

Reducción de dimensión

Aprendizaje automático



Juan David Martínez

jdmartinev@eafit.edu.co

2023

Agenda

- Reducción de dimensión
- Análisis de componentes principales (PCA)
- Otras formas de reducción de dimensión

Reducción de dimensión

Muchos problemas de **Machine Learning** implican **millones de características** para cada ejemplo (instancia de entrenamiento)

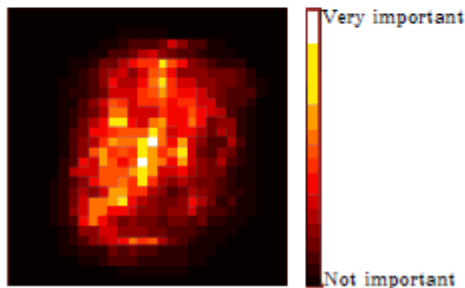
- Extremadamente lento
- Difícil de encontrar una buena solución

Este problema se conoce como la maldición de la dimensionalidad



Reducción de dimensión

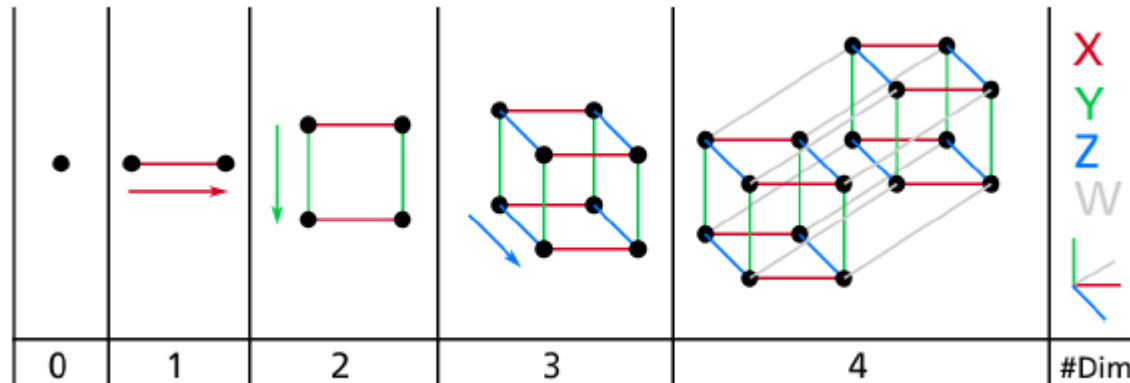
Es posible reducir considerablemente el número de características



- Los píxeles en el borde generalmente son blancos
- Se pueden eliminar sin perder mucha información
- En el proceso de reducción de dimensión **se pierde algo de información**
- Filtra ruidos y detalles innecesarios y puede mejorar el rendimiento
- Acelera el entrenamiento y facilita la visualización

La maldición de la dimensión

Estamos acostumbrados a vivir en **tres dimensiones**, la intuición nos falla cuando intentamos imaginarnos un espacio de alta dimensión

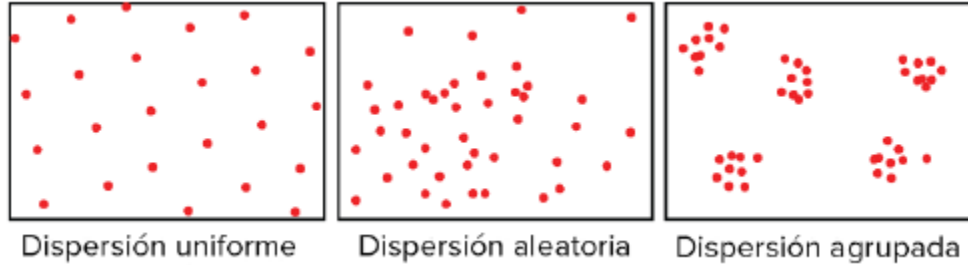


La maldición de la dimensión

- En un cuadrado de lado 1, la distancia entre dos puntos será en promedio 0,52.
- En un cubo de lado 1, la distancia promedio será 0,66
- En un hipercubo de lado 1 de 1 millón de dimensiones, la distancia promedio será de 408,25. Es decir, la mayoría de muestras están muy lejos una de la otra
- ¡Entre más dimensiones, mayor riesgo de sobre-entrenamiento!
- Solución: Aumenta el tamaño de la muestra.
- Problema: El número de muestras requeridas para alcanzar una densidad dada crece exponencialmente con el número de dimensiones.
- Con 100 características, se necesitarían más instancias que átomos en el universo
- Solución: Reducir el número de características

Enfoques principales: Proyección

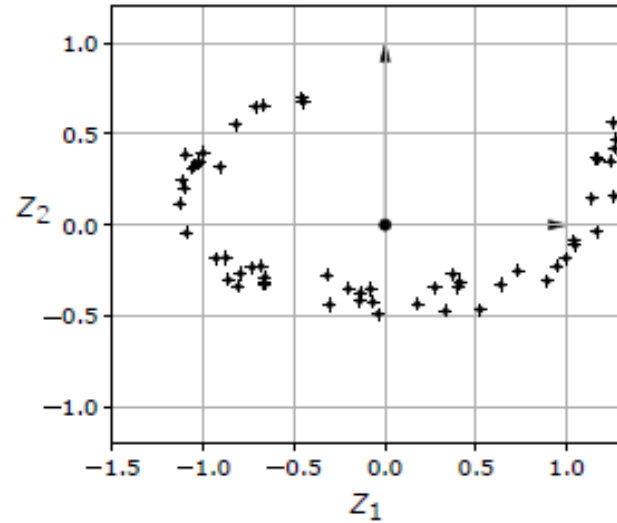
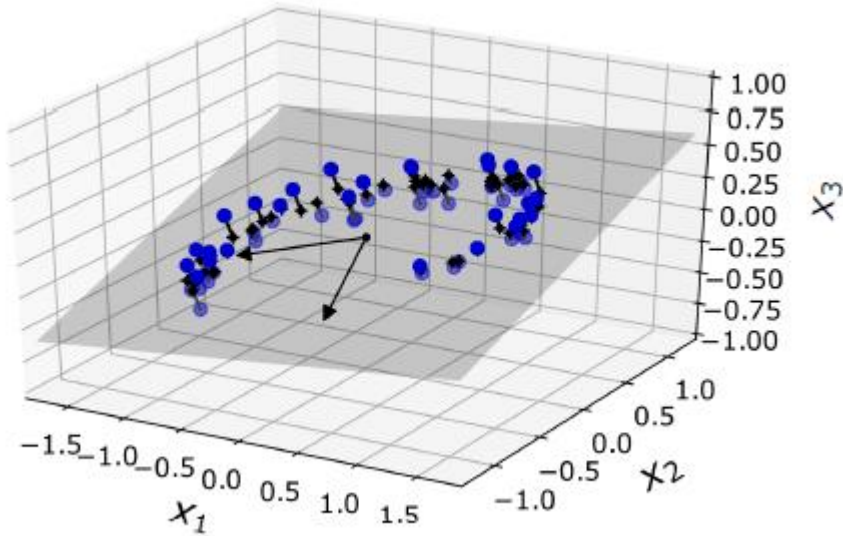
- Generalmente los datos no se distribuyen uniformemente en todas las dimensiones



