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Nuts and bolts of neighbour embeddings

Dmitry Kobak

28 November 2025

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Everything you always wanted to know about *t*-SNE but were afraid to ask

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Much more than you ever
~~Everything you always~~ wanted to know about *t*-SNE but were afraid to ask

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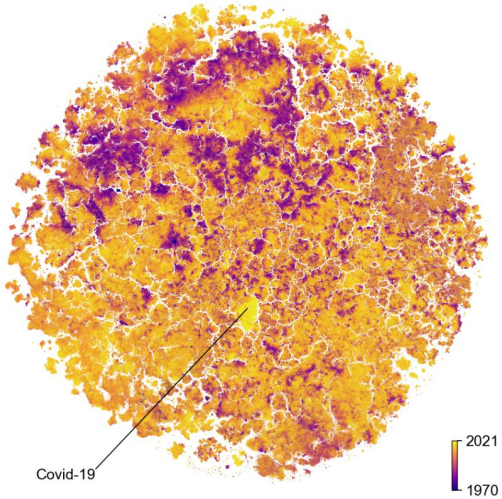
Covid-19
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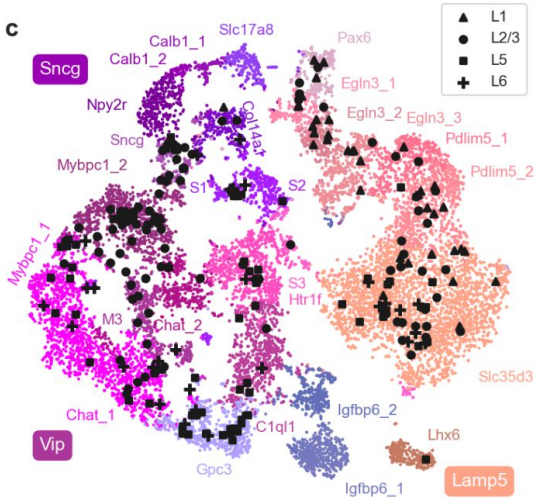
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Sncg
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Calb1_2
Slc17a8
Pax6
Npy2r
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Egln3_2
Egln3_3
Sncg
Pdlim5_1
Mybpc1_2
Pdlim5_2
S1
S2
Mybpc1_1
S3
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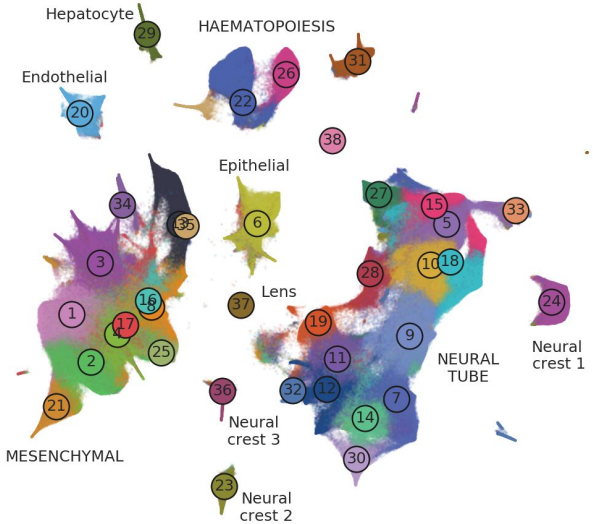
Hepatocyte
HAEMATOPOIESIS
Endothelial
Epithelial
Lens
NEURAL TUBE
Neural crest 1
Neural crest 3
MESENCHYMAL
Neural crest 2

La Manno et al., Nature 2021

Neighbor embeddings

identify similar objects and embed them close to each other

Neighbor embeddings

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[PDF] **Stochastic neighbor embedding**

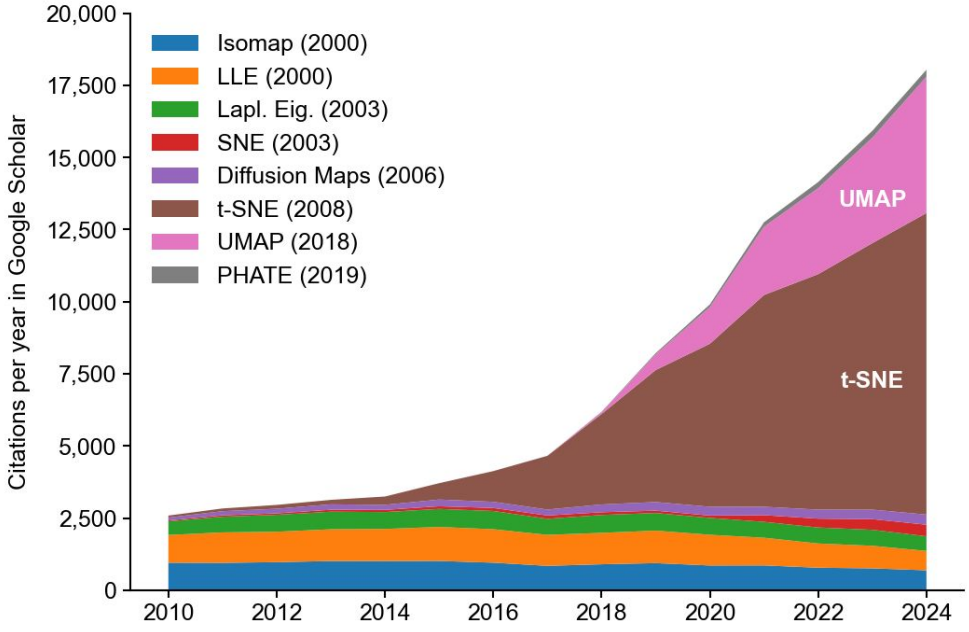
G Hinton, ST Roweis - NIPS, 2002 - Citeseer

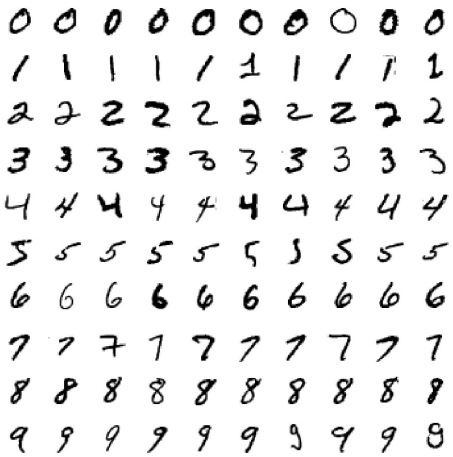
We describe a probabilistic approach to the task of placing objects, described by high-dimensional vectors or by pairwise dissimilarities, in a low-dimensional space in a way that preserves neighbor identities. A Gaussian is centered on each object in the high …

[PDF] Visualizing data using **t-SNE**.

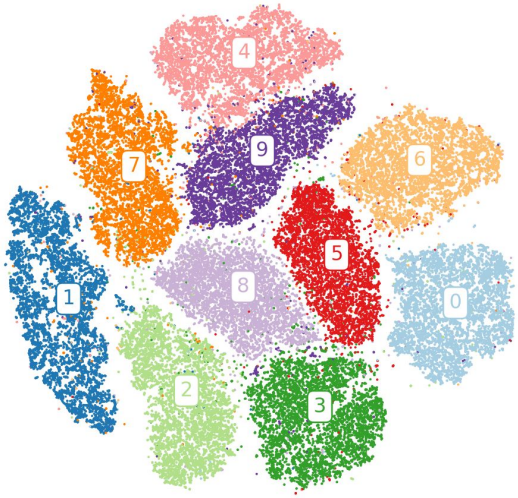
L Van der Maaten, G Hinton - Journal of machine learning research, 2008 - jmlr.org

We present a new technique called "**t-SNE**" that visualizes high-dimensional data by giving each datapoint a location in a two or three-dimensional map. The technique is a variation of Stochastic Neighbor Embedding (Hinton and Roweis, 2002) that is much easier to optimize …

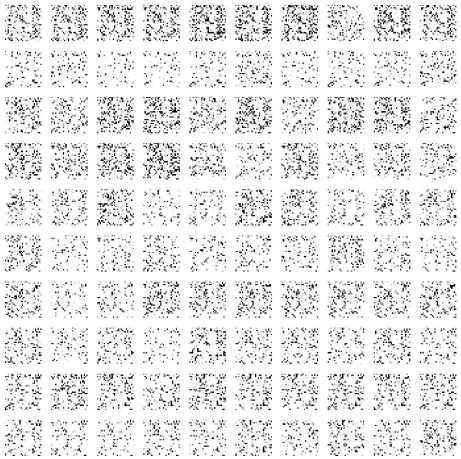




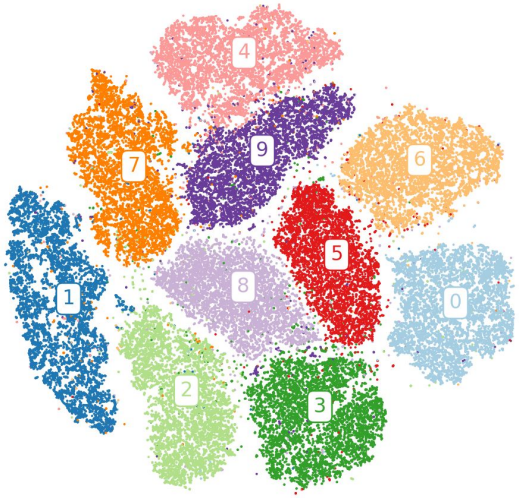
MNIST



t-SNE

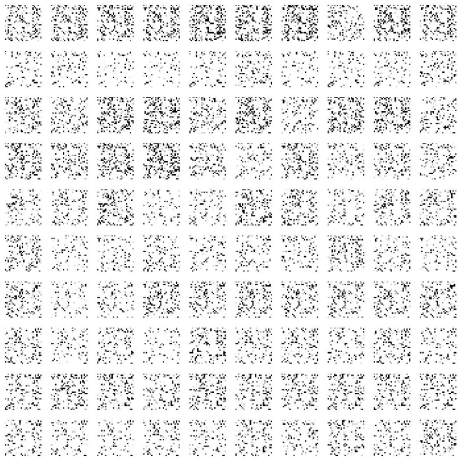


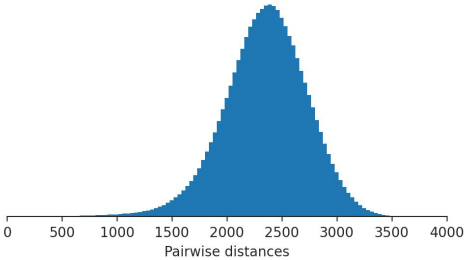
MNIST

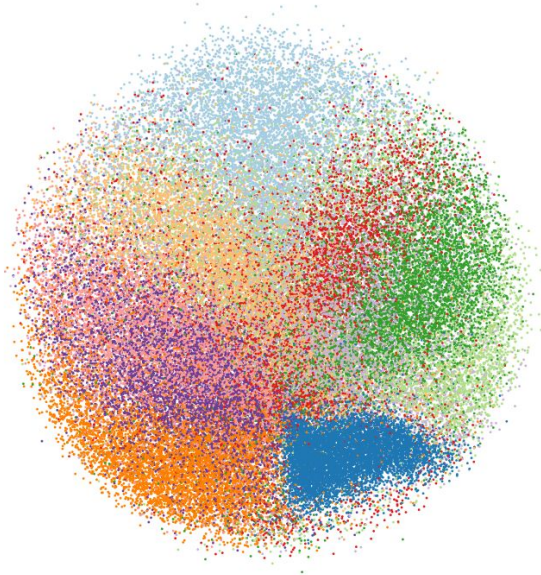


t-SNE

$$\mathcal{L} = \sum_{i<j} (d_{ij} - \|\mathbf{y}_i - \mathbf{y}_j\|)^2$$

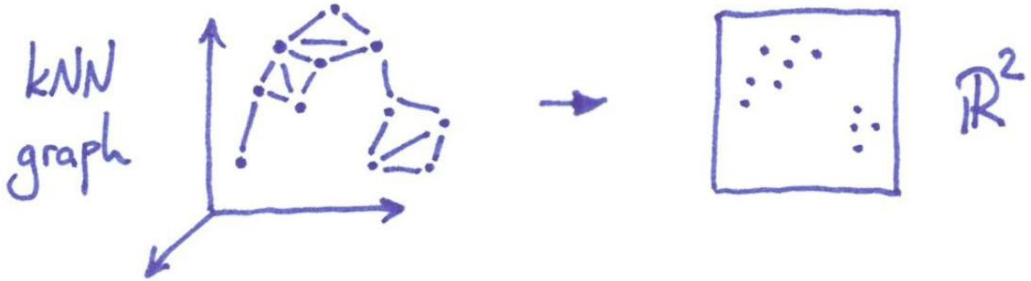




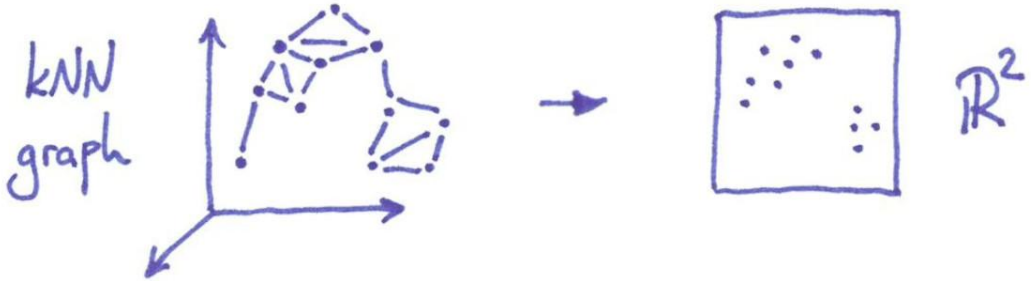


MDS

Neighbor embeddings



t-SNE



$$\mathcal{L}_{\text{t-SNE}} = \sum_{ij} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

p_{ij} can be normalized symmetrized adjacency matrix of the kNN graph.

