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UMAP

Uniform Manifold Approximation and Projection for dimension reduction

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Who am I?

I am a research mathematician at the Tutte Institute for Mathematics and Computing

My Ph.D. was in Profinite Lie Rings
(no, you don't care)

I now work on applying topological techniques to unsupervised learning problems

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What is Dimension Reduction?

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Find the “latent” features in your data

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Matrix Factorization

Neighbour Graphs

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Matrix Factorization

Principal Component Analysis

Linear Autoencoder

Latent Dirichlet Allocation

Non-negative Matrix Factorization

Generalised Low Rank Models

Word2Vec

GloVe

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Neighbour Graphs

Laplacian Eigenmaps

Hessian Eigenmaps

Local Tangent Space Alignment

JSE

Isomap

t-SNE

Locally Linear Embedding

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PCA is the prototypical matrix factorization

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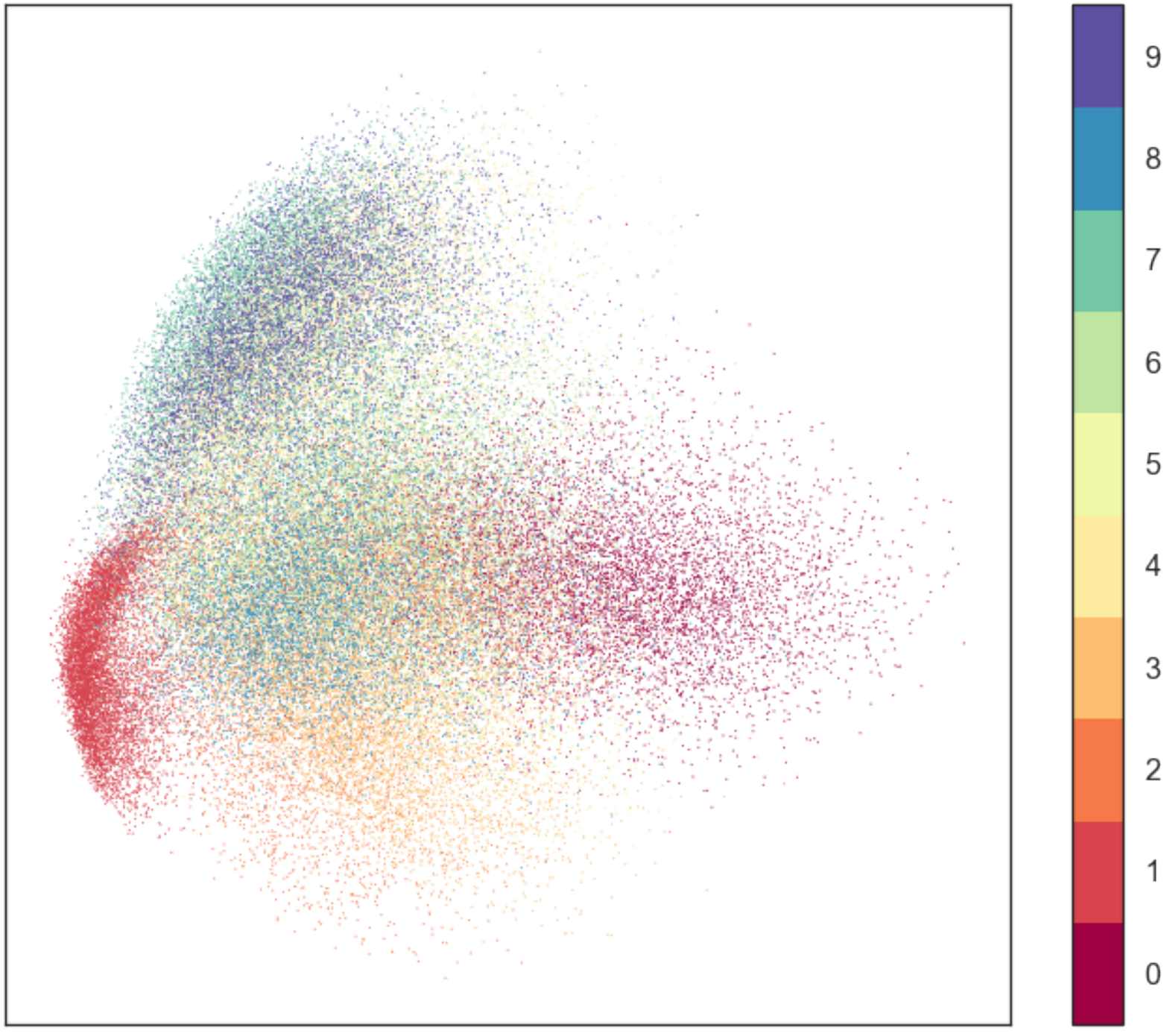
PCA on MNIST digits



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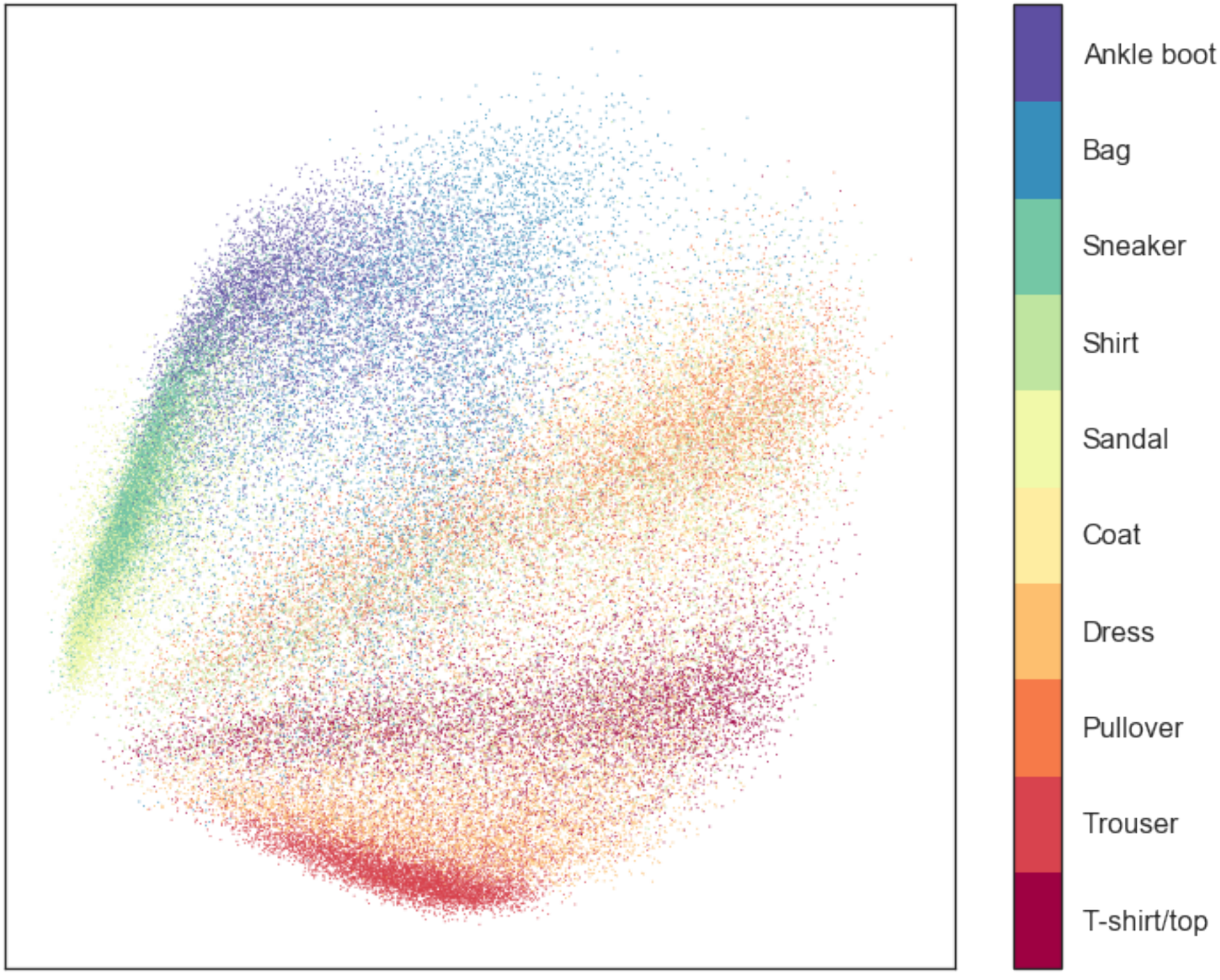
PCA on Fashion MNIST



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t-SNE is the current state-of-the art for neighbour graphs

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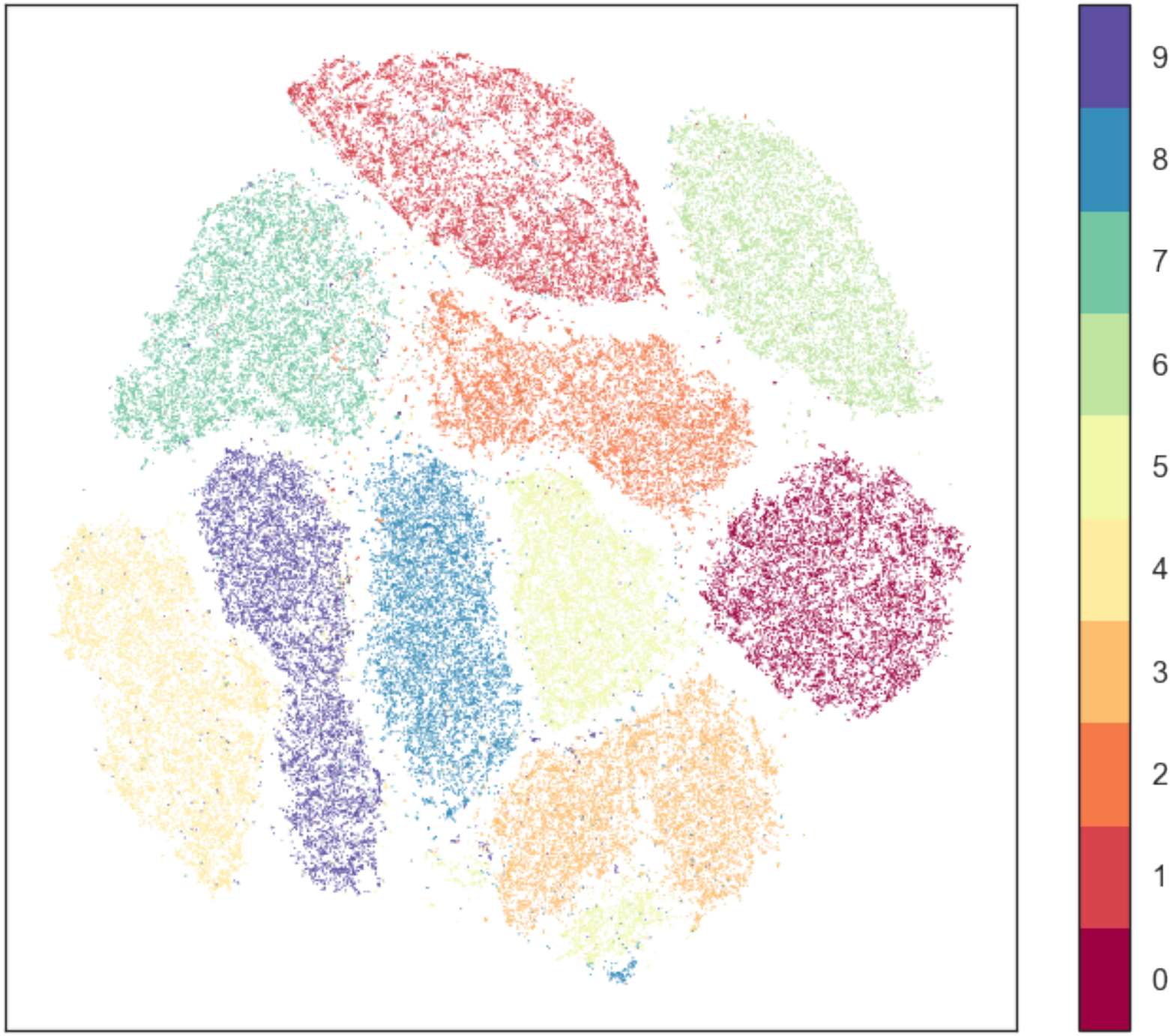
t-SNE on MNIST digits



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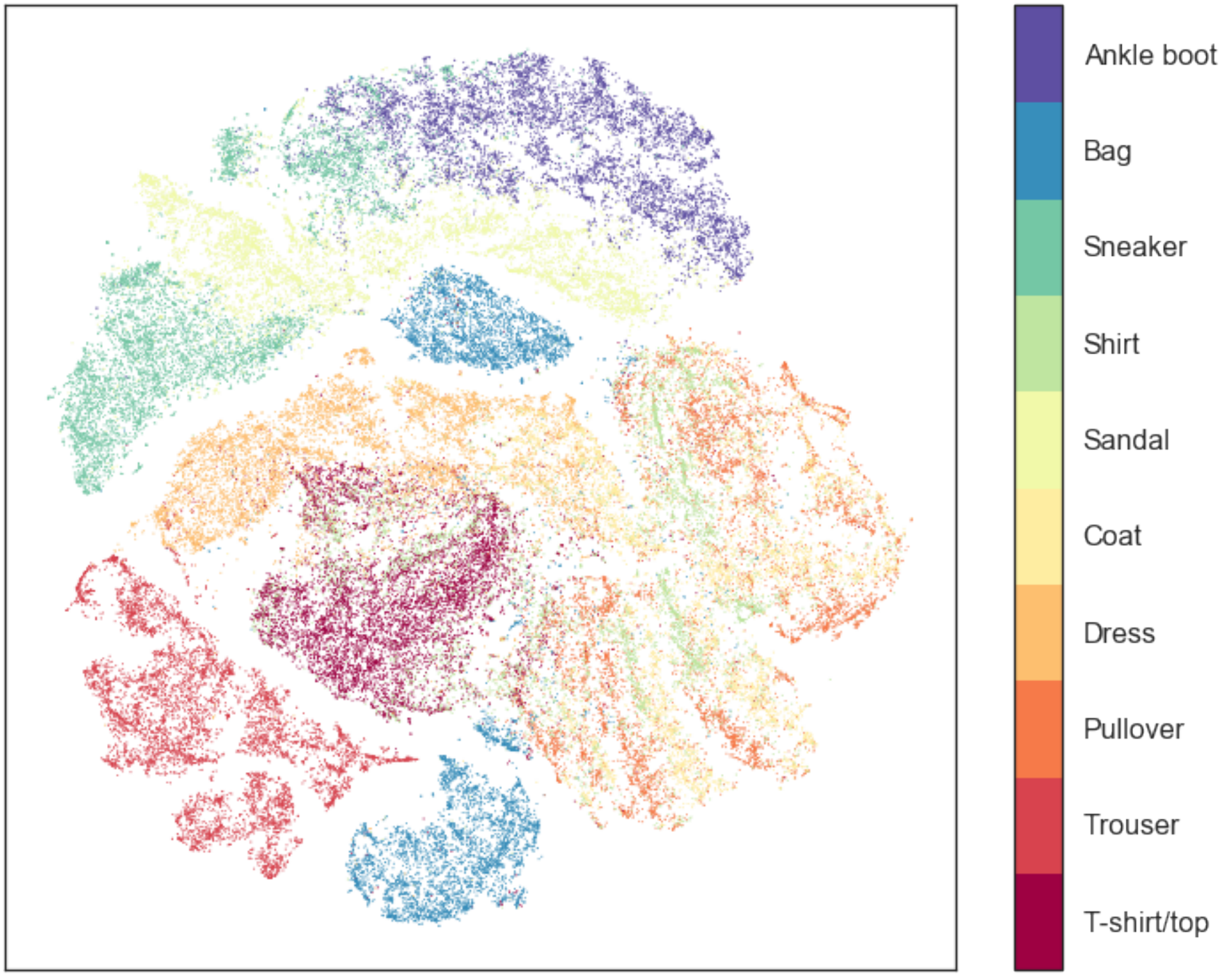
t-SNE on Fashion MNIST



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Uniform Manifold Approximation and Projection

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UMAP builds mathematical theory to justify the graph based approach

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First, a little bit of topological data analysis...

