Lecture 9

Dimensionality Reduction

ISLR 12, ESL 14, tSNE

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Supervised vs. Unsupervised Learning

We focused mostly on supervised learning methods such as regression and classification

- The goal was to predict an outcome Y, from a set of features $X_1, X_2, \dots, X_p$

In unsupervised learning we are only given the features $X_1, X_2, \dots, X_p$ and we are interested in findings some interesting about the data or hidden (latent) structure

- Informative ways to visualize the data
- Discover subgroups (clusters) among the variables or observations
- Project the data from a high- to a low-dimensional space
- Anomaly detection

Other learning paradigms (out of scope for the lecture):

- reinforcement learning
- self-supervised learning (e.g. reducing unsupervised to supervised learning)

Unsupervised Learning

Unsupervised learning is more exploratory and thus more challenging

- we have no clear target question – no output guides our predictions
- therefore, it is difficult to assess the quality of our results
- compared to supervised where we could just look at e.g. the test error

Big advantage: Much easier to obtain large amounts of unlabeled data

Examples

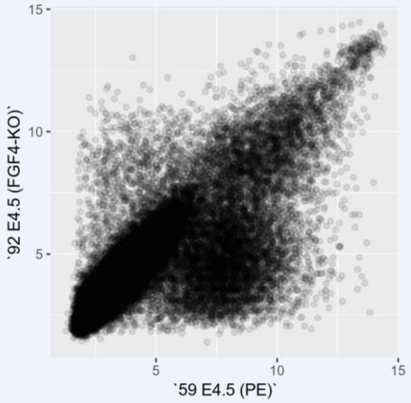
- grouping genomic signatures of cancer samples by subtype
- characterizing shoppers browsing and purchasing habits
- movies grouped by the ratings assigned by movie viewers

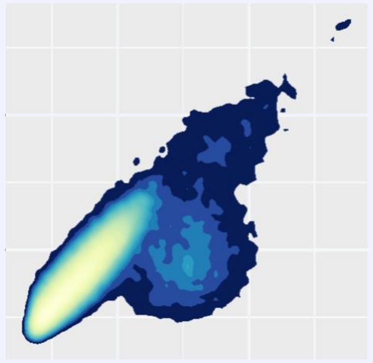
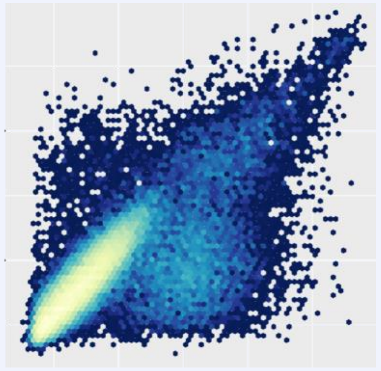
Visual Data Exploration (Tutorial)

1D data: compute summary statistics: mean, mode, median, quartiles, box-whiskers plot

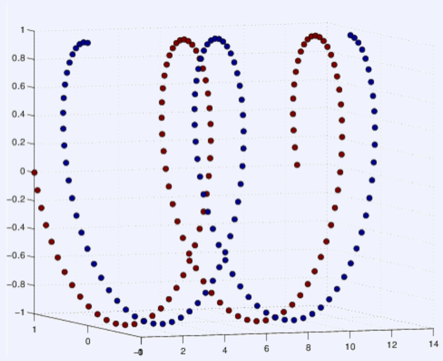
1D data distribution: histograms, dots and beeswarm plot, kernel density estimation, violin plot