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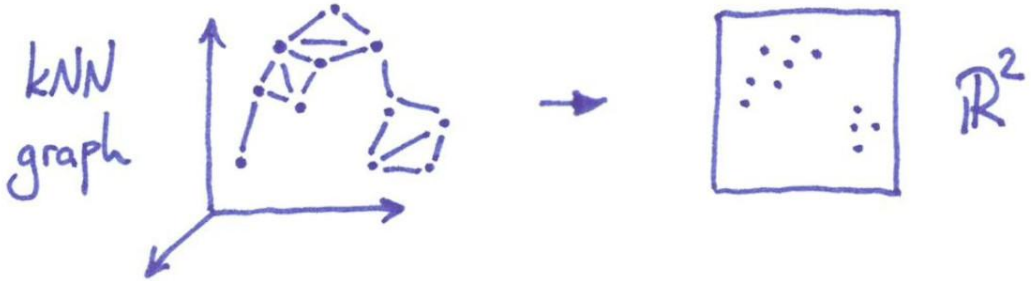
t-SNE



$$\mathcal{L}_{\text{t-SNE}} = \sum_{ij} p_{ij} \log \frac{p_{ij}}{q_{ij}} \sim -\sum_{ij} p_{ij} \log q_{ij} = -\sum_{ij} p_{ij} \log \frac{w_{ij}}{Z} = \underbrace{-\sum_{ij} p_{ij} \log w_{ij}}_{\text{attraction}} + \underbrace{\log \sum_{ij} w_{ij}}_{\text{repulsion}}.$$

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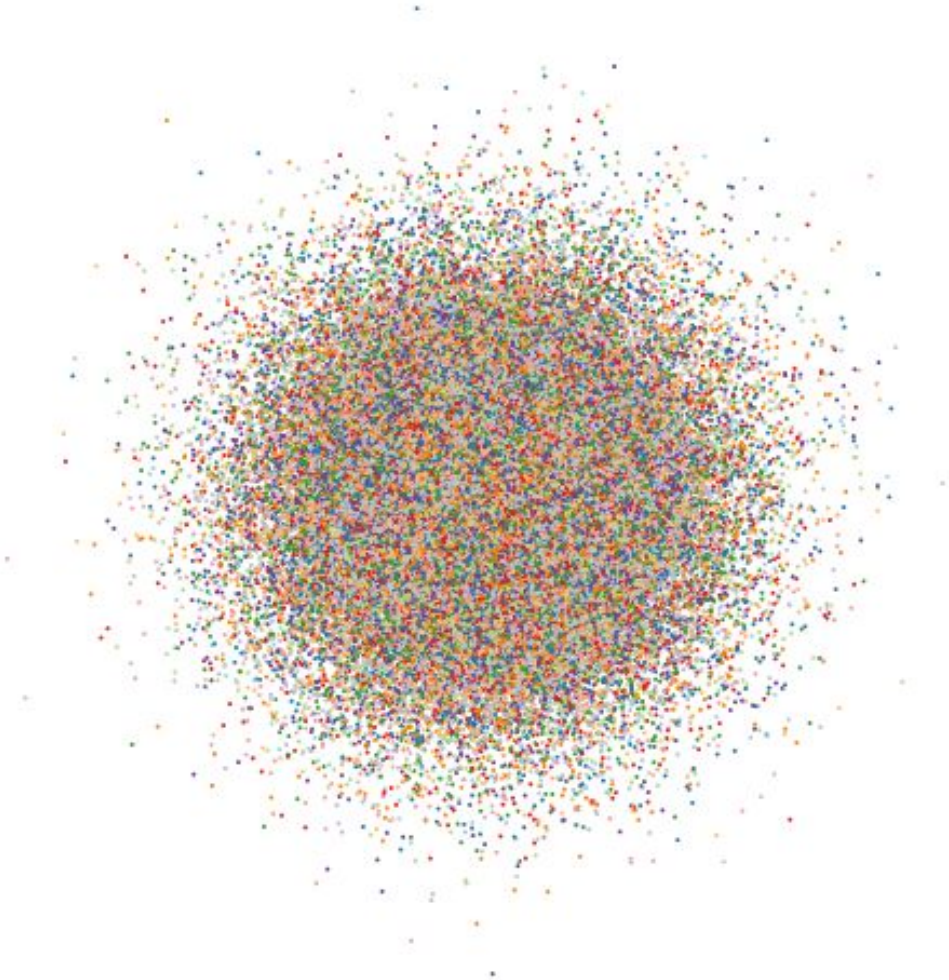
Gradient descent

Gradient descent starting
from a random configuration.

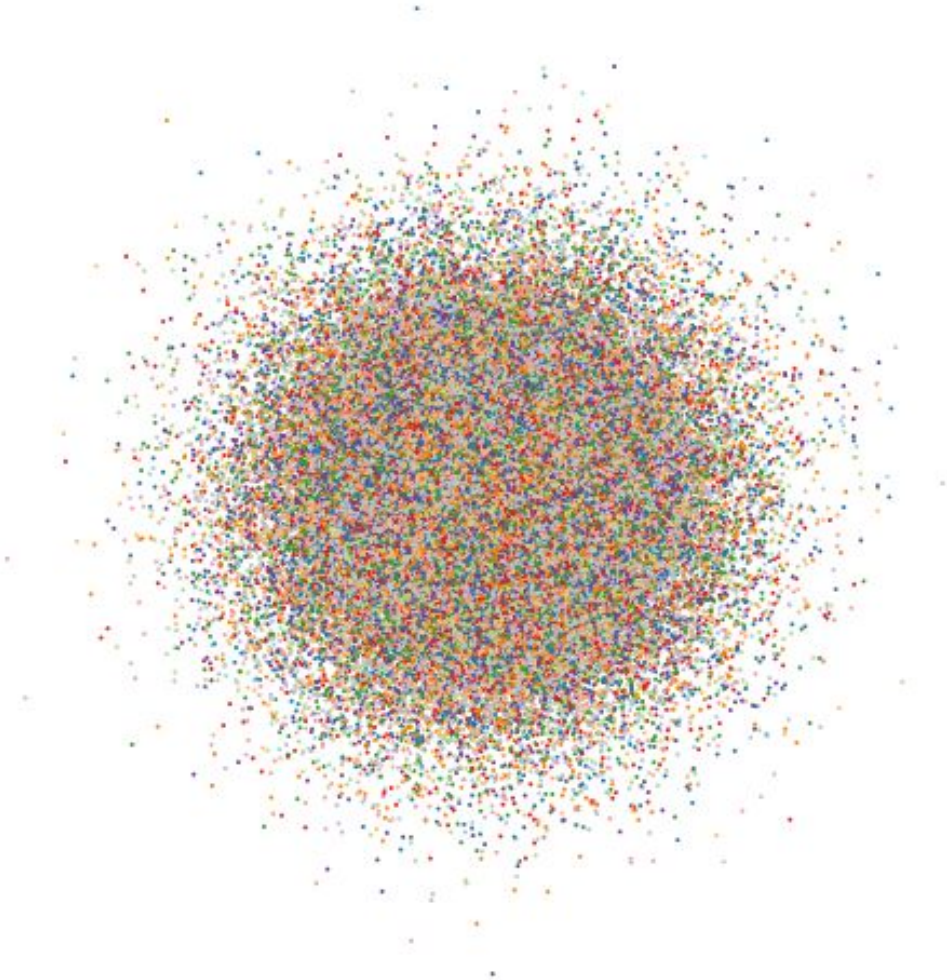
Each frame is scaled
(in reality embedding is
initialized small and slowly
grows in size).



Gradient descent

Optimization issues:

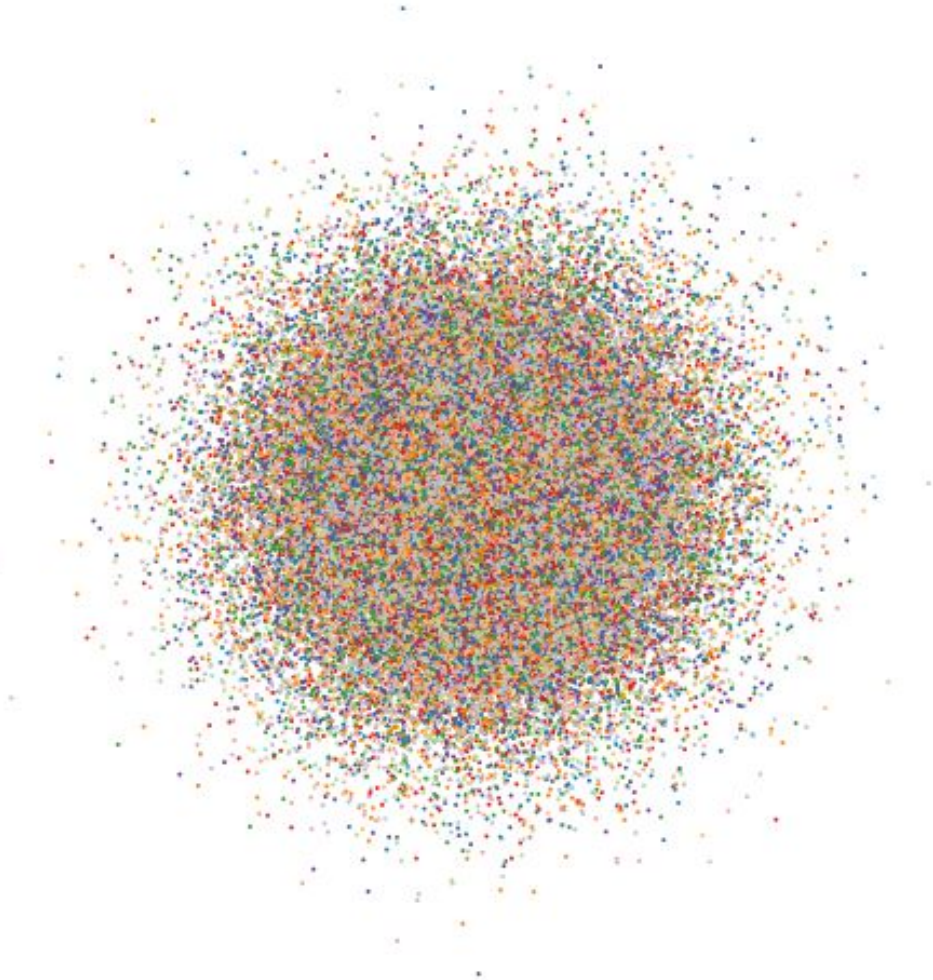
1) Initialization
2) Learning rate
3) Local minima
4) Runtime



Early exaggeration

Multiply all attractive forces by 12 for 250 iterations.

$$-\underbrace{\sum_{ij} p_{ij} \log w_{ij}}_{\text{attraction}} + \underbrace{\log \sum_{ij} w_{ij}}_{\text{repulsion}}$$



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Multiply all attractive forces by 12 for 250 iterations.

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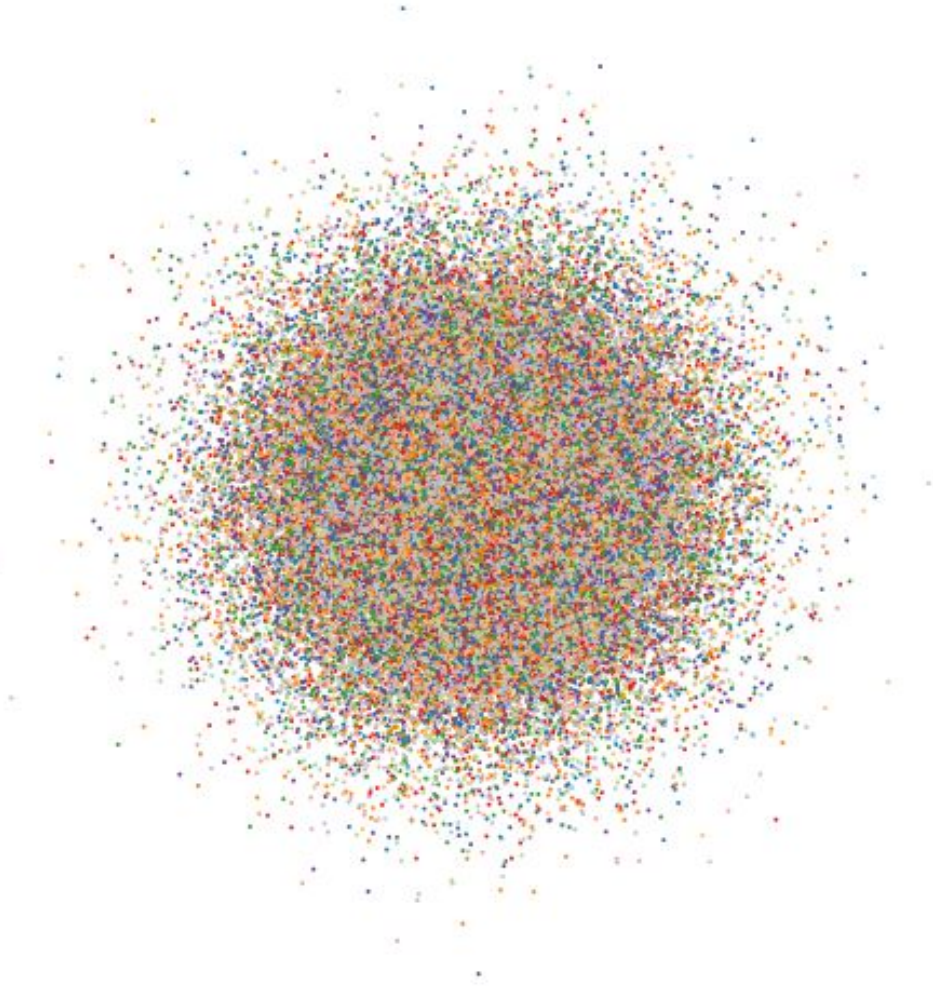
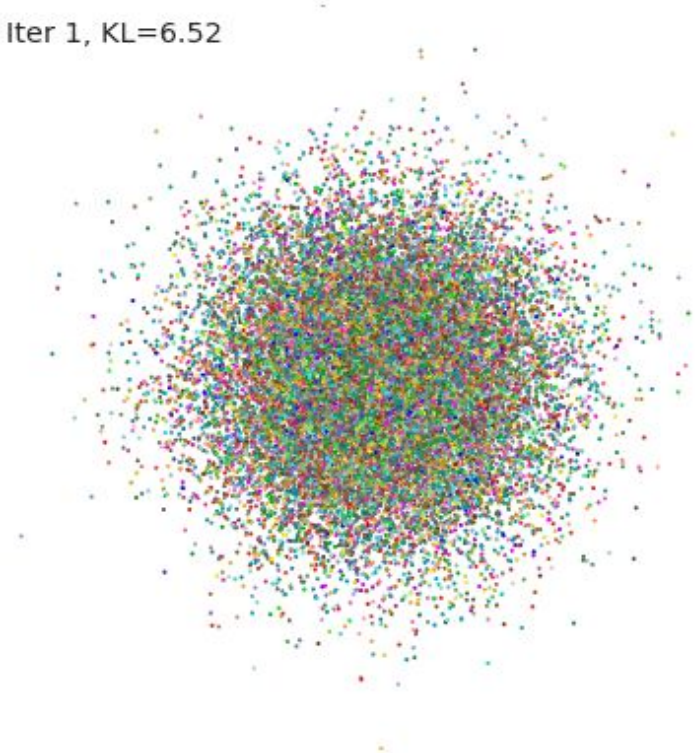
The learning rate should grow with sample size:

