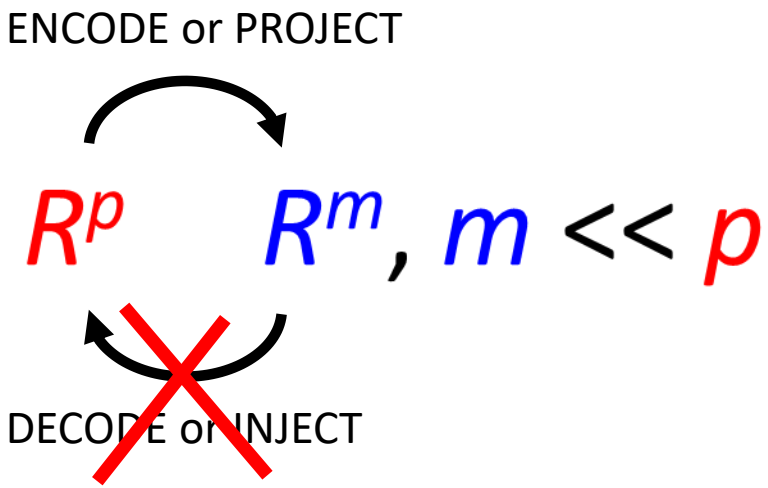
Two killer applications in manifold learning/dimred

- t-distributed stochastic neighbor embedding (t-SNE)
- Uniform manifold approximation and projection (UMAP)

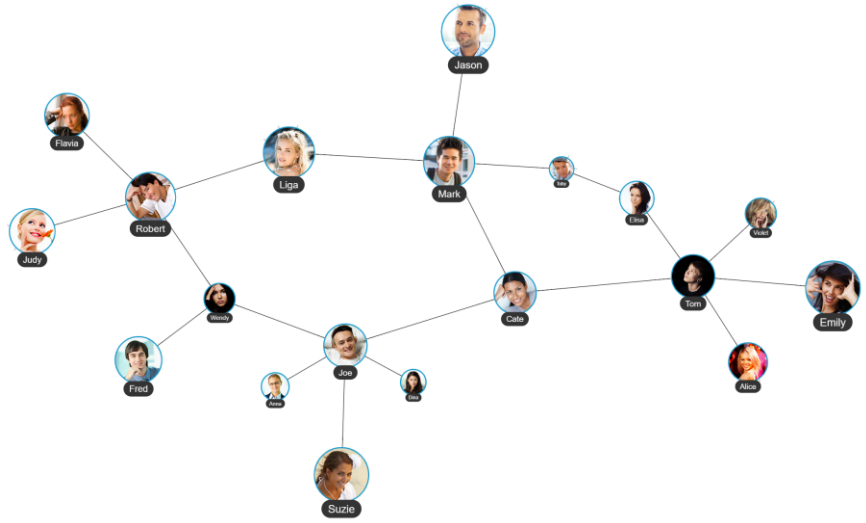
t-SNE and UMAP are projective methods



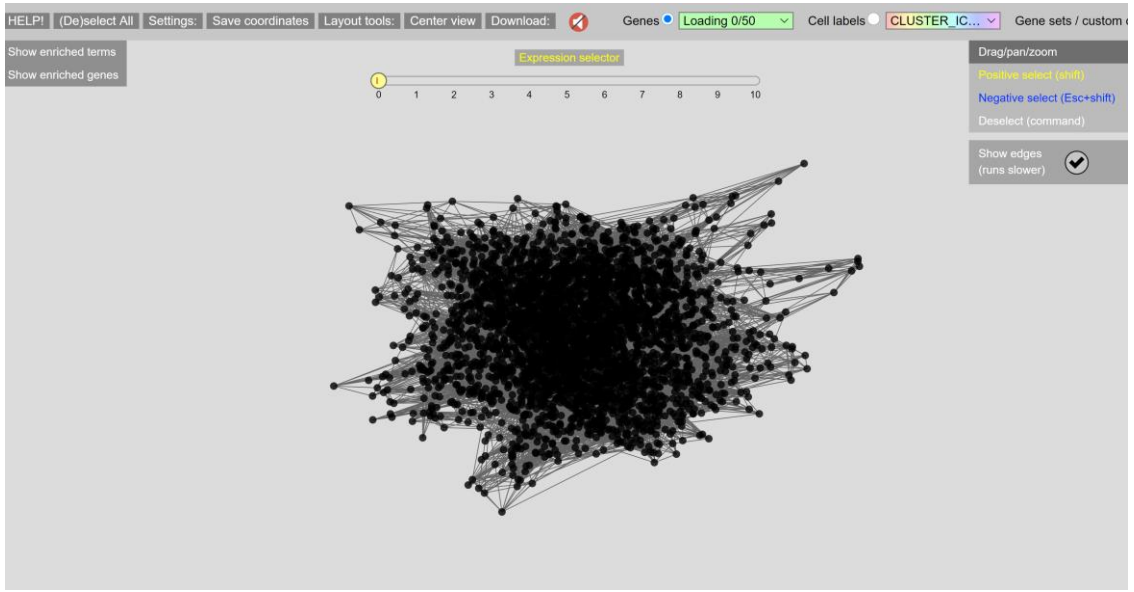
Variant 2: The projector is know only for $\boldsymbol{y} \in \boldsymbol{X}$

Using graph layouts to reduce data dimensionality

- Simple algorithm:
  - Compute the KNN-graph
  - Apply graph drawing (layouting) algorithm to visualize it in 2D (3D)
  - Force-directed layout (e.g., Fruchterman–Reingold's algorithm)



https://demo.zoomcharts.com/net-chart/examples/layout/layout-forced.html



https://www.ihes.fr/~zinovyev/mosaic/SPRING/springViewer.html?datasets/CHLA9_nufp

Problems with drawing knn-graphs

- In many situations, it is already a usefull solution for visualizing the data, but…