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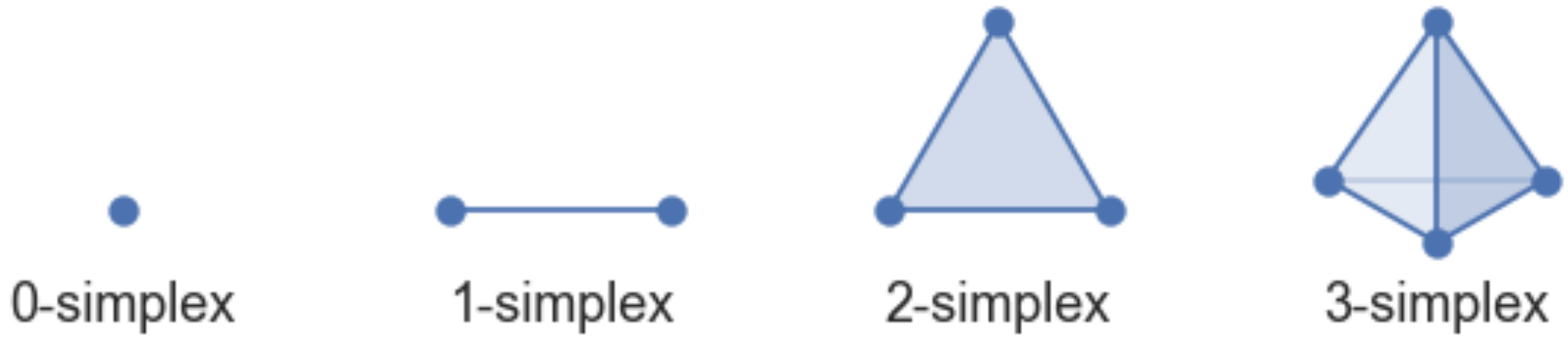
Simplices



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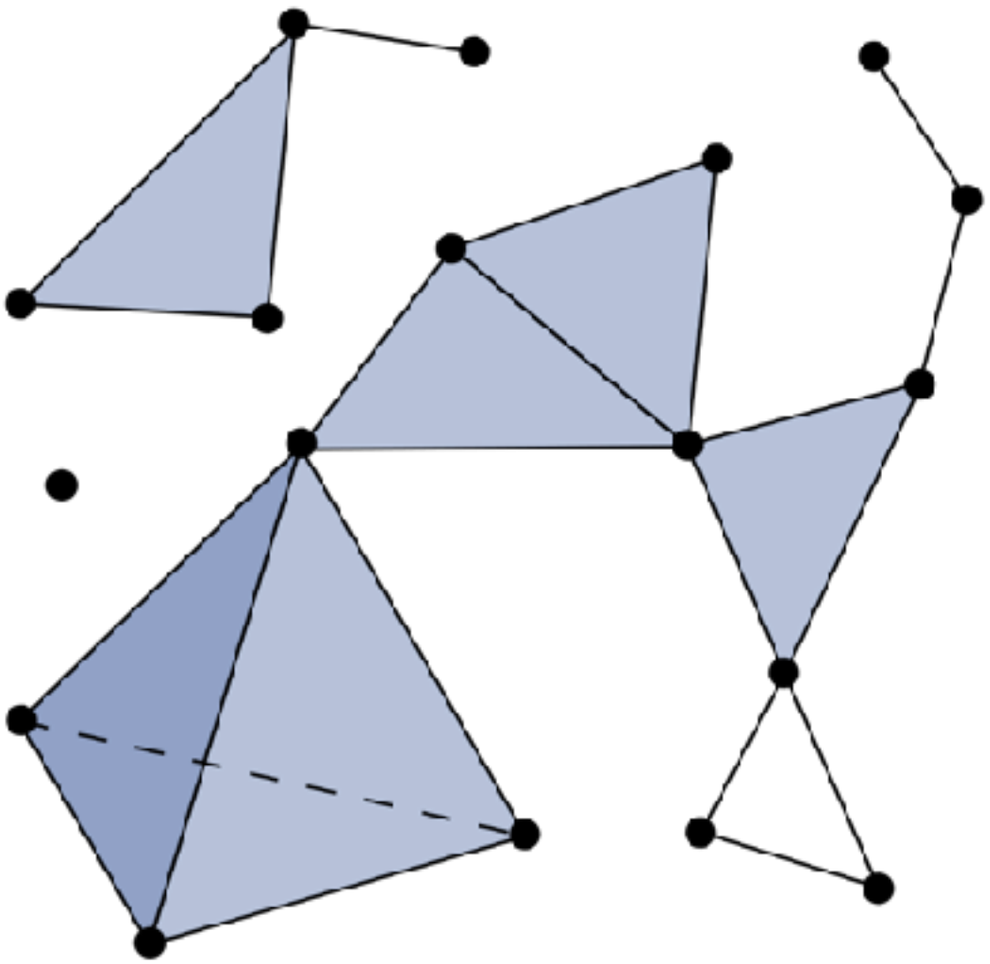
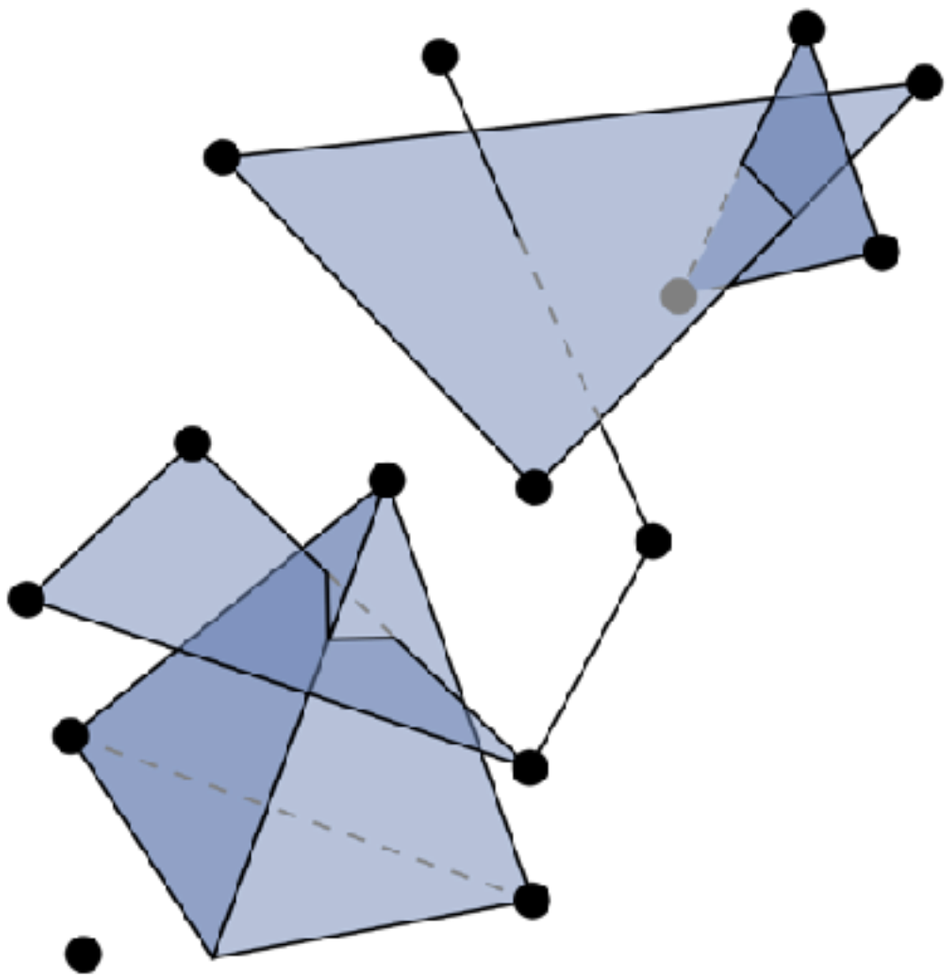
Simplicial complex



Collection of Simplices



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Theorem 1 (Nerve theorem)**.** *Let $\mathcal{U} = \{U_i\}_{i \in I}$ be a cover of a topological space X. If, for all $\sigma \subset I$ $\bigcap_{i \in \sigma} U_i$ is either contractible or empty, then $\mathcal{N}(\mathcal{U})$ is homtopically equivalent to X.*

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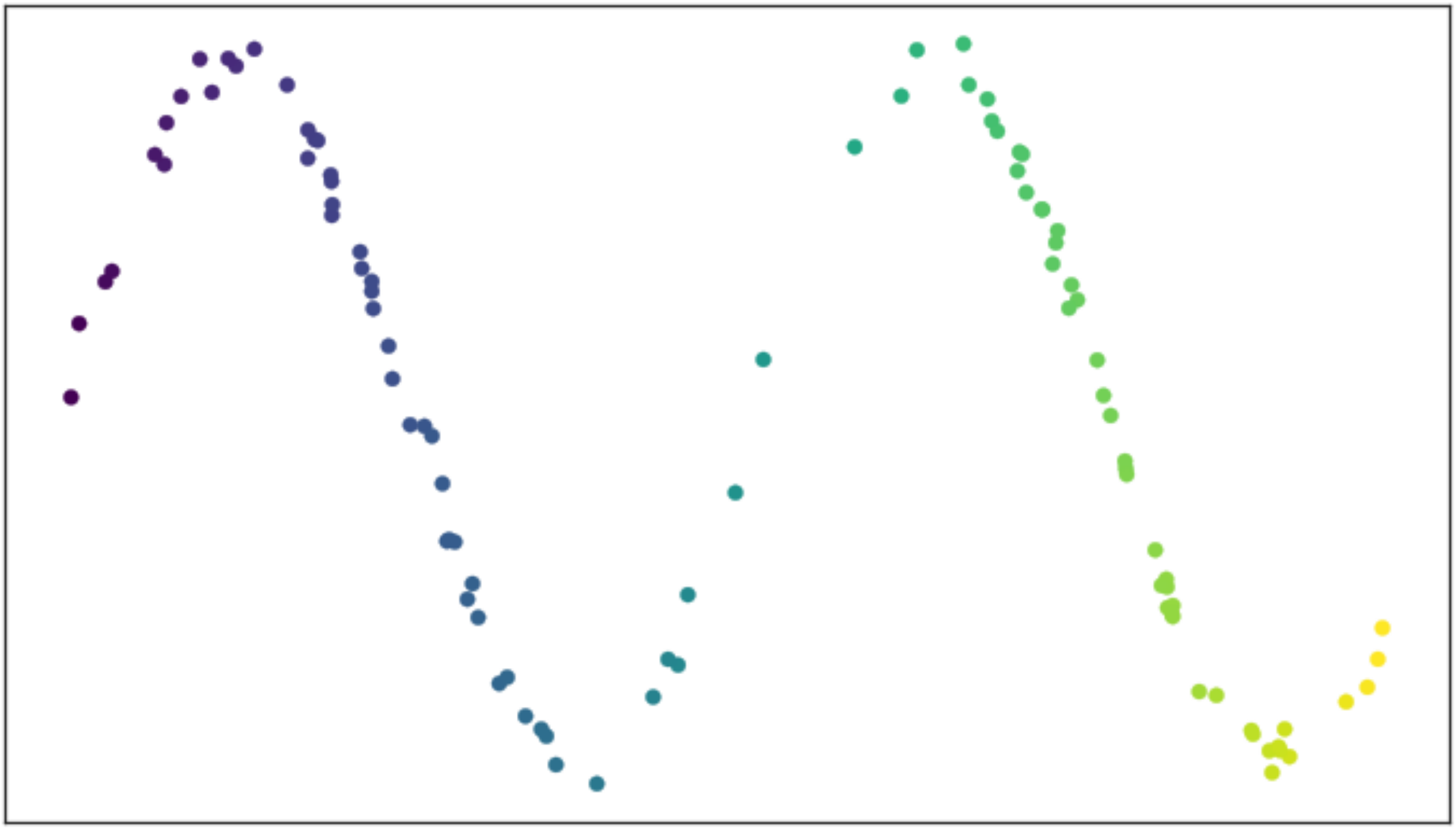