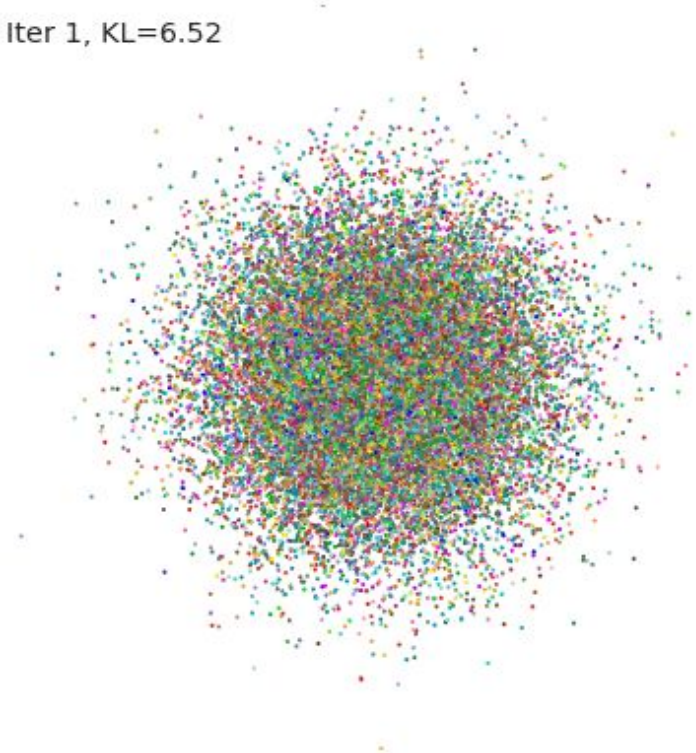
$$\eta = n \,/\, \text{exagg.}$$

Belkina et al. (2019) based on Linderman & Steinerberger (2019)



Early exaggeration: scRNA-seq data

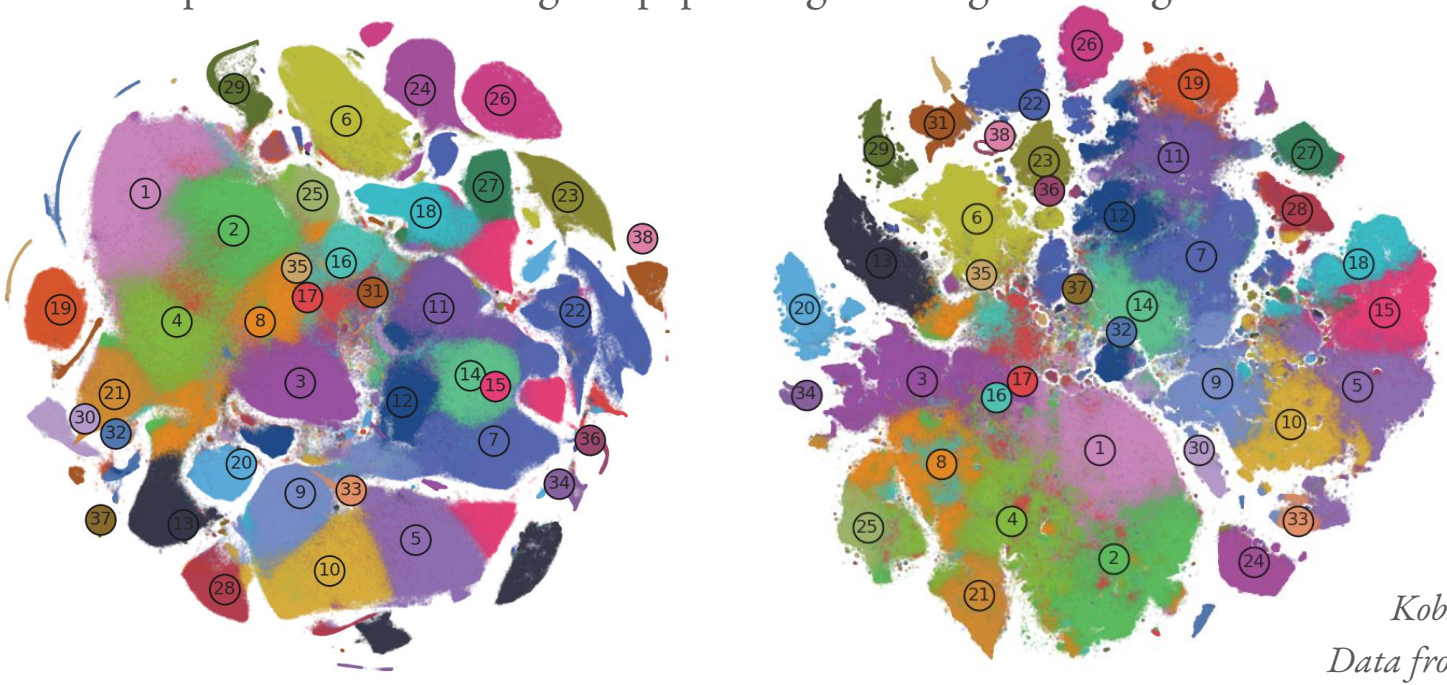




Data from Tasic et al. (2018)

Early exaggeration and the learning rate: real-world example

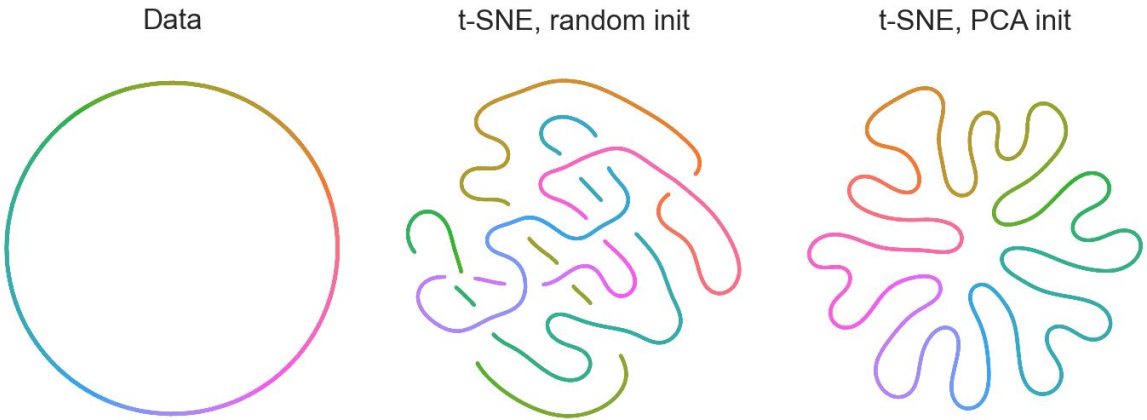
Single-cell transcriptomic study of mouse embryogenesis ($n \approx 2{,}000{,}000$).
Left — t-SNE published in the original paper. Right — high learning rate.



Kobak & Berens (2019)
Data from Cao et al. (2019)

Initialization

The loss function has many local minima. Even with early exaggeration, initialization can play a big role. With random initialization, t-SNE will often struggle to preserve global structure.



Kobak & Linderman, Nature Biotech 2021

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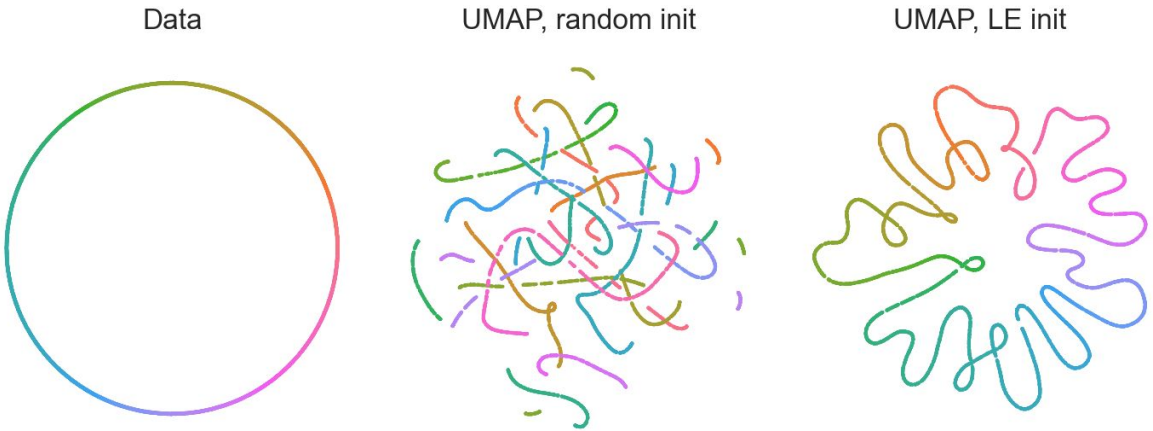
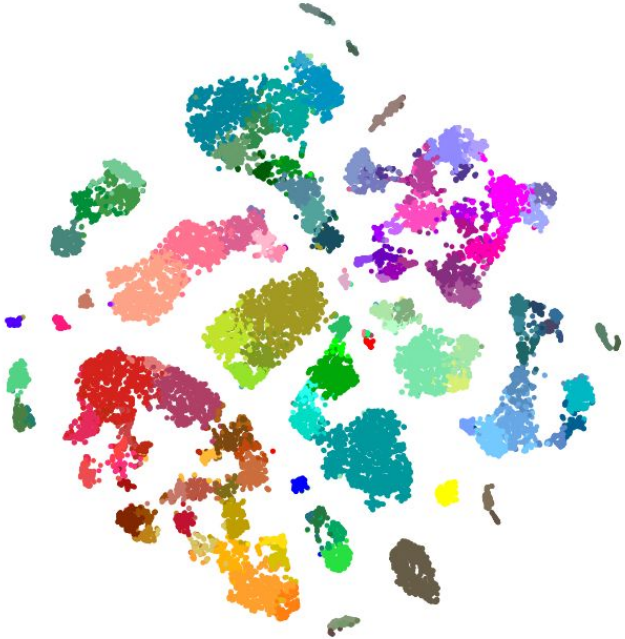


Kobak & Linderman, Nature Biotech 2021

Initialization: real-world example

t-SNE (random initialization)



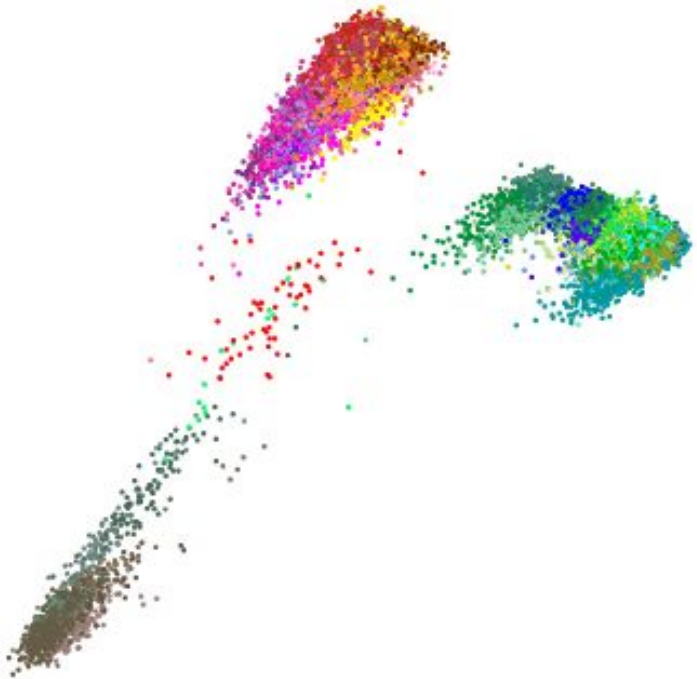
PCA

Single-cell RNA-seq data from mouse cortex

Kobak & Berens, Nature Comms 2019)

Data from Tasic et al. (2018)

Initialization:
real-world example



Single-cell RNA-seq data from mouse cortex

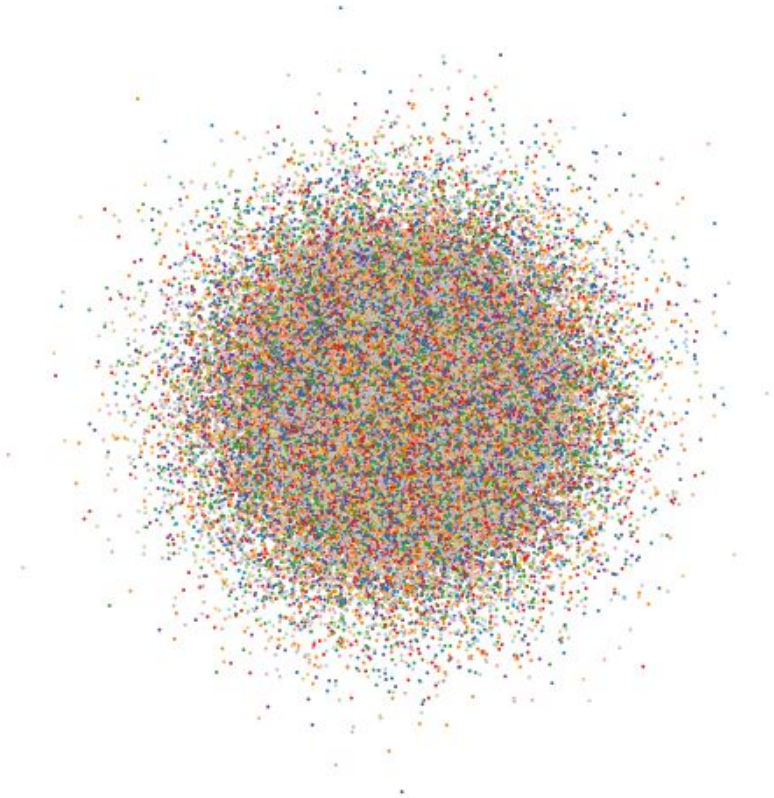
Kobak & Berens, Nature Comms 2019)
Data from Tasic et al. (2018)

Approximations

$$-\underbrace{\sum_{ij} p_{ij} \log w_{ij}}_{\text{attraction}} + \underbrace{\log \sum_{ij} w_{ij}}_{\text{repulsion}}$$

Approximate kNN graph with small k

Approximations:
* Barnes–Hut
* Fourier interpolation
* Sampling



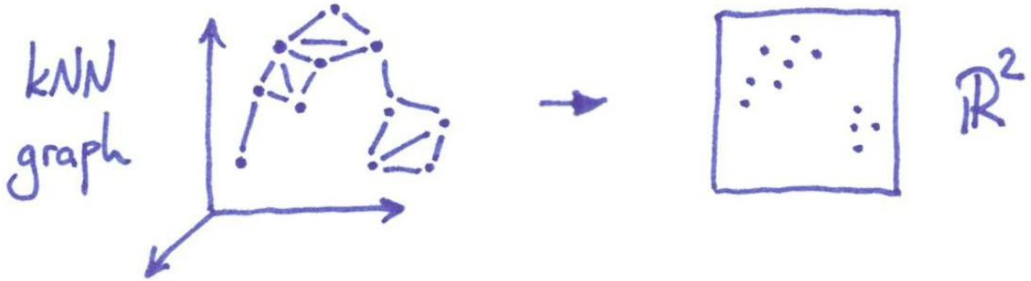
Optimization issues

A good t-SNE implementation should:

1. use informative initialization by default;
2. set appropriate optimization parameters (learning rate set to n);
3. support approximate nearest neighbors and $O(n)$ approximation of repulsive forces.