2D data: scatter plots, density plots, hexagon plots

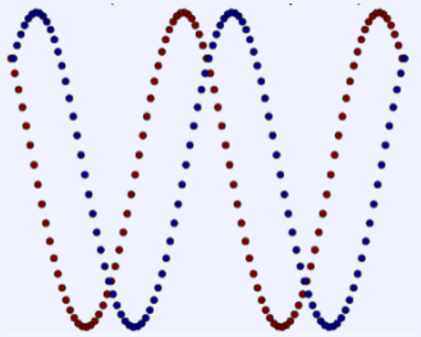


Visualizing more than two dimensions

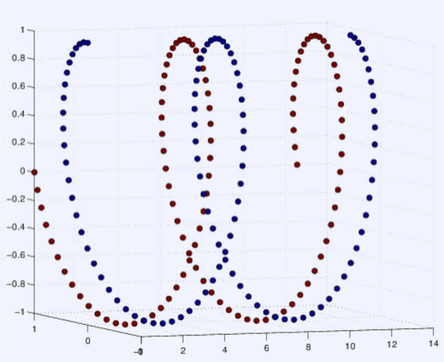


original 3D data



2D reduction with PCA

Visualizing more than two dimensions



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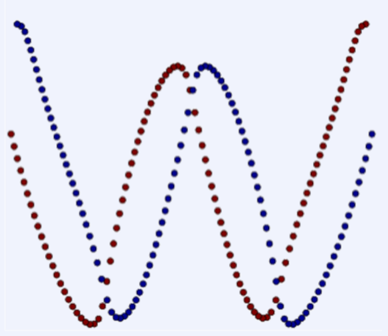
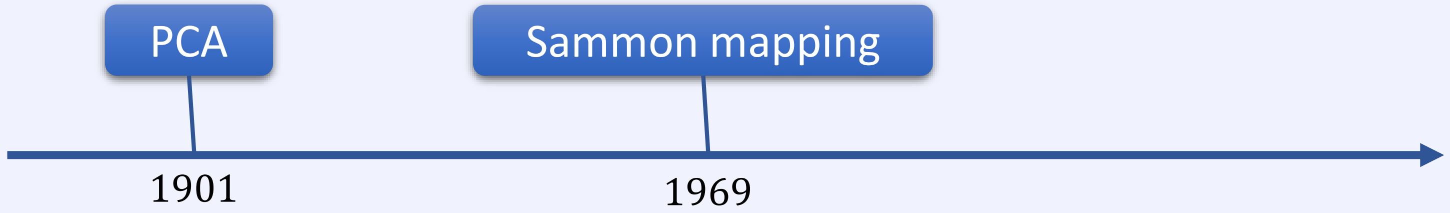
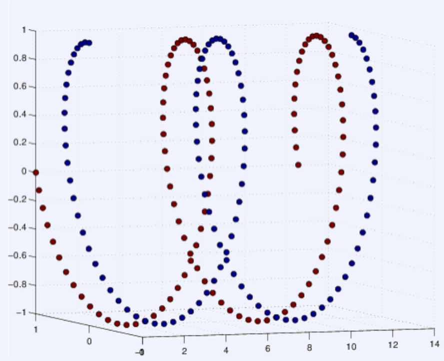


2D reduction with Sammon mapping



Visualizing more than two dimensions



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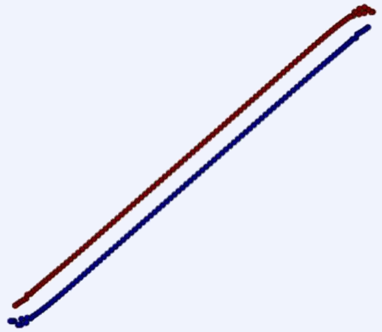
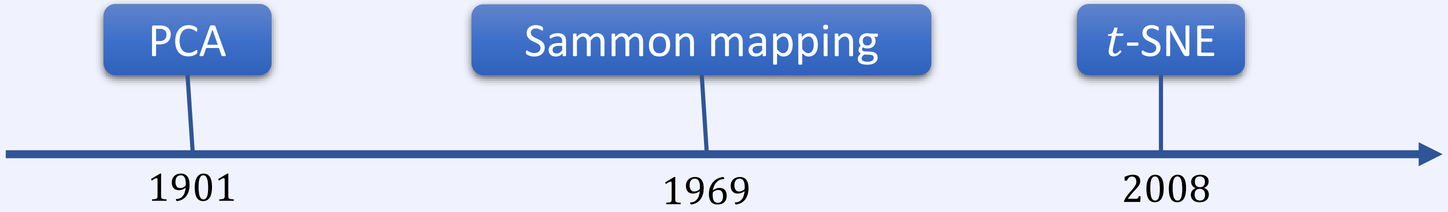


2D reduction with t-SNE



Dimensionality Reduction: Further Motivation

High-dimensional data is challenging:

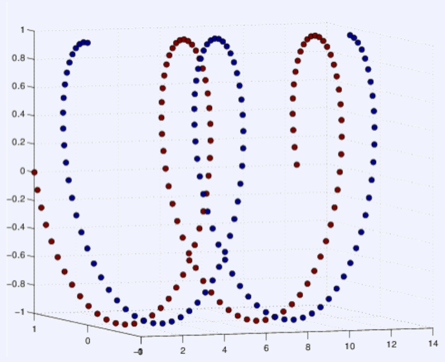
- hard to visualize high-dimensional data
- highly correlated dimension could cause trouble for some algorithms
- curse of dimensionality: we need exponential amounts of data to characterize the density as the dimensionality goes up
- computation is expensive because of high complexity of distance functions

Often the data lies on a low-dimensional manifold, embedded in a high-dimensional space

Goal: Reduce the dimensionality while avoiding information loss and preserving the structure

- computational or memory savings
- uncover the intrinsic dimensionality of the data