- Muchas características son casi constantes mientras que otras están altamente correlacionadas
- Las muestras se encuentran dentro o cerca de un subespacio de dimensiones mucho más bajas

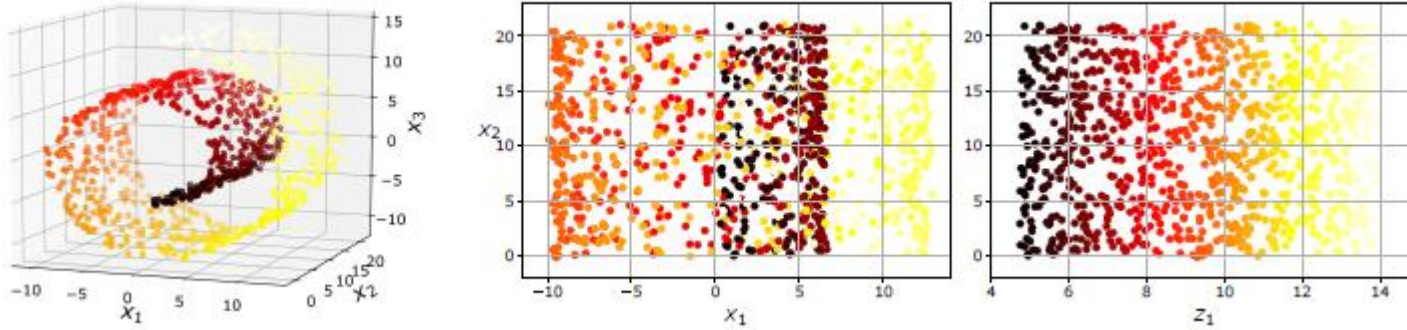
Proyección: Ejemplo 1

Todas las muestras se encuentran cerca de un plano de menor dimensión (2D)



Proyectamos todas las muestras al nuevo espacio de representación z_1 y z_2

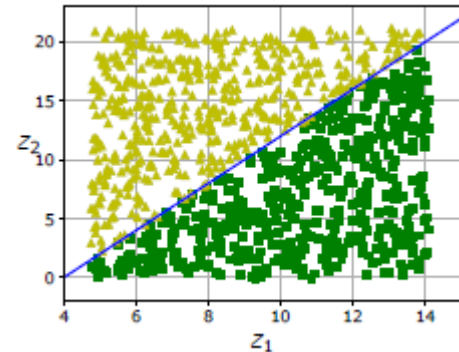
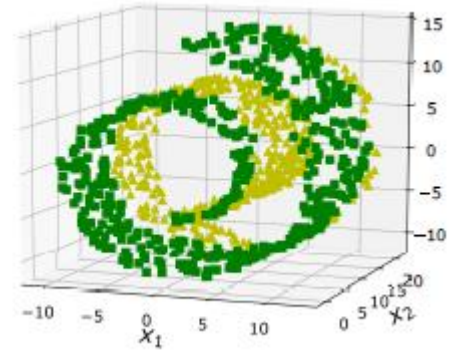
Proyección: Ejemplo 2



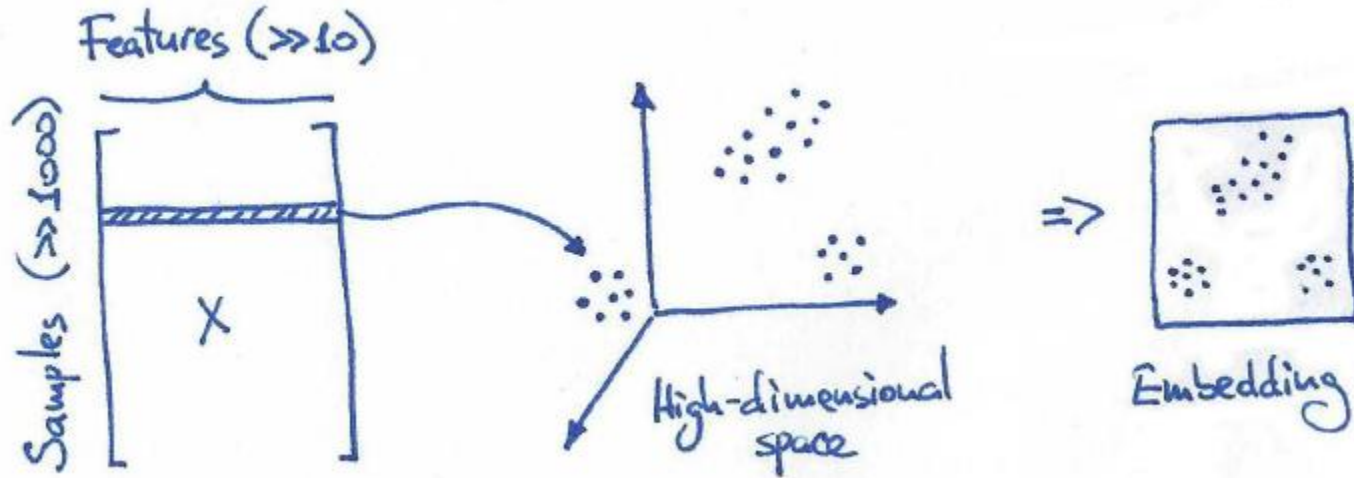
- La proyección en un plano (por ejemplo quitando x_3) aplastaría capas del rollo suizo (centro)
- Lo que deseamos es desenrollar el rollo (derecha)

Enfoques principales: Manifold learning

- El rollo suizo es un ejemplo de una variedad 2D
- Una variedad d –dimensional es una parte de un espacio n –dimensional ($d \ll n$) que localmente se parece a un hiperplano d –dimensional
- Manifold assumption: La mayoría de los conjuntos de datos de alta dimensión se encuentran cerca de un manifold de mucha más baja dimensión
- La tarea a resolver (clasificación, regresión) será más simple en este nuevo espacio



