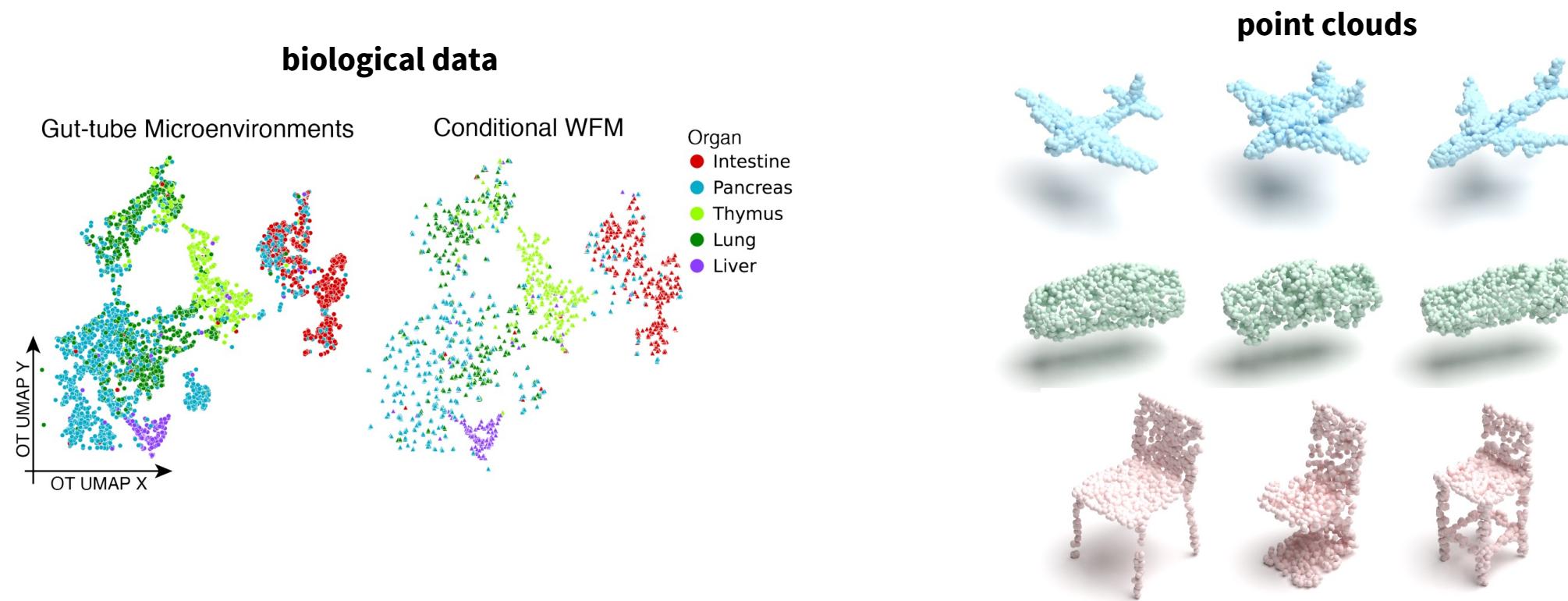
Still can **learn a flow** between them

(we also can't simply flatten them into a mixture)



Why would we have unpaired distributions?