PCA



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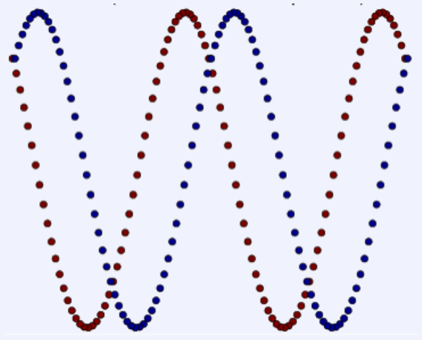
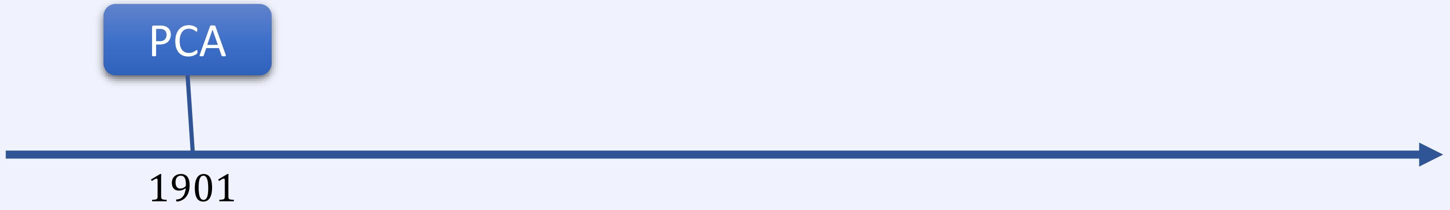


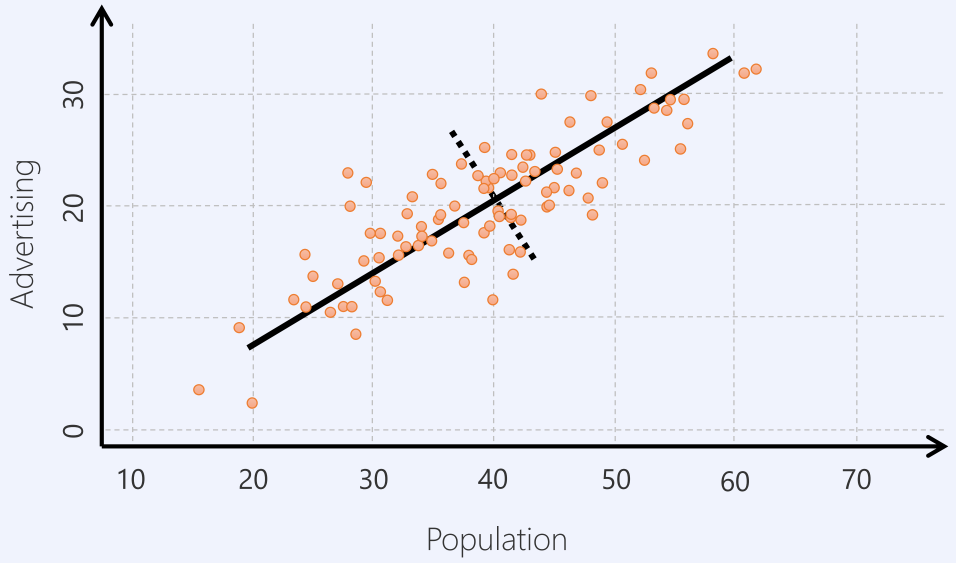
2D reduction with PCA



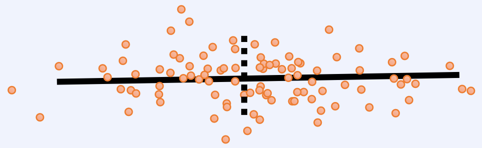
Principal Component Analysis

Example: population and ad spending for 100 different cities shown as circles

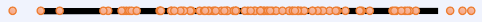
- Data are roughly linear along one direction with a small variance along a second direction
- Solid line indicates the first principal component (PC) direction, and dotted line the second PC
- Most of the variation is along the first PC



- The PCs define a new coordinate system



- Project points onto the first PC



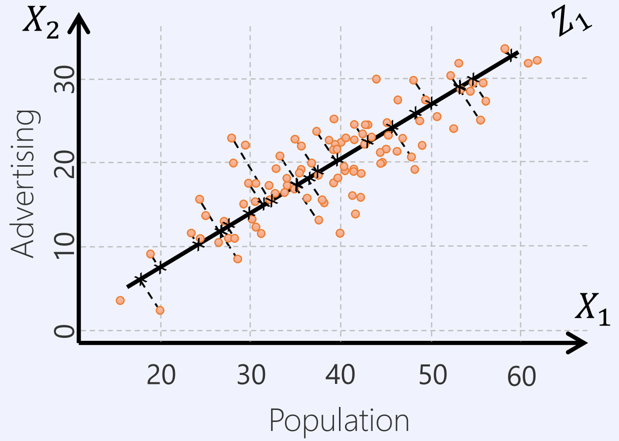
Principal Component Analysis

The first PC is the direction in space along which **variance** of data is **greatest**

