Generative modeling on the space of empirical measures

Nic Fishman and Gokul Gowri

2025.10.17

roadmap

1. ***distribution encoders:*** achieving a CLT for encoders

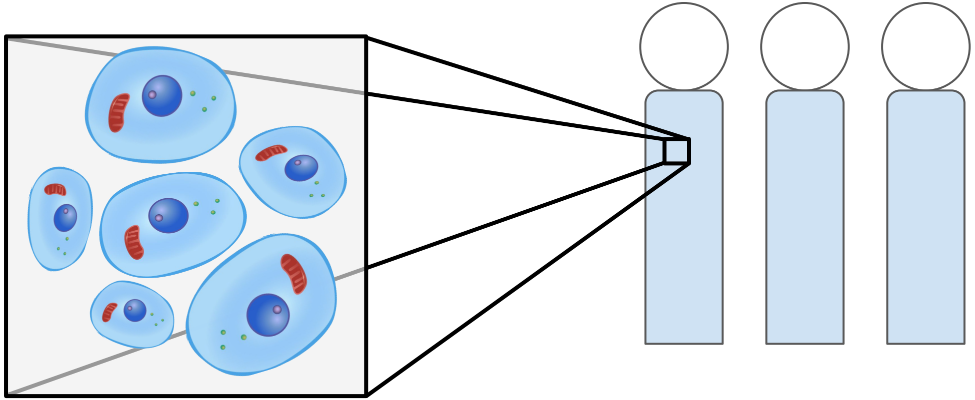
2. ***unsupervised distribution embeddings:*** distribution representations using conditional generators

3. ***any-to-any transport:*** learning transport maps between any pair of distributions, using dist. encoders

4. ***outlook:*** what's next?

distribution embeddings

many complex systems are *multiscale*



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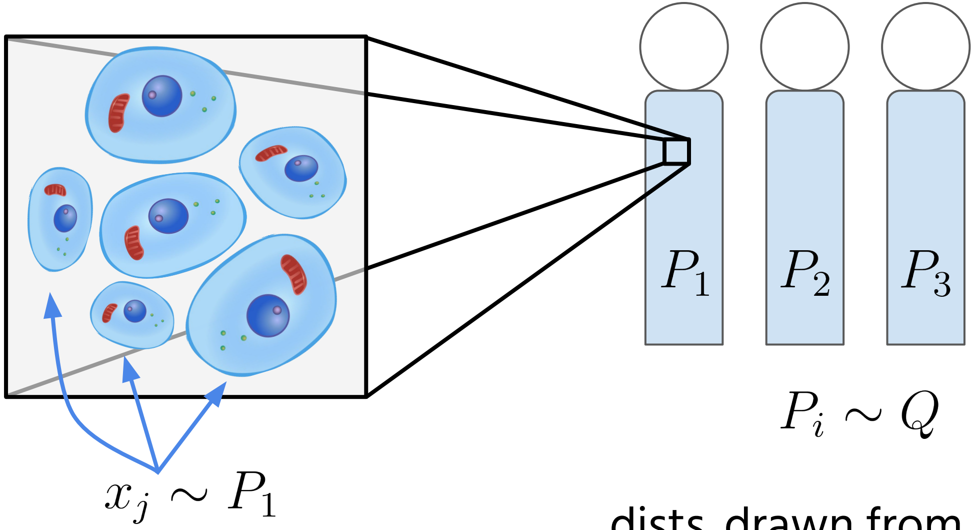

sets of samples
drawn from a dist.

dists. drawn from a metadist.

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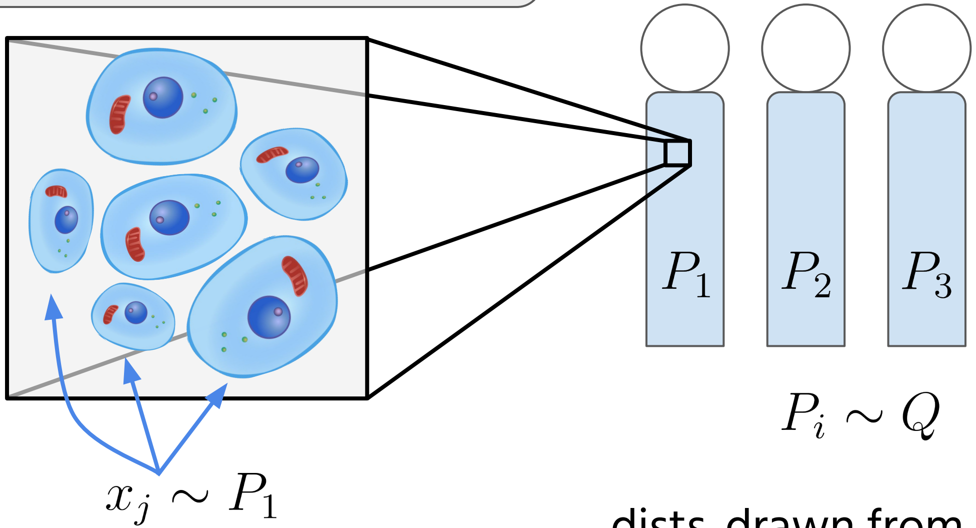
how do we get an embedding of $\boldsymbol{P}$ from samples $\boldsymbol{x} \sim \boldsymbol{P}$?



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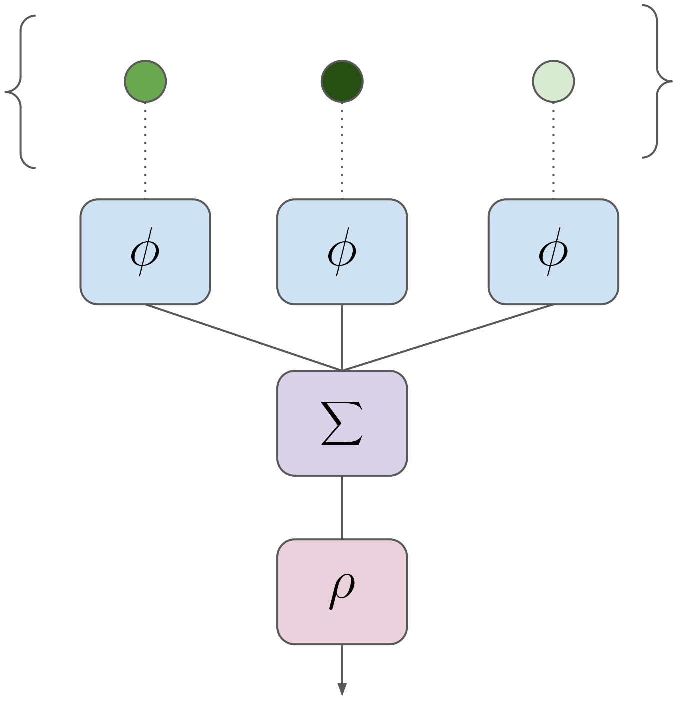
deep sets (and related) offer tools for representing sets



Zaheer et al., 2017

what properties do we want for a distribution encoder?

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we want the encoding to concentrate around its population value:

$$\sqrt{m}(\mathcal{E}(S) - \phi(P)) \xrightarrow{d} \mathcal{N}(0, \Sigma)$$

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so that any plug-in loss becomes an unbiased, asymptotically normal estimator

$$\sqrt{m}\,\left(\ell\left(\mathcal{E}(S)\right) - \ell\left(\phi(P)\right)\right) \xrightarrow{d} \mathcal{N}(0, \sigma^2)$$

distributional invariance enables a CLT for encoders

we call an encoder satisfying the following properties *distributionally invariant*