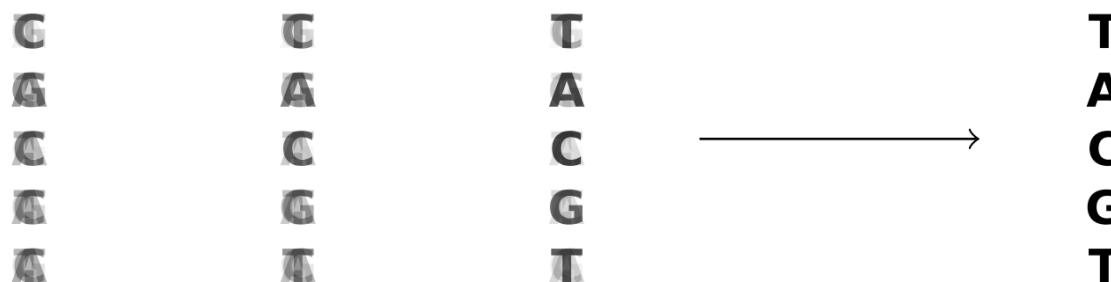
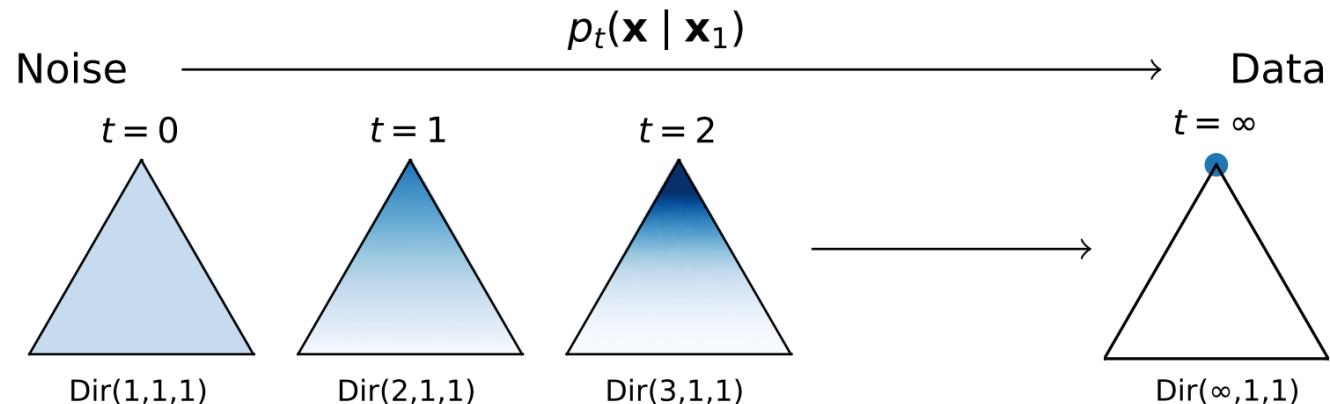
Want to do generative modeling where the data points are inherently distributions



Related: flows for categorical distributions

📚 Dirichlet Flow Matching. Stark et al., NeurIPS 2024.

📚 Fisher Flow Matching. Davis et al., ICML 2024.



How to flow on the Wasserstein manifold?



Riemannian Flow Matching. Chen and Lipman, ICLR 2024.

Use **Riemannian flow matching** with the geodesics (OT paths) on the Wasserstein manifold

Algorithm 1: Wasserstein FM Training

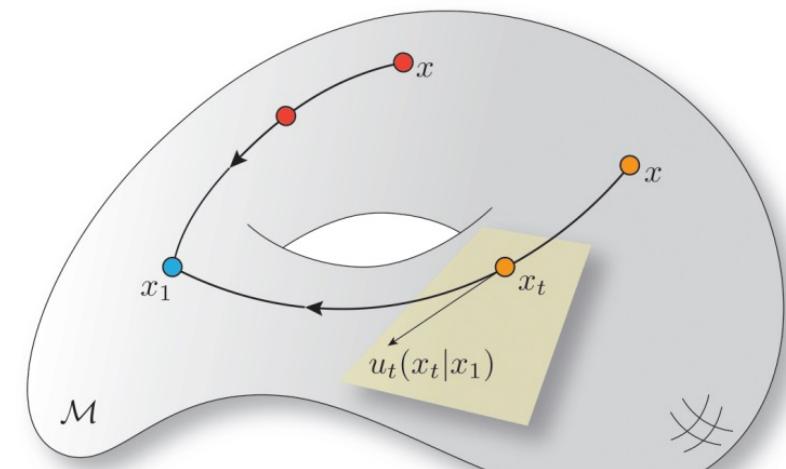
Data: base $\mathbf{p}_0 \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$, target $\mathbf{p}_1 \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$, geo $\in \{\text{BW}, \text{PC}\}$
Init: Parameters θ of f_θ^{geo}
while not converged **do**
 Sample time $t \sim \mathcal{U}(0, 1)$
 Sample source measure $\mu \sim \mathbf{p}_0$
 Sample target measure $\nu \sim \mathbf{p}_1$
 if geo is BW **then**
 $\mu_t \leftarrow (m_t, \Sigma_t)$ via equation 8
 $v_t \leftarrow (\dot{m}_t, \Sigma_t^{\text{BW}})$ via equation 9
 else
 $\mu_t \leftarrow$ Approximate via equation 4
 $v_t \leftarrow$ Approximate via equation 7
 $\ell(\theta) \leftarrow \|f_\theta^{\text{geo}}(\mu_t, t) - v_t\|_{L^2(\mu_t)}^2$
 $\theta \leftarrow \text{optimizer_step}(\theta, \ell(\theta), \nabla_\theta \ell(\theta))$