- if projected onto this direction the resulting one-dimensional dataset has the largest possible variance
- The $\boldsymbol{j^{th}}$ PC is the direction orthogonal to all previous PCs, on which the remaining variance is largest

At the same time the first PC **minimizes** the sum of squared distances (dashed lines)

- the line that is closest to all the observations



Principal Component Analysis

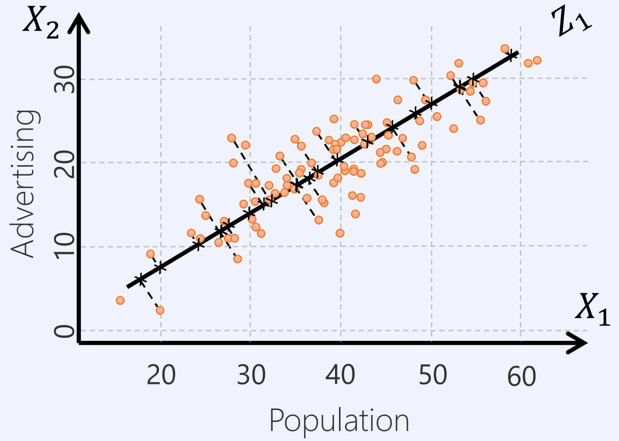
Formally we define the first PC Z_1 as a **linear combination** of mean-centered X_j

$$Z_1 = \sum_{j=1}^{p} \phi_{j1}(X_j - \bar{X}_j) \text{ for constants } \phi_{11}, \phi_{21}, \dots, \phi_{p1} \text{ and means } \bar{X}_j$$

- we require $\phi_{11} + \phi_{21} + \cdots + \phi_{p1} = 1$ to prevent arbitrary scaling
- find ϕ_{j1} such that variance is maximized / distance is minimized
- Z_1 is a n-dimensional vector
- its components z_{i1} are called the **PC scores**

- Solve the following problem subject to the scaling constraint

$$\max_{\phi_{11},\phi_{21},\dots,\phi_{p1}} \underbrace{\frac{1}{n}\sum_{i=1}^{n} z_{i1}^2}_{\text{variance}} = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{j1}(X_j - \bar{X}_j)\right)^2$$



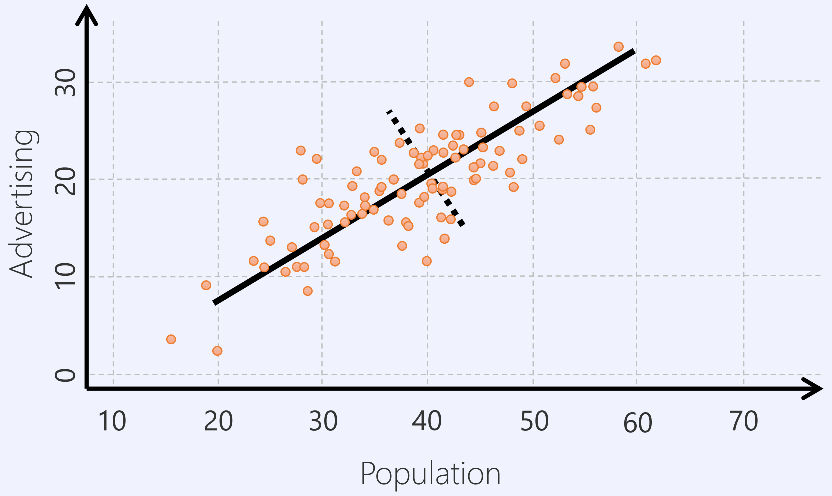
Principal Component Analysis

Example:

- first PC $Z_1 = 0.839(\mathbf{pop} - \overline{\mathbf{pop}}) + 0.544(\mathbf{ad} - \overline{\mathbf{ad}})$
- $\phi_{11} = 0.839, \phi_{21} = 0.544$ component loadings

- out of every linear combination of **pop** and **ad** with $\phi_{11}^2 + \phi_{21}^2 = 1$ the first PC has the highest variance i.e. $Var(\phi_{11}(\mathbf{pop} - \overline{\mathbf{pop}}) + \phi_{21}(\mathbf{ad} - \overline{\mathbf{ad}}))$ is maximum
- at the same time first PC is the closest line to the data

- second PC $Z_2 = 0.544(\mathbf{pop} - \overline{\mathbf{pop}}) - 0.839(\mathbf{ad} - \overline{\mathbf{ad}})$