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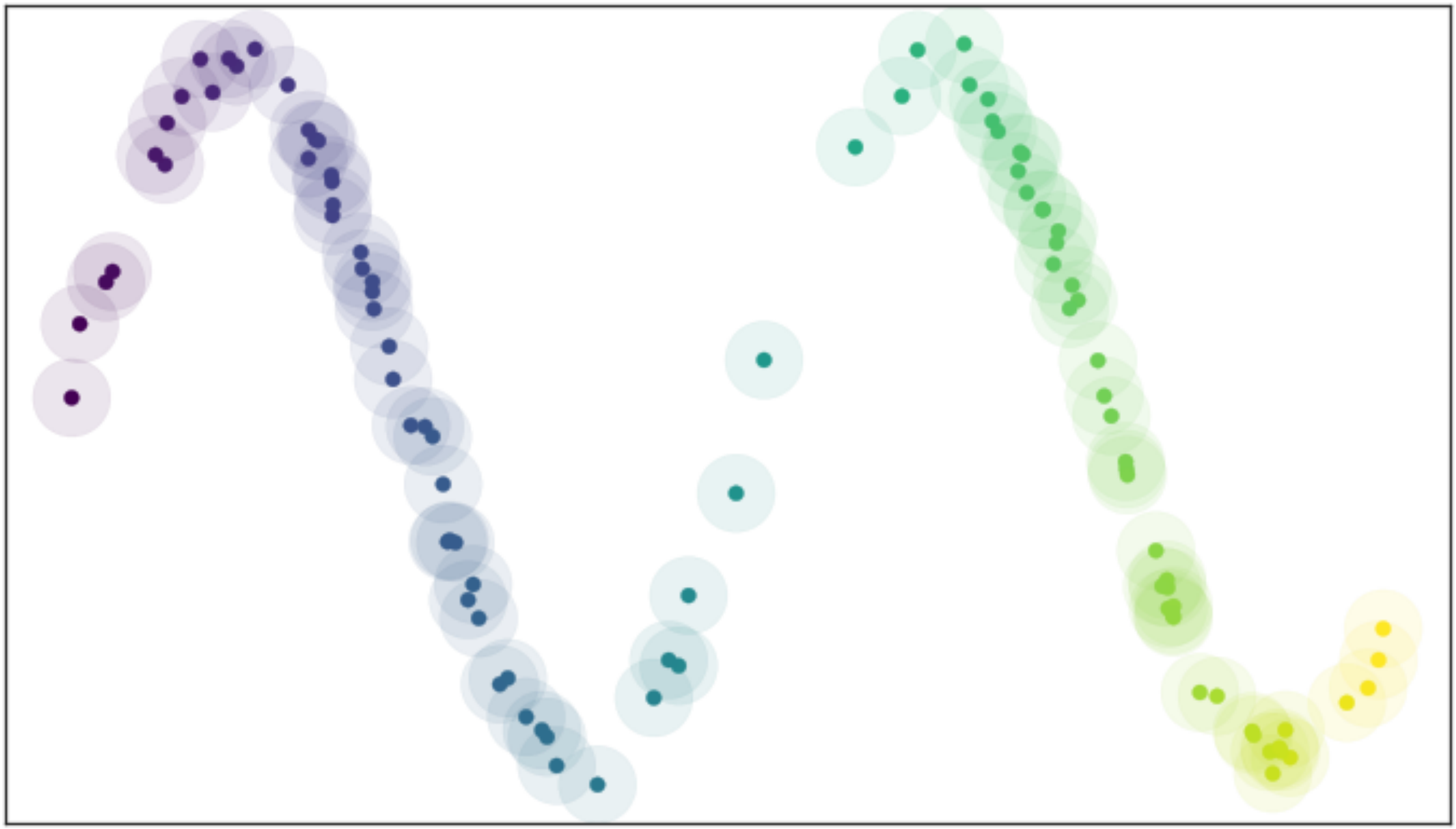

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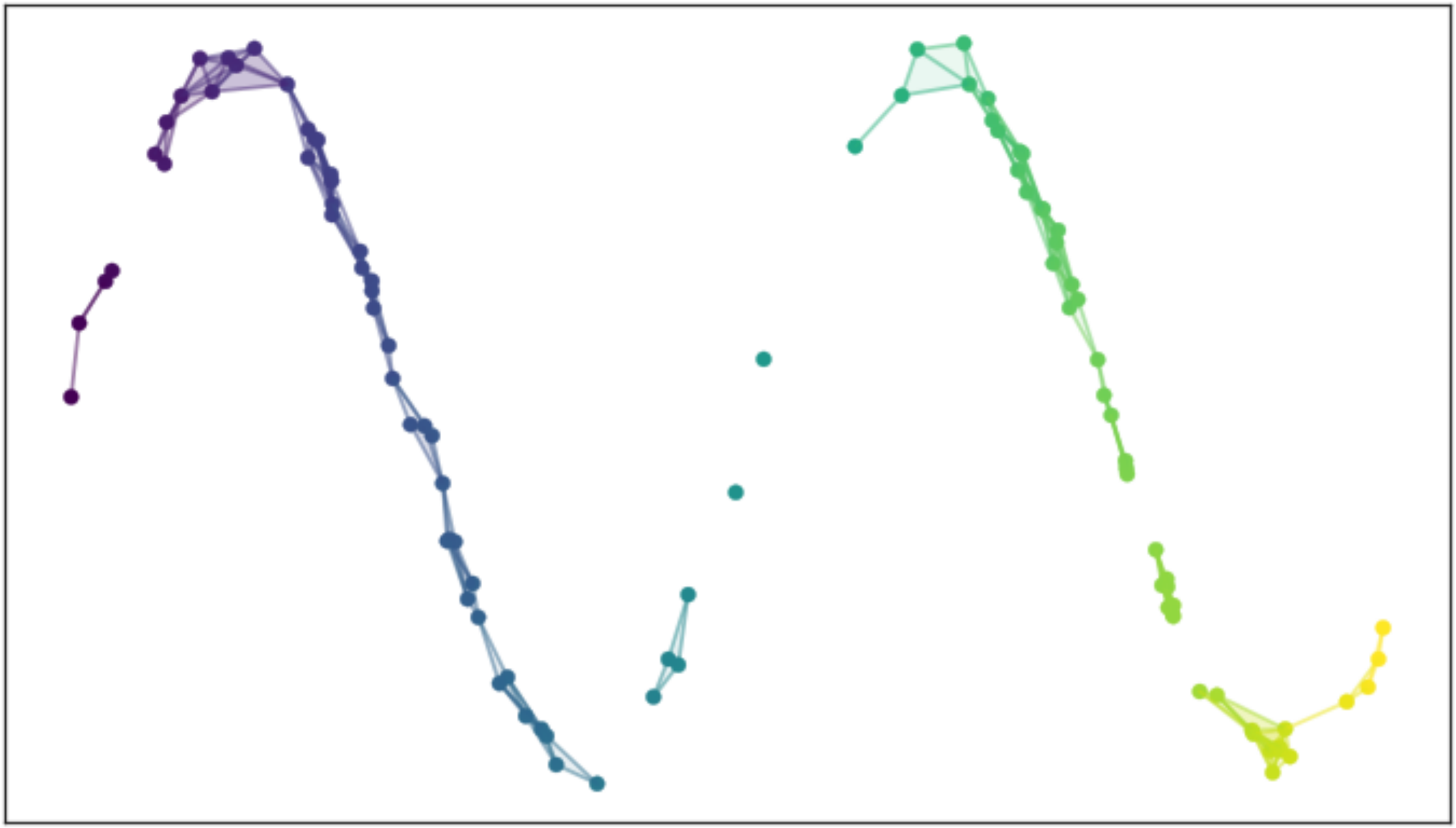

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If the data is uniformly distributed on the manifold then the cover will be “good”

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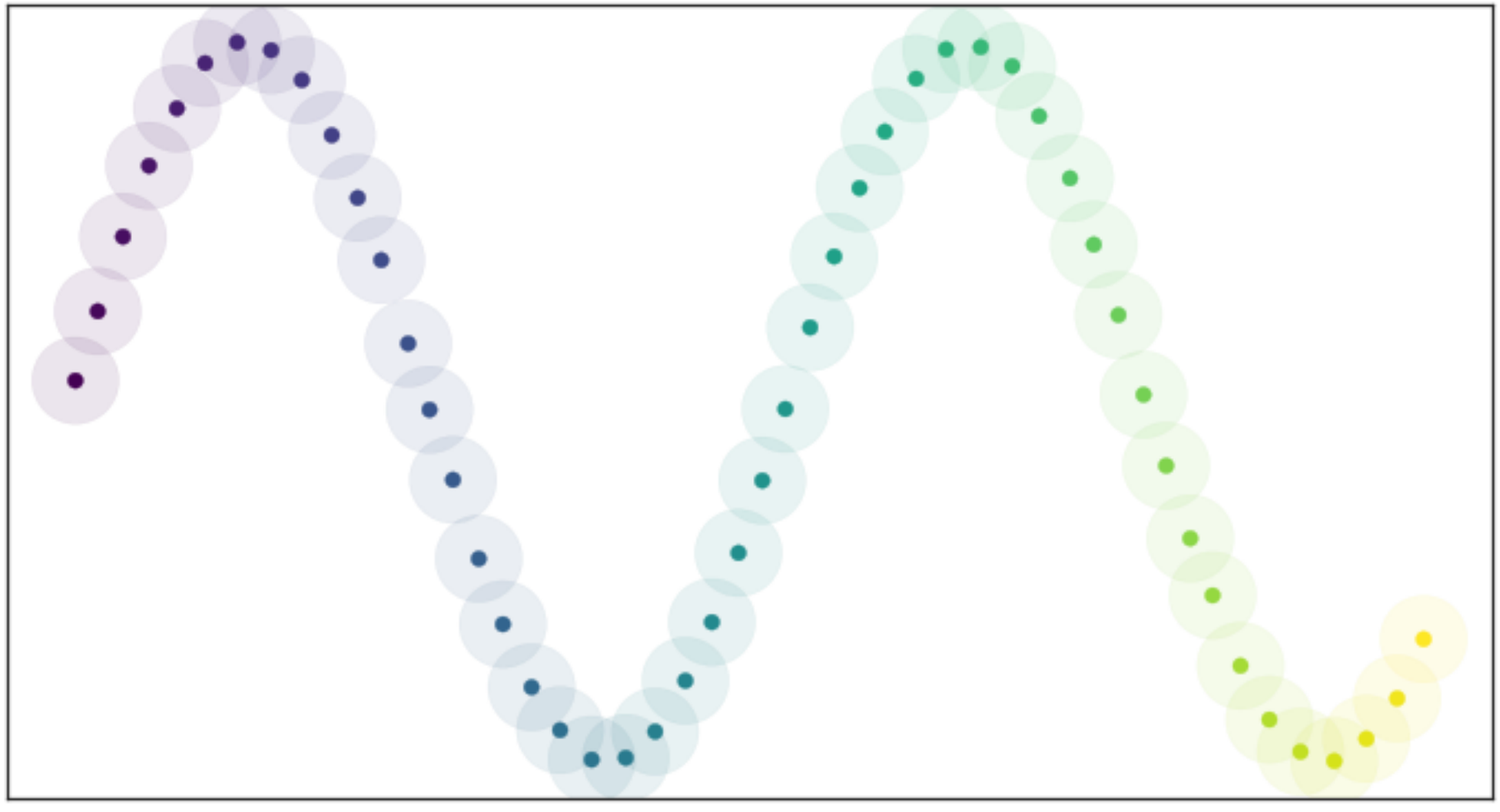

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When is data that nicely behaved?

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Assumption:

Data is uniformly distributed on the manifold

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Define a Riemannian metric on the manifold to make this assumption true

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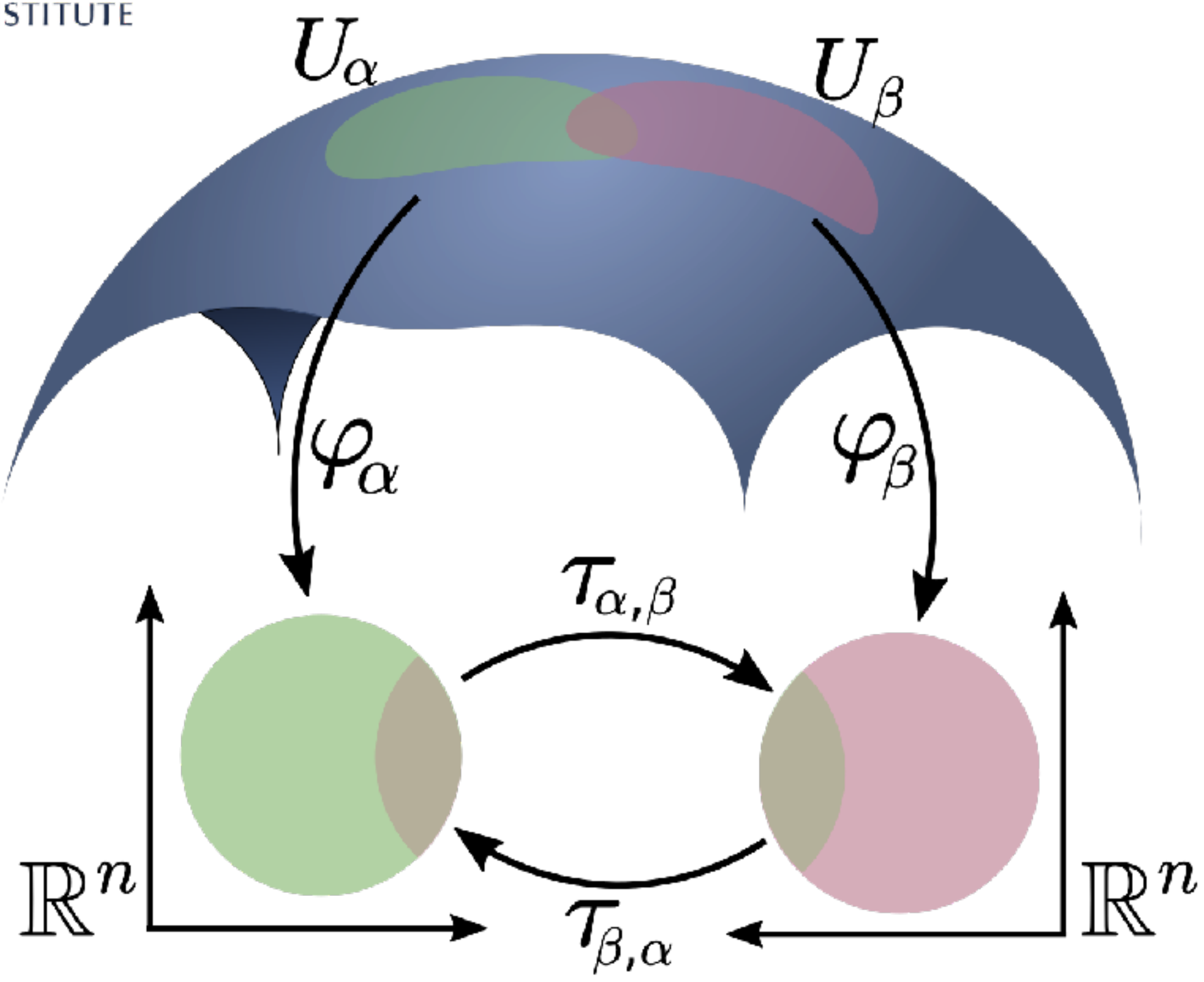