=> In Python, use `openTSNE` *(Poličar et al., 2024)*.

t-SNE



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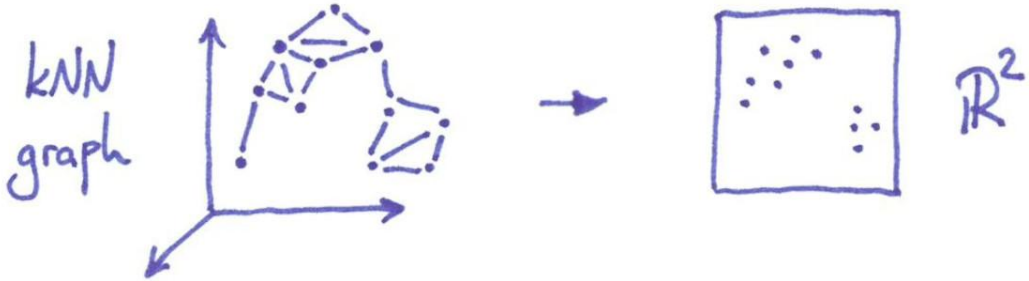
t-SNE



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Usually high-dim affinities are obtained with a Gaussian kernel via *perplexity* parameter

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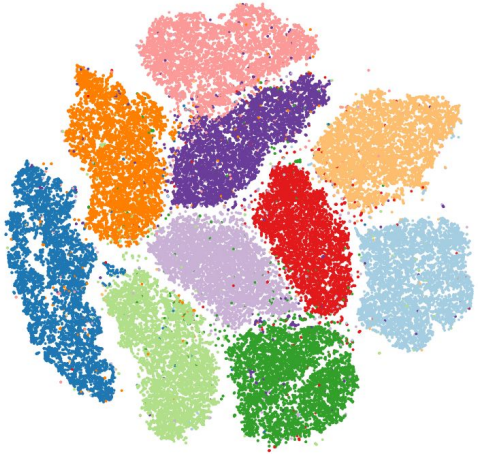
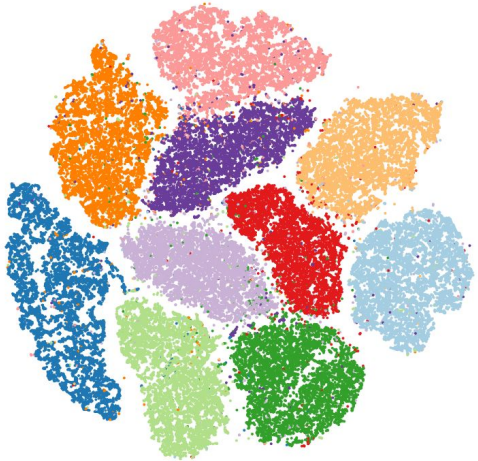
t-SNE with perplexity 30



t-SNE with a kNN kernel (k=10)



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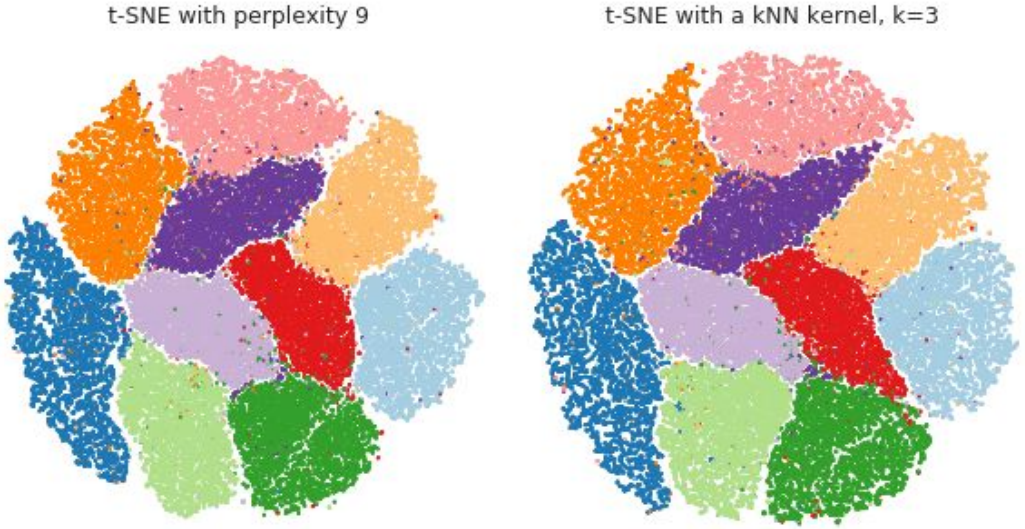

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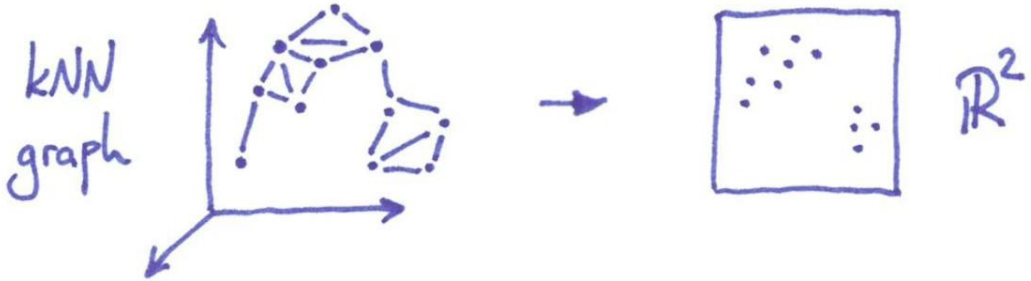
t-SNE



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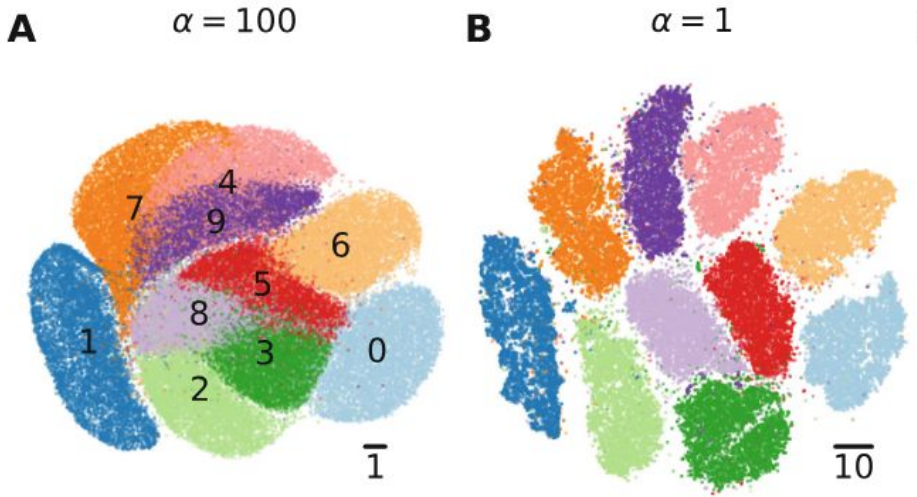
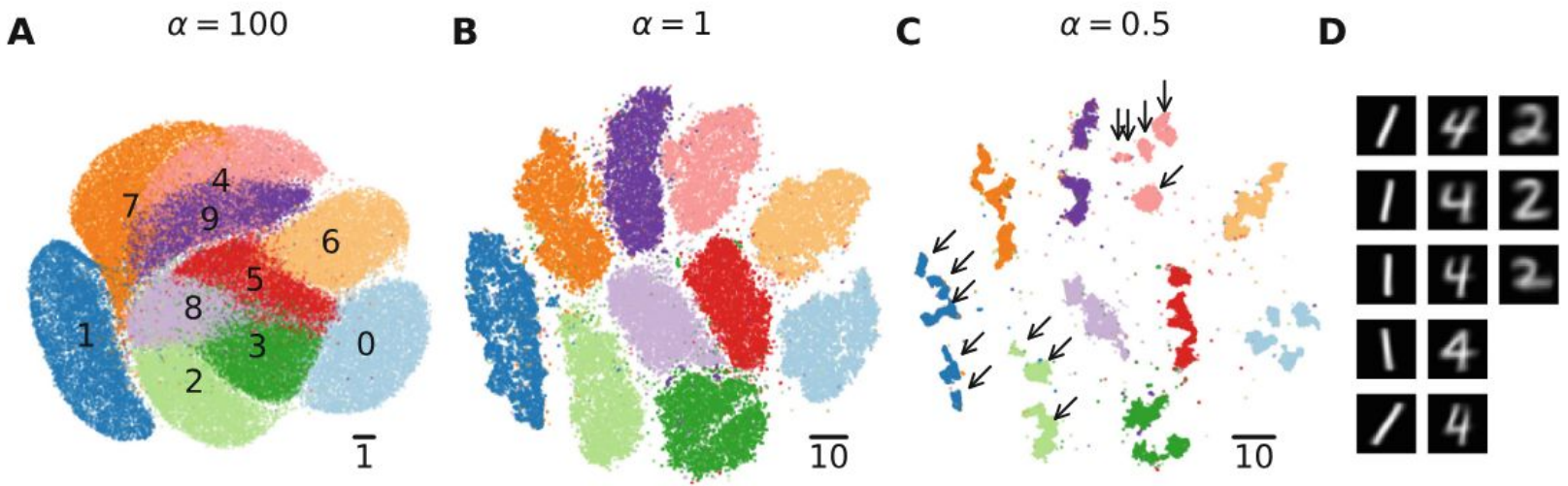
The *t*-distribution kernel: from SNE to *t*-SNE



$$k(d) = \frac{1}{(1 + d^2/\alpha)^\alpha}$$

Kobak et al., ECML 2019

The *t*-distribution kernel: beyond *t*-SNE



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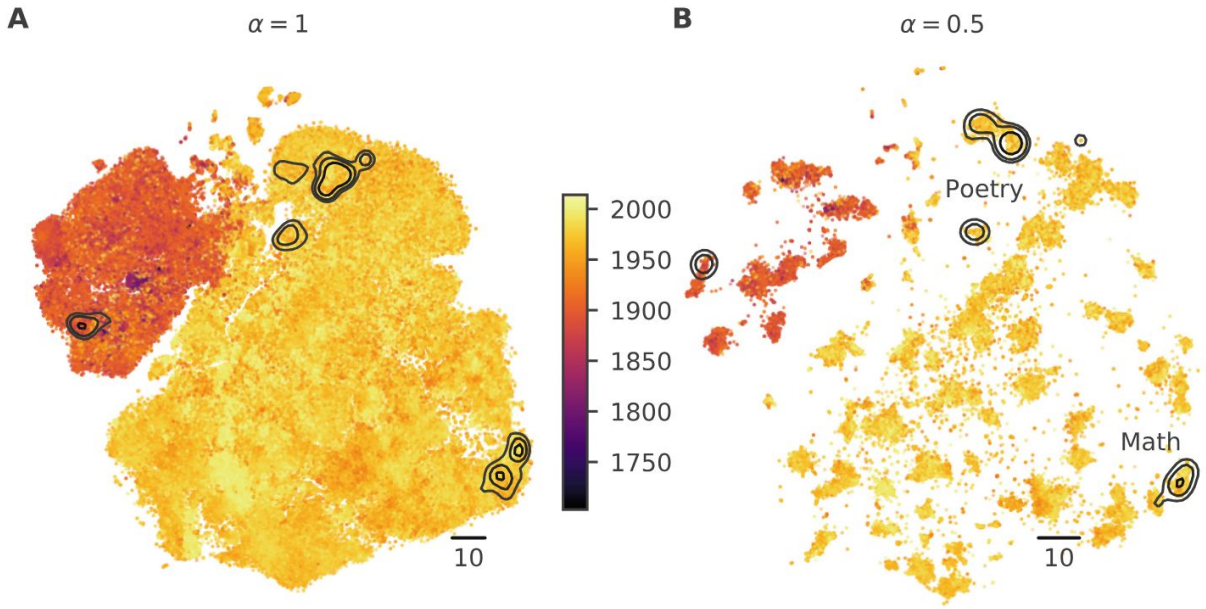
Kobak et al., ECML 2019

The *t*-distribution kernel: beyond *t*-SNE

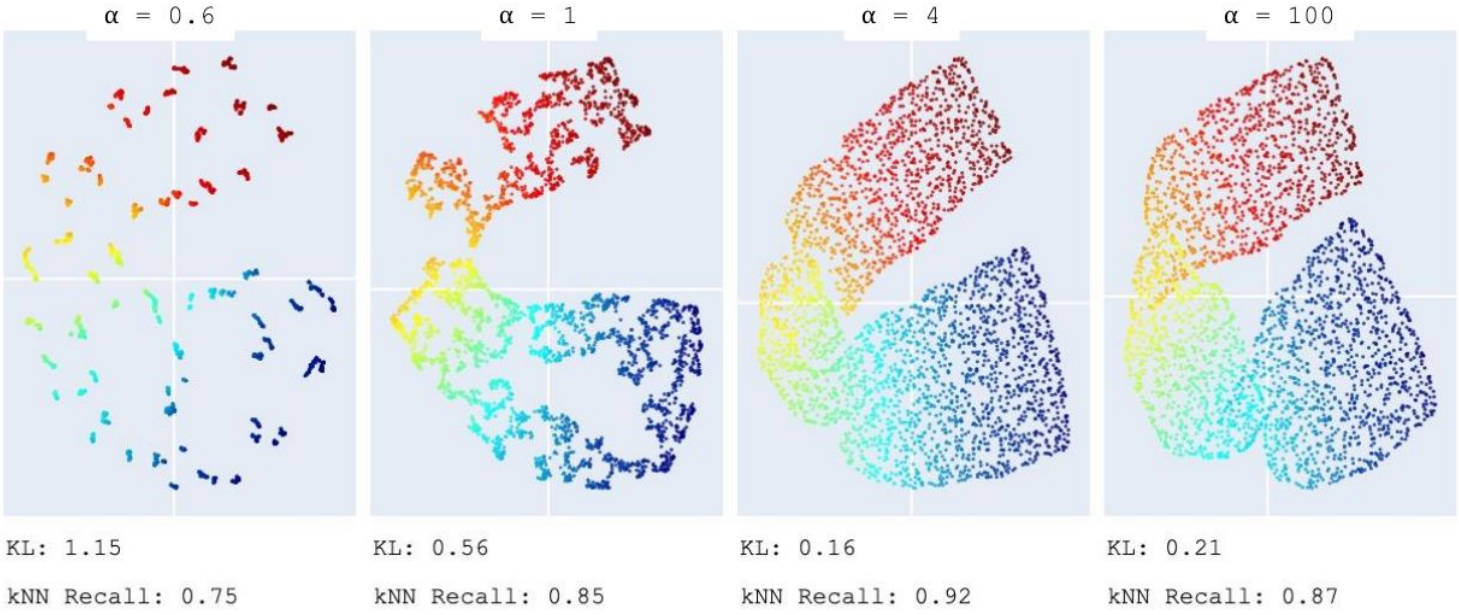


Russian language part of the HathiTrust library ($n = 408\,291$).