Algorithm 2: BW(\mathbb{R}^d) generation

Data: Trained f_θ^{BW} , step size $h = 1/N$
Init: $\mathcal{N}(m_0, \Sigma_0) \sim \mathbf{p}_0$
for $k = 0, \dots, N - 1$ **do**
 $(s_k, S_k) \leftarrow f_\theta^{\text{BW}}((m_{kh}, \Sigma_{kh}), kh)$
 $m_{(k+1)h} \leftarrow m_k + hs_k$
 $U_k \leftarrow (I + hS_k)$
 $\Sigma_{(k+1)h} \leftarrow U_k \Sigma_{kh} U_k$
Return: $\mathcal{N}(m_{Nh}, \Sigma_{Nh})$

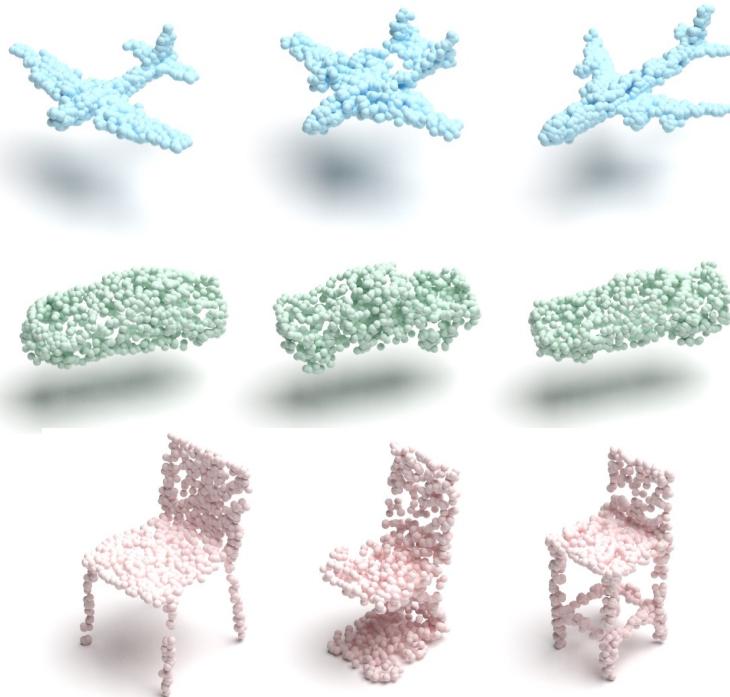
Algorithm 3: Point-cloud generation

Data: Trained f_θ^{PC} , step size $h = 1/N$
Init: $\hat{\mathbf{X}}_0 = \{X_1, \dots, X_n\} \sim \mathbf{p}_0$
for $k = 0, \dots, N - 1$ **do**
 $\hat{\mathbf{X}}_{(k+1)h} \leftarrow \hat{\mathbf{X}}_{kh} + h f_\theta^{\text{PC}}(\hat{\mathbf{X}}_{kh}, kh)$
Return: $\hat{\mathbf{X}}_{Nh}$



Point cloud generation results

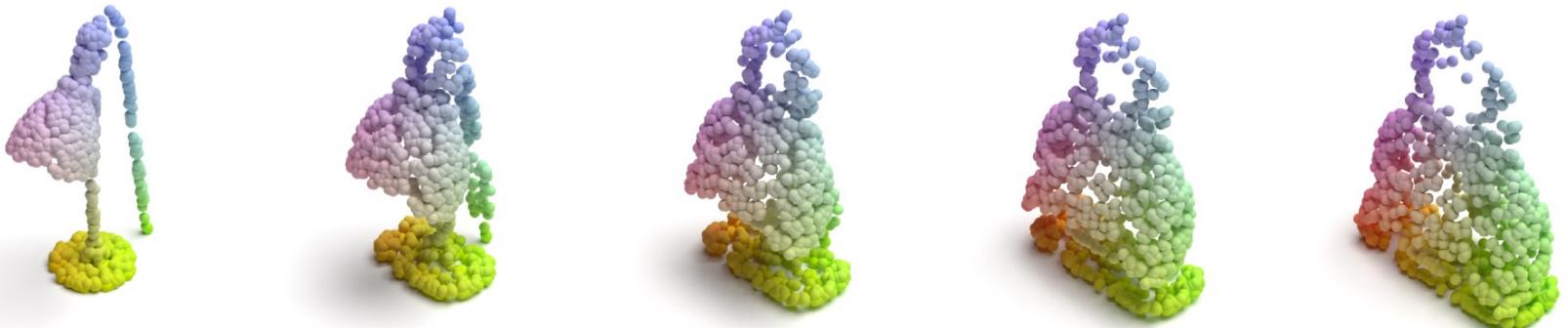
Competitive and **don't require spatially discretizing** the domain like most of the baselines