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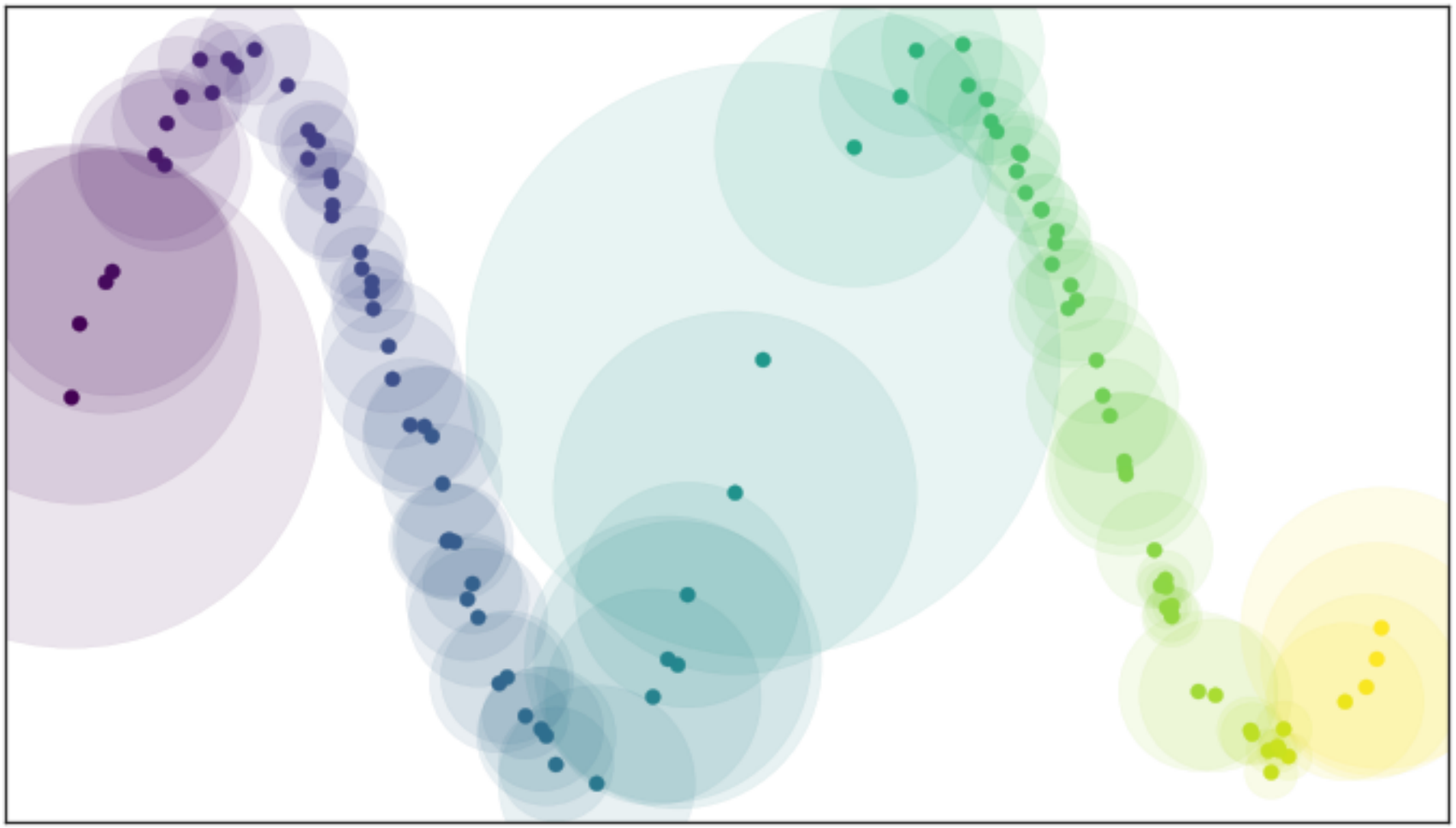

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Why choose a fixed radius? Why not have a fuzzy cover?

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Theorem 2 (UMAP Adjunction)**.** *The functors* FinReal : **sFuzz** $\to$ **FinEPMet** *and* FinSing : **FinEPMet** $\to$ **sFuzz** *form an adjunction* FinReal $\dashv$ FinSing.

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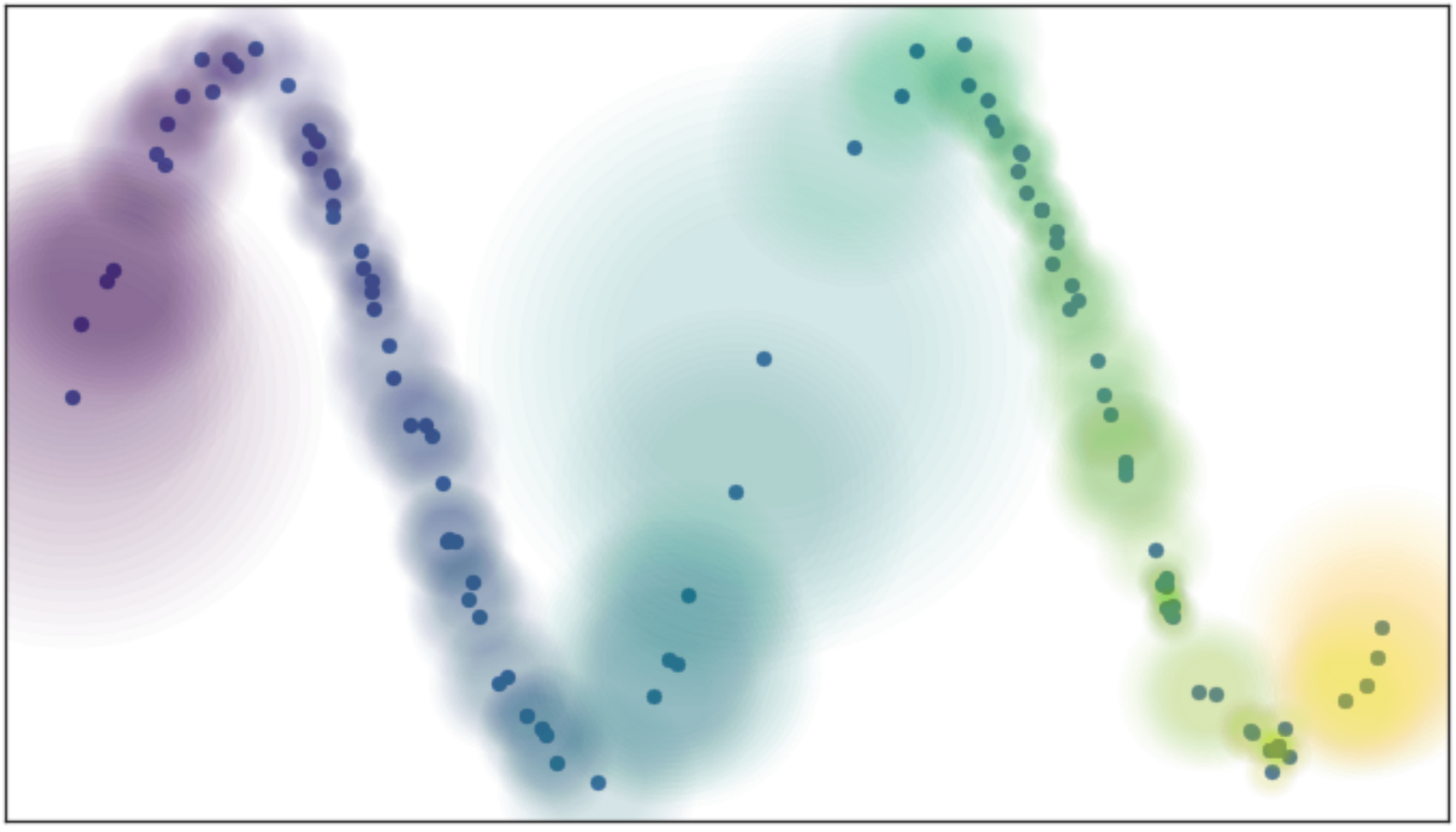

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Assumption:

The manifold is locally connected

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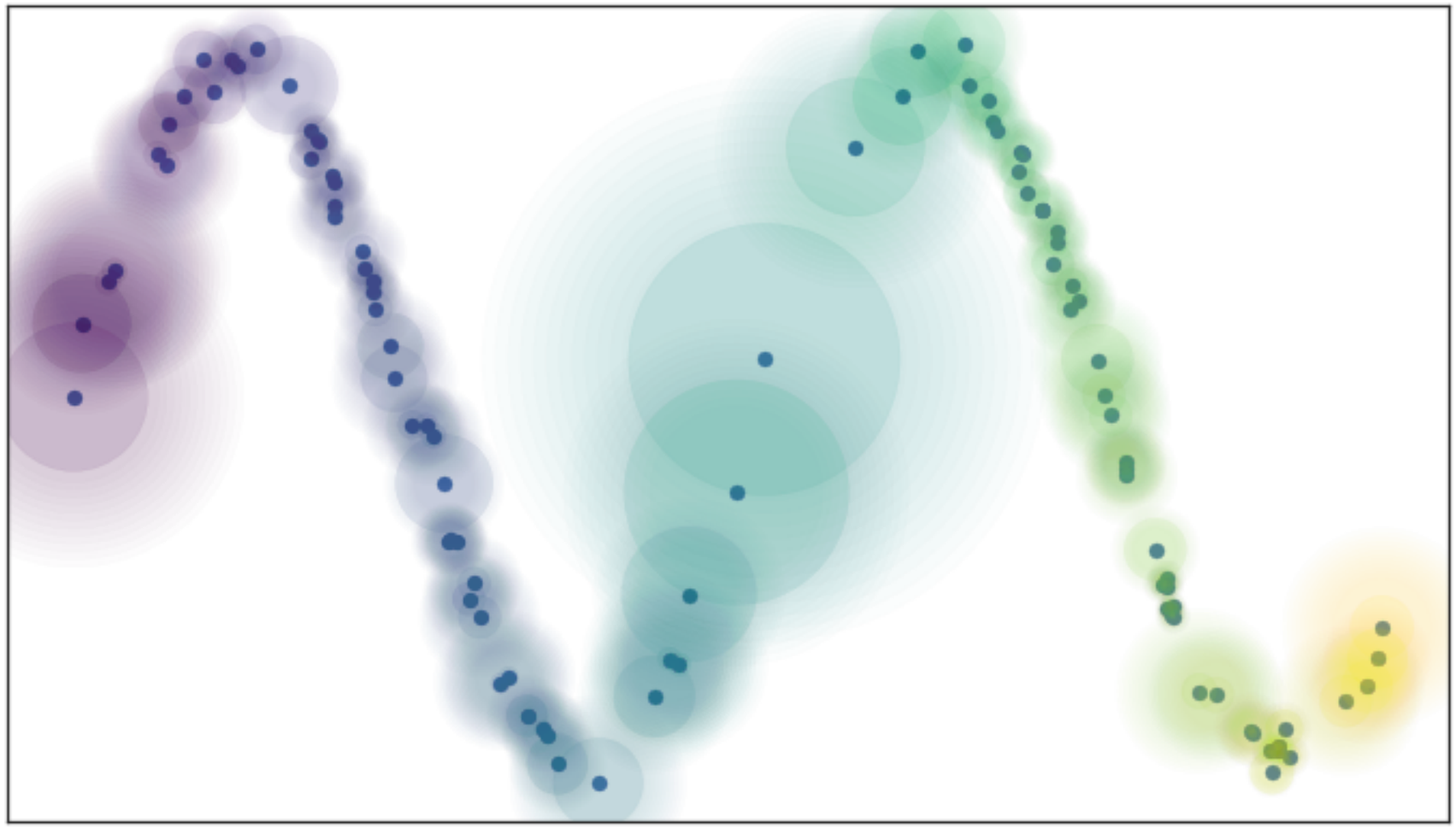