Kobak et al., ECML 2019

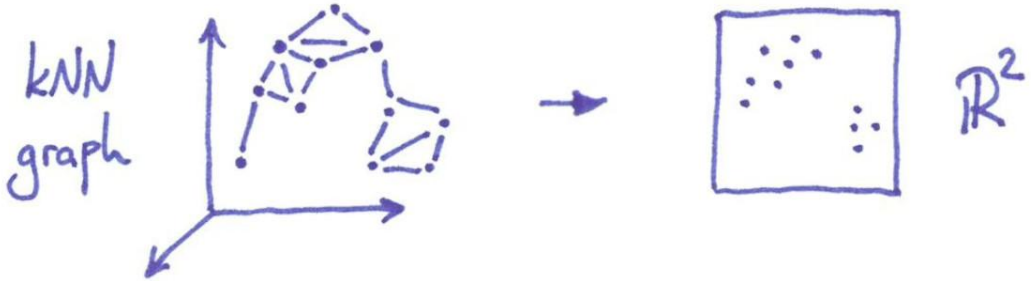
The *t*-distribution kernel: optimizing the α

$$\frac{\partial L}{\partial \alpha} = \sum_{i,j} (p_{i,j} - q_{i,j}) \left(\log \left(1 + \frac{d_{i,j}^2}{\alpha} \right) - \frac{d_{i,j}^2}{\alpha + d_{i,j}^2} \right)$$



Artemii Schlychkov, work in progress

t-SNE



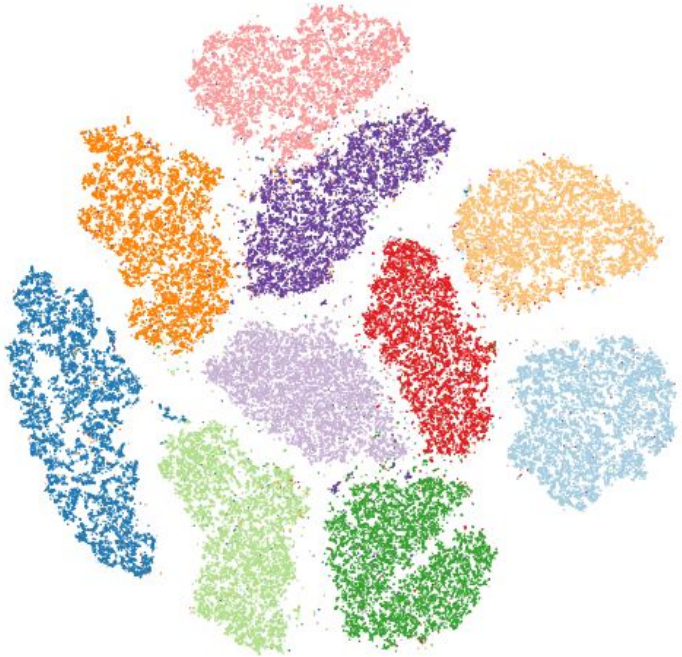
$$\mathcal{L}_{\text{t-SNE}} = \sum_{ij} p_{ij} \log \frac{p_{ij}}{q_{ij}} \sim -\sum_{ij} p_{ij} \log q_{ij} = -\sum_{ij} p_{ij} \log \frac{w_{ij}}{Z} = \underbrace{-\sum_{ij} p_{ij} \log w_{ij}}_{\text{attraction}} + \underbrace{\log \sum_{ij} w_{ij}}_{\text{repulsion}}.$$

p_{ij} can be normalized symmetrized adjacency matrix of the kNN graph.

$$q_{ij} = \frac{w_{ij}}{Z} = \frac{w_{ij}}{\sum w_{ij}} \text{ with } w_{ij} = \frac{1}{1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2}.$$

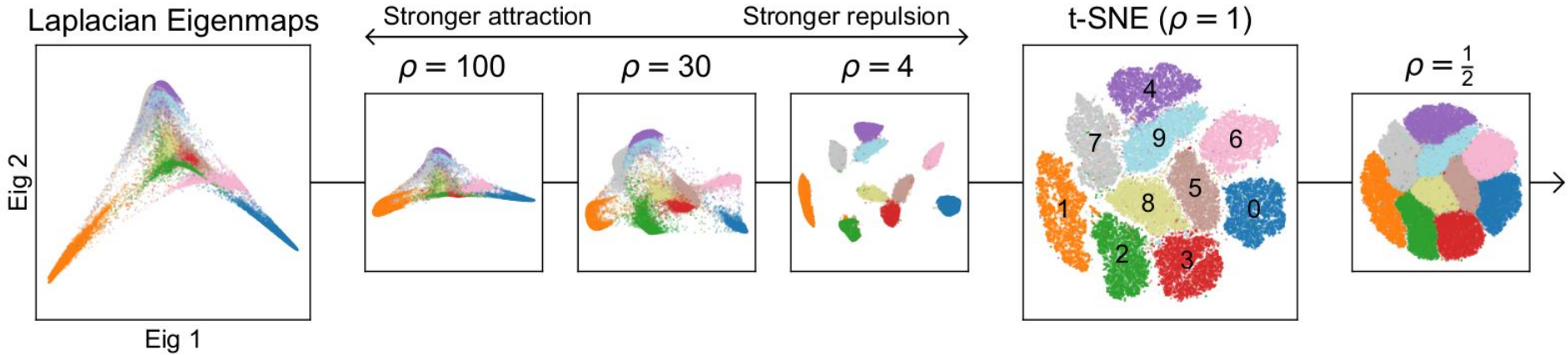
Attraction-repulsion spectrum

Niklas Böhm



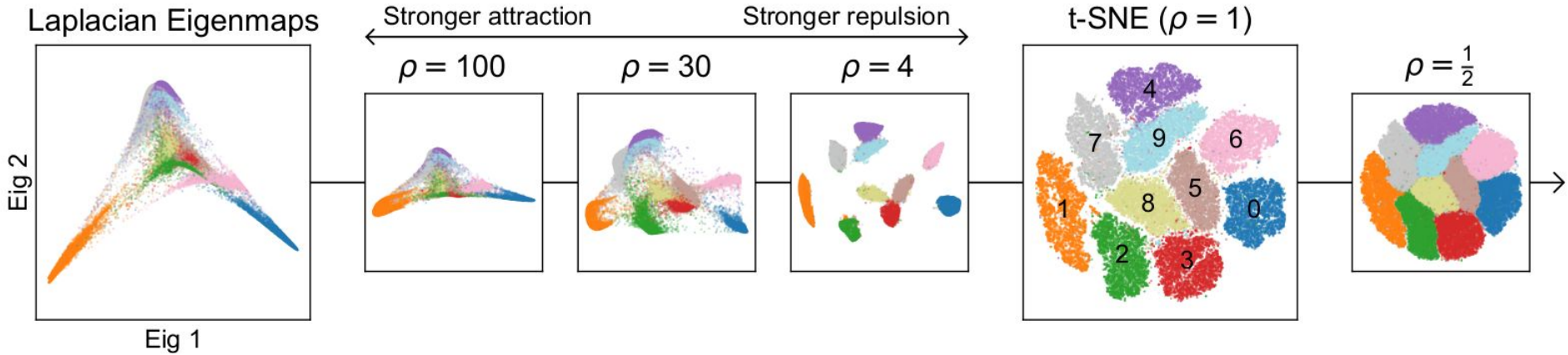
Böhm et al., JMLR 2022

Attraction-repulsion spectrum



Böhm et al., JMLR 2022

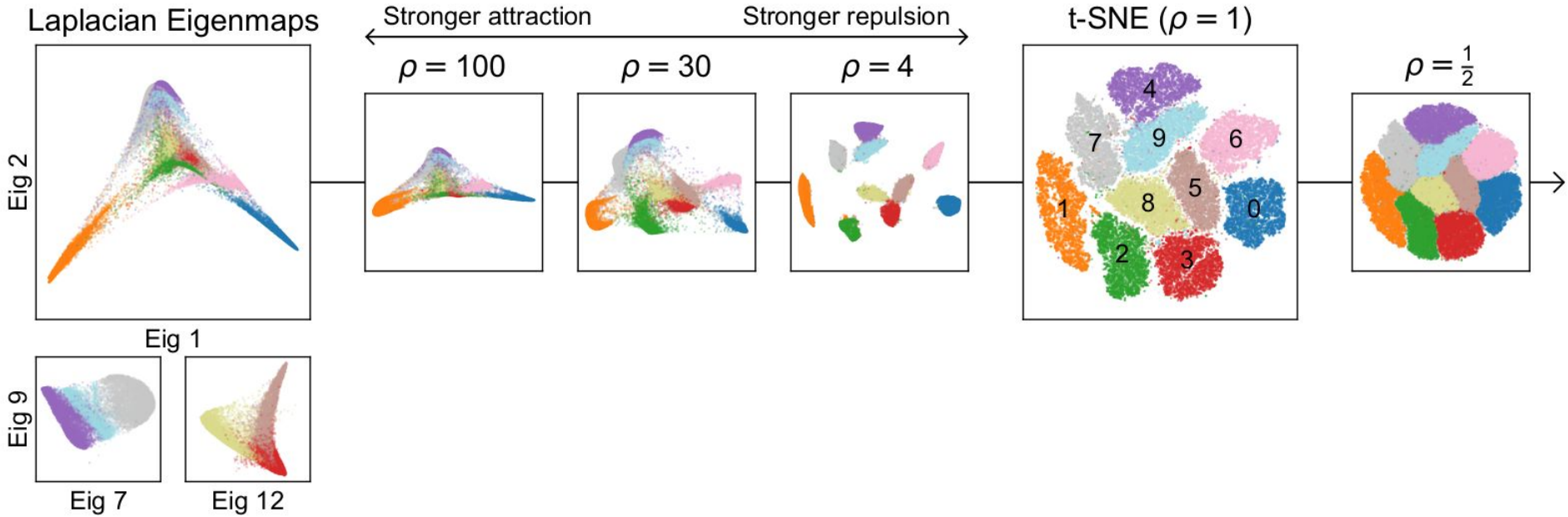
Attraction-repulsion spectrum



For very strong exaggeration, t-SNE approximates Laplacian Eigenmaps of the affinity matrix *(Linderman & Steinerberger, 2020).*

Böhm et al., JMLR 2022

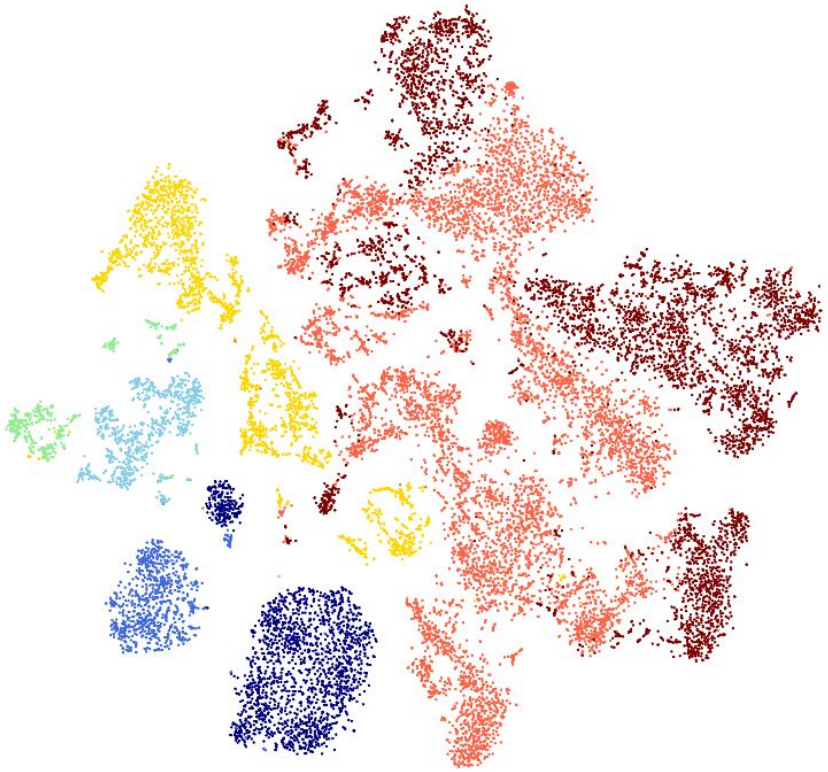
Attraction-repulsion spectrum



The ‘data-agnostic’ repulsion term brings our information from higher Laplacian eigenvectors.