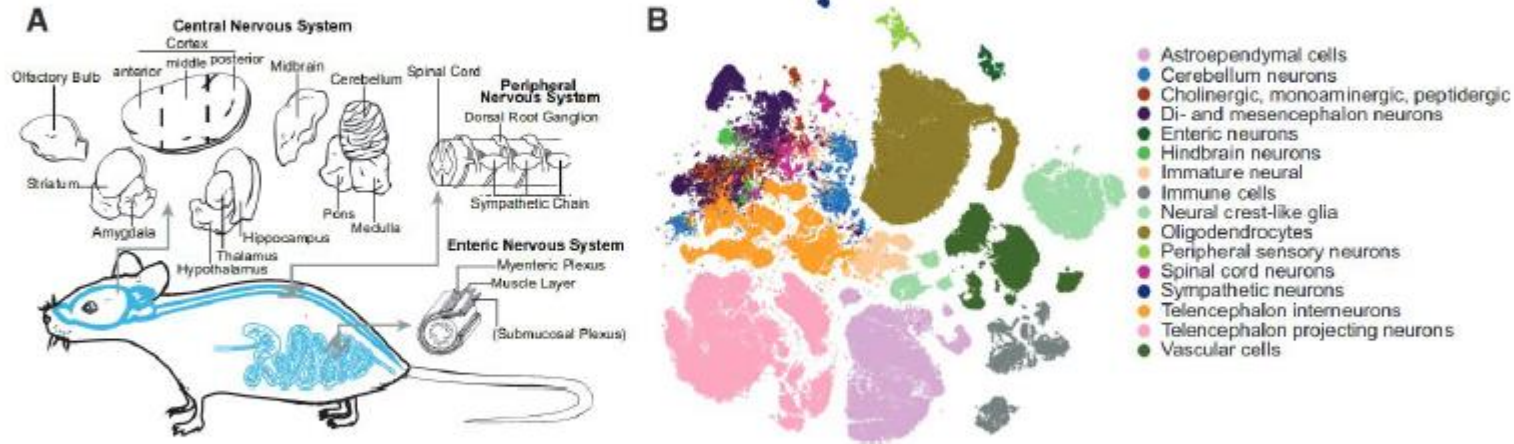
Visualización de datos t-SNE



- Unsupervised non-parametric methods for dimensionality reduction (non-linear methods)

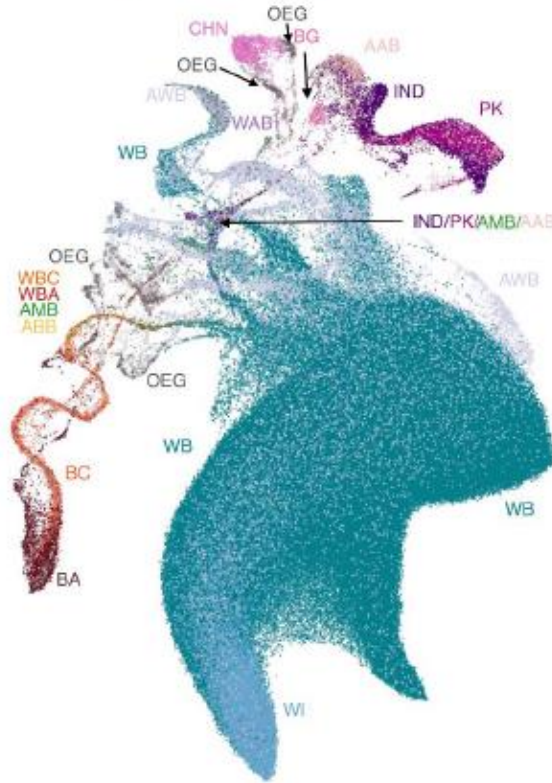
Visualización de datos t-SNE

Single-cell transcriptomics (single-cell RNA sequencing): samples are cells, features are genes.



Visualización de datos t-SNE

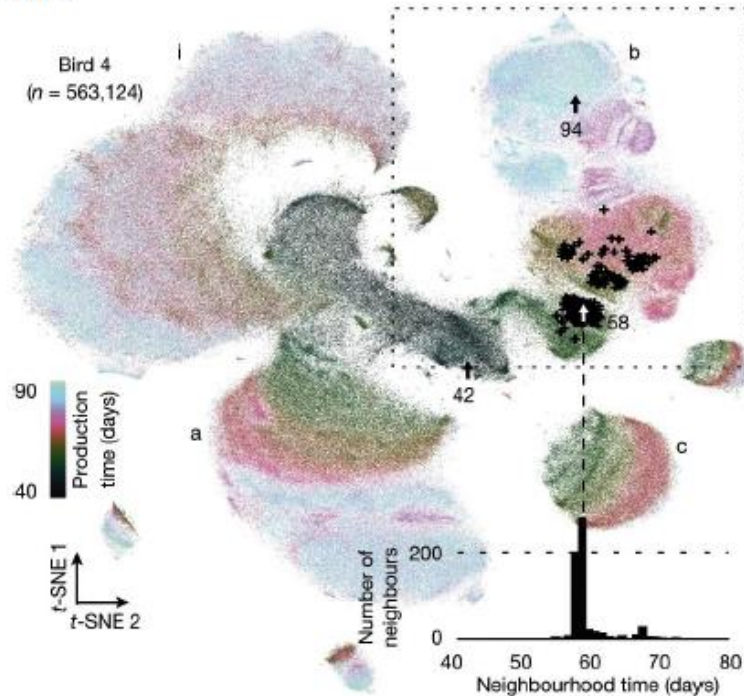
Population genomics: samples are people, features are single-nucleotide polymorphisms.



Diaz-Papkovich et al. (2019)
 $n \approx 500,000$

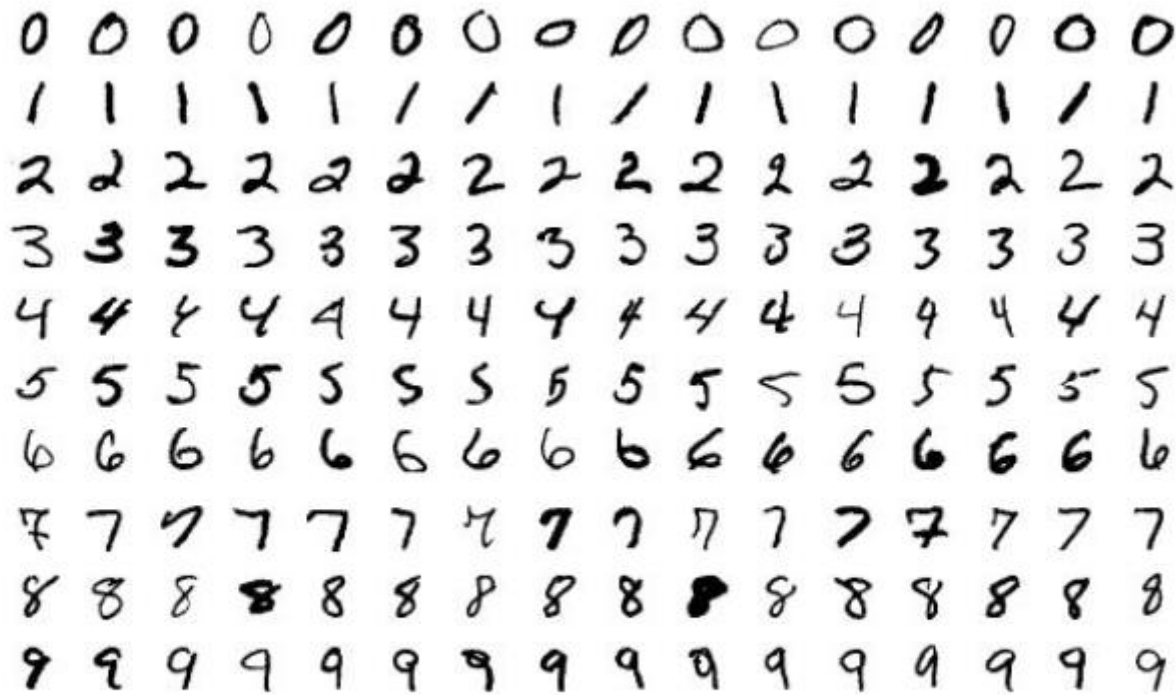
Visualización de datos t-SNE

Behavioural physiology: samples are syllable renditions, features are spectrogram bins.