1. ***permutation invariance:*** reordering samples does not change the embedding

$$\mathcal{E}(S) = \mathcal{E}(\pi(S))$$

2. ***proportional invariance:*** duplicating every sample *K* times does not change the embedding

$$\mathcal{E}(S) = \mathcal{E}(\cup_{k=1}^{K} S)$$

3. ***smooth pooling:*** Hadamard differentiability of the pooling operator

embeddings are normally distributed

we run the following experiment:

with a mean-pooled GNN

fix a distribution P_i

for different set sizes *m*

1. sample many size *m* sets
2. visualize embeddings

we see normality as m becomes large

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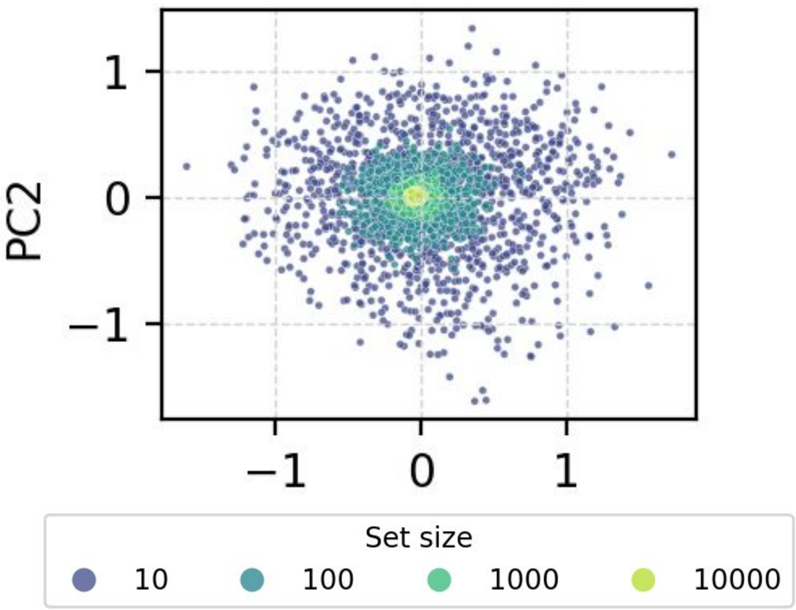


what about when we have additional, unlabeled data?

we have shown how to build distribution encoders

but often we have a small amount of labeled and a large amount of unlabeled data.

how can we build unsupervised distribution embeddings?

unsupervised distribution embeddings

generative distribution embeddings

intuition: the ideal distribution embedding should provide enough information to generate samples from the corresponding distribution

$$\mathcal{G}(\mathcal{E}(S_{i,m})) \xrightarrow{d} P_i \quad \text{as} \quad m \to \infty$$

implementing generative distribution embeddings

to build a GDE, all you need to do is combine

1. a distributionally invariant encoder

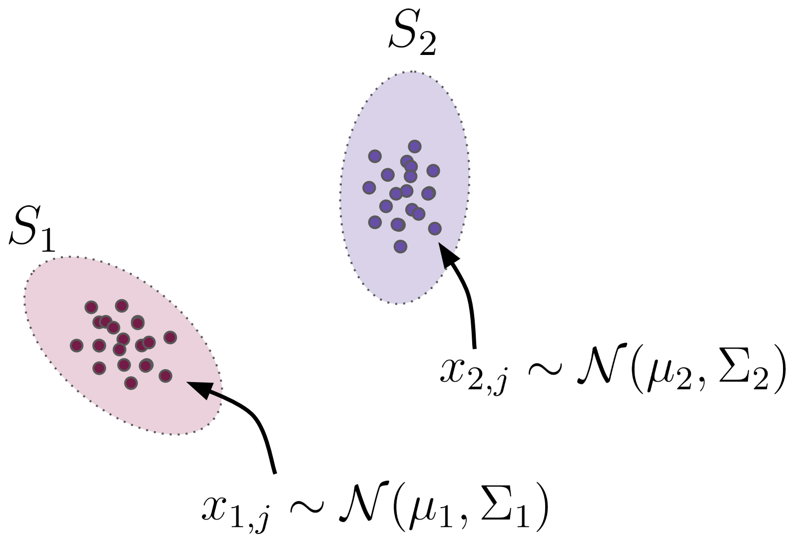
    e.g., a mean-pooled GNN, a mean-pooled self-attention

2. a conditional generator

    e.g., a diffusion model, an autoregressive LLM

and train end-to-end using the conditional generator loss

a toy example with Gaussians



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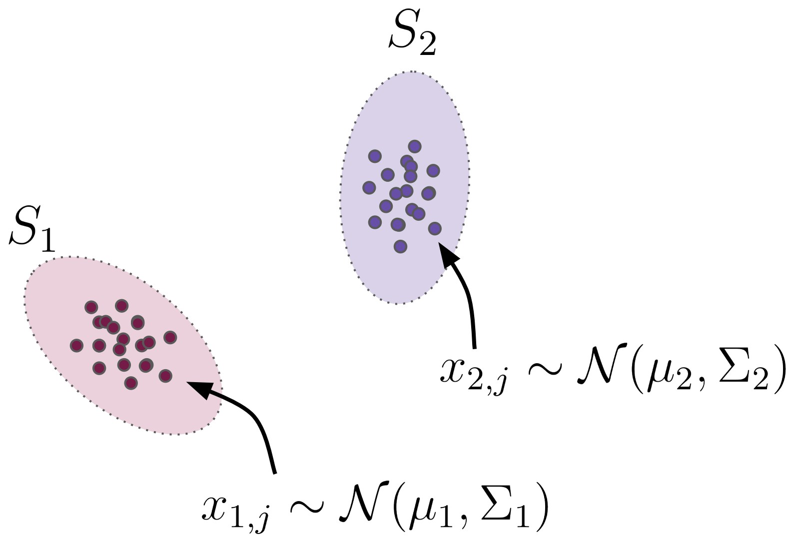

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$$\Sigma_i \sim \mathcal{W}^{-1}(\Phi, \nu)$$
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$$\mathcal{D} = \left\{ S_i = \{x_{ij}\}_{j=1}^{m} \right\}_{i=1}^{n}$$

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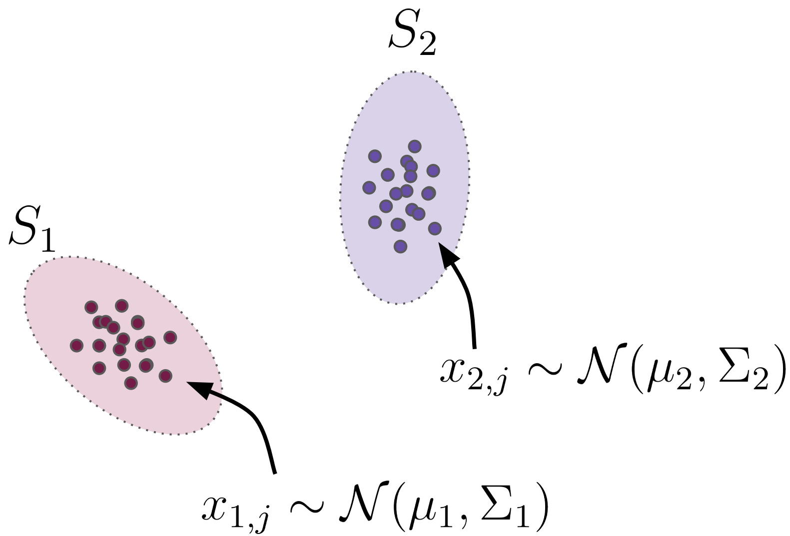

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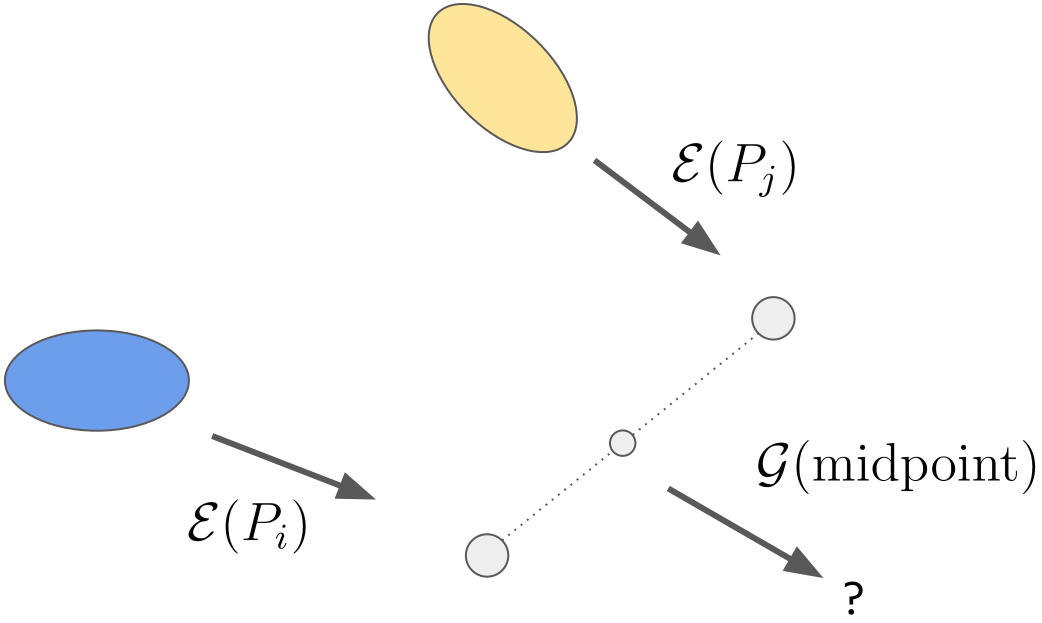
we will learn representations of distributions using
encoder: a mean-pooled deep sets
generator: conditional diffusion