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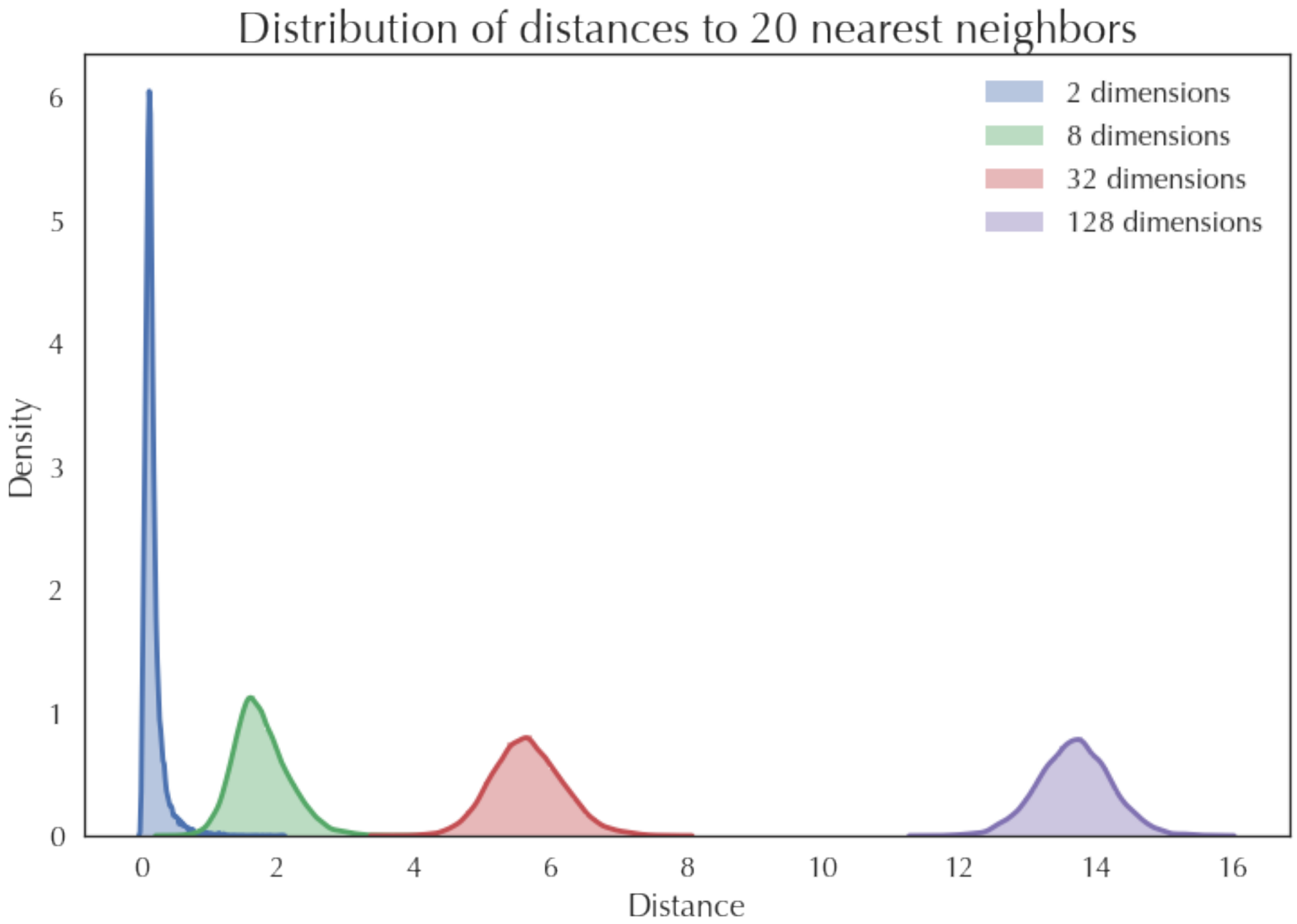

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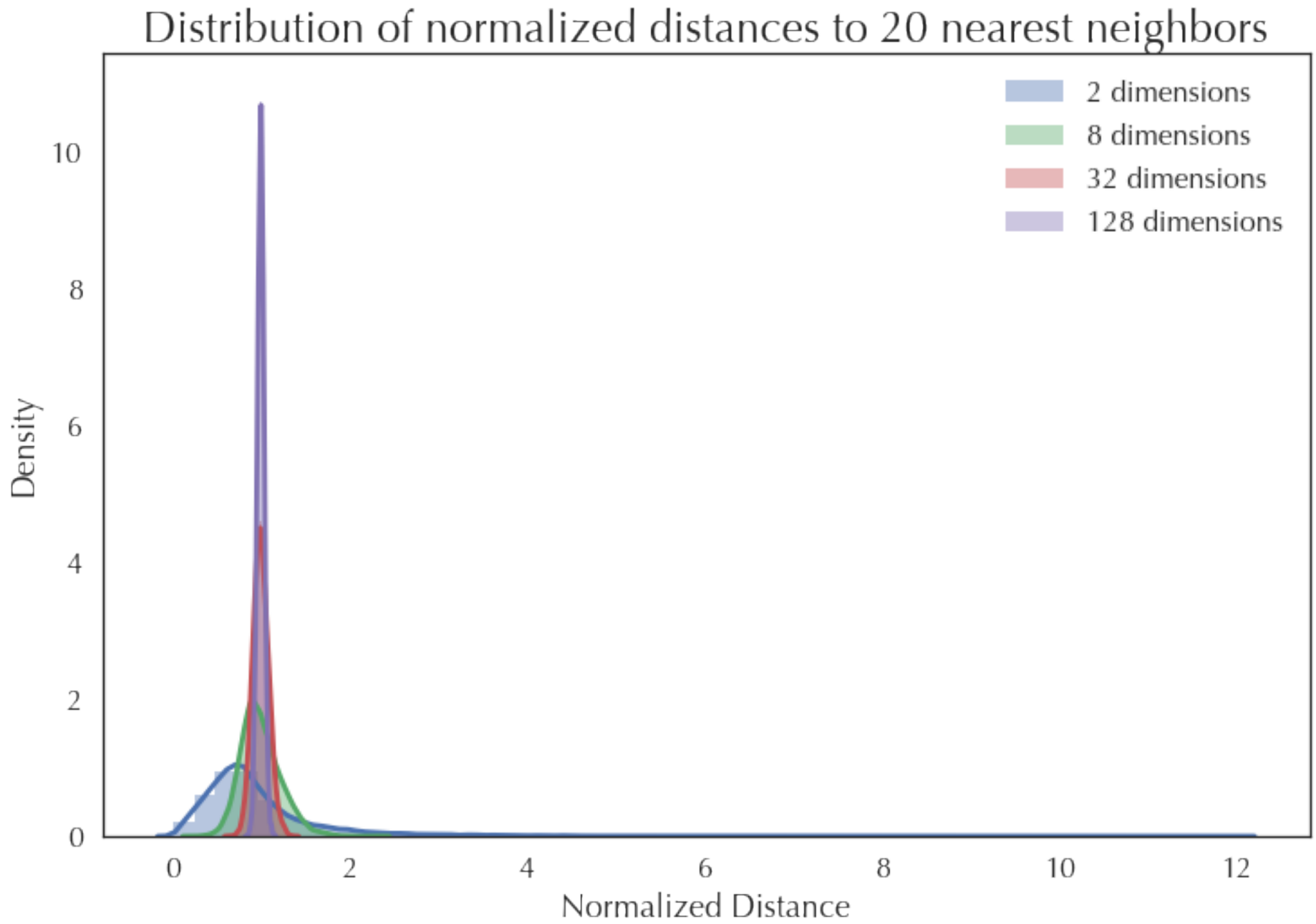

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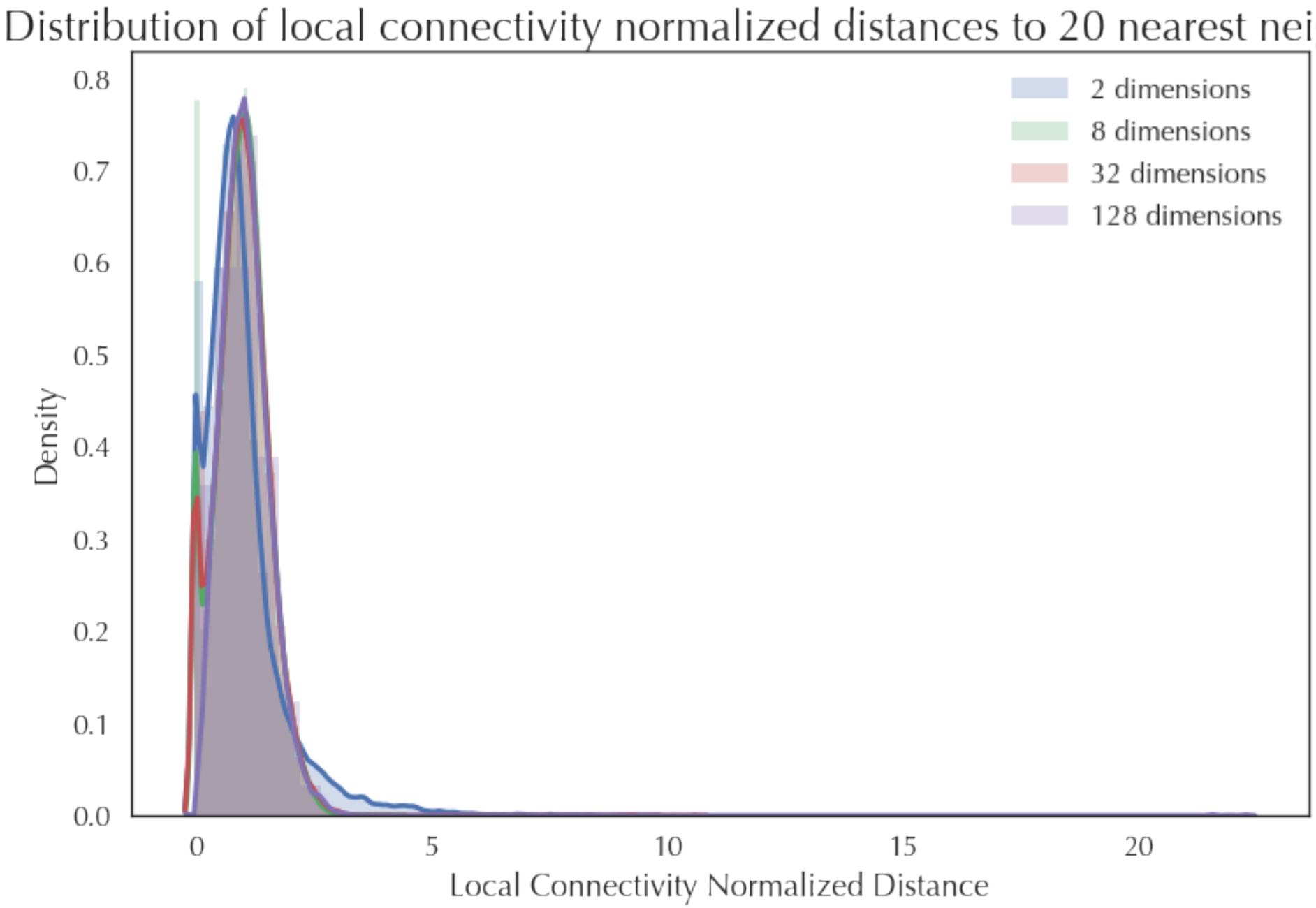

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But our local metrics are all incompatible!

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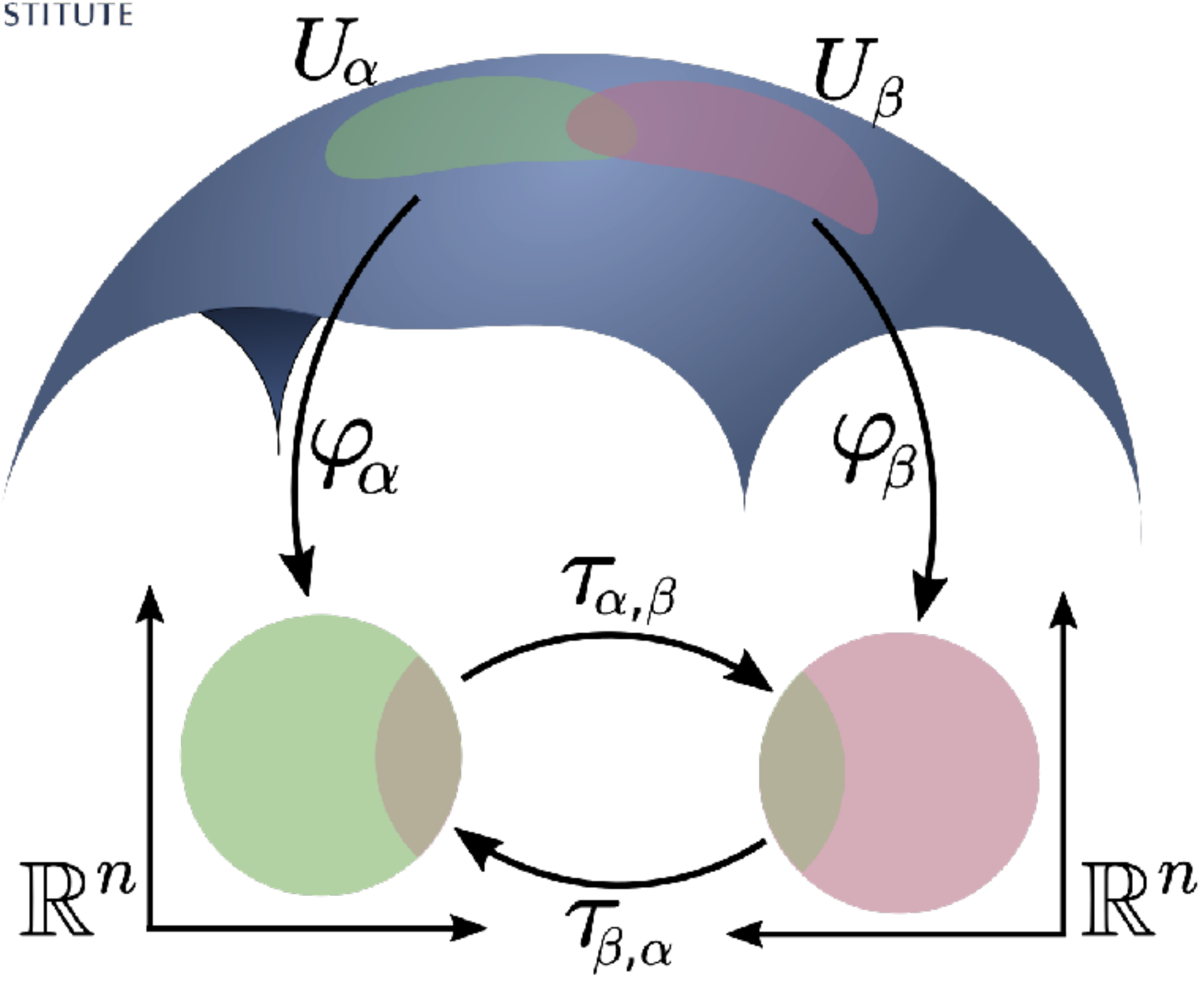