- The structure of knn graph heavily depends on the local density
- Point crowding
- The graph is very ‘rigid’

- Solutions:
  - Makes the structure of the neighbourhood graph more adapted to the density variations
  - Introduce a ‘softer’ probabilistic model in constructing the neighborhood graph – instead of a ‘hard’ connection a probability of being connected

- Two methods have become famous for this in recent years: t-SNE and UMAP

Stochastic neighbor embedding (SNE and t-SNE)

t-SNE uses the Kullback-Leibler (KL) divergence

- **Reminder:**

$$D_{\mathrm{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$

- KL measures ‘distance’ from distribution P to Q
- Not a metric function - not symmetric!
- Measures how much more information is contained in P with respect to Q

t-distributed stochastic neighbor embedding (t-SNE)

- SNE by Sam Roweis and Geoffrey Hinton in 2002
- Laurens van der Maaten proposed the t-distributed variant (t-SNE) in 2008

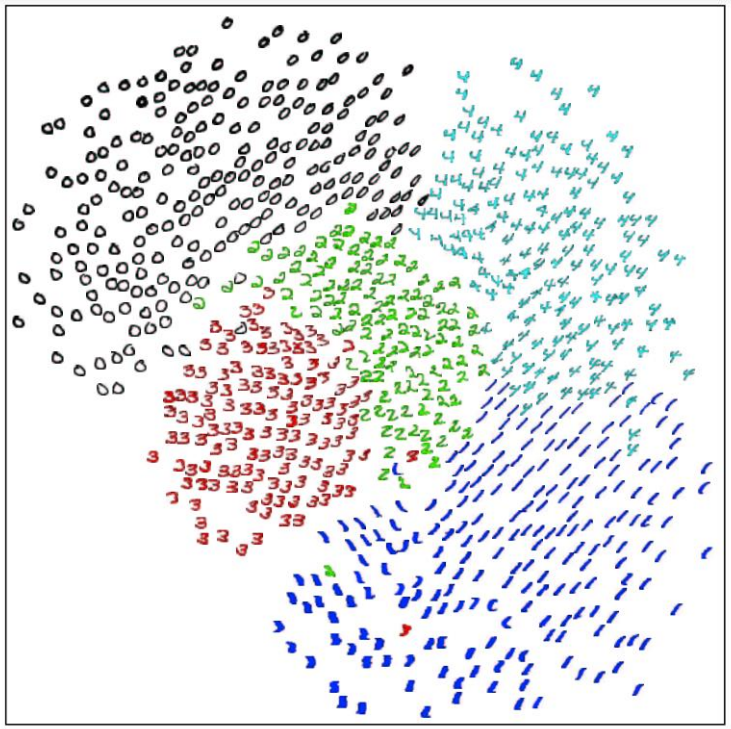
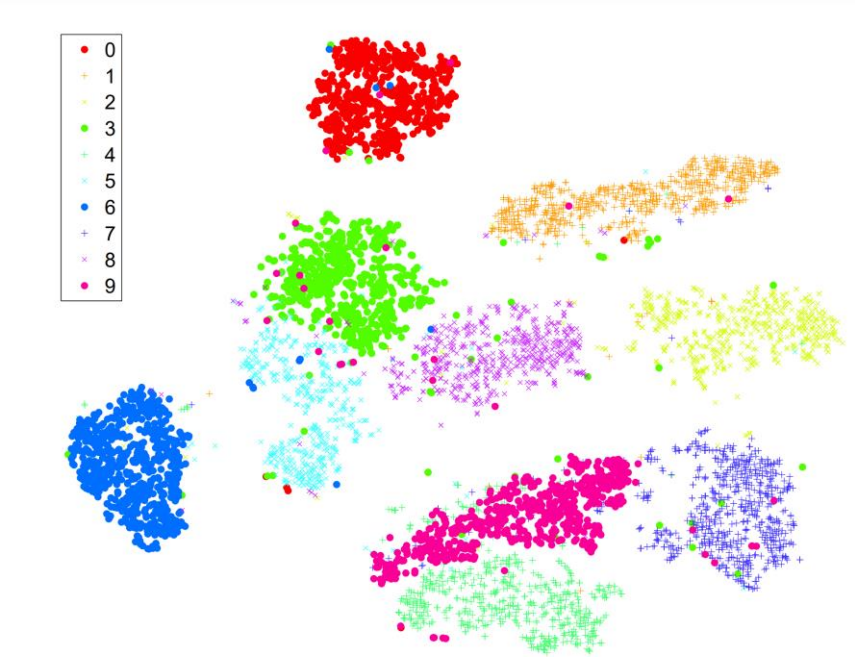


Figure 1: The result of running the SNE algorithm on 3000 256-dimensional grayscale images of handwritten digits. Pictures of the original data vectors $\mathbf{x}_i$ (scans of handwritten digit) are shown at the location corresponding to their low-dimensional images $\mathbf{y}_i$ as found by SNE. The classes are quite well separated even though SNE had no information about class labels. Furthermore, within each class, properties like orientation, skew and stroke-thickness tend to vary smoothly across the space. Not all points are shown: to produce this display, digits are chosen in random order and are only displayed if a 16 x 16 region of the display centered on the 2-D location of the digit in the embedding does not overlap any of the 16 x16 regions for digits that have already been displayed.



(a) Visualization by t-SNE.