probing the geometry of the latent space



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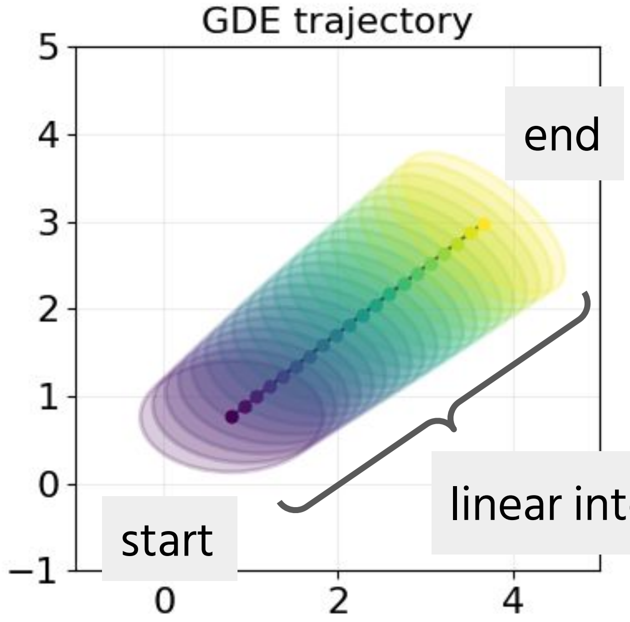

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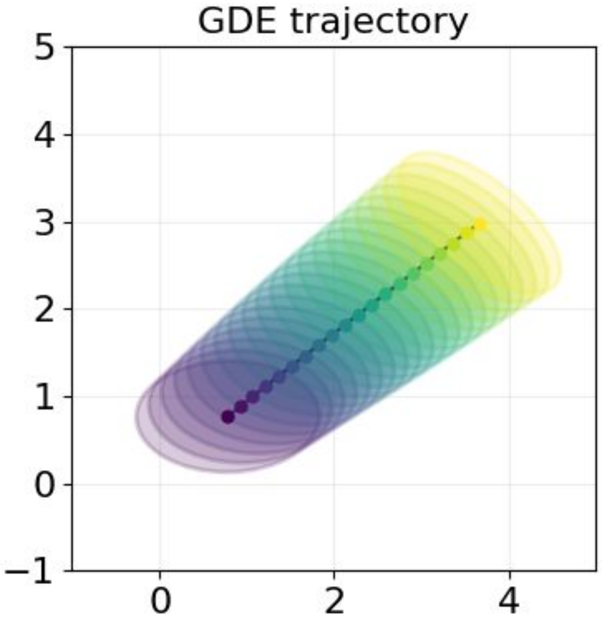

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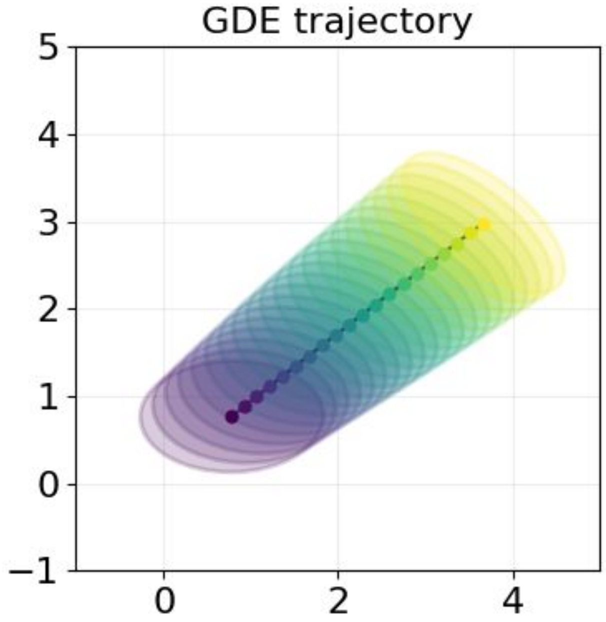

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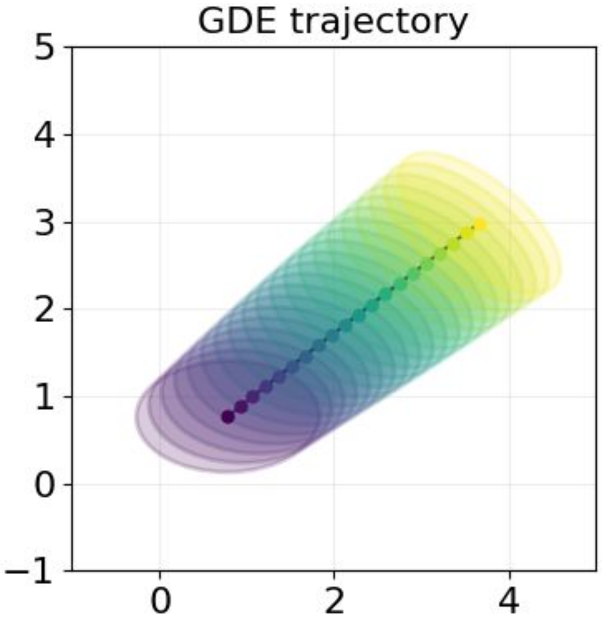

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it is! this is almost exactly the optimal transport under the wasserstein 2 distance

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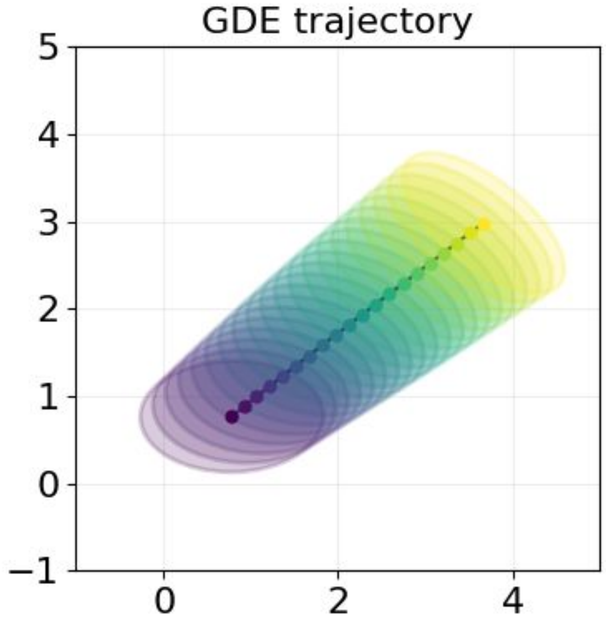
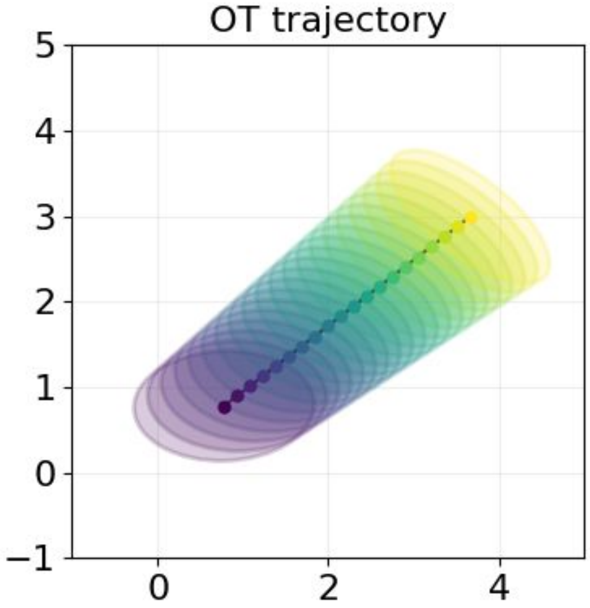