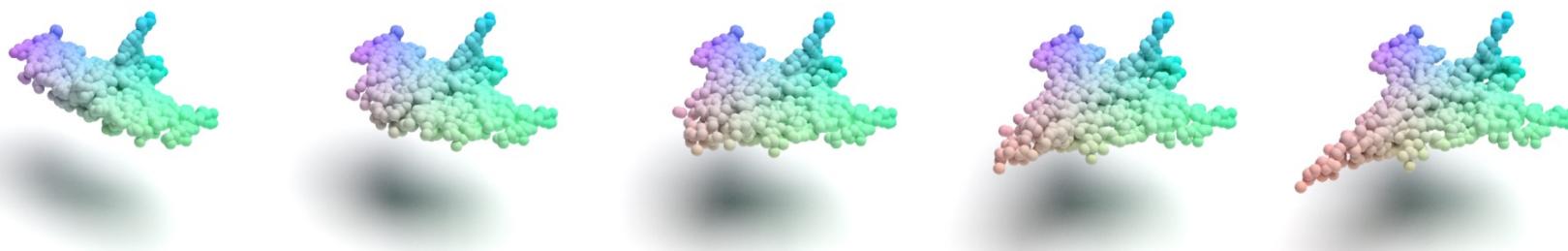
	Airplane		Chair		Car	
	CD ↓	EMD ↓	CD ↓	EMD ↓	CD ↓	EMD ↓
PointFlow	75.68	70.74	62.84	60.57	58.10	56.25
SoftFlow	76.05	65.80	59.21	60.05	64.77	60.09
DPF-Net	75.18	65.55	62.00	58.53	62.35	54.48
Shape-GF	80.00	76.17	68.96	65.48	63.20	56.53
PVD	73.82	64.81	56.26	53.32	54.55	53.83
PSF	71.11	61.09	58.92	54.45	57.19	56.07
WFM (ours)	73.45	71.72	58.98	57.77	56.53	57.95

WFM also does interpolations and completions

Flow from a **distribution over lamps** to a **distribution over handbags**



Completion using a flow trained over a **distribution of planes**



Transport and flows between distributions over distributions

Brandon Amos • Meta, NYC

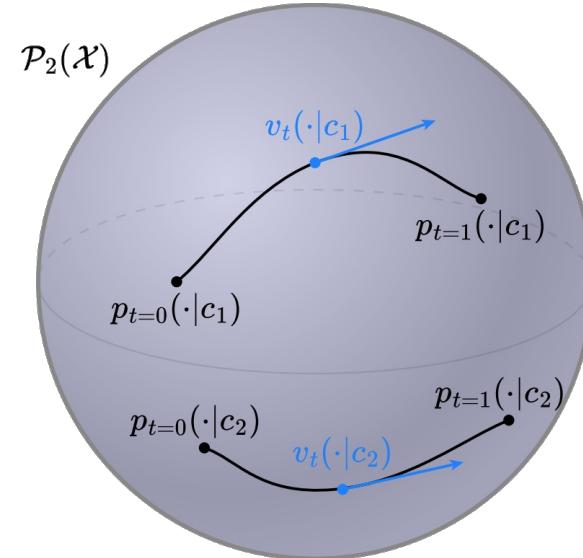
📚 **Meta Optimal Transport** [ICML 2023]



📚 **Meta Flow Matching** [2024]



📚 **Wasserstein Flow Matching** [2024]



slides



bamos.github.io/presentations