Notion of perplexity

- In information theory, perplexity is a measurement of how well a probability distribution or probability model predicts a sample
- It may be used to compare probability models.
- A low perplexity indicates the probability distribution is good at predicting the sample
- The perplexity PP of a discrete probability distribution *p* is defined as

$$PP(p) := 2^{H(p)} = 2^{-\sum_x p(x) \log_2 p(x)}$$

- For Gaussian distribution *PP(p)* = $\frac{1}{2}\ln(\sqrt{2\pi e}\sigma)$

Stochastic neighbor embedding (SNE)

- Conditional probability

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$$

Reminds Kernel Density Estimate of PDF in point *i* , but σ_i depends on *i!* (adaptive KDE)

Conditional probability of that x_i would pick x_j as its neighbor if neighbors were picked in proportion to their probability density under a Gaussian centered at x_i

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N}$$

Stochastic neighbor embedding (SNE)
evaluating σ_i

- Perplexity of distribution PP($p_{j|i}$) must be the same for each *i*

PP($p_{j|i}$) = PP = const

- Perplexity PP is the main parameter of the method
- Large perplexity -> larger σs
- Maximum perplexity is *N* – 1, corresponding to $\sigma = \infty$ (in this case the similarities are distributed uniformly)

Stochastic neighbor embedding (SNE)

R^p $\qquad\qquad$ R^m, $m << p$

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)} \qquad q_{ij} = \frac{\exp(-||\mathbf{y}_i - \mathbf{y}_j||^2)}{\sum_{k\neq i}\exp(-||\mathbf{y}_i - \mathbf{y}_k||^2)}$$

We try to minimize Kullback-Leibler divergence between *p* and *q*

$$C = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}} = \sum_i KL(P_i||Q_i)$$

Expression for the gradient of *C*:

$$\frac{\partial C}{\partial \mathbf{y}_i} = 2\sum_j (\mathbf{y}_i - \mathbf{y}_j)(p_{ij} - q_{ij} + p_{ji} - q_{ji})$$

t-distributed Stochastic neighbor embedding (t-SNE)

R^p $\qquad$ R^m, $m << p$

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)} \qquad q_{ij} = \frac{\left(1+\|y_i - y_j\|^2\right)^{-1}}{\sum_{k\neq l}\left(1+\|y_k - y_l\|^2\right)^{-1}}$$

We try to minimize Kullback-Leibler divergence between *p* and *q*

$$C = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}} = \sum_i KL(P_i||Q_i)$$

Expression for the gradient of *C*:

$$\frac{\delta C}{\delta y_i} = 4\sum_j (p_{ij} - q_{ij})(y_i - y_j)\left(1+\|y_i - y_j\|^2\right)^{-1}.$$

Discussion on t-SNE

- Some remarks:

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$$

- if $||x_i - x_j|| \gg \sigma_i$ then $p_{i|j} \approx 0$

- if $||x_i - x_j|| \ll \sigma_i$ (large perplexity) then

$p_{i|j} \approx 1 - \frac{\left||x_i - x_j|\right|^2}{2\sigma_i^2} / \sum_k (1 - \frac{\left||x_i - x_j|\right|^2}{2\sigma_i^2})$

and t-SNE becomes very close to Multi-Dimensional Scaling (PCA)

Point ‘crowding problem’

- In high dimension we have more room, points can have a lot of different neighbors
- In 2D a point can have a few neighbors at distance one all far from each other
- This is the ”crowding problem” - we don’t have enough room to accommodate all neighbors
- This is a problem with SNE (and other dimensionality reduction methods such as MDS)
- t-SNE solution: change the Gaussian in q to a heavy tailed distribution (Student distribution)

Gradient for SNE

$$\frac{\partial C}{\partial \mathbf{y}_i} = 2\sum_j (\mathbf{y}_i - \mathbf{y}_j)(p_{ij} - q_{ij} + p_{ji} - q_{ji})$$

Gradient for t-SNE – less attractive

$$\frac{\delta C}{\delta y_i} = 4\sum_j (p_{ij} - q_{ij})(y_i - y_j)\left(1 + \|y_i - y_j\|^2\right)^{-1}.$$

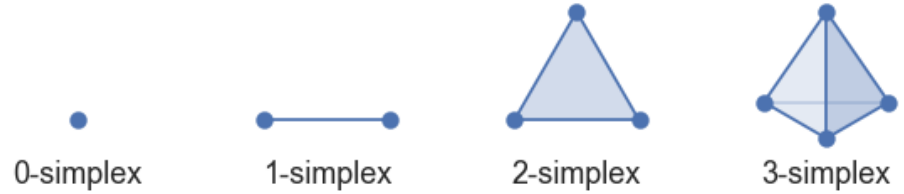
Discussion on t-SNE

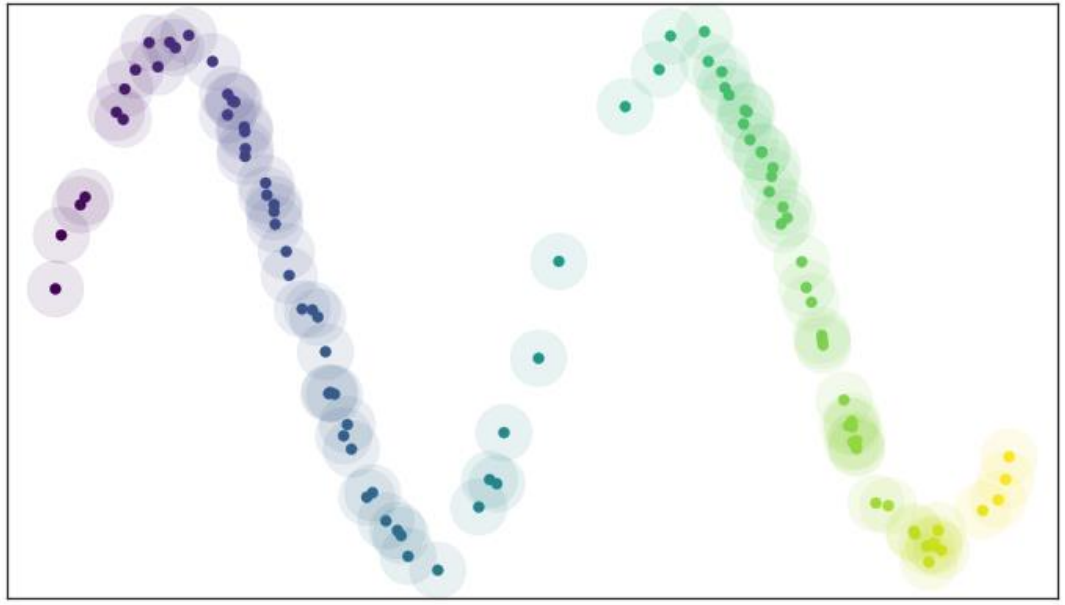
- Low values of perplexity will unveil the local structure in the data, whereas high values of perplexity will enhance the emergence of the global structure at the cost of blurring the local structure
- Short and long distances
- Pro: In linear and non-linear principal manifolds, distant points can become close after projection; in t-SNE it usually does not happen
- Cons: Exaggerated clustering (sometimes)