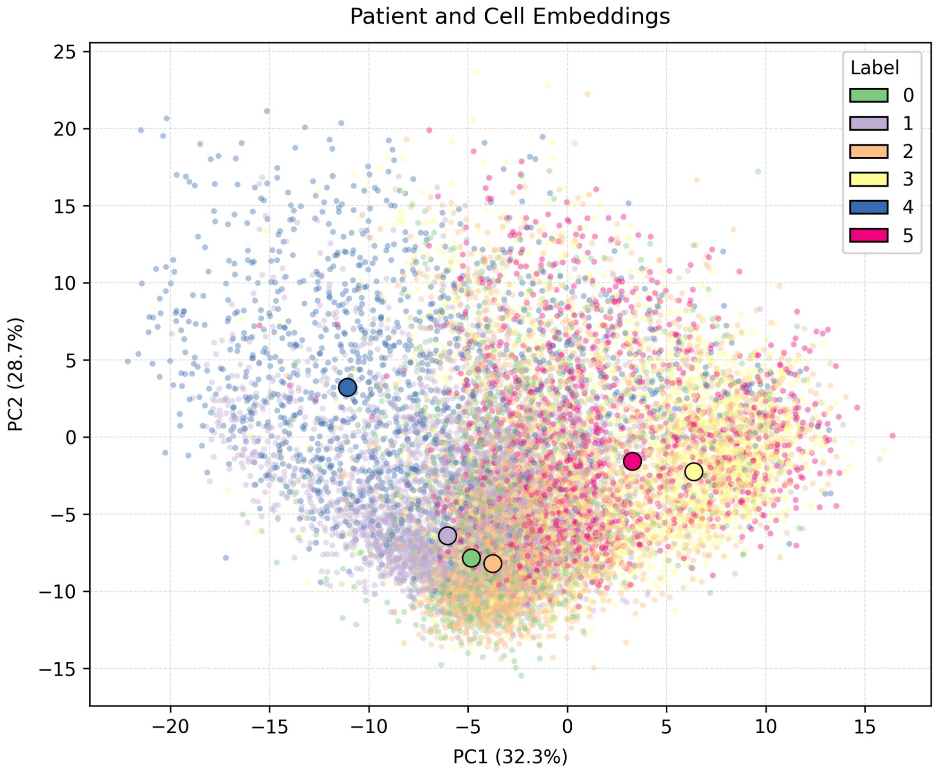
notes on the geometry of GDE latent spaces

1. GDE interpolants are not exactly optimal transport interpolants in general, in practice they are OT-like but restricted to a family of distributions

2. GDE latent spaces can be warped by metadistribution-induced weighting on the statistical manifold

3. while GDE interpolants resemble OT interpolants at the population level, they don't directly provide information about unit level trajectories

example: donor-level representations from cell-level data



data from Fullard et al., 2025

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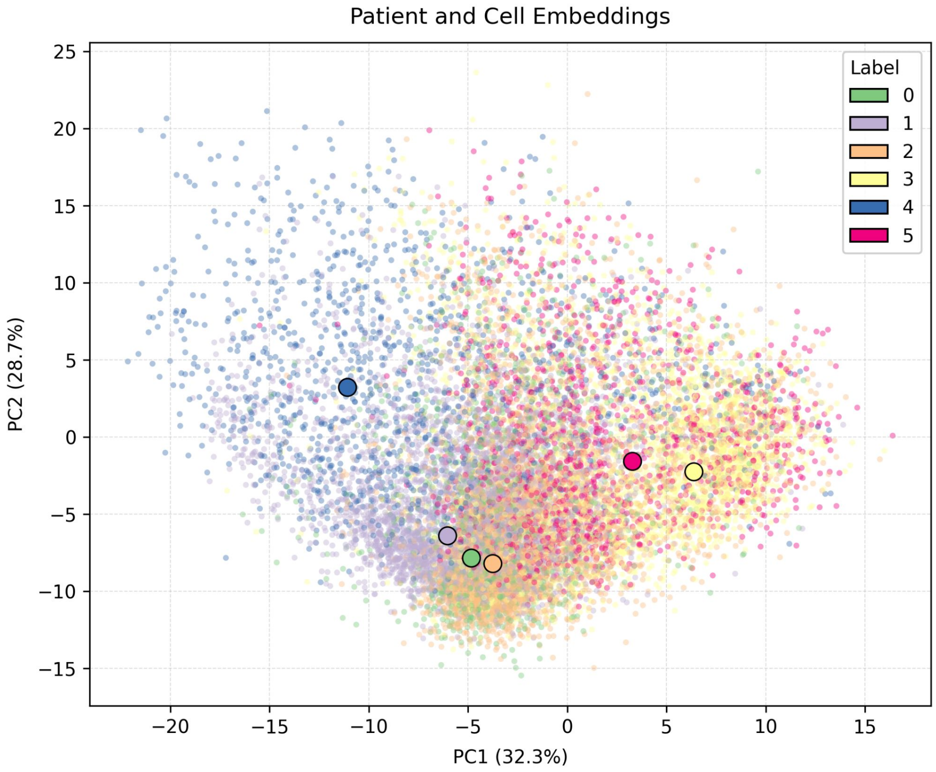

We construct a model to predict donor attributes based on single cells.

For the supervised task we use 10% of the donors, for the semisupervised we use that 10% as labeled data and the remaining 90% unlabeled.

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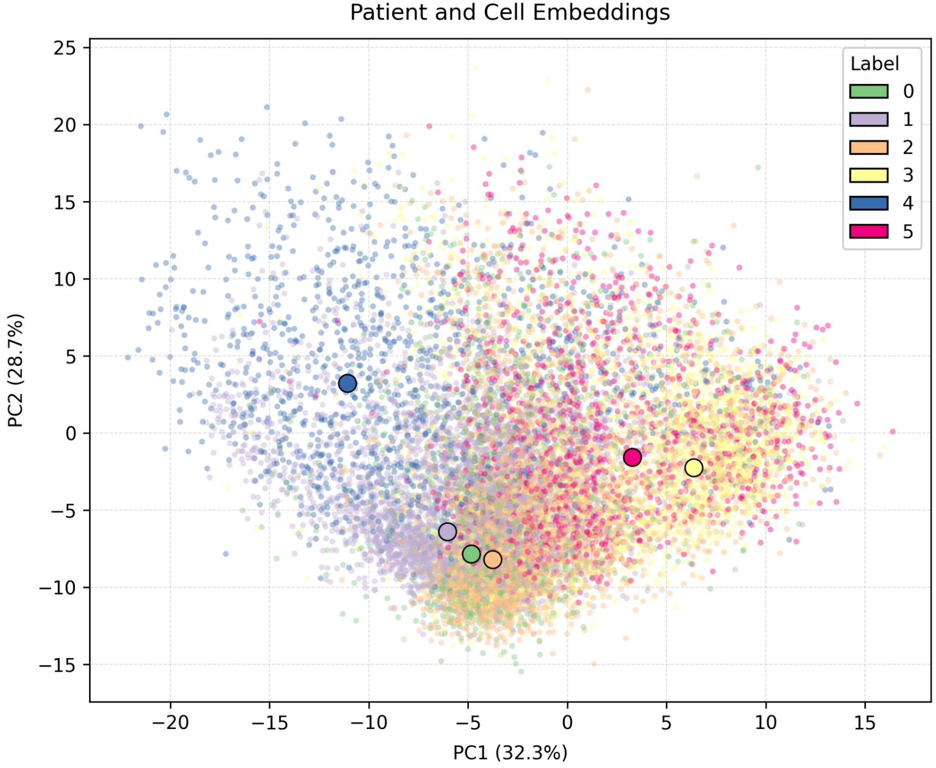

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Metric	Semi-Supervised	Supervised
Accuracy	**0.8887**	0.8791
Balanced Accuracy	**0.5383**	0.5291
Roc Auc	**0.5131**	0.4872
F1 Score	**0.1479**	0.1293

data from Fullard et al., 2025

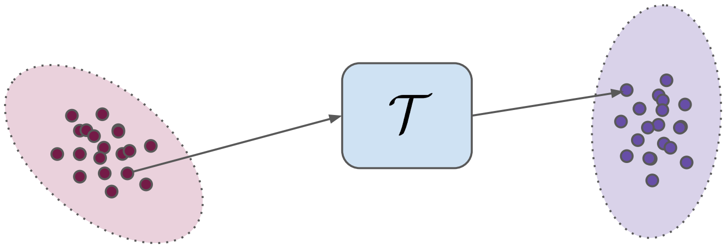
GDEs are applicable in many real world settings

GDEs can also be useful for modelling...