Kollmorgen et al. (2020)
 $n \approx 600,000$

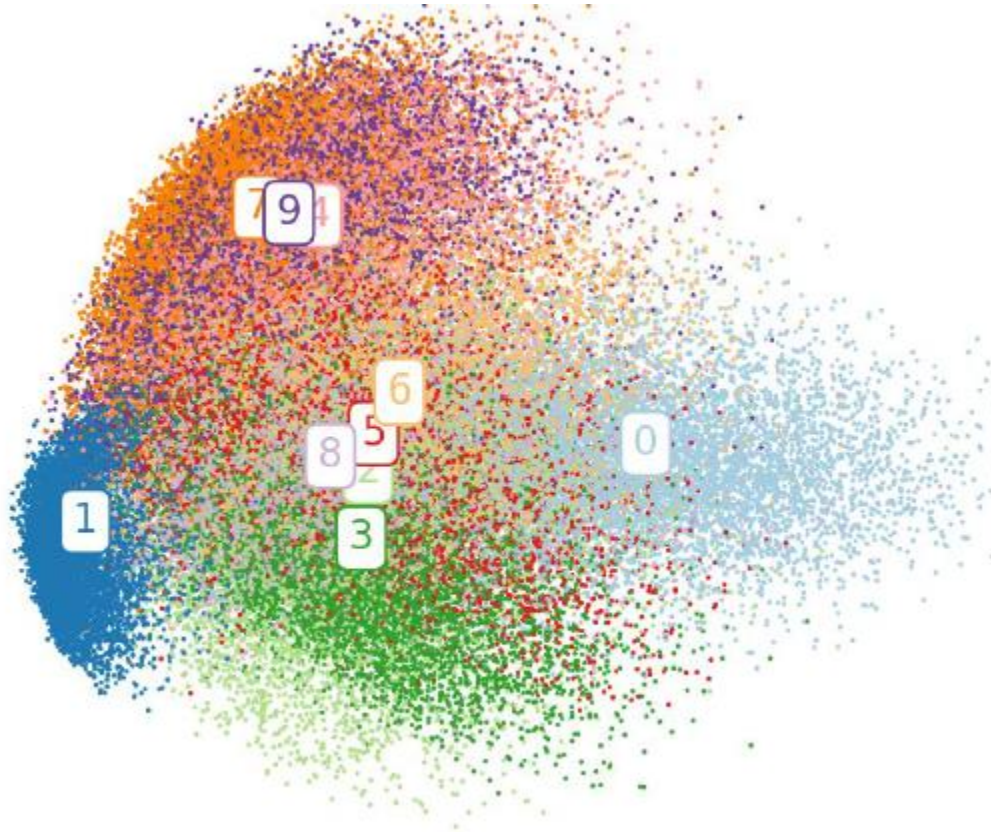
t-SNE MNIST



$n = 70,000$

28×28 images = 784 pixels

t-SNE MNIST



0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9

Multidimensional scaling MDS

- MSD: Arrange points in 2D to approximate high-dimensional pairwise distances

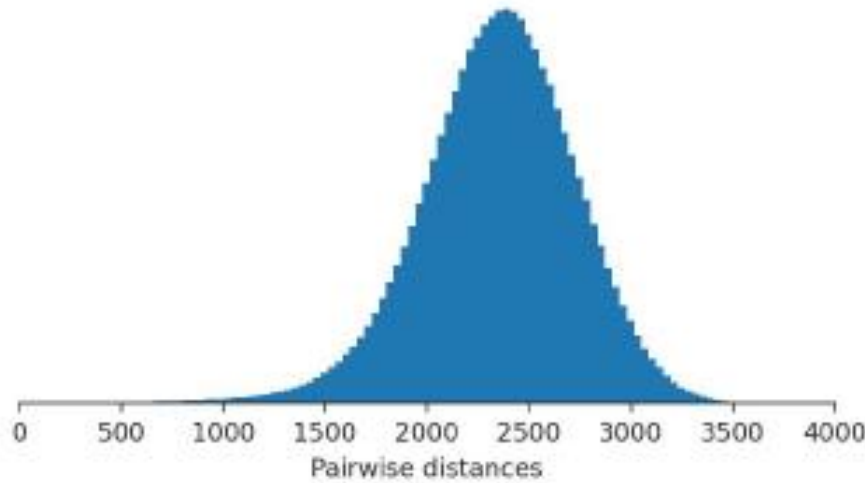


$$\mathcal{L} = \sum_{i < j} (d_{ij} - \|\mathbf{y}_i - \mathbf{y}_j\|)^2$$

Here $n = 5,000$.

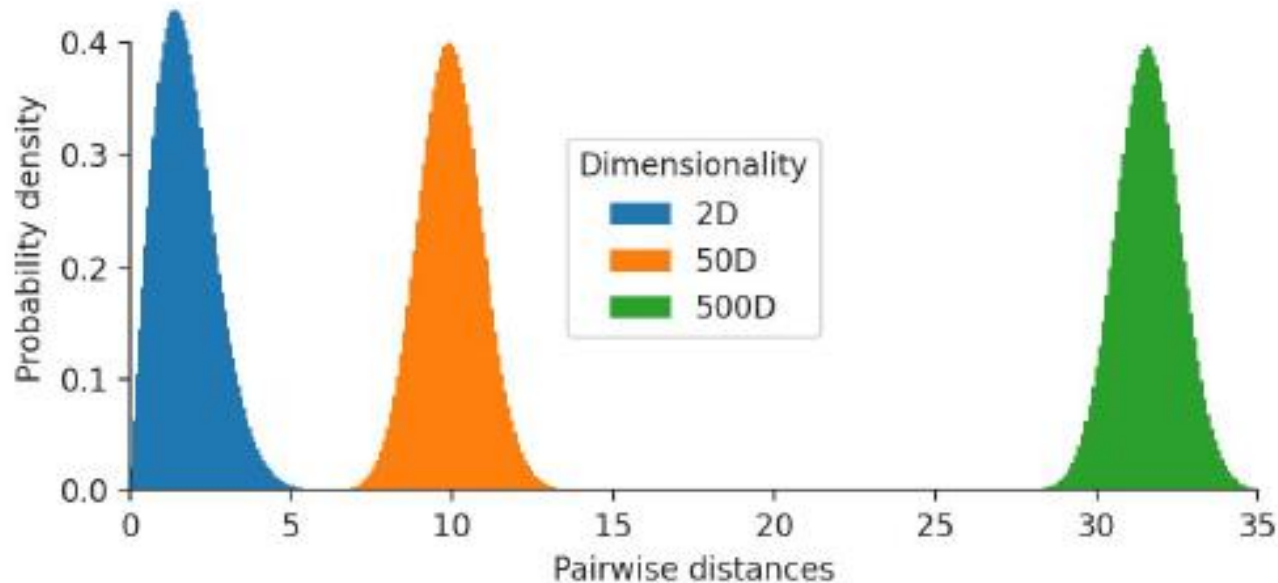
¿Por qué MSD falla?