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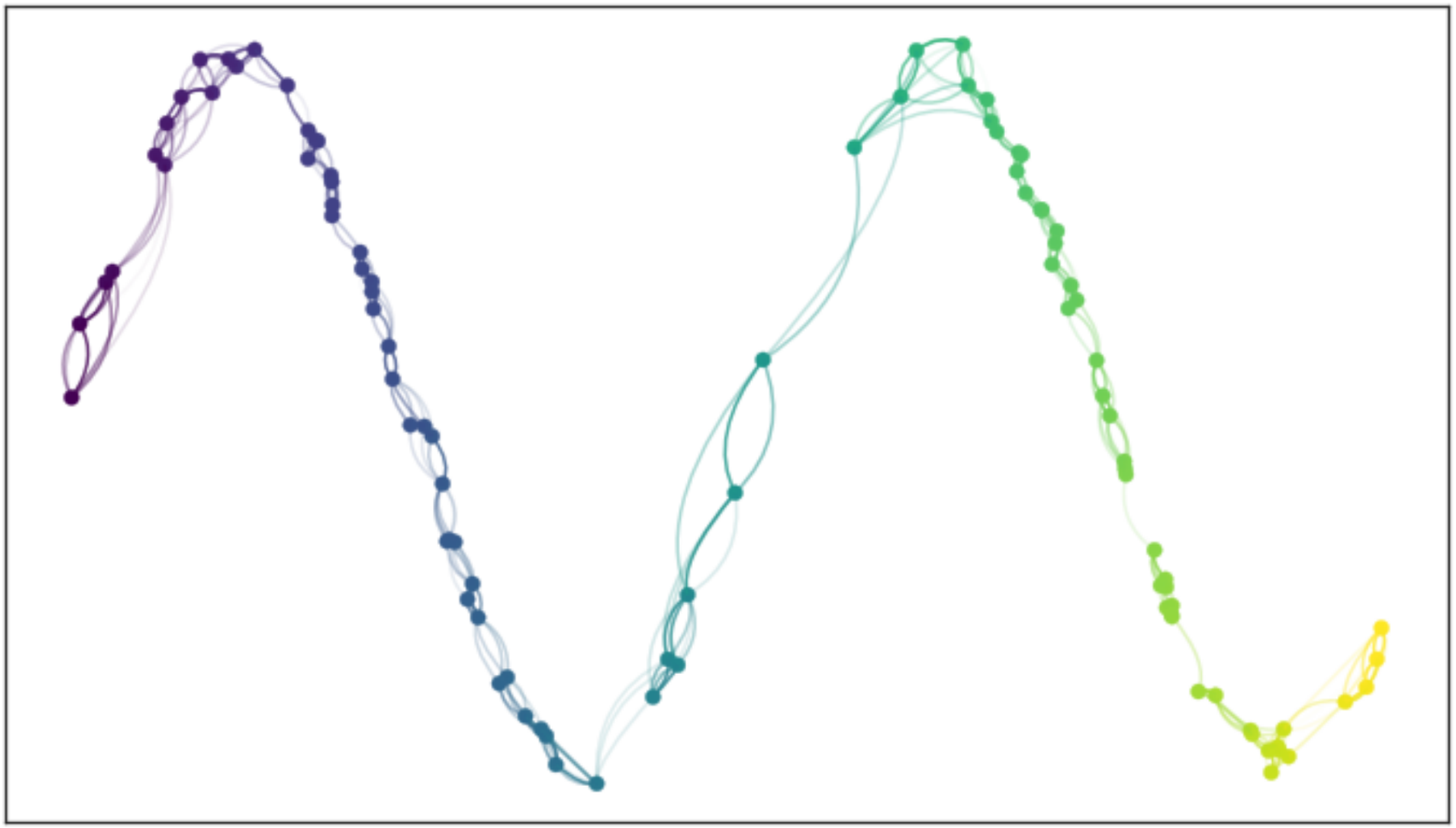

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Theorem 2 (UMAP Adjunction)**.** *The functors* FinReal : **sFuzz** $\to$ **FinEPMet** *and* FinSing : **FinEPMet** $\to$ **sFuzz** *form an adjunction* FinReal $\dashv$ FinSing.

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Under a probabilistic fuzzy union the combination of weights on edges is given by

$$f(\alpha, \beta) = \alpha + \beta - \alpha \cdot \beta$$

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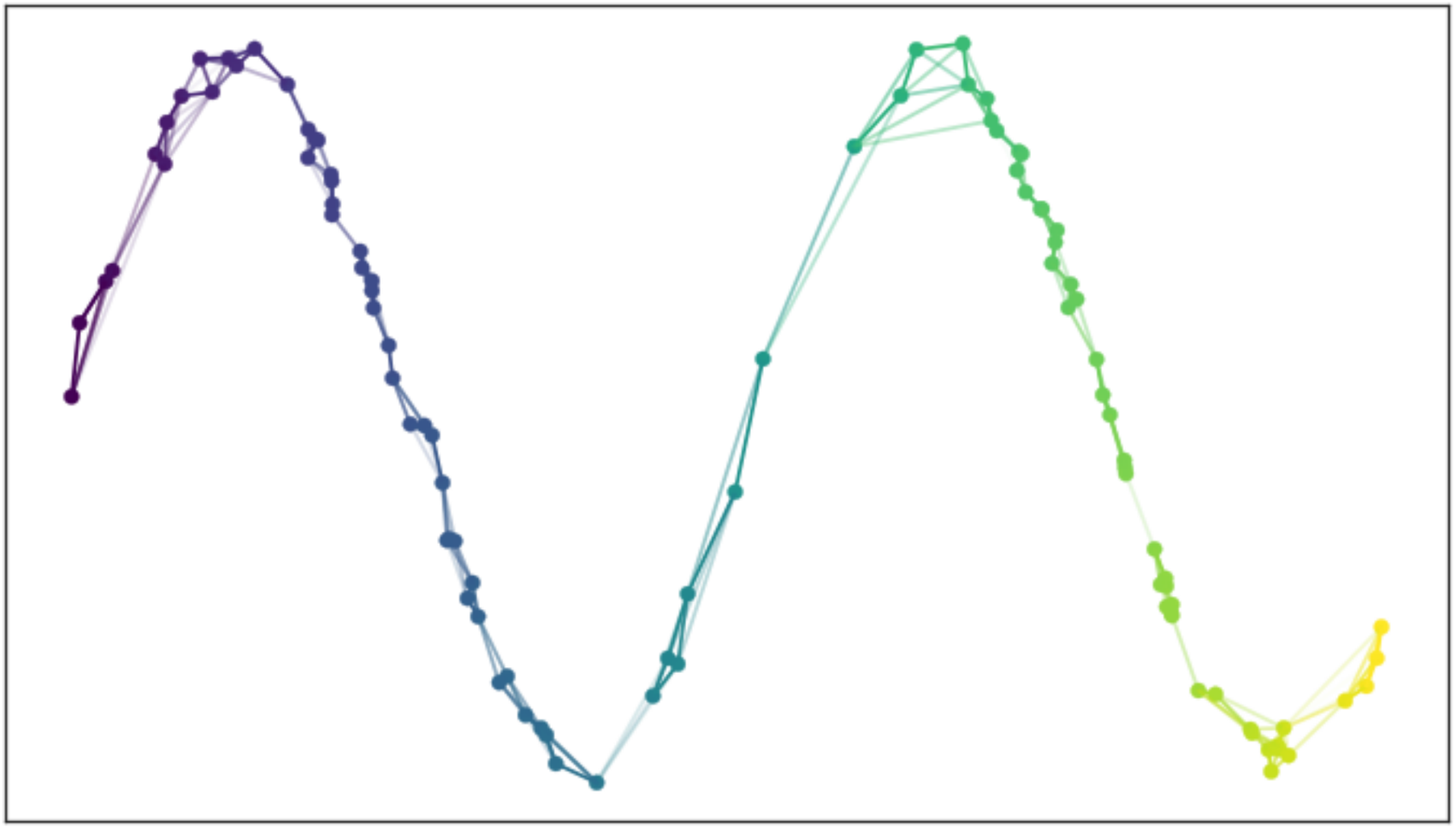

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Suppose we were given a low dimensional representation

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We can apply the same process to get a fuzzy graph!

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Except we *know* the manifold, and *don't know* the "correct" nearest neighbour distance

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Now measure the distance between the graphs using cross-entropy and optimize

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$$\sum_{a \in A} \mu(a) \log\left(\frac{\mu(a)}{\nu(a)}\right) + (1-\mu(a)) \log\left(\frac{1-\mu(a)}{1-\nu(a)}\right)$$

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We are just embedding the graph

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Get the clumps right

$$\sum_{a \in A} \mu(a) \log\left(\frac{\mu(a)}{\nu(a)}\right) + (1-\mu(a)) \log\left(\frac{1-\mu(a)}{1-\nu(a)}\right)$$

Get the gaps right

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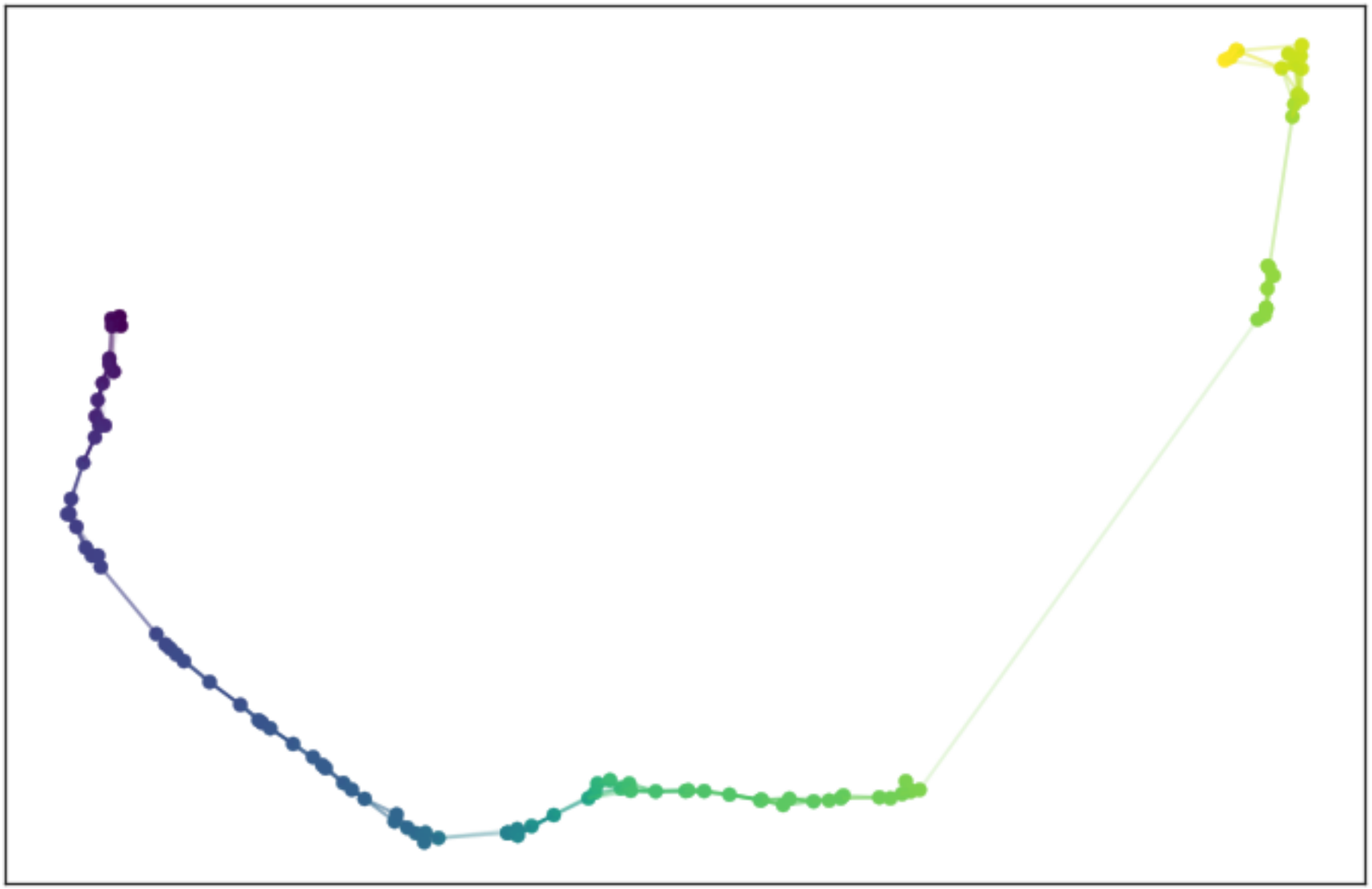

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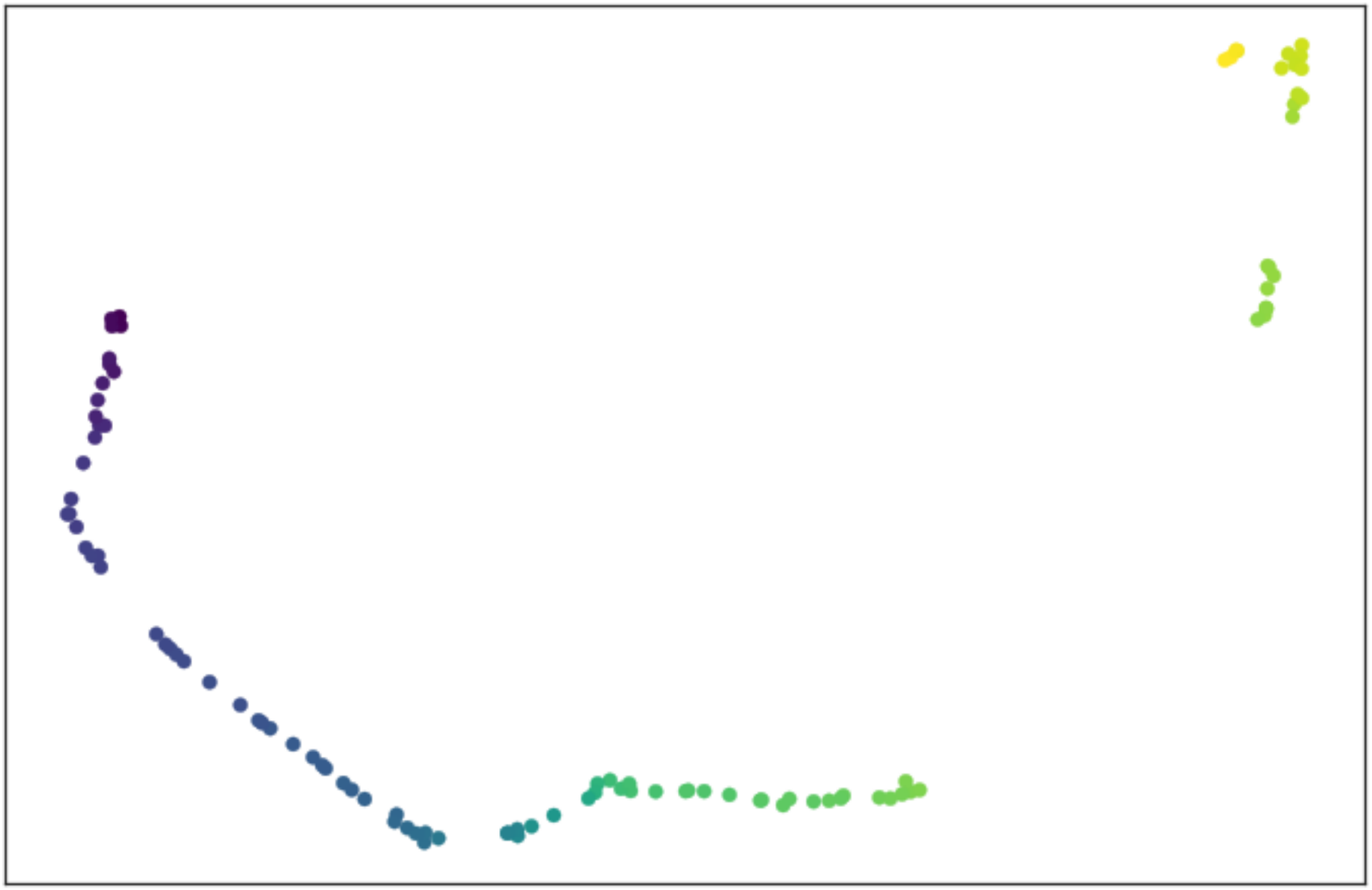