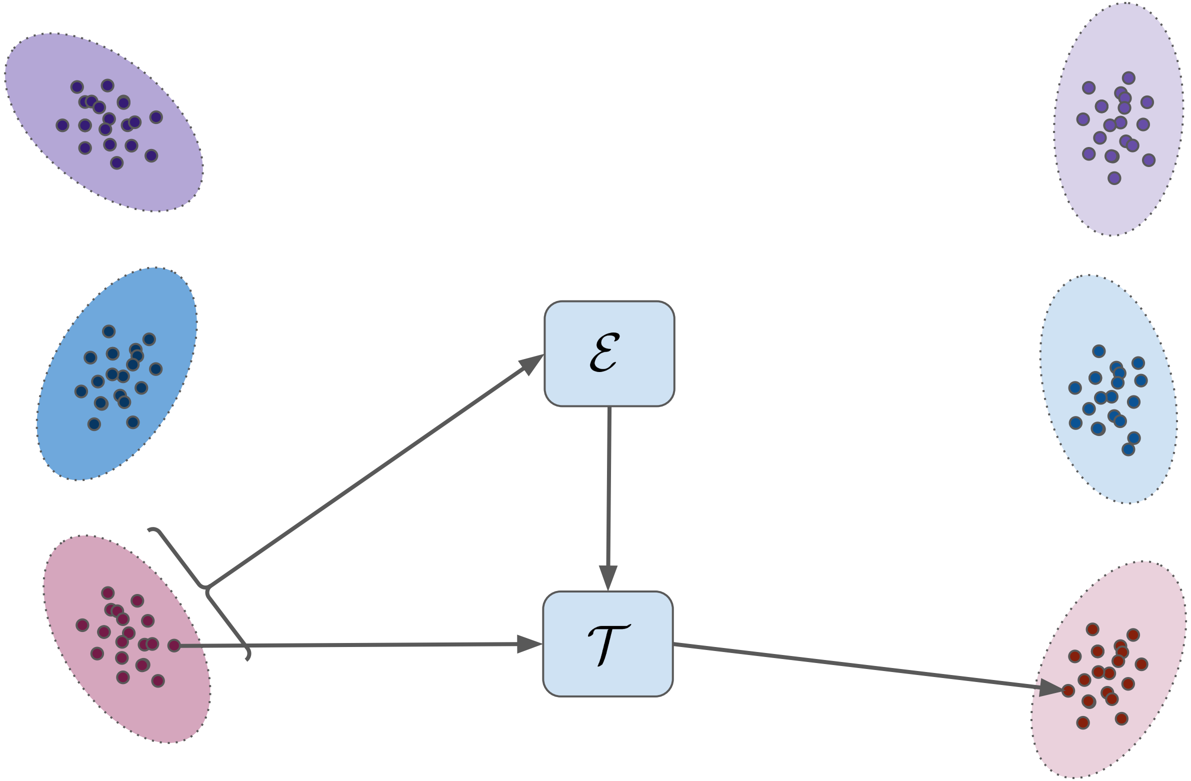
- high throughput genetic perturbation screens
- clonal properties in lineage traced scRNA-seq data
- promoter expression screens
- viral sequence evolution

see Generative Distribution Embeddings, arXiv; NeurIPS 2025 transport

many models transport from one distribution to another



Goodfellow et al., 2014; Genevay et al., 2018; Lipman et al., 2022; Albergo et al., 2022 source conditioning provides tools for simultaneously solving many transport problems



Atanackovic et al., 2024

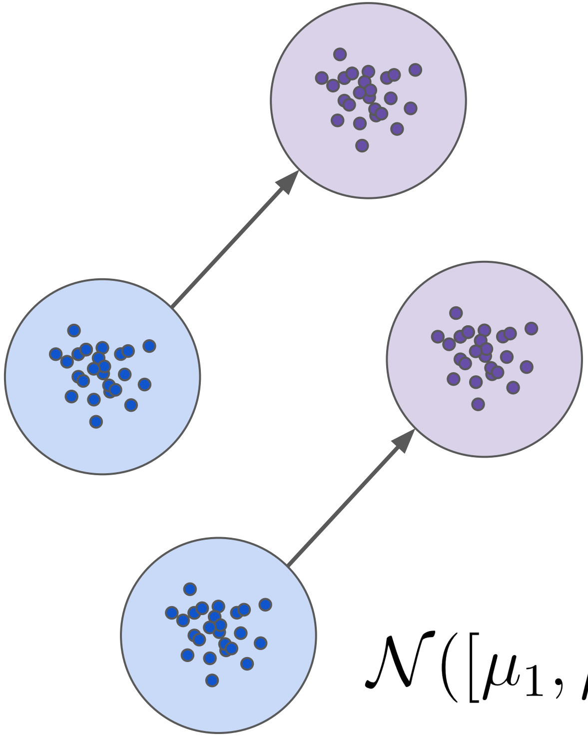
what if we want to make use of unpaired data?

source-conditioning is applicable only when we have explicit source-target pairs

what if we have access to many "orphan" marginals without source/target labels?

this happens in real data (we'll show some examples)

a toy example with Gaussians



$$\mathcal{N}([\mu_1 + 3, \mu_2 + 3], I_2)$$

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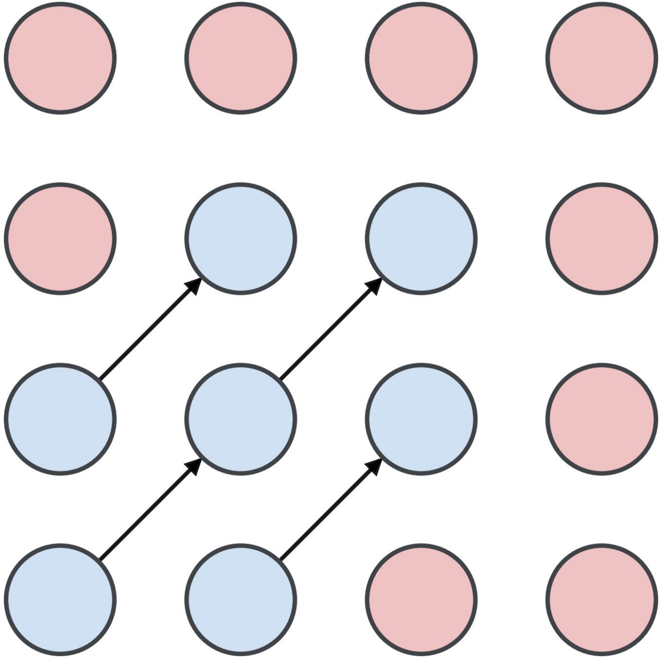

source-target pairing observed for

$$\mu_1, \mu_2 \in [0, 3]$$

orphan marginals observed for

$$\mu_1, \mu_2 \in [3, 5]$$

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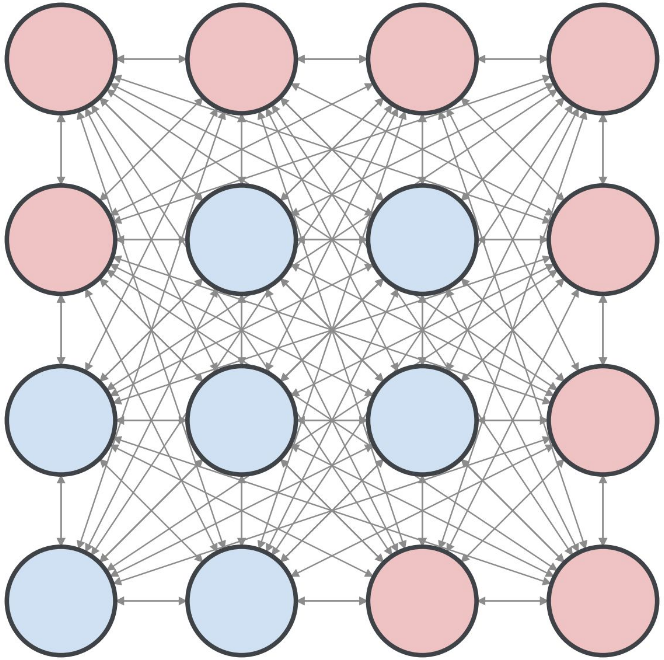


1. use all pairings to train an "unsupervised" any-to-any model

2. train a small "latent predictor" to predict the target latent given the source latent

transport with distribution embeddings

goal: learn a model which can transport between any pair of distributions by conditioning on source and target distribution embeddings