- Preserving high-dimensional distances is usually a bad idea because it is not possible to preserve them (curse of dimensionality)



¿Por qué MSD falla?

- Pairwise distances between points in a standard Gaussian:



Neighbour embeddings

- Idea: Preserve nearest neighbours instead of preserving distances

[\[PDF\] 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 ...

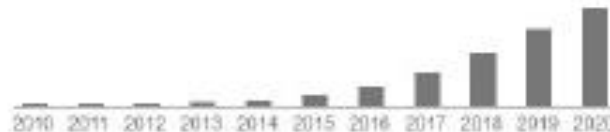
☆ 99 Cited by 1464 Related articles All 17 versions 🔗

[\[PDF\] Visualizing data using t-SNE.](#)

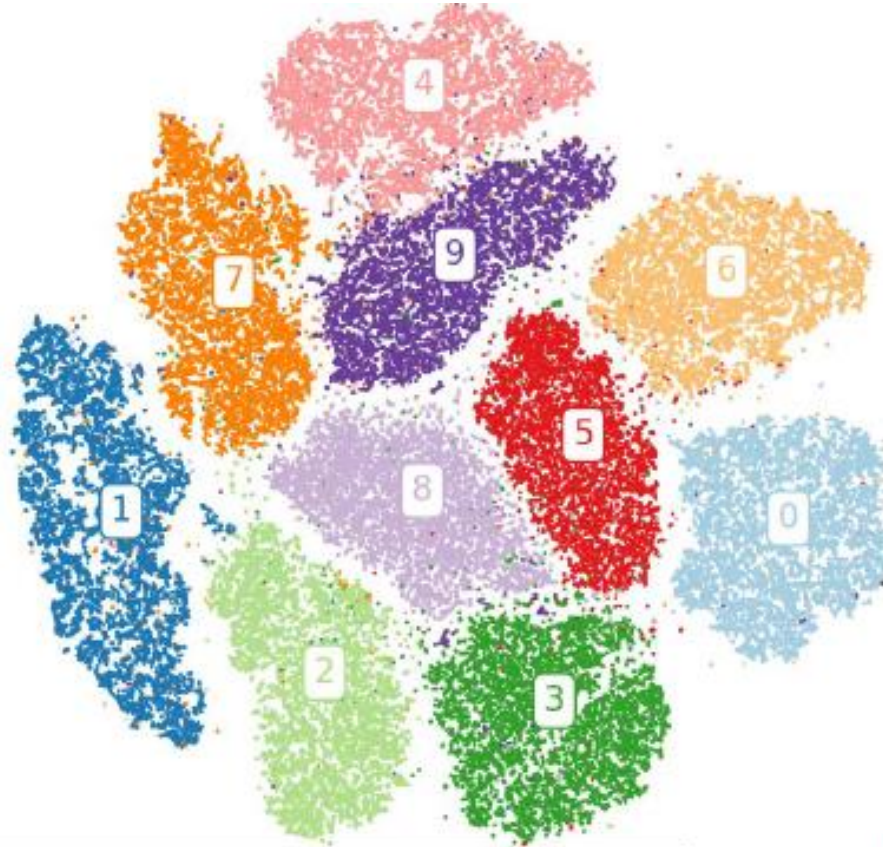
[L Van der Maaten](#), [G Hinton](#) - Journal of machine learning research, 2008 - jmlr.org

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 ...