Attraction-repulsion spectrum

Niklas Böhm

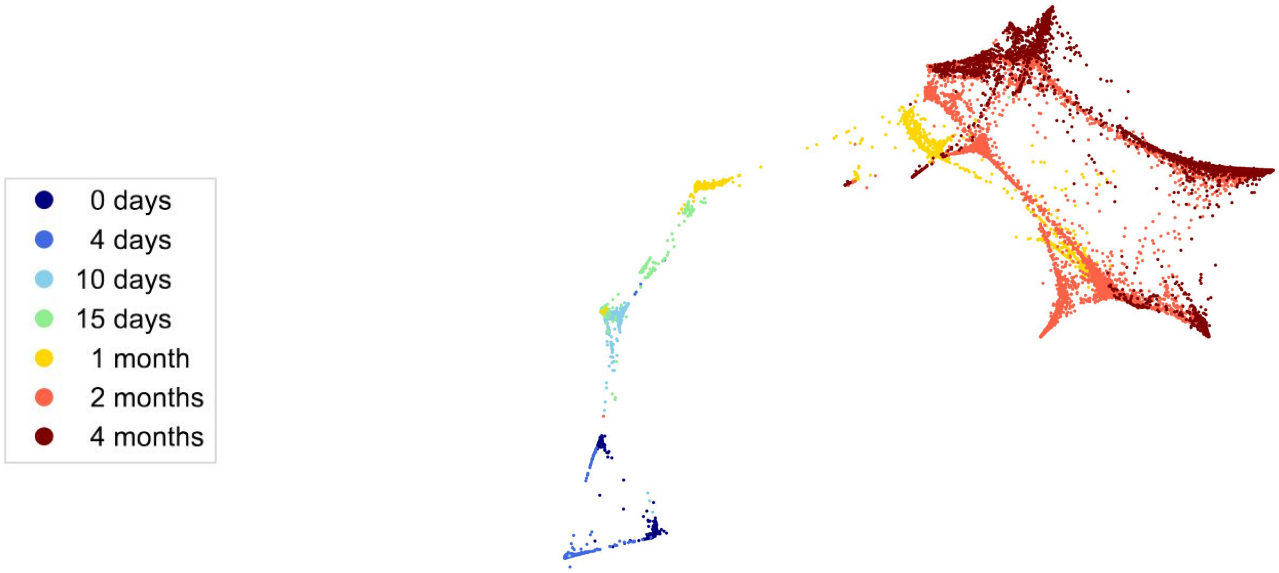


Brain organoid scRNA-seq data
from *Kanton et al., Nature 2019*

Böhm et al., JMLR 2022

Attraction-repulsion spectrum

Niklas Böhm



Brain organoid scRNA-seq data
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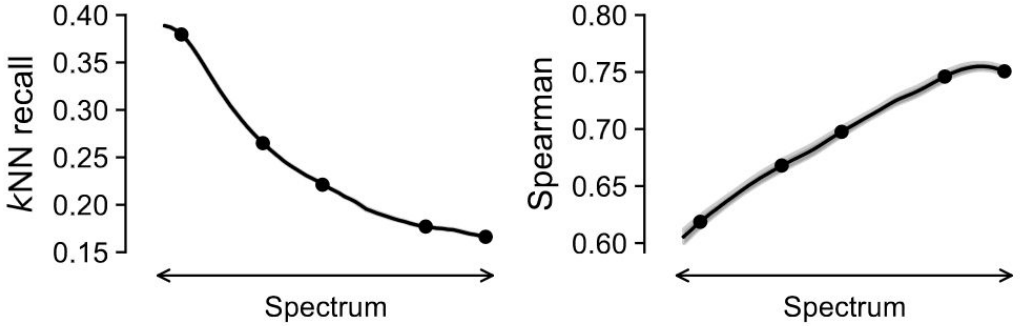
Böhm et al., JMLR 2022

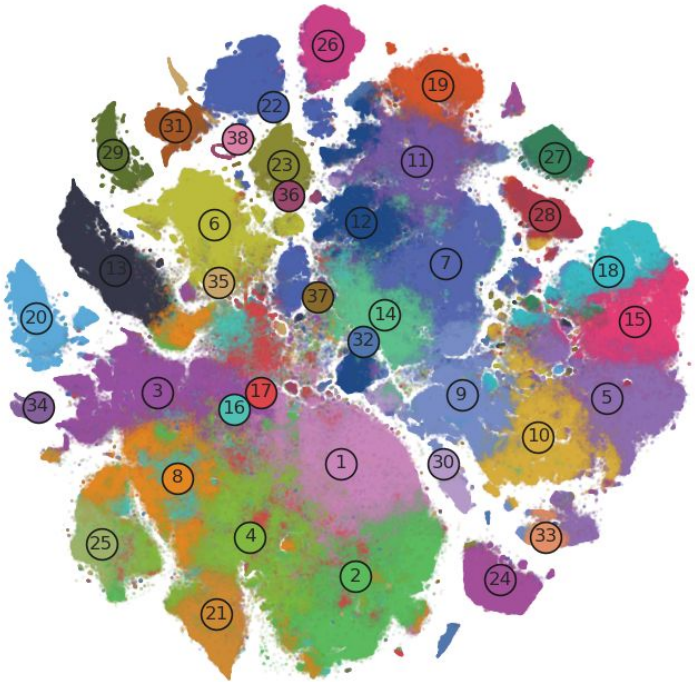
Local-global trade-off

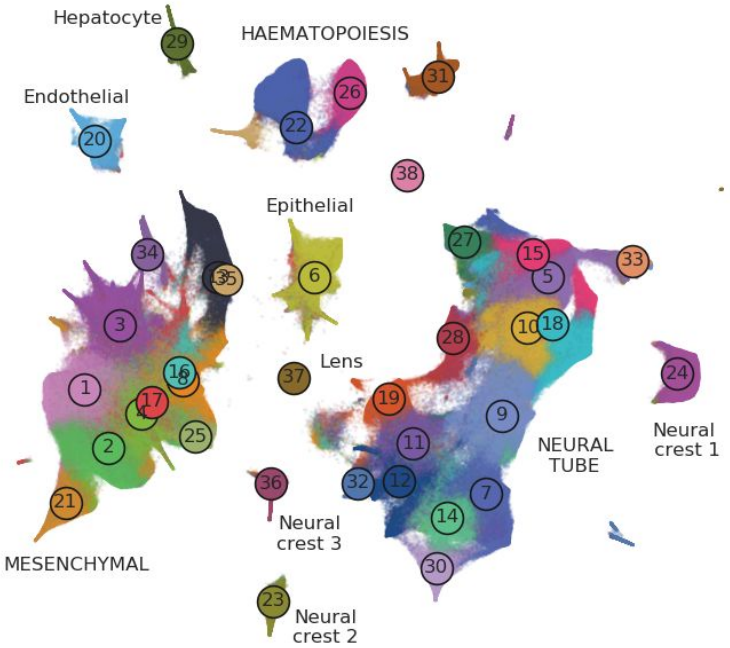
Sebastian Damrich



Damrich et al., bioRxiv 2023

Local-global trade-off (n = 2 mln)



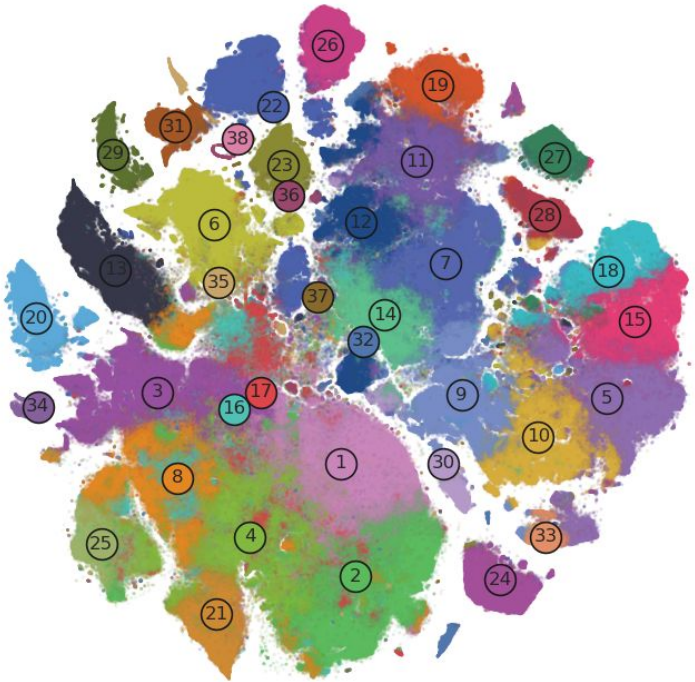


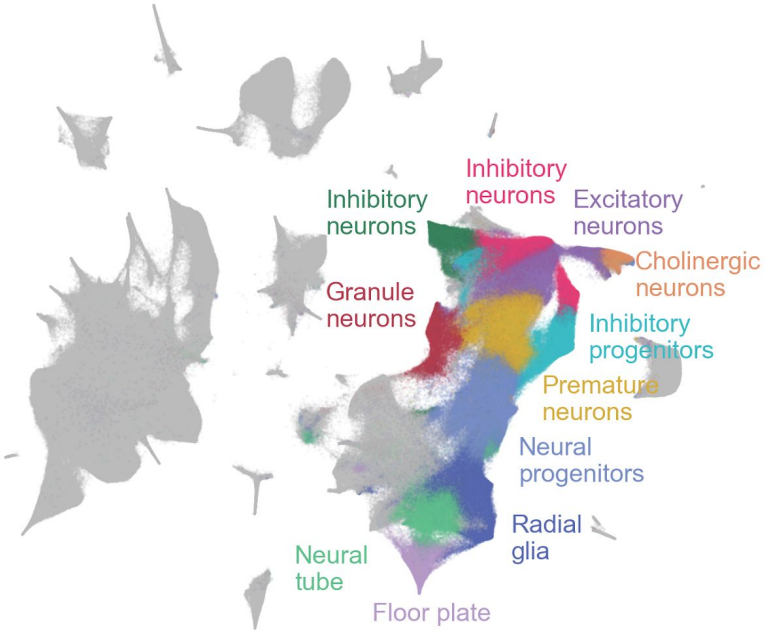
Data from

Cao et al., Nature 2019

Kobak & Berens, Nature Comms 2019

Local-global trade-off (n = 2 mln)





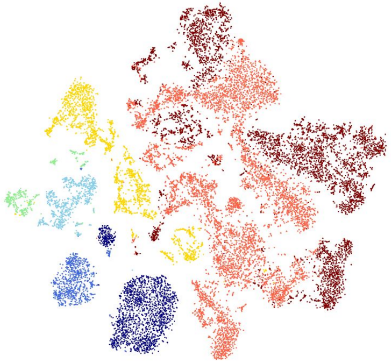
Data from

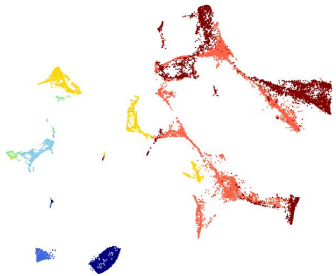
Cao et al., Nature 2019

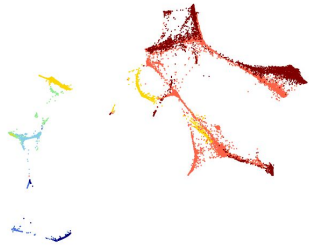
Kobak & Berens, Nature Comms 2019

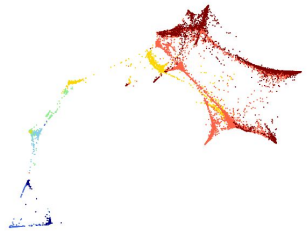
UMAP is equivalent to *t*-SNE with increased attraction

Sebastian Damrich







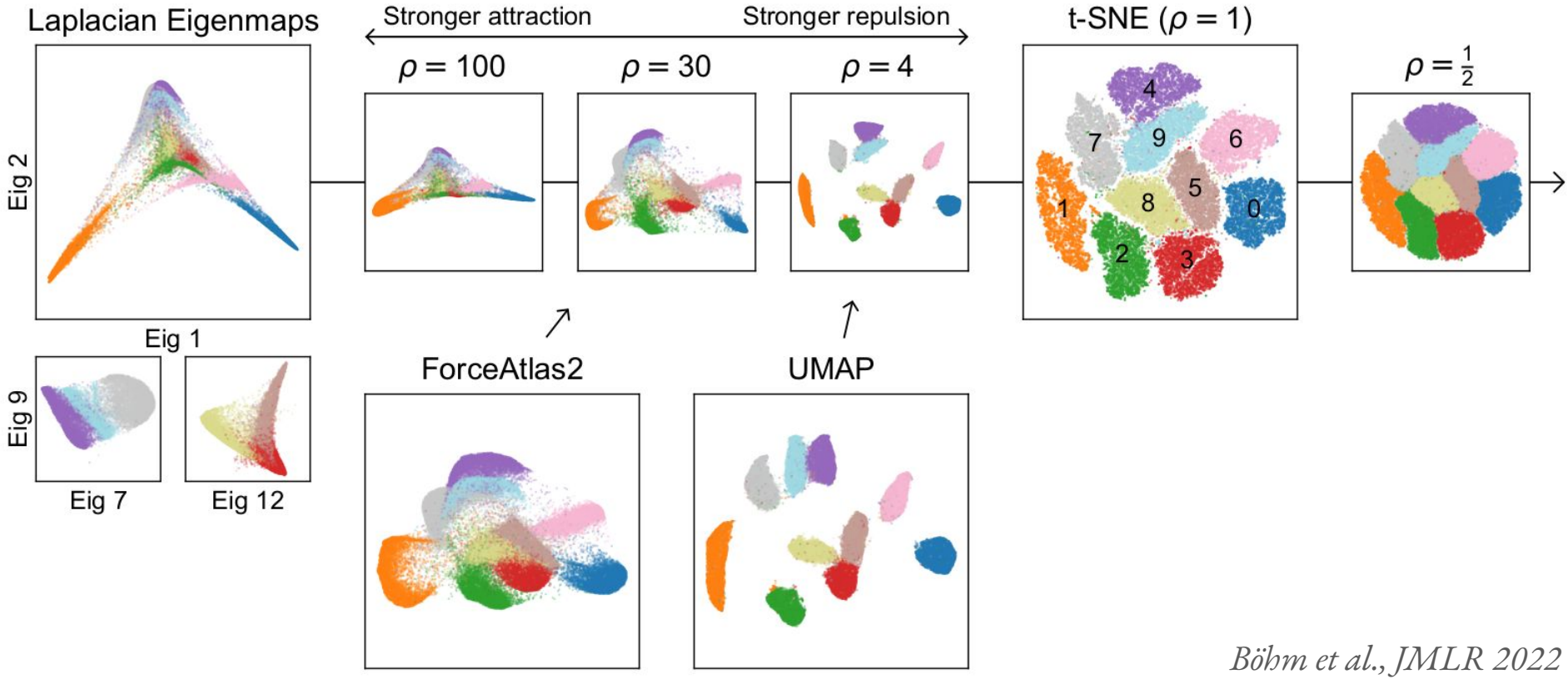


UMAP

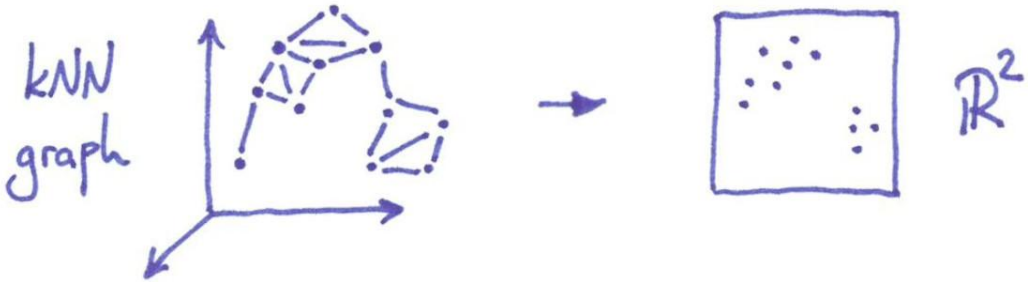
ForceAtlas2

Damrich et al., ICLR 2023

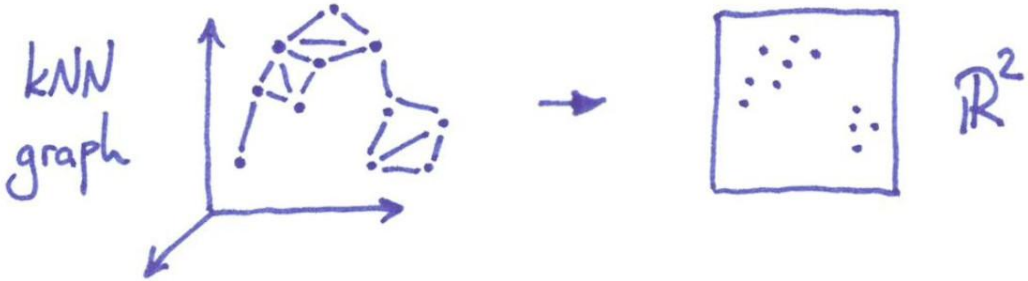
Other neighbour embedding algorithms



Böhm et al., JMLR 2022



1. What if my graph is not a *k*NN graph?
2. What if I want higher embedding dimensionality?



1. What if my graph is not a *k*NN graph?
2. What if I want higher embedding dimensionality?

$$-\sum_{ij} p_{ij} \log \frac{w_{ij}}{Z} \qquad -\sum_{ij} p_{ij} \log \left(\frac{w_{ij}}{w_{ij} + \sum_{k \in \mathcal{I}_m} w_{ik}} \right)$$