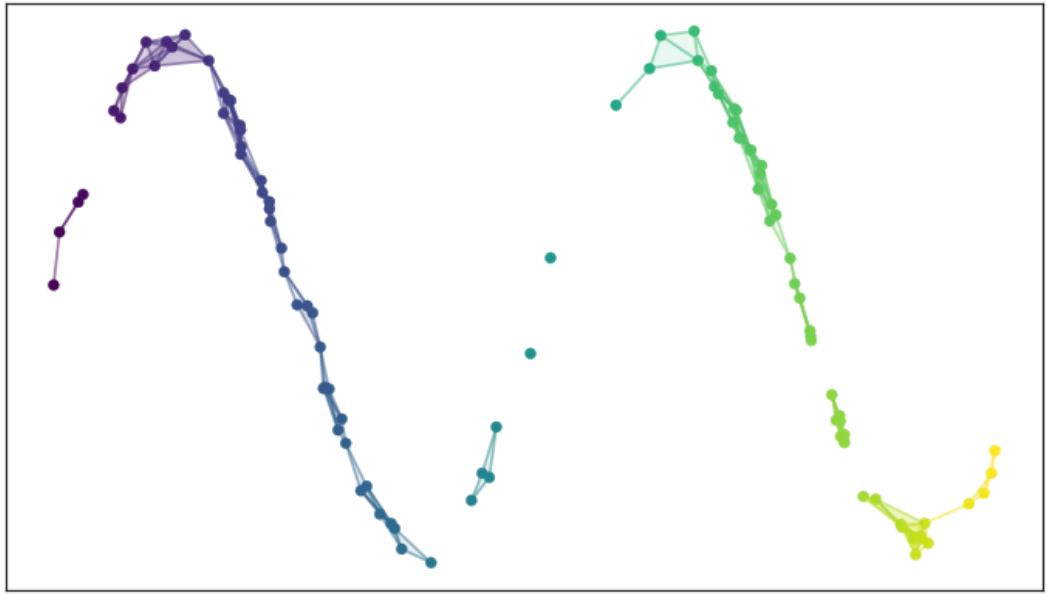
Uniform Manifold Approximation and Projection (UMAP)

Uniform Manifold Approximation and Projection (UMAP)

- Starts with a ‘fuzzy simplicial complex’ (weighted KNN graph, in simple words) but ends with a simple weighted neighbourhood graph







https://umap-learn.readthedocs.io/en/latest/how_umap_works.html

Constructing weighted neighbourhood graph

For each point *i,* define distance to the nearest neighbour

$$\rho_i = \min\{d(x_i, x_{i_j}) \mid 1 \leq j \leq k, d(x_i, x_{i_j}) > 0\},$$

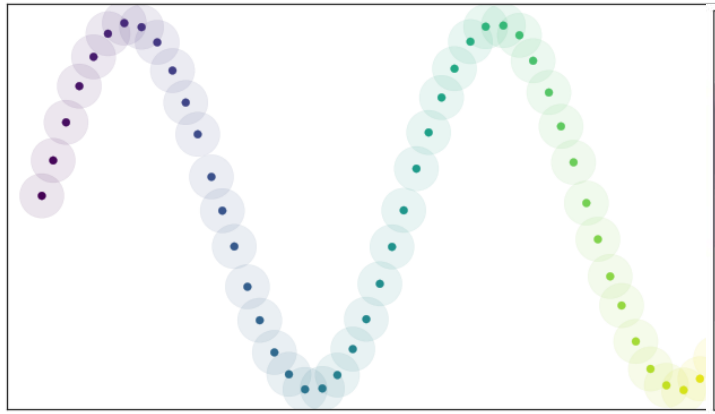
Define σ_i using the following equation (local dispersion)

$$\sum_{j=1}^{k} \exp\left(\frac{-\max(0, d(x_i, x_{i_j}) - \rho_i)}{\sigma_i}\right) = \log_2(k)$$

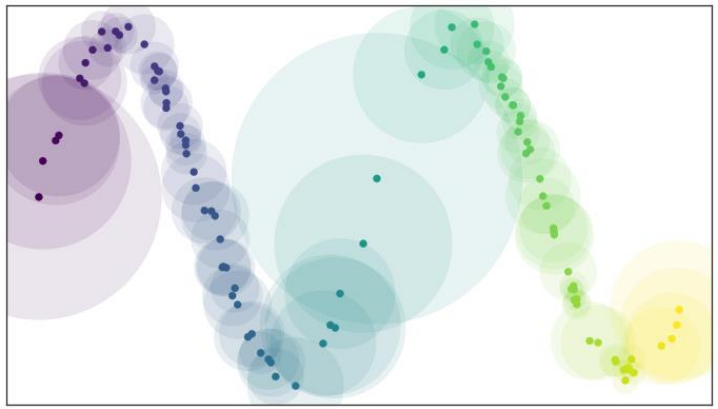
Weight of the neighbourhood graph

$$w((x_i, x_{i_j})) = \exp\left(\frac{-\max(0, d(x_i, x_{i_j}) - \rho_i)}{\sigma_i}\right)$$