☆ 99 Cited by 18533 Related articles All 32 versions 🔗

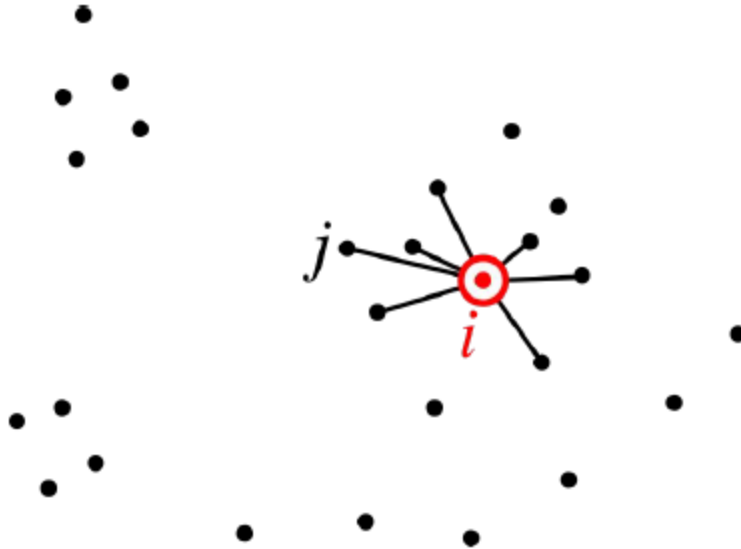


MNIST t-SNE



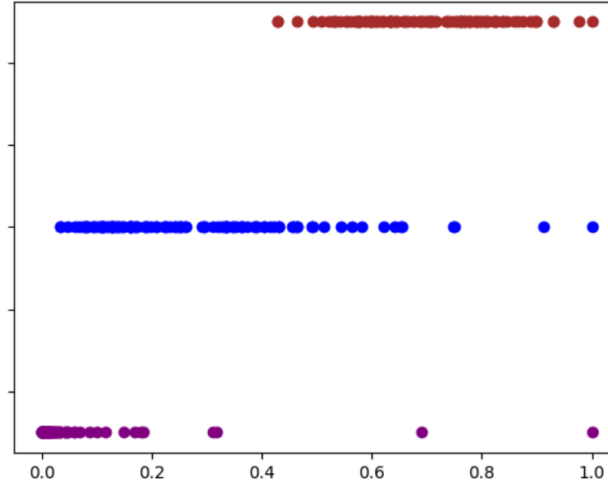
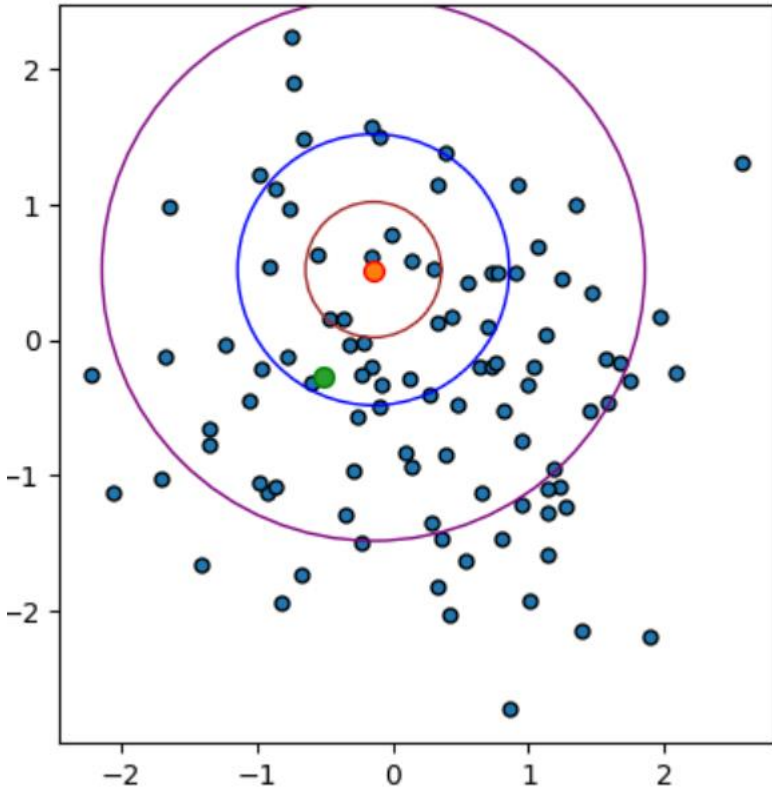
Stochastic neighbour embedding

- Loss function: Kullback-Leibler divergence between pairwise similarities (affinities) in the high-dimensional and in the low-dimensional spaces. Similarities are defined such that they sum to 1



$$\mathcal{L} = \sum_{i,j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Similarity



$$\text{sim}_{ij} = \exp\left(-\frac{1}{2\sigma^2}\|x_i - x_j\|^2\right)$$

$\sigma^2 = 1$, $d = 0.8780828489462678$

$\sigma^2 = 2$, $d = 0.21952071223656694$

$\sigma^2 = 0.5$, $d = 3.512331395785071$

Stochastic neighbour embedding

- High dimensional similarities

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

- Kernel width is adaptively chosen to achieve the desired perplexity (default: 30)

$$\mathcal{P} = 2^{\mathcal{H}}, \text{ where } \mathcal{H} = -\sum_{j \neq i} p_{j|i} \log_2 p_{j|i}.$$

- Symmetrize and normalize to sum 1

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

- This defines similarities as non-zero, but most will be ≈ 0 and can be set to 0 without affecting the result. Uniform similarities can be also used

$$p_{j|i} = 1/k \text{ for } k \text{ nearest neighbours}$$

Stochastic neighbour embedding

- Low dimensional similarities

$$q_{ij} = \frac{w_{ij}}{Z}, \quad w_{ij} = k(\|\mathbf{y}_i - \mathbf{y}_j\|), \quad Z = \sum_{k \neq l} w_{kl}$$

- Similarity kernel in SNE:

$$k(d) = \exp(-d^2)$$

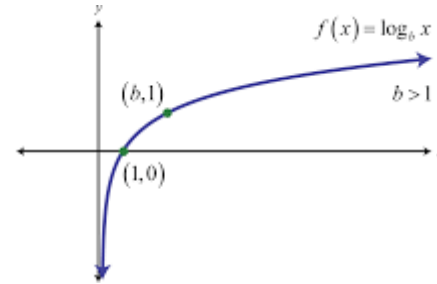
- Similarity kernel in t-SNE

$$k(d) = 1/(1 + d^2)$$

Gradient descent

- The loss is optimized via gradient descent starting from a random set of points

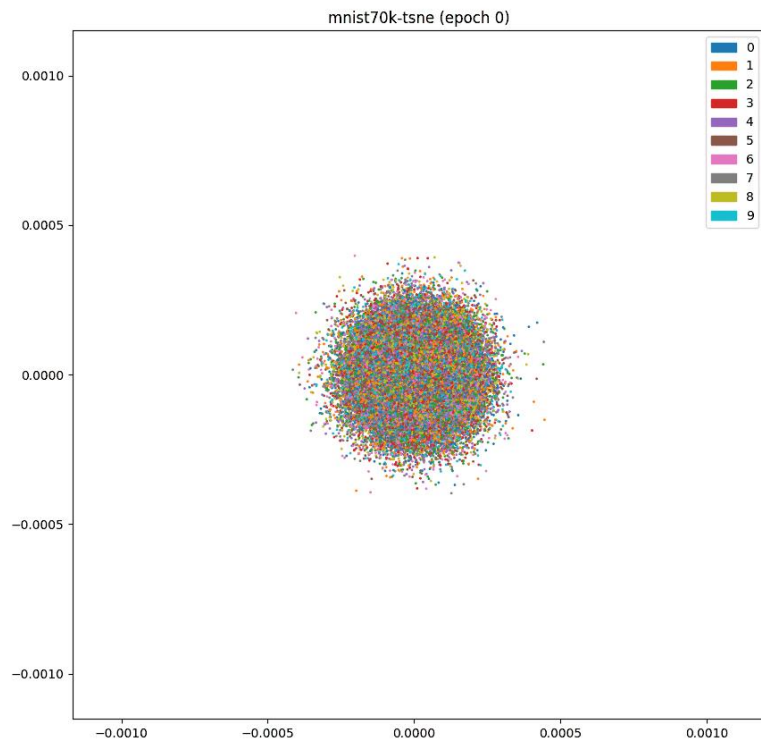
$$\begin{aligned}\mathcal{L} &= -\sum_{i,j} p_{ij} \log q_{ij} = -\sum_{i,j} p_{ij} \log \frac{w_{ij}}{Z} \\ &= -\sum_{i,j} p_{ij} \log w_{ij} + \log \sum_{i,j} w_{ij},\end{aligned}$$



- This works as a many-body simulation: close neighbours attract each other while all points repulse each other

$$\begin{aligned}\frac{\partial \mathcal{L}_{\text{t-SNE}}}{\partial \mathbf{y}_i} &= -2 \sum_j p_{ij} \frac{1}{w_{ij}} \frac{\partial w_{ij}}{\partial \mathbf{y}_i} + 2 \frac{1}{Z} \sum_j \frac{\partial w_{ij}}{\partial \mathbf{y}_i} \\ &\sim \sum_j p_{ij} w_{ij} (\mathbf{y}_i - \mathbf{y}_j) - \frac{1}{Z} \sum_j w_{ij}^2 (\mathbf{y}_i - \mathbf{y}_j)\end{aligned}$$