Sebastian Damrich

Damrich et al., ICLR 2023

InfoNC-t-SNE: sampling-based approximation

Can be optimized by SGD in batches for any output dimensionality.

$$\mathcal{L}_{\text{InfoNCE}} = -\sum_{ij} p_{ij} \log \left(\frac{w_{ij}}{w_{ij} + \sum_{k \in \mathcal{I}_m} w_{ik}} \right).$$

Damrich et al., ICLR 2023

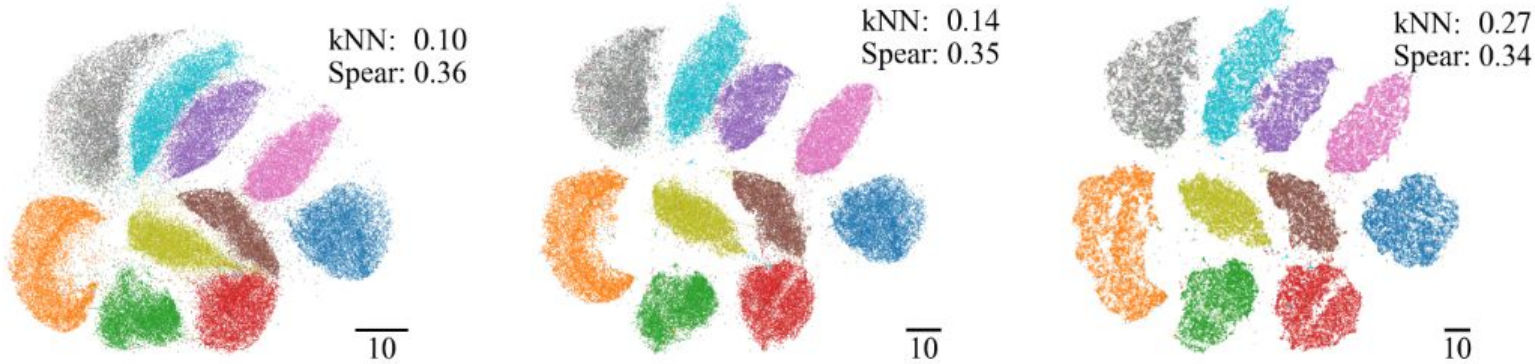
InfoNC-t-SNE

$$\mathcal{L}_{\text{InfoNCE}} = -\sum_{ij} p_{ij} \log \left(\frac{w_{ij}}{w_{ij} + \sum_{k \in \mathcal{I}_m} w_{ik}} \right).$$

Damrich et al., ICLR 2023

InfoNC-t-SNE

$$\mathcal{L}_{\text{InfoNCE}} = -\sum_{ij} p_{ij} \log \left(\frac{w_{ij}}{w_{ij} + \sum_{k \in \mathcal{I}_m} w_{ik}} \right).$$



(i) $m = 5$ (j) $m = 50$ (k) $m = 500$

Damrich et al., ICLR 2023

Parametric InfoNC-t-SNE

$$\mathcal{L}_{\text{InfoNCE}} = -\sum_{ij} p_{ij} \log \left(\frac{w_{ij}}{w_{ij} + \sum_{k \in \mathcal{I}_m} w_{ik}} \right).$$

Can optimize a parametric mapping (e.g. MLP) with the same loss!

(c) InfoNC-t-SNE

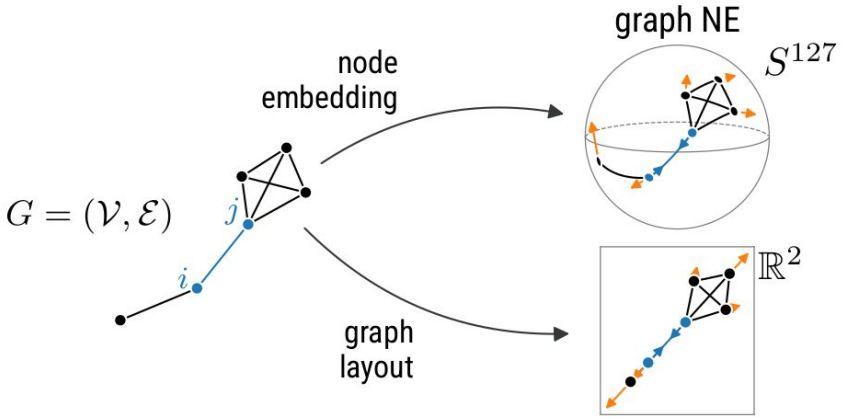
(f) Param. InfoNC-t-SNE

Damrich et al., ICLR 2023

Graph layouts & node embeddings via NE algorithms

Niklas Böhm

Marius Keute



InfoNCE

$$\ell_{ij} = -\log \frac{\exp(\mathbf{y}_i^\top \mathbf{y}_j/\tau)}{\sum_k \exp(\mathbf{y}_i^\top \mathbf{y}_k/\tau)}$$

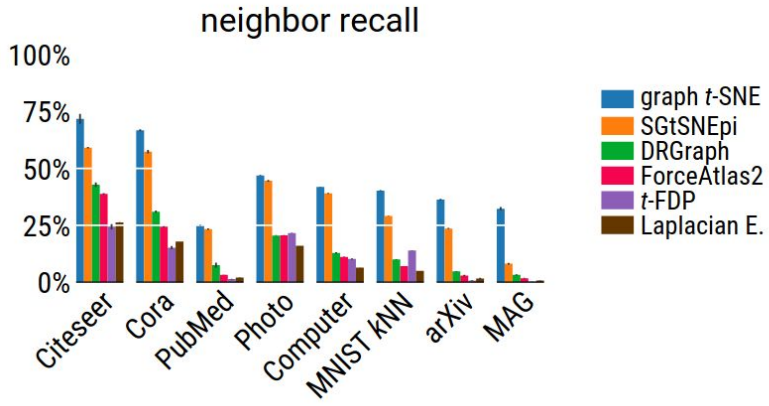
KL divergence

$$\ell_{ij} = -\log \frac{(1+\|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{kl}(1+\|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

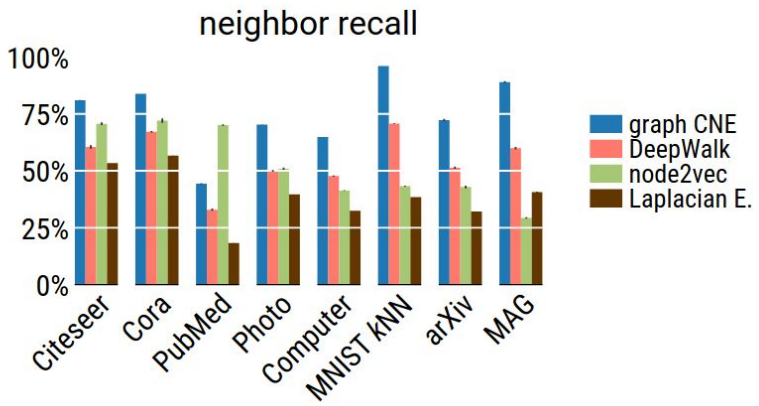
Böhm & Keute et al., TMLR 2025

Graph layouts & node embeddings via NE algorithms

2D embeddings



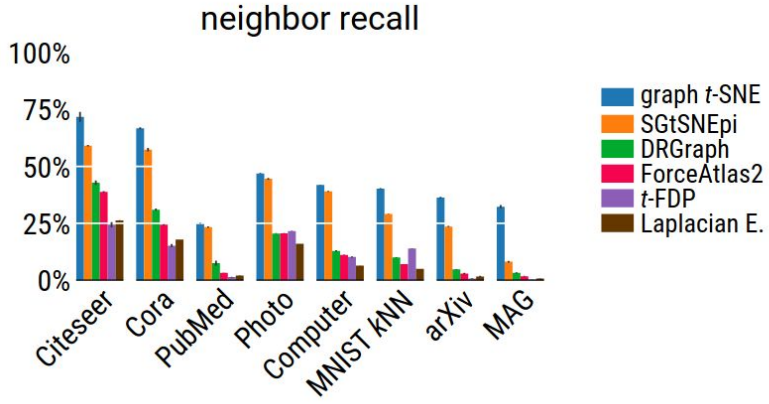
128D embeddings

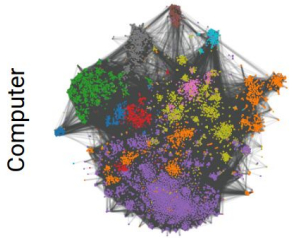


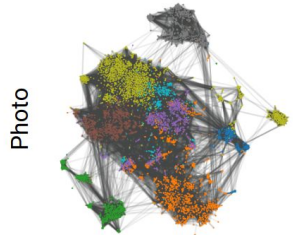
Böhm & Keute et al., TMLR 2025

Graph layouts & node embeddings via NE algorithms

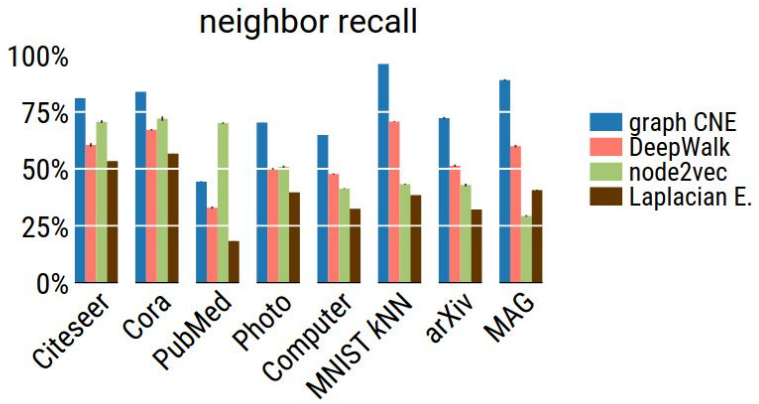
2D embeddings





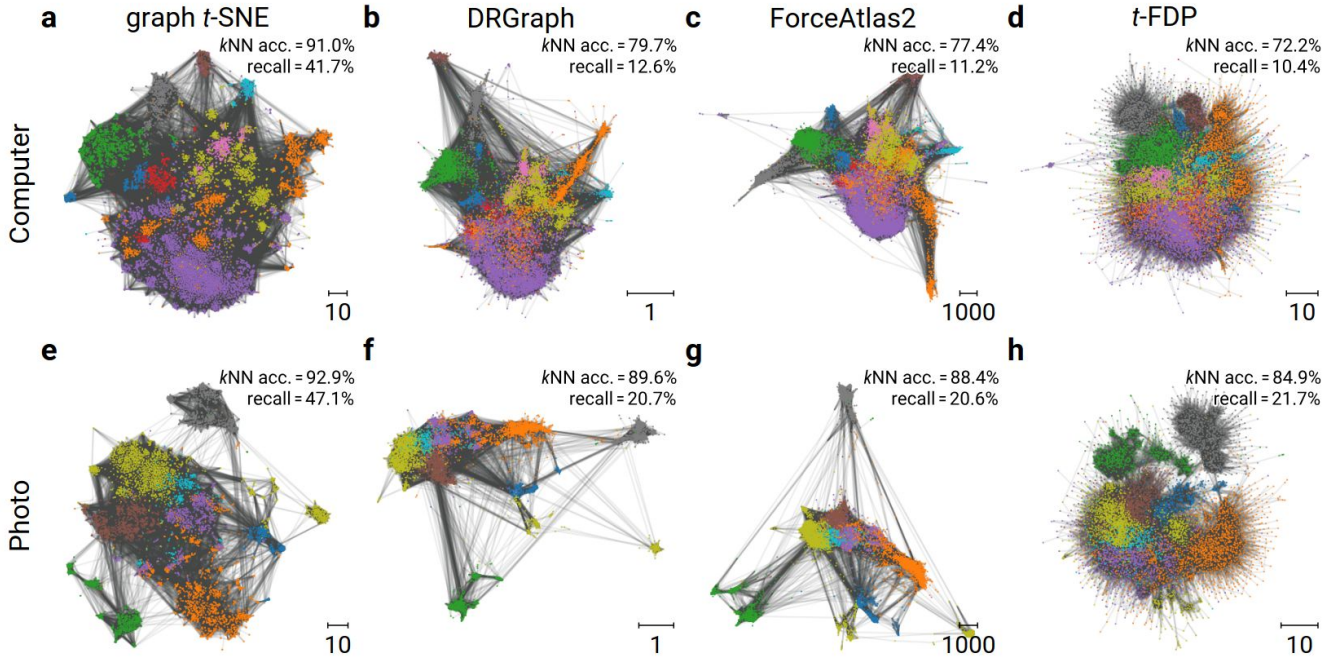


128D embeddings



Böhm & Keute et al., TMLR 2025

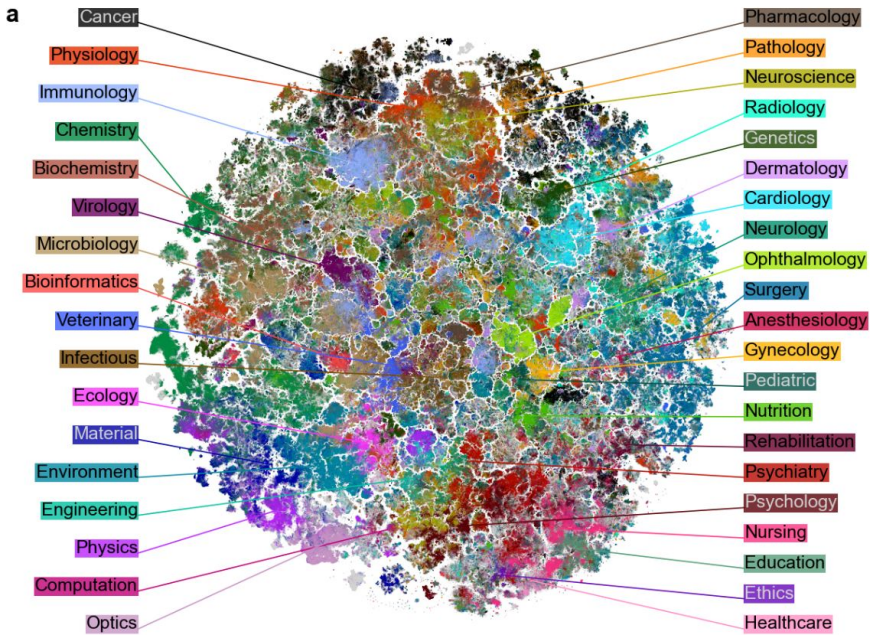
Graph layouts & node embeddings via NE algorithms