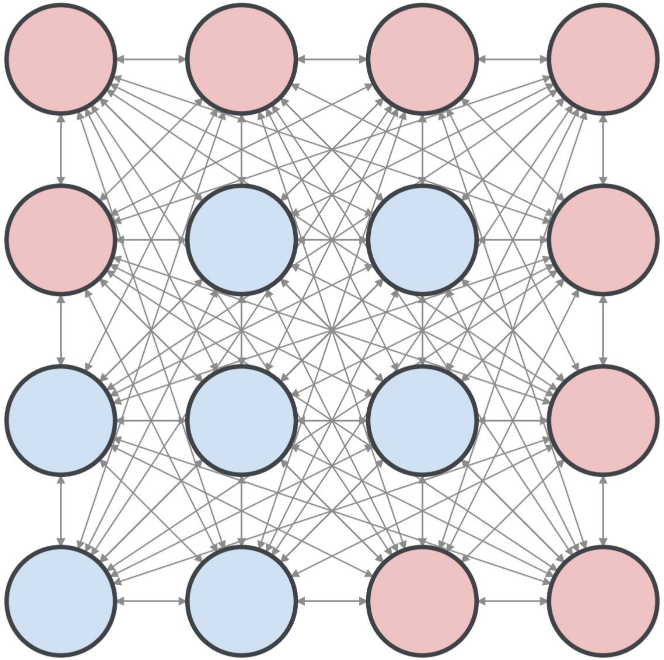
we sample two distributions and two sets of samples

$$P_i \sim Q \quad x_{jk} \sim P_j \quad S_{i,m} = \{x_{ik}\}_{k=1}^m$$
$$P_j \sim Q \quad x_{ik} \sim P_i \quad S_{j,m} = \{x_{jk}\}_{k=1}^m$$

our goal is to learn an any-to-any transport map

$$\mathcal{T}\big(S_{i,m},\, \mathcal{E}(S_{i,m}),\, \mathcal{E}(S_{j,m})\big) \xrightarrow{d} P_j \quad \text{as } m \to \infty.$$

a toy example with gaussians



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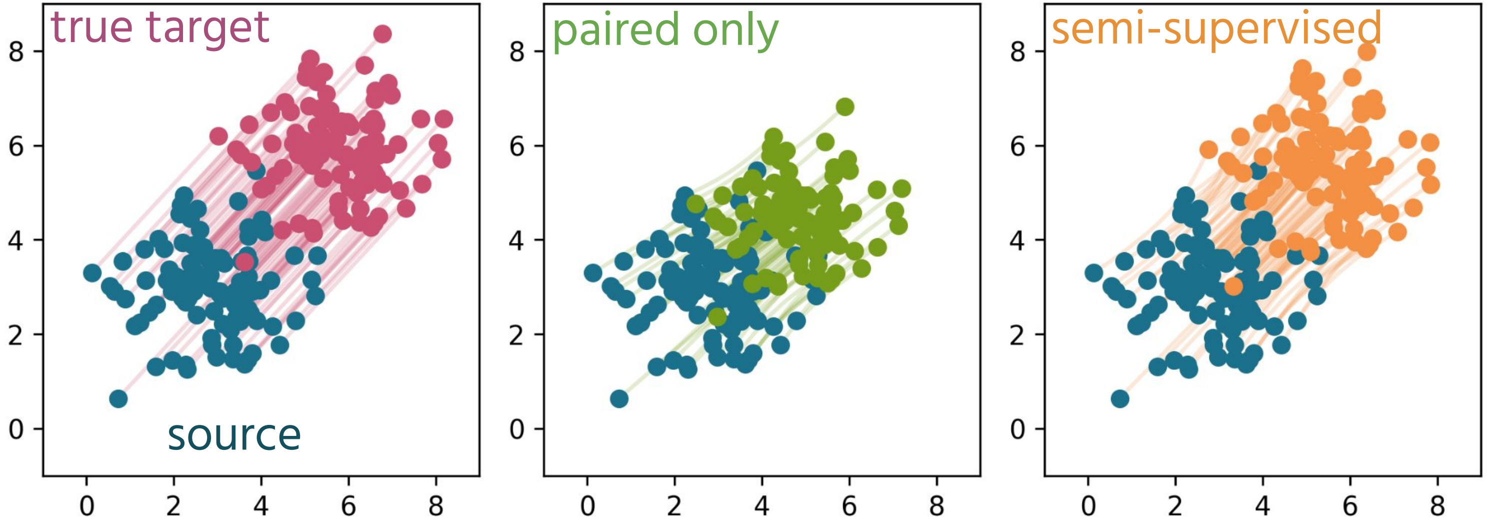
we learn any-to-any transport using
encoder: mean pooled deep sets
transport model: flow matching

TDEs rescue performance outside of paired data distribution



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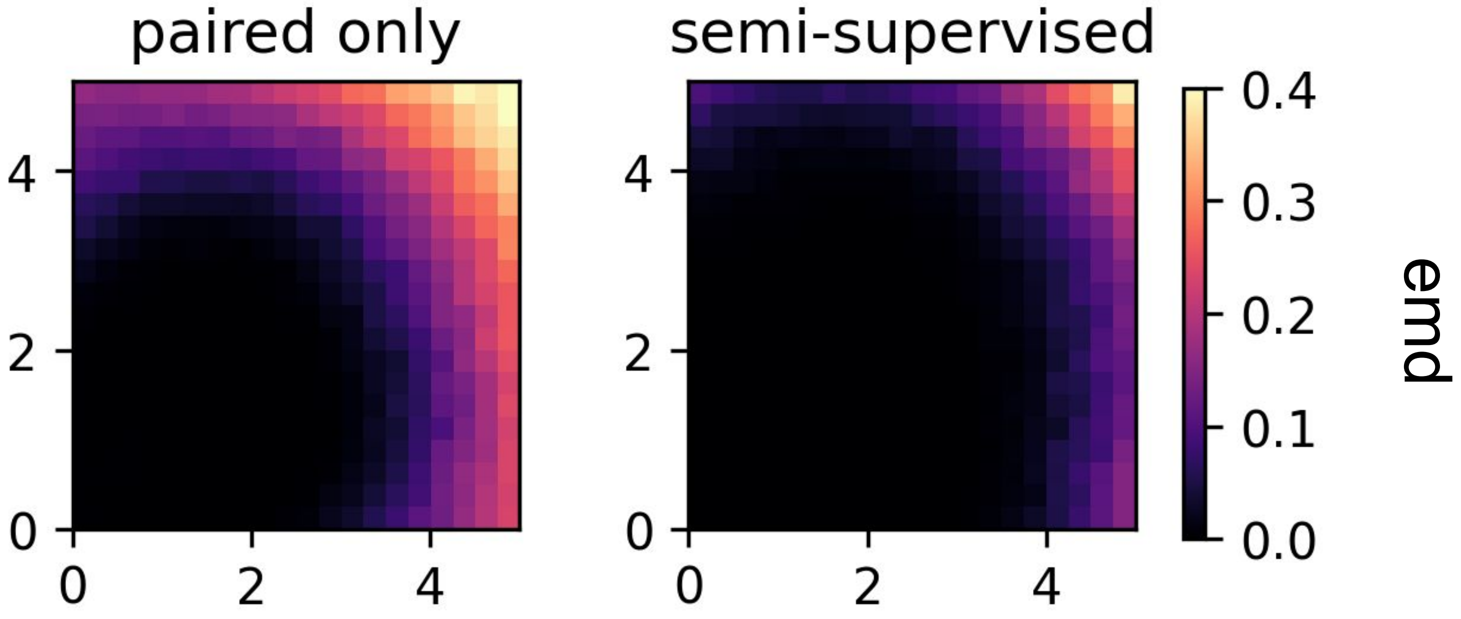
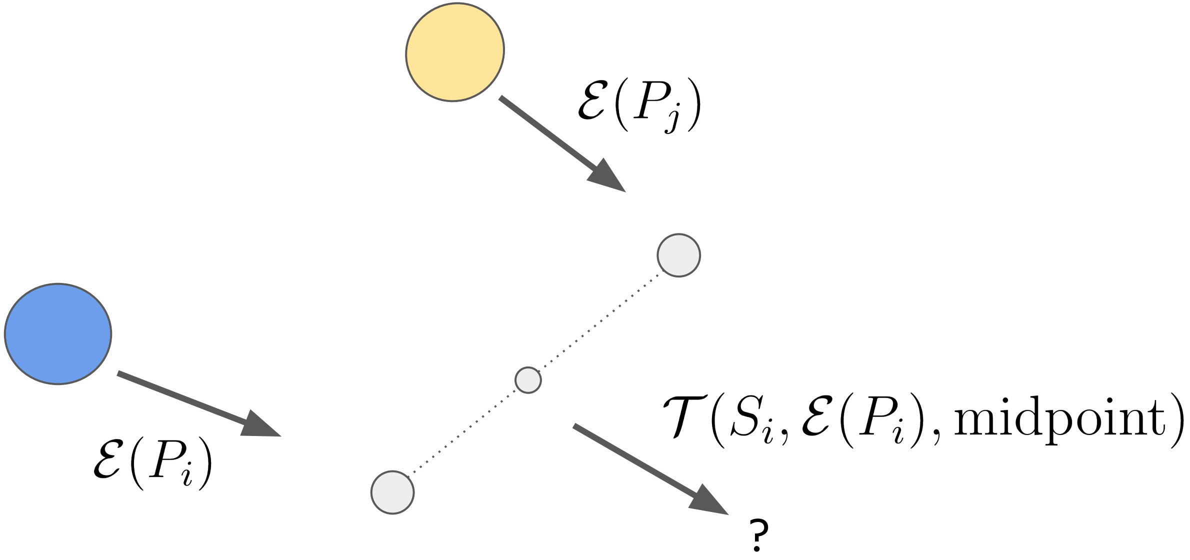


probing the latent geometry (again)