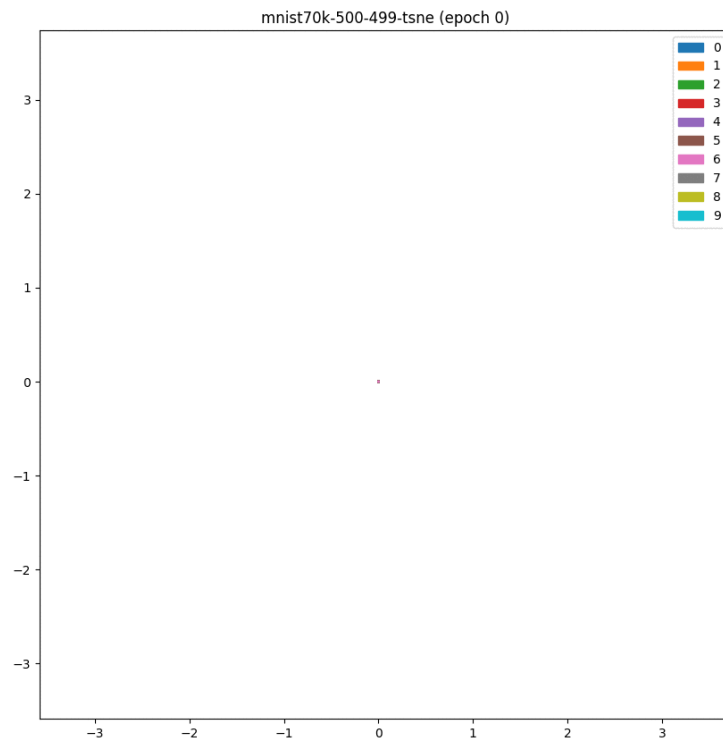
Early exaggeration



er

h

blk



Perplexity and the number of neighbours

- Perplexity can be seen as the 'effective' number of neighbours that enter the loss function. Default is 30
- Smaller values are rarely useful, higher values are computationally unfeasible

Perplexity 300



Perplexity 30

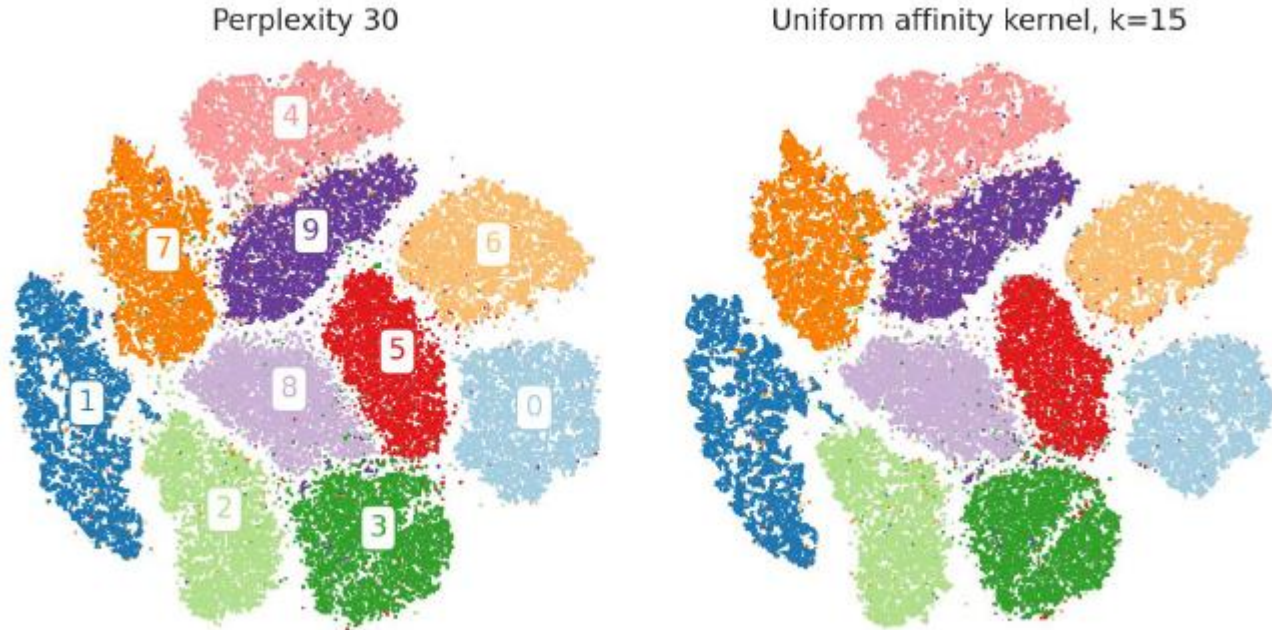


Perplexity 3



Uniform affinities

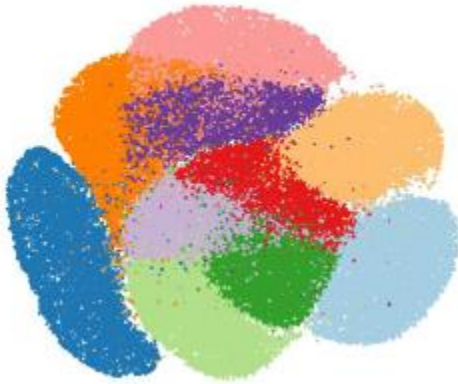
- Gaussian affinities with perplexity P can be replaced with uniform affinities with $k = P/2$



Low-dimensional similarity kernel

- The main innovation of tSNE with respect to SNE was the Cauchy kernel, addressing the crowding problema of SNE
- Even heavier-tailed kernels can bring out even finer cluster structure.