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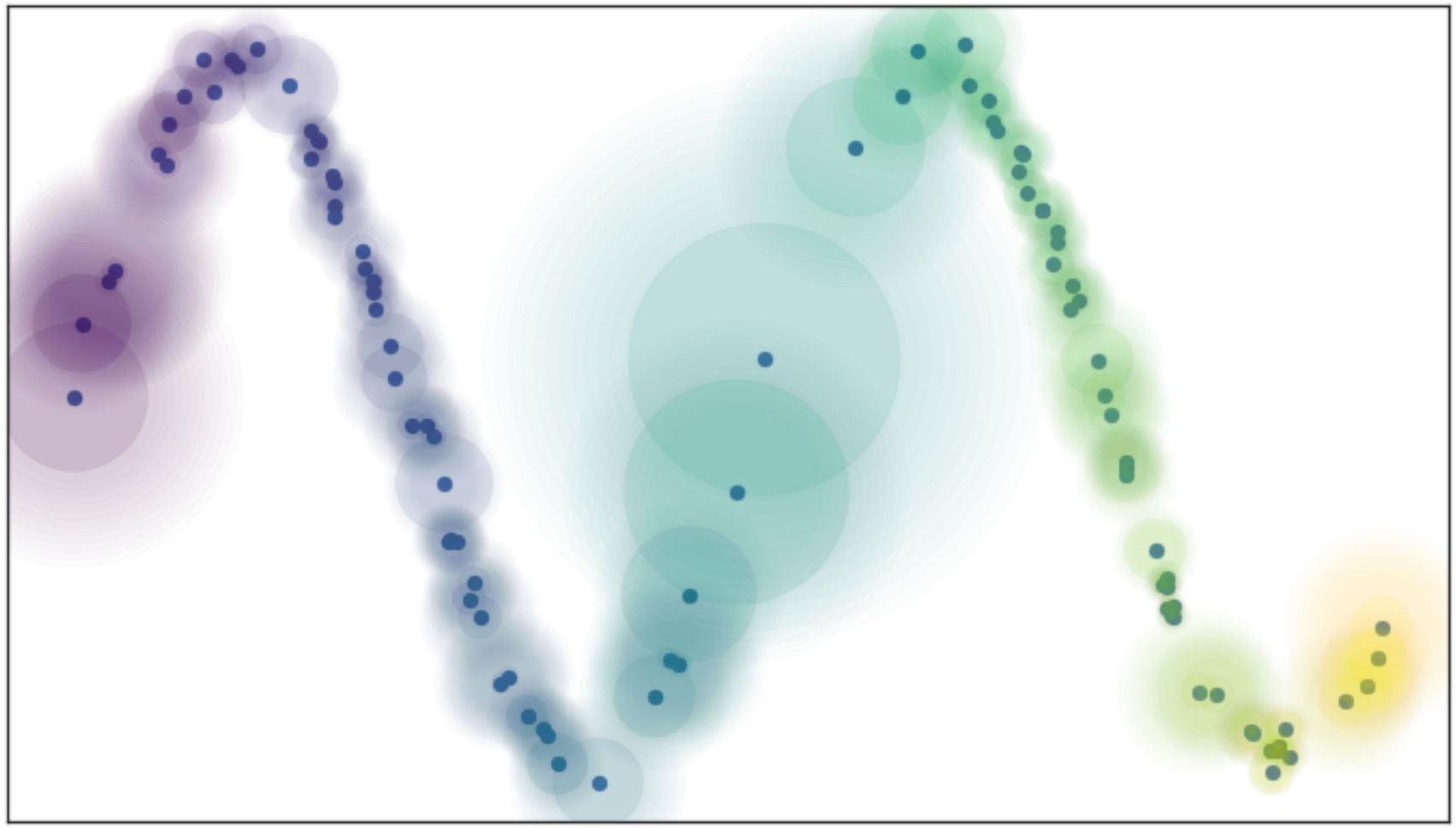

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On real data?

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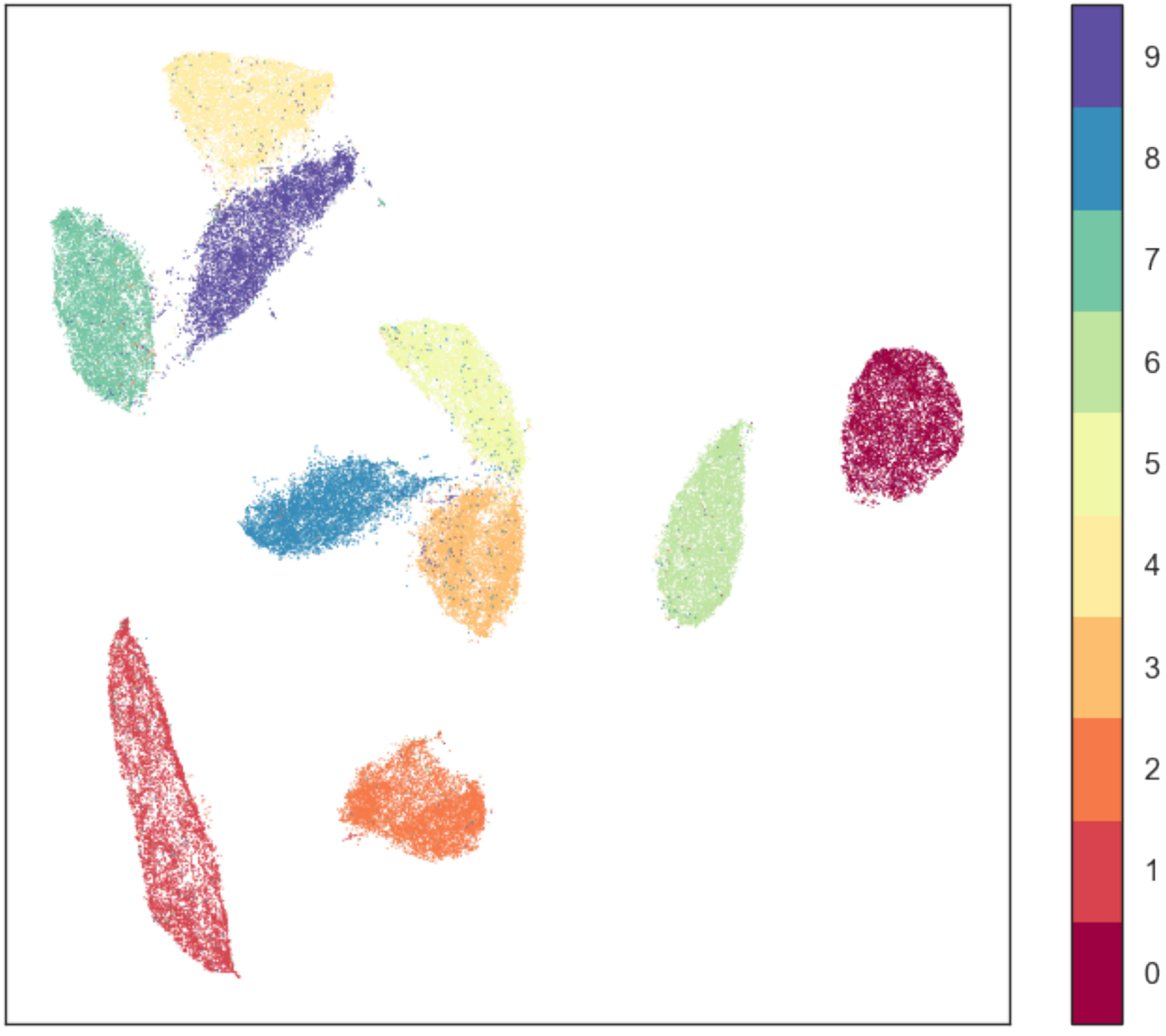
UMAP on MNIST digits



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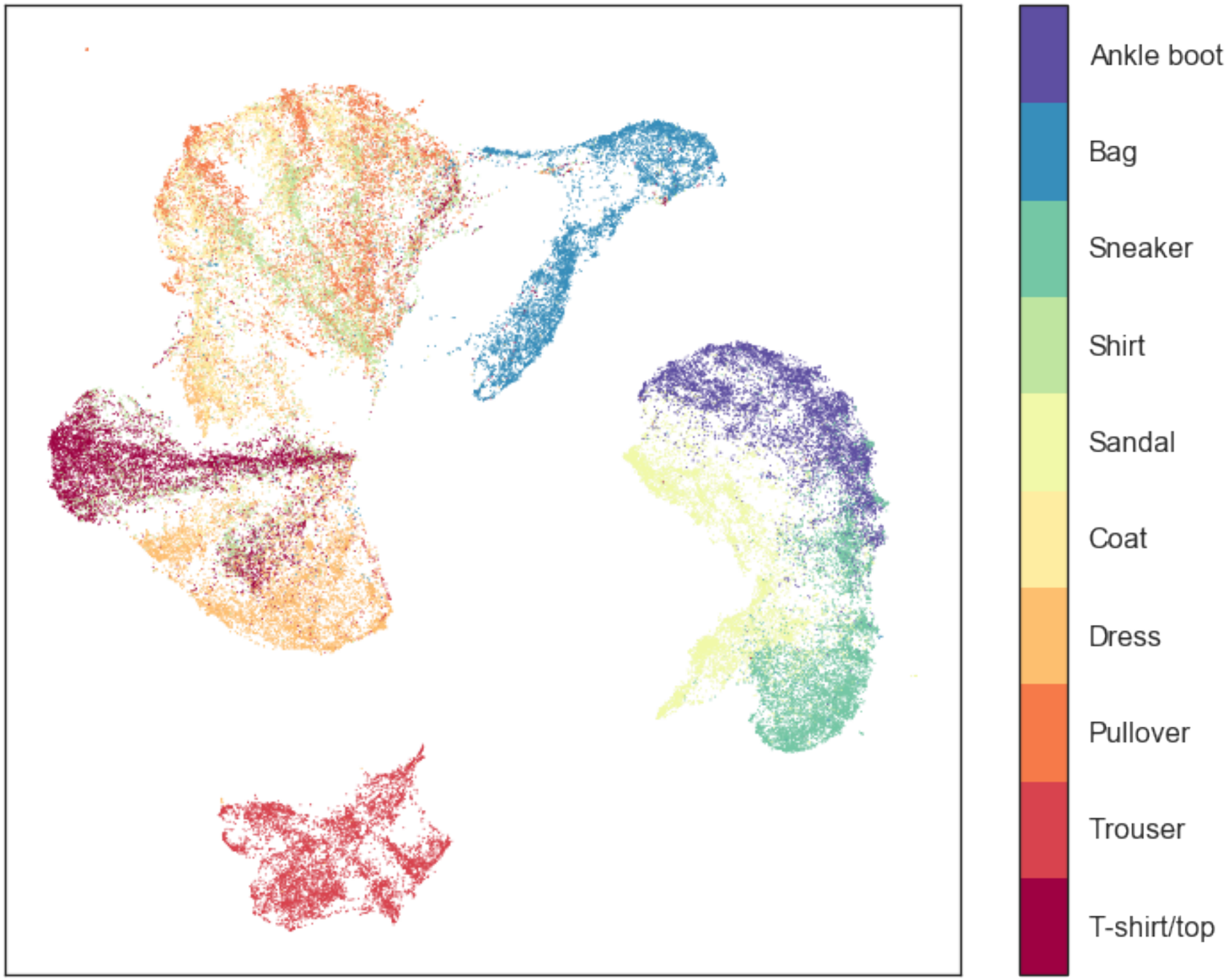
UMAP on Fashion MNIST



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Implementation

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Need to find (approximate) nearest neighbours very efficiently

Even in high dimensional space

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RP-trees + NN-descent

Dasgupta + Freund 2008

Dong, Charikar + Li 2011

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Need to optimize the layout subquadratically

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SGD + negative sampling

Mikolov et al 2013
Tang et al 2016

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Need to be high level but still fast

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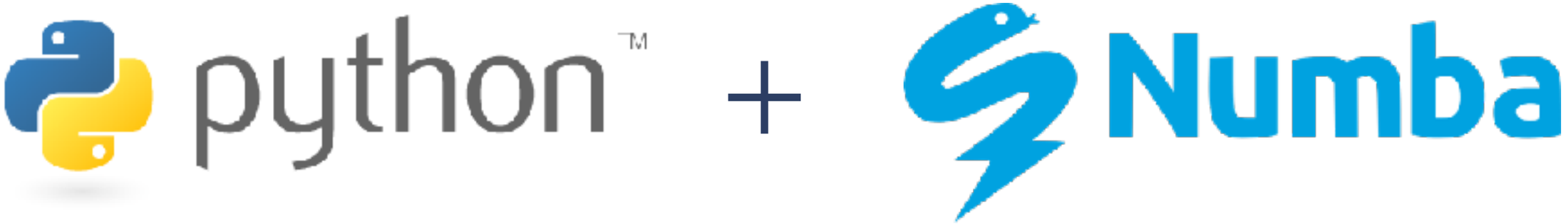

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Numba is awesome!