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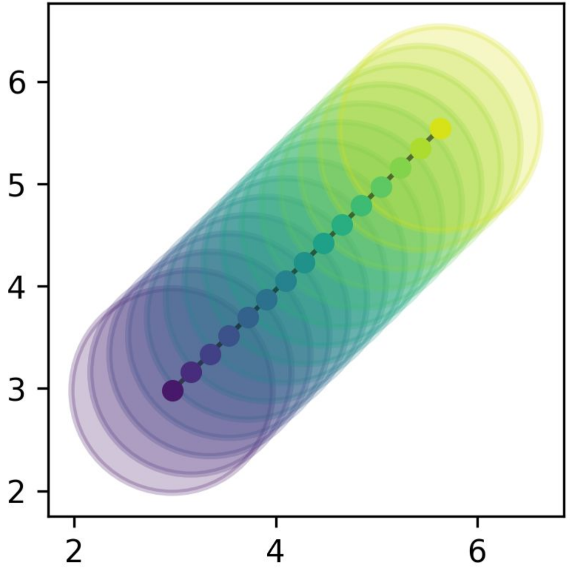
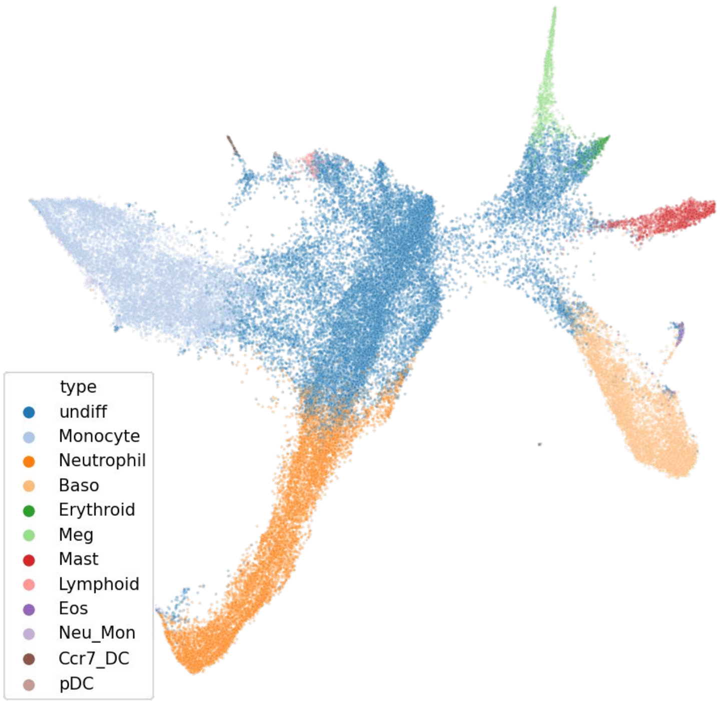


and again, we closely match the OT

but this time with unit-level trajectories!

Lineage-traced scRNAseq measures dynamics of clones



lineage traced scRNA-seq data from Weinreb et al., 2020

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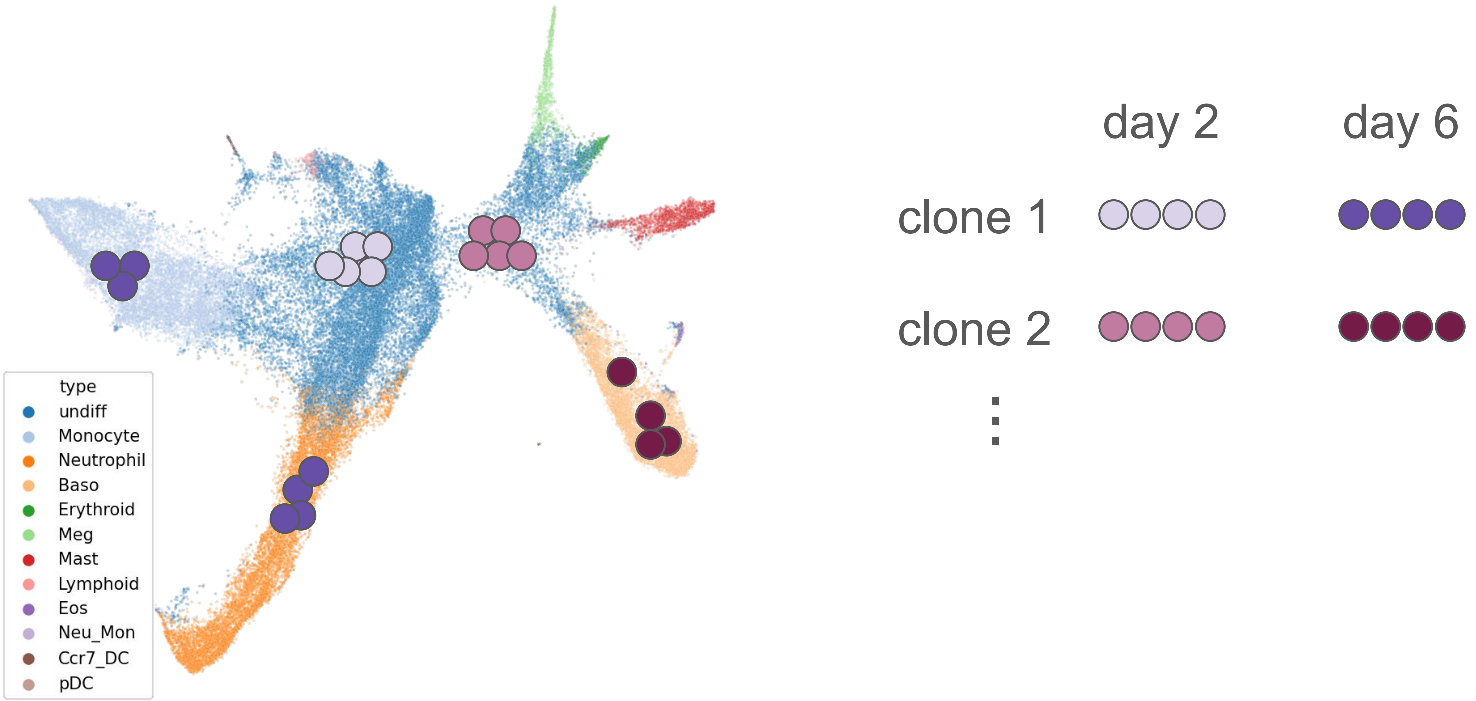

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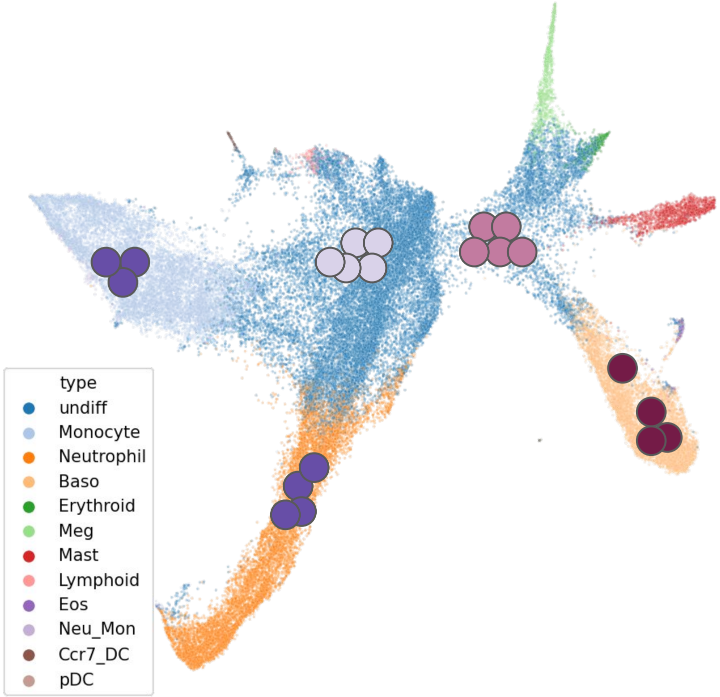
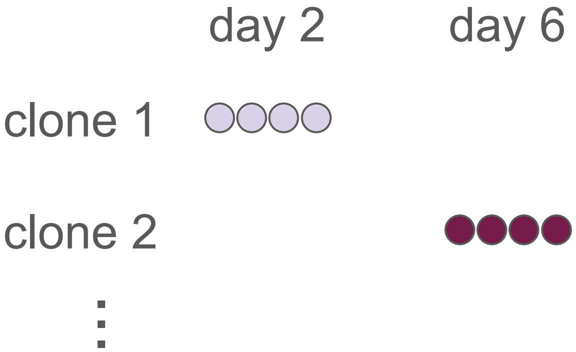
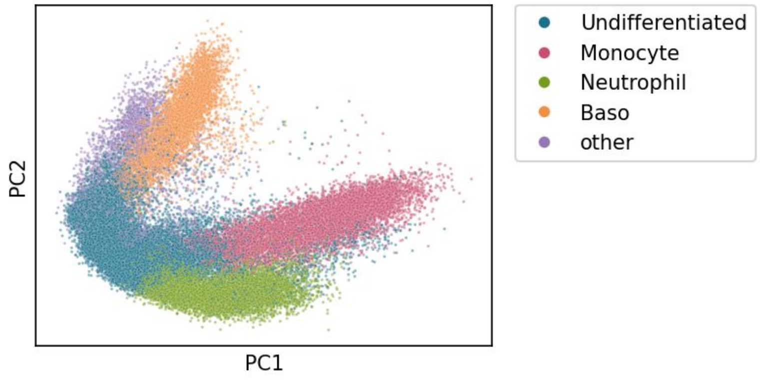