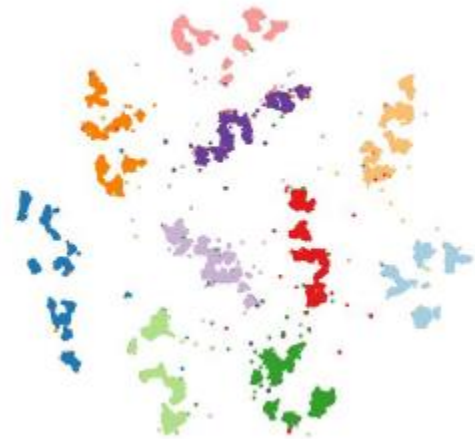
Gaussian kernel



Cauchy kernel

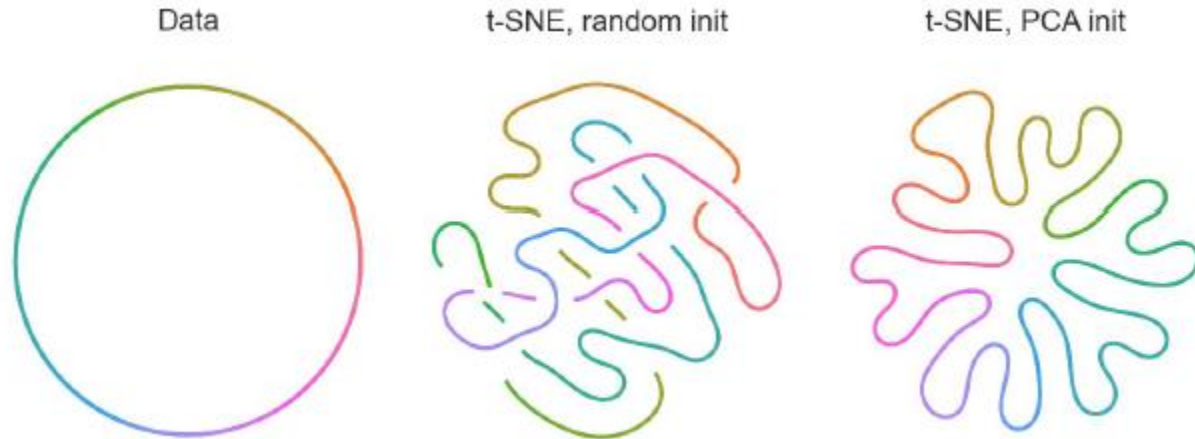


Heavier-tailed kernel



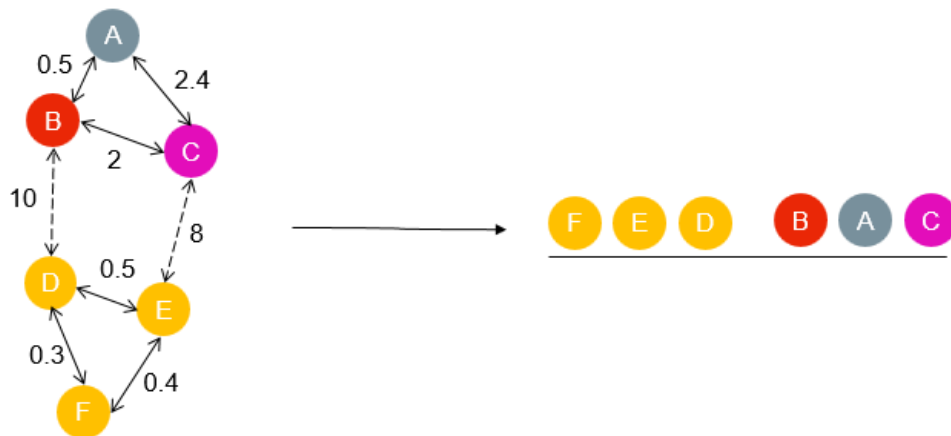
The role of initialization

- tSNE preserves local structure but fails preserving global structure. The cost function has a lot of local mínimos and initialization plays an important role.
- Always use informative initialization like PCA



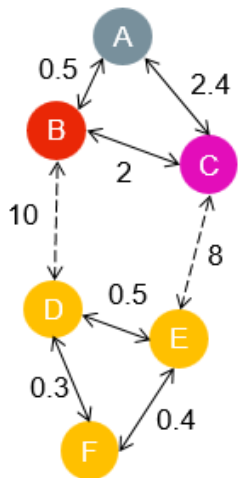
UMAP

- UMAP is a dimensionality reduction technique that preserves as much of the data's local and global structure as possible.

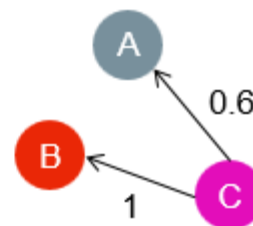
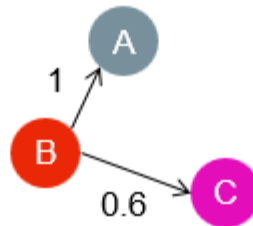
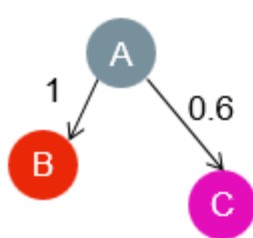


UMAP

- **High-Dimensional Graph Construction:** UMAP begins by constructing a weighted graph in the high-dimensional space. Each data point is connected to its nearest neighbors, creating a local neighborhood graph. The connections (edges) are weighted by similarity, with closer points having stronger connections.

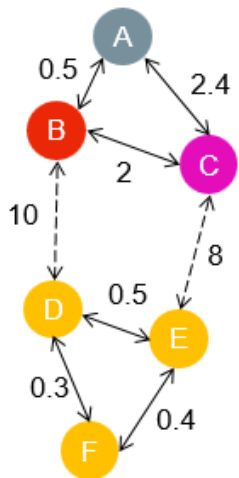


$$v_{j|i} = \exp[(-d(x_i, x_j) - \rho_i)/\sigma_i]$$



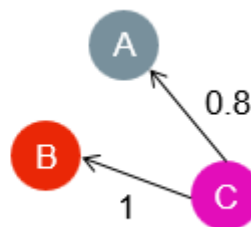
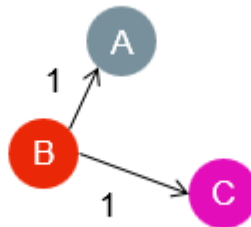
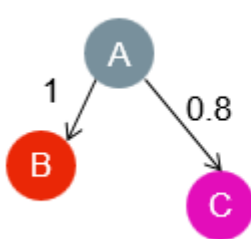
UMAP

- High-Dimensional Graph Construction:** UMAP begins by constructing a weighted graph in the high-dimensional space. Each data point is connected to its nearest neighbors, creating a local neighborhood graph. The connections (edges) are weighted by similarity, with closer points having stronger connections.



$$v_{j|i} = \exp[(-d(x_i, x_j) - \rho_i)/\sigma_i]$$

$$v_{ij} = (v_{j|i} + v_{i|j}) - v_{j|i}v_{i|j}$$



- Number of neighbors and σ

Algorithm 3 Compute the normalizing factor for distances σ

function SMOOTHKNNDIST(knn-dists, n , ρ)

Binary search for σ such that $\sum_{i=1}^n \exp(-(knn-dists_i - \rho)/\sigma) = \log_2(n)$

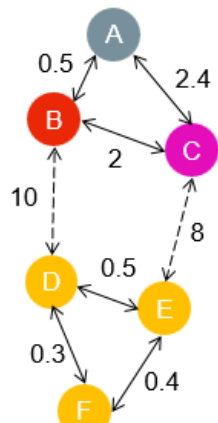
return σ

UMAP

Optimization: UMAP then uses a force-directed graph layout algorithm in lower-dimensional space to find a representation that is as structurally similar as possible to the high-dimensional graph. The low dimensional similarities are given by:

$$w_{ij} = \left(1 + a \|y_i - y_j\|_2^{2b}\right)^{-1} \quad a \approx 1.929 \text{ and } b \approx 0.7915$$

$$C_{UMAP} = \sum_{i \neq j} v_{ij} \log v_{ij} + (1 - v_{ij}) \log (1 - v_{ij}) \\ - v_{ij} \log w_{ij} - (1 - v_{ij}) \log (1 - w_{ij})$$



UMAP - MNIST