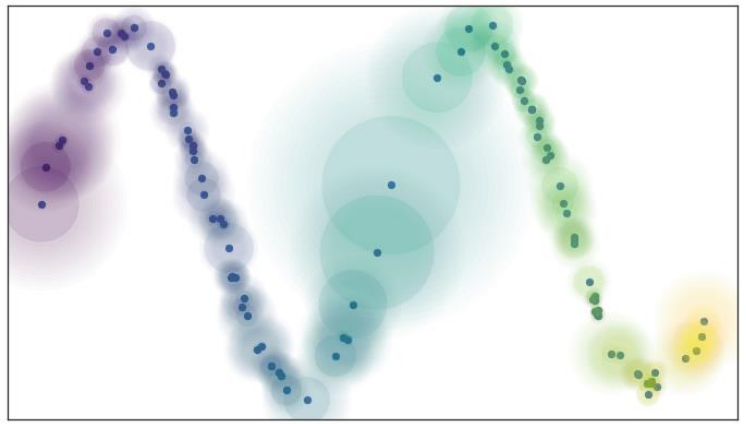
‘Uniform’ case



kNN graph

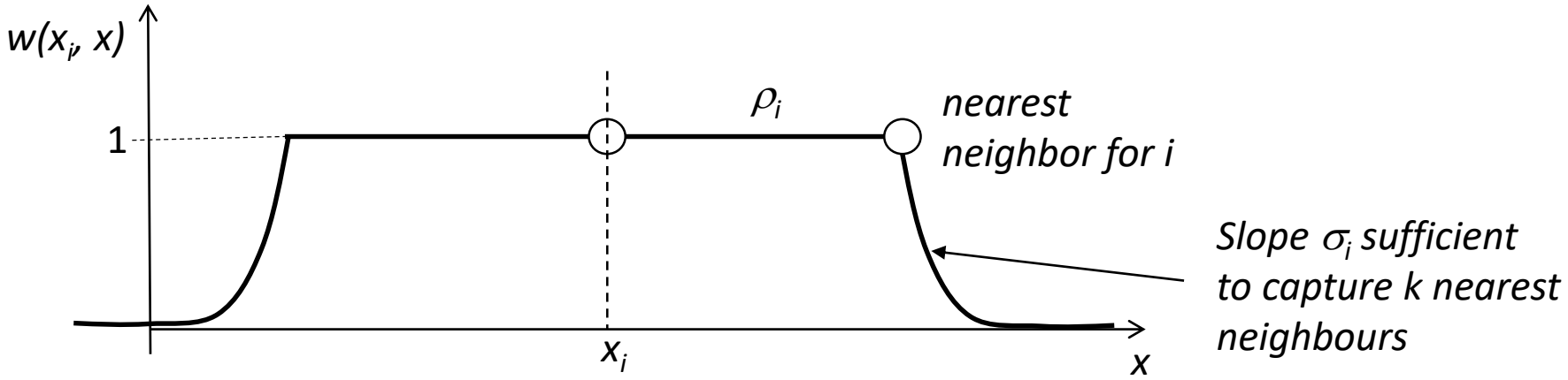


Fuzzy weighted neighbourhood graph (‘UMAP-modified kNN’)

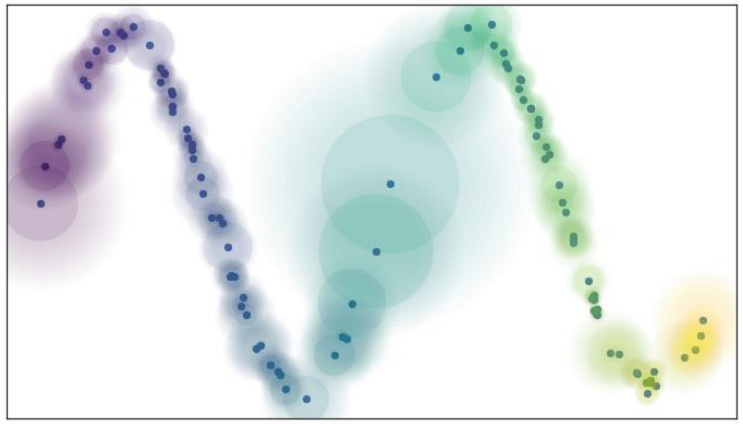


k=4

$$w((x_i, x_{i_j})) = \exp\left(\frac{-\max(0, d(x_i, x_{i_j}) - \rho_i)}{\sigma_i}\right)$$



Fuzzy weighted neighbourhood graph ('UMAP-modified kNN')



Minimizing ‘cross-entropy’

Preservation of small distances

Preservation of large distances

$$\sum_{e \in E} \left[w_h(e) \log \left(\frac{w_h(e)}{w_l(e)} \right) + (1 - w_h(e)) \log \left(\frac{1 - w_h(e)}{1 - w_l(e)} \right) \right]$$