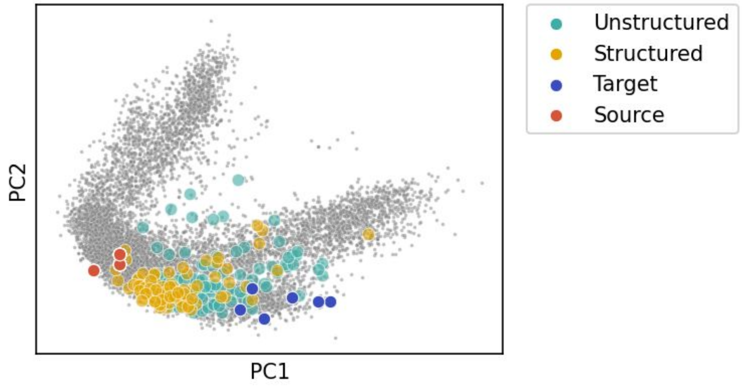


~90% of clones appear at only one timepoint!

lineage traced scRNA-seq data from Weinreb et al., 2020

TDEs improve performance by using "orphan" clones





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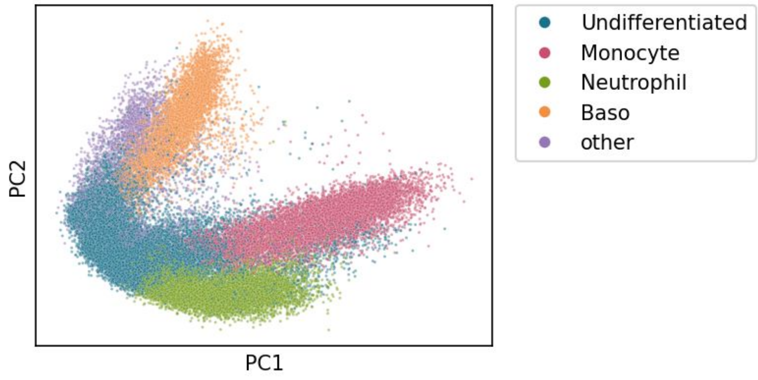

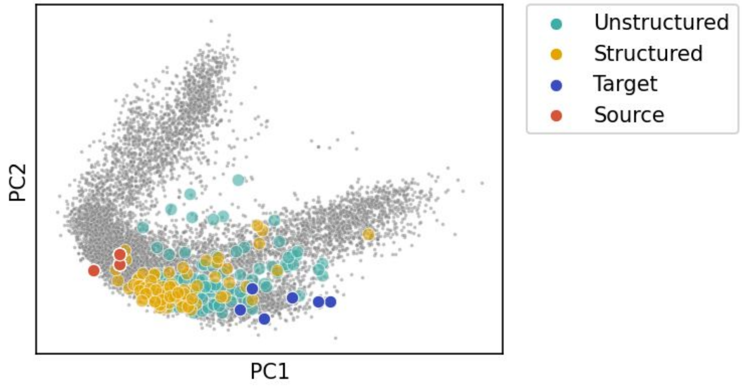

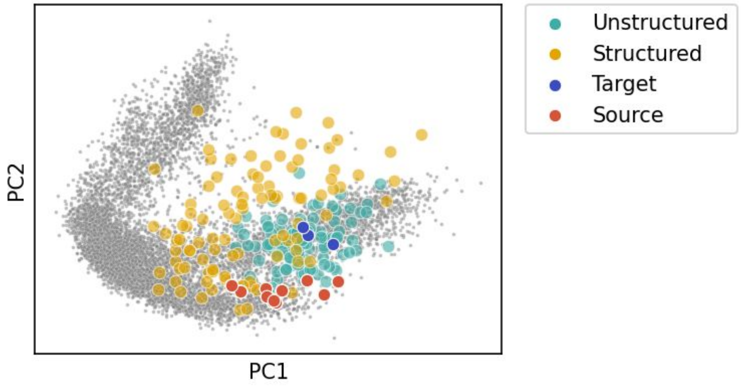

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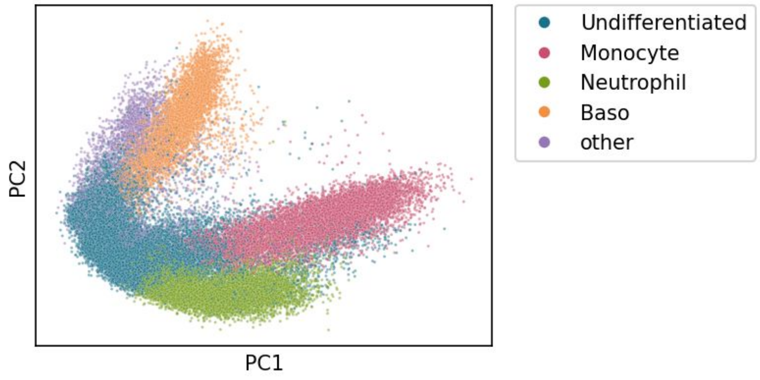
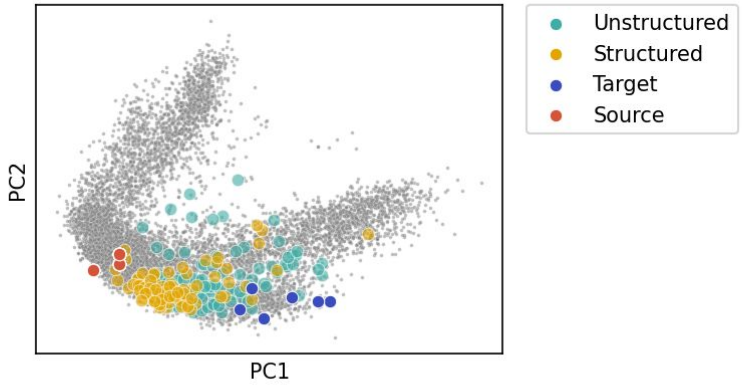
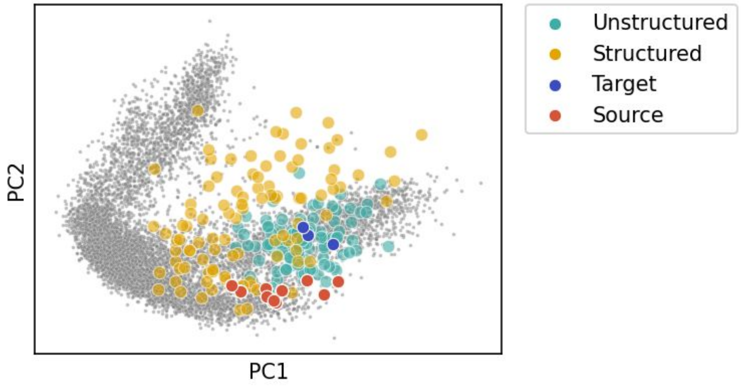




Method	Energy Distance
Source-conditioned	3.34
TDE	**3.20**



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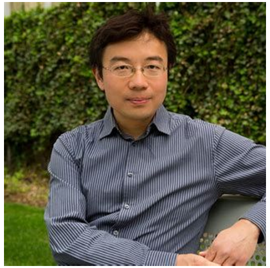
- what is the relationship between the complexity of a family of distributions and the resources required for a model to learn any-to-any transport?
- can we build a foundation model for transport between any and all distributions? who wants to give us a trillion dollars to try

thank you!

Paolo
Fischer



Peng
Yin

Omar
Abudayyeh

Jonathan
Gootenberg

the workshop organizers
and
all of you :)