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- High performance
- Clean code
- Custom distance metrics

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Performance Comparison

	UMAP speed up over t-SNE
COIL20	3x
MNIST	13x
Fashion MNIST	11x
GoogleNews	19x

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Where Next?

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Given the mathematical foundation, a number of options are available

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Embed new unseen points into an existing embedding

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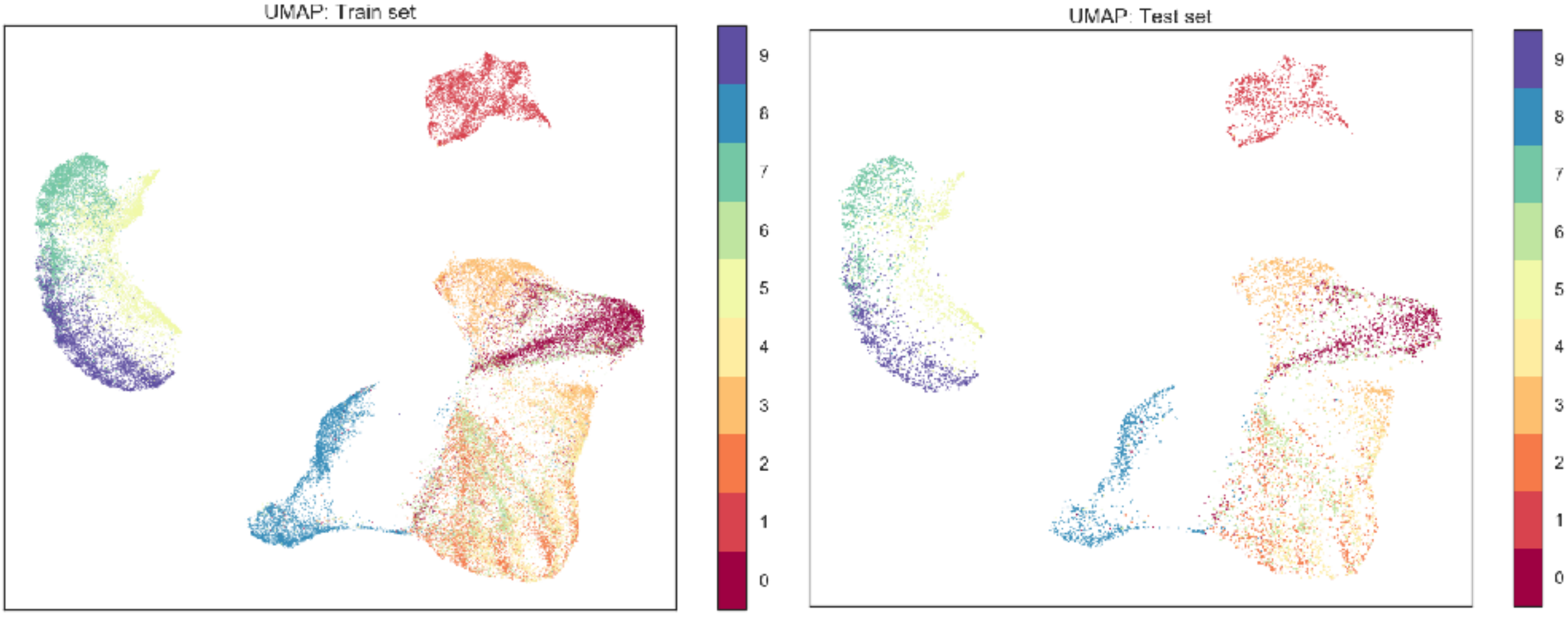

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Make use of labels for supervised dimension reduction

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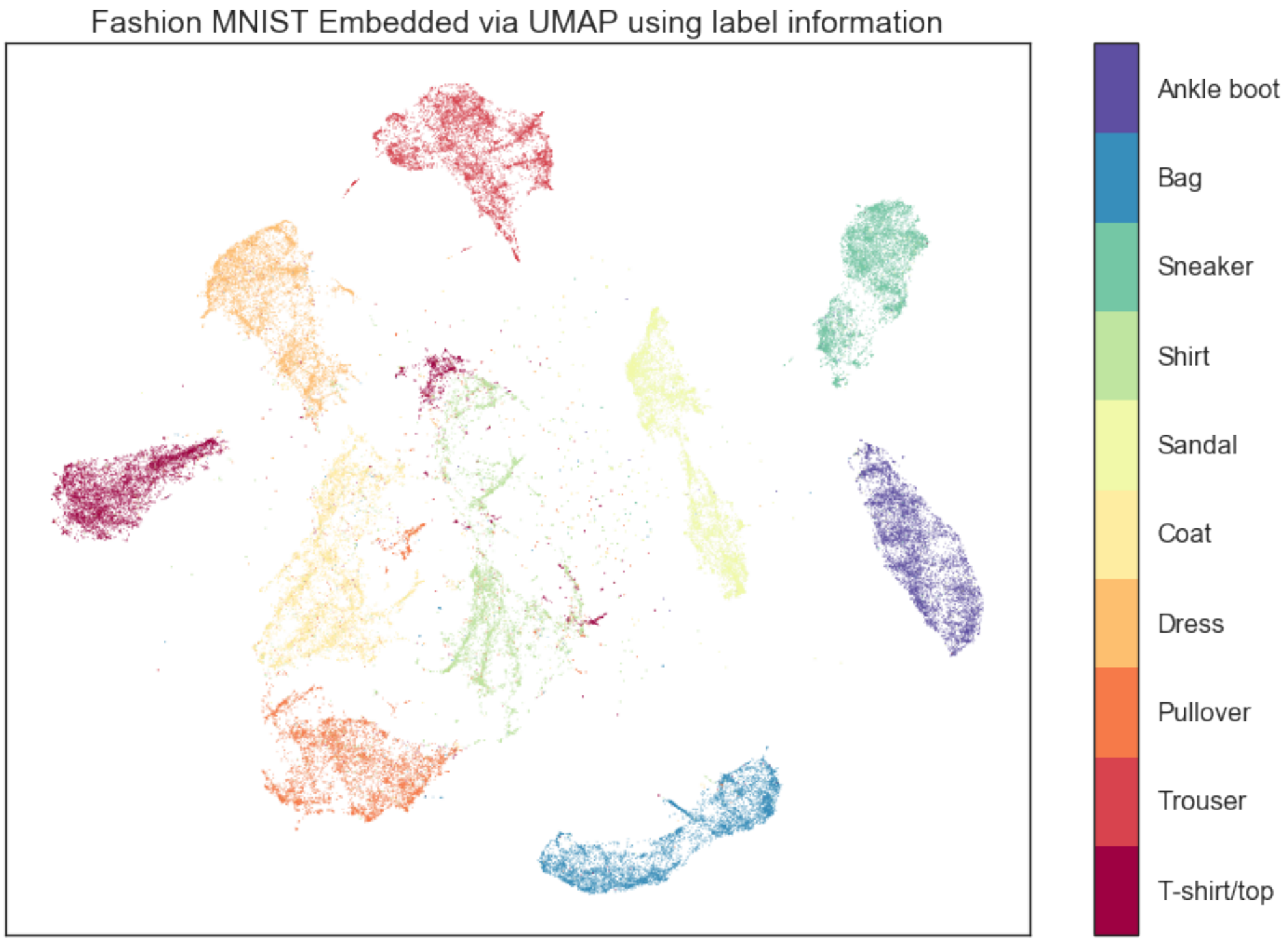

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And combine those for metric learning

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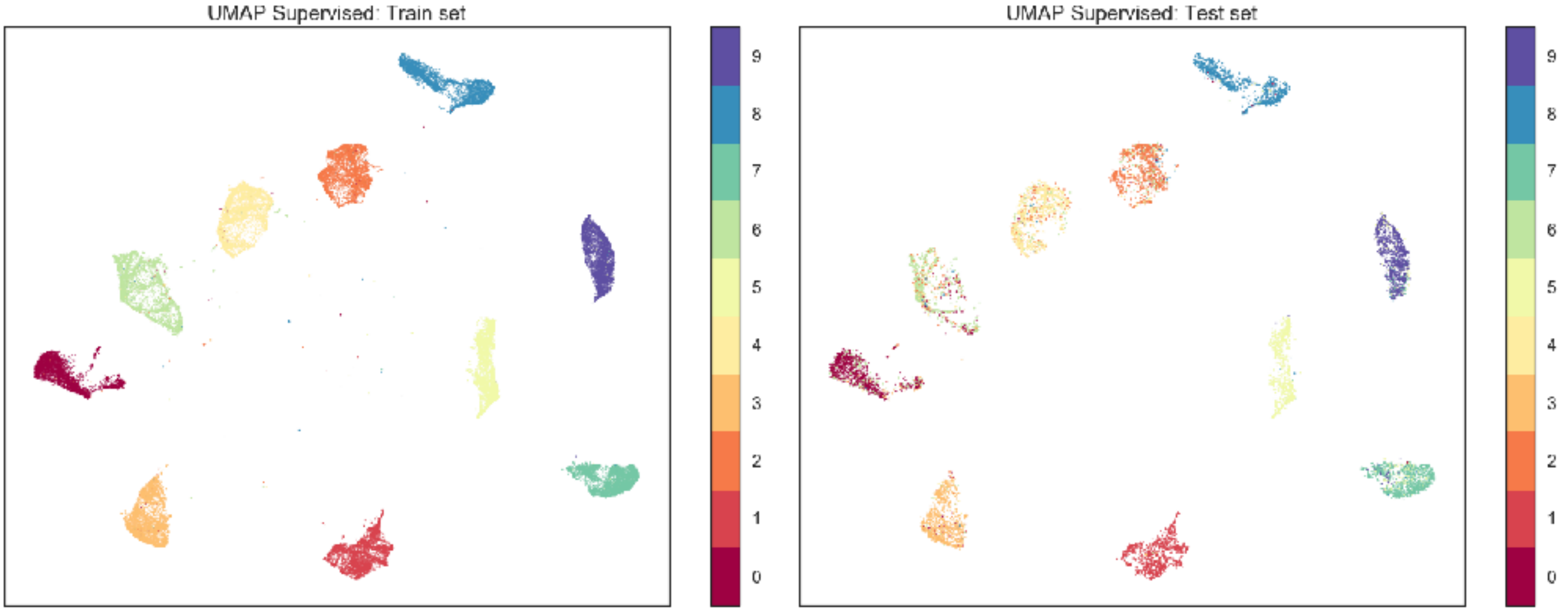

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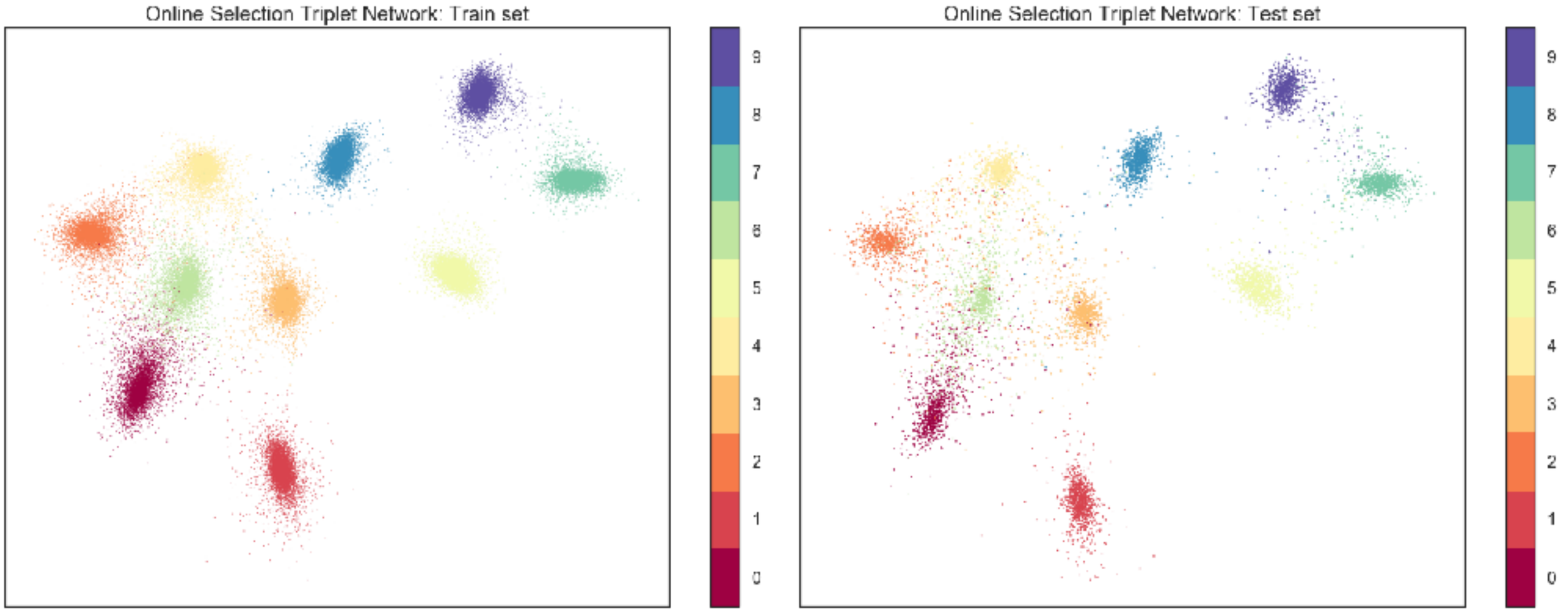

Derived from Adam Bielski's Siamese/Triplet repository:
https://github.com/adambielski/siamese-triplet

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Adding one categorical variable is no harder theoretically than adding many

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Combine spaces with different metrics

Continuous, categorical, ordinal, Haversine, Levenstein, and more …

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As long as you can provide a metric for the datatype UMAP can combine it with other datatypes!

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UMAP for pandas dataframes!

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https://github.com/lmcinnes/umap

conda install -c conda-forge umap-learn

pip install umap-learn

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@leland_mcinnes