$1 \geq w_h > 0$ – weights in high-dimensional space

$1 \geq w_l > 0$ – weights in low-dimensional space

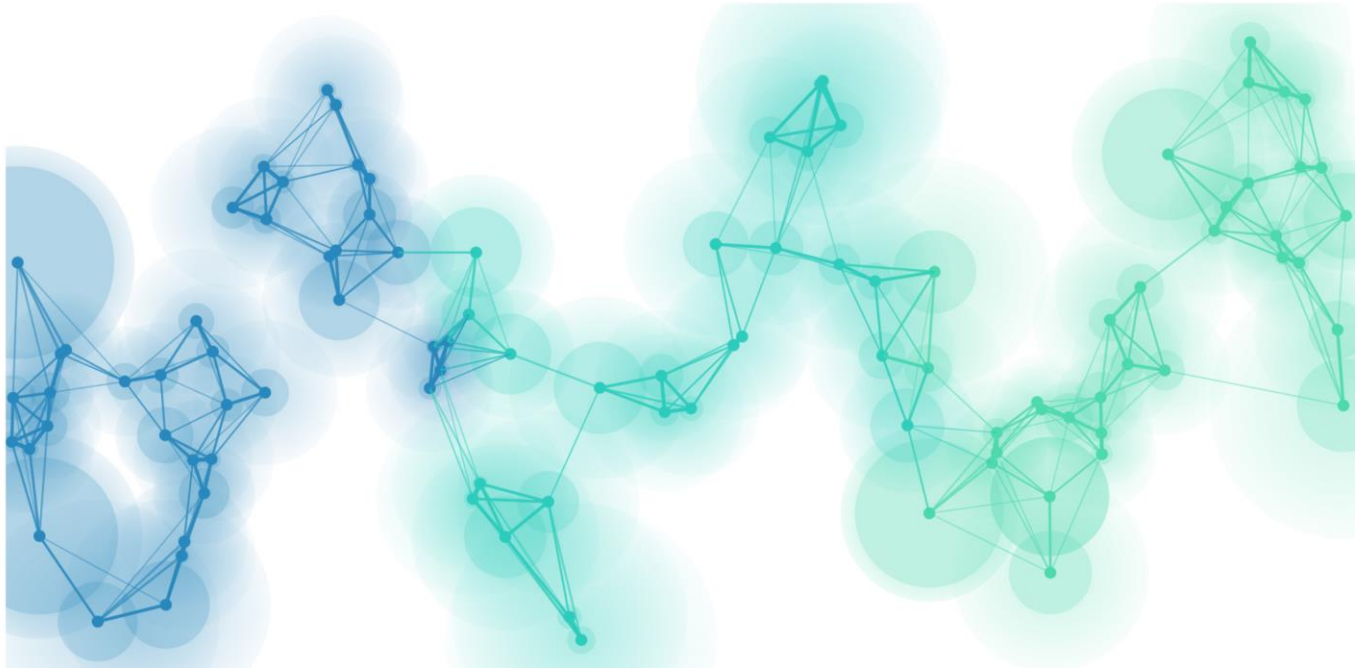
Actual algorithm is very close to force-directed layout algorithm

Hyperparameters of UMAP

- Min-dist:

minimal distance between

points in low-dimensional space

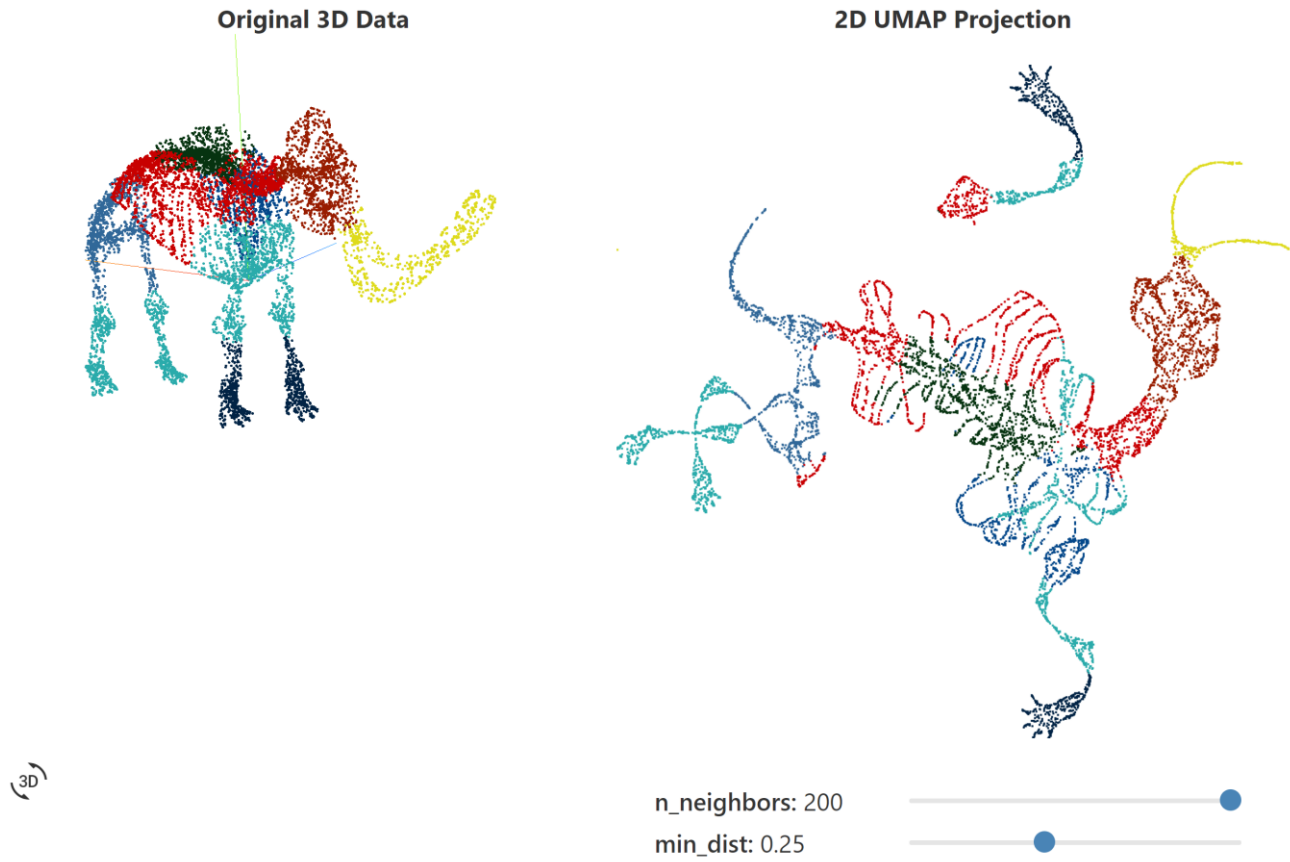


- N_neighbours:

k in the kNN graph

https://pair-code.github.io/understanding-umap/supplement.html

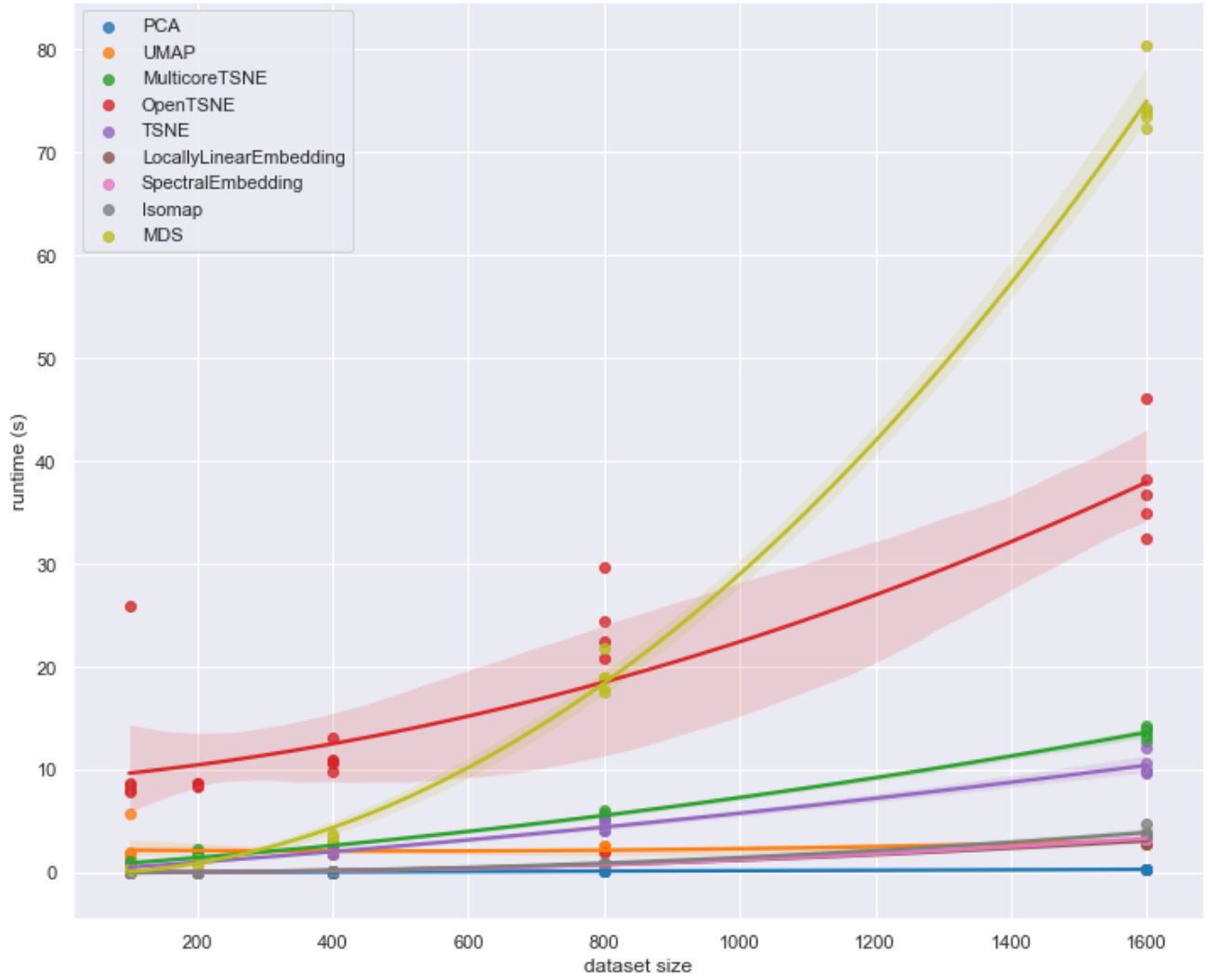
Toy example to play with parameters: *Projecting a mammoth from 3D to 2D*