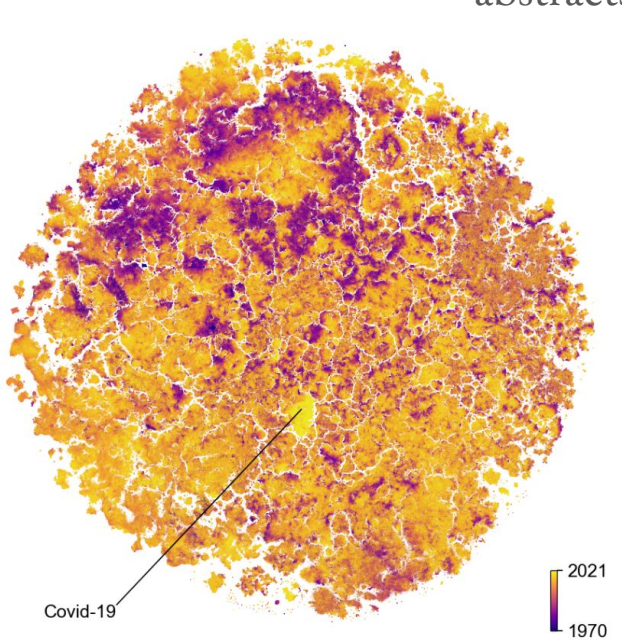


Böhm & Keute et al., TMLR 2025

LLM-based embeddings of text data

All 21 million English abstracts from PubMed



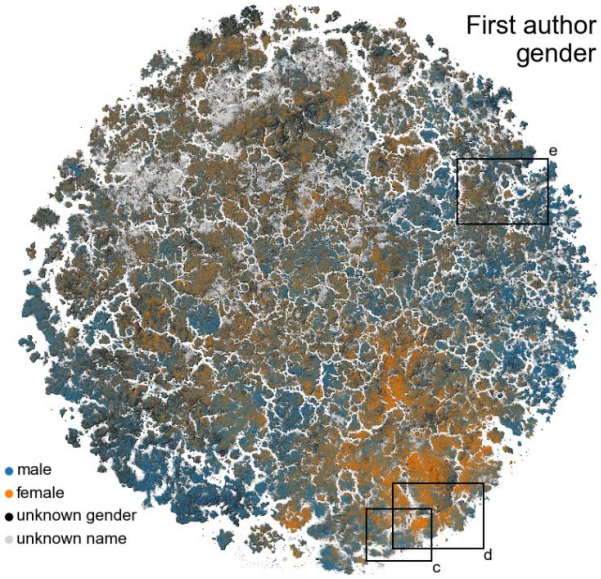


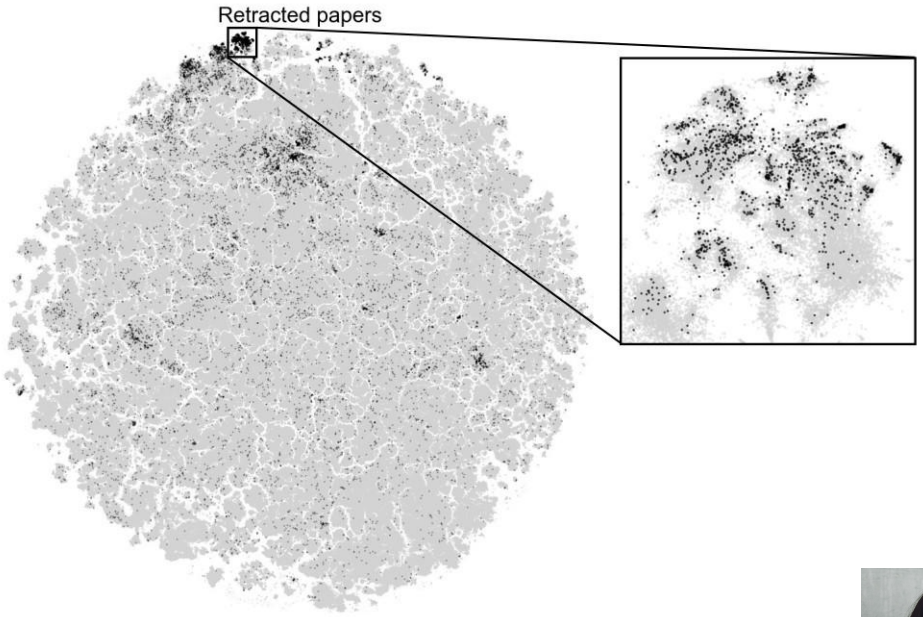
https://static.nomic.ai/pubmed.html

González-Márquez et al., Patterns 2024

Rita González Márquez

LLM-based embeddings of text data

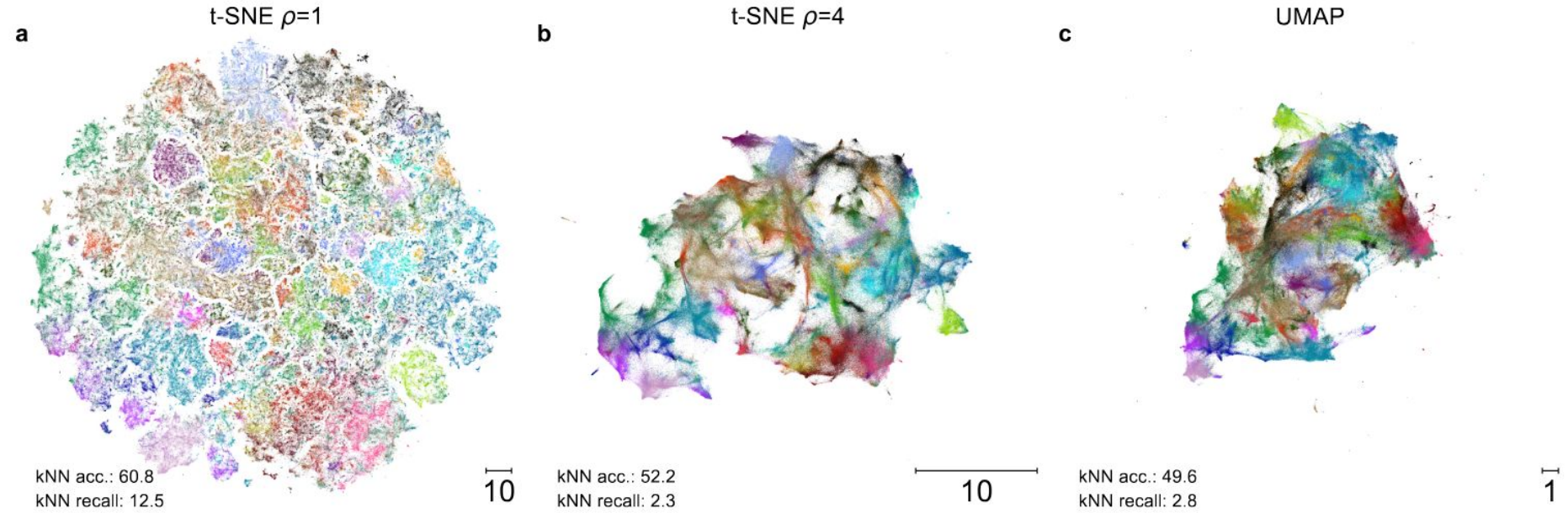




González-Márquez et al., Patterns 2024

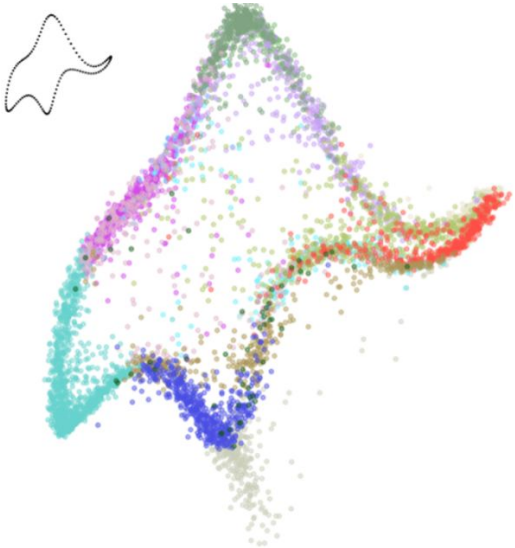
Rita González Márquez

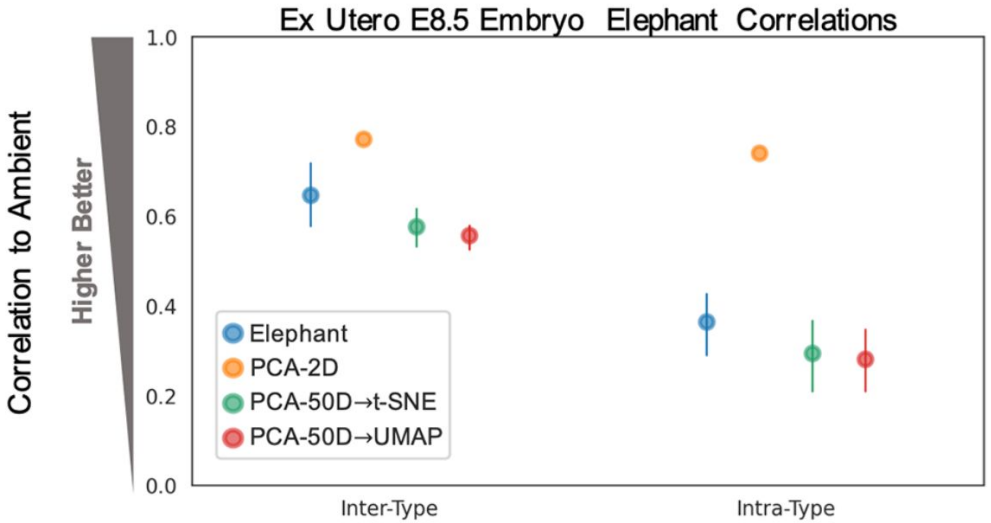
Attraction-repulsion spectrum (*t*-SNE/UMAP) for PubMed



Embeddings of a subset of the PubMed dataset using different neighbor embedding methods. Subset size: 1,000,000 labeled papers.

“All embeddings are wrong …”

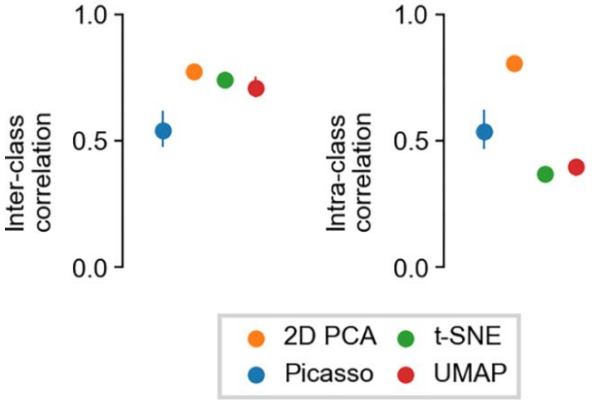




Chari & Pachter, PLoS Comp Bio 2023

“... but some are useful”

Jan Lause



Lause et al., PLoS Comp Bio 2024

“... but some are useful”

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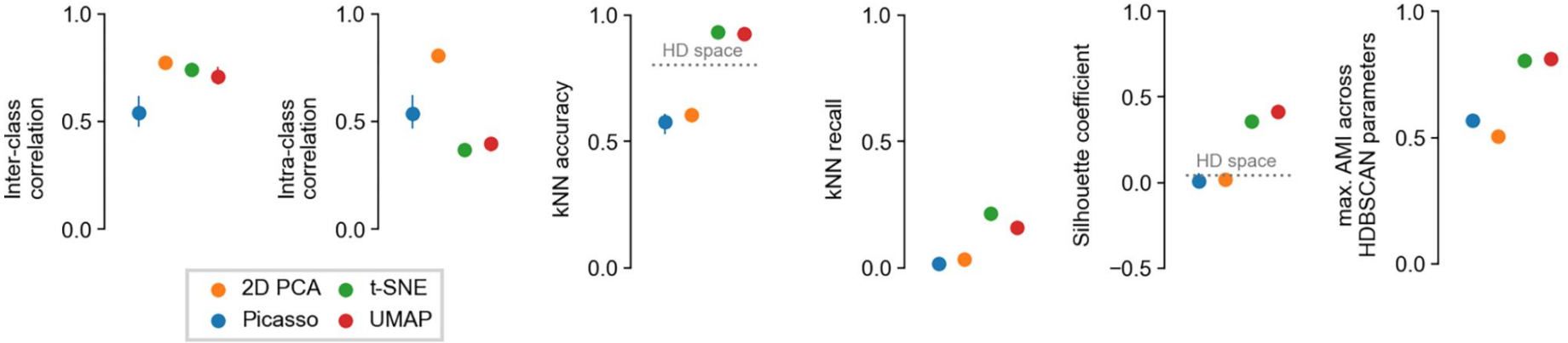

Lause et al., PLoS Comp Bio 2024