https://pair-code.github.io/understanding-umap/

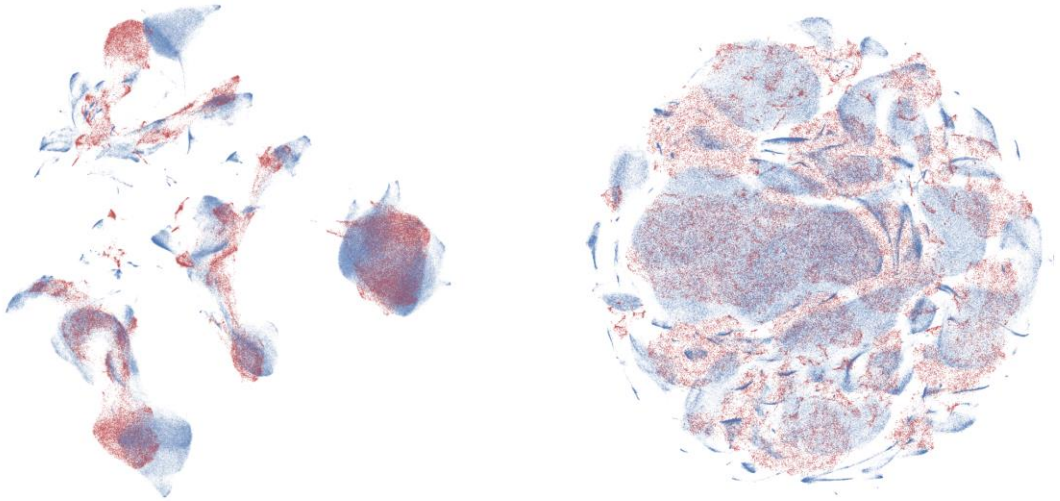
Comparing tSNE and UMAP

- Speed



Comparing tSNE and UMAP

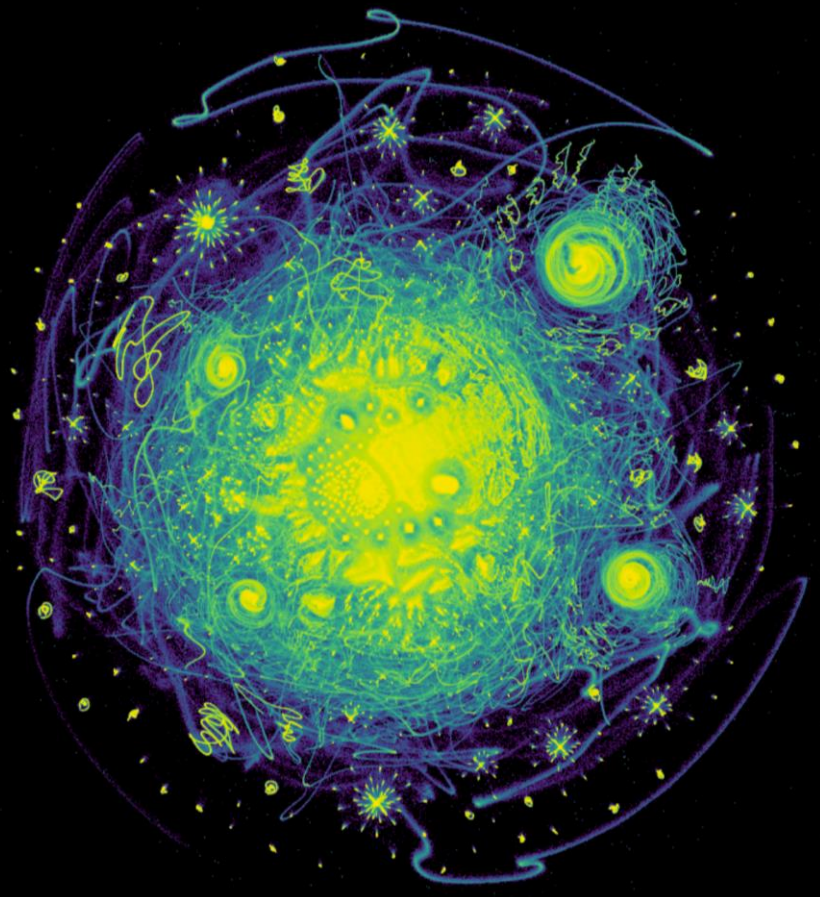
- UMAP better represents the global structure of the dataset
- UMAP is way faster than t-SNE
- UMAP is more stable to subsampling than t-SNE
- UMAP can work directly in very high ambient dimensionalities (>10^6)



(a) UMAP (b) t-SNE

Figure 7: Procrustes based alignment of a 10% subsample (red) against the full dataset (blue) for the flow cytometry dataset for both UMAP and t-SNE.

from https://arxiv.org/pdf/1802.03426.pdf



igure 13: Visualization of 30,000,000 integers as represented by binary vector
f prime divisibility, colored by density of points.

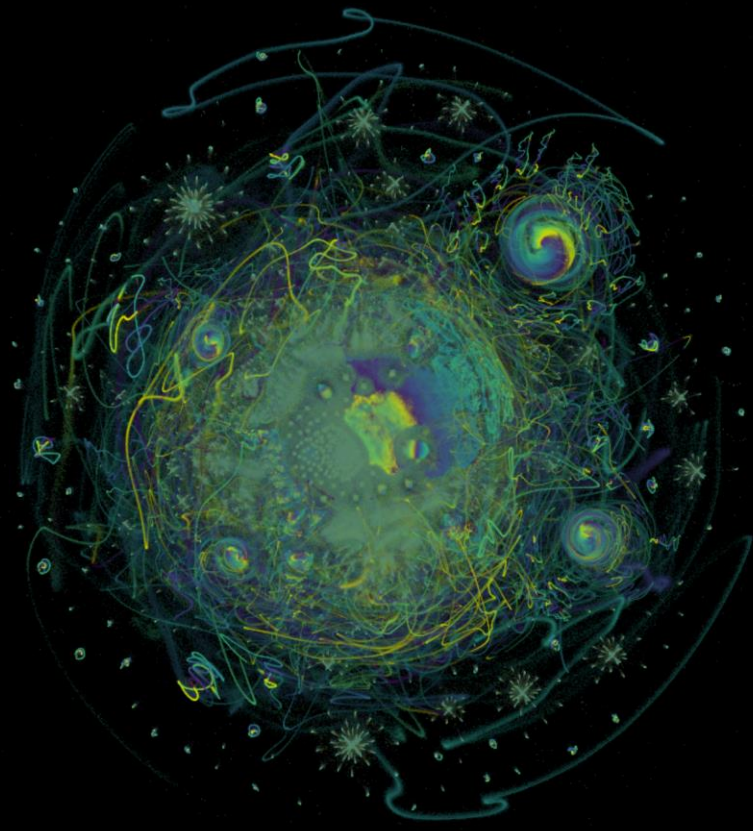


Figure 14: Visualization of 30,000,000 integers as represented by binary vectors of prime divisibility, colored by integer value of the point (larger values are green or yellow, smaller values are blue or purple).

from https://arxiv.org/pdf/1802.03426.pdf

Comments to both t-SNE and UMAP methods

- Hyperparameters really matter
- Cluster sizes in a UMAP plot mean nothing
- Distances between clusters might not mean anything
- Random noise doesn’t always look random
- You may need more than one plot
- For large ‘neighbourhood’ parameters, both methods give results similar to Multi-dimensional scaling
- Both can work with non-Euclidean metrics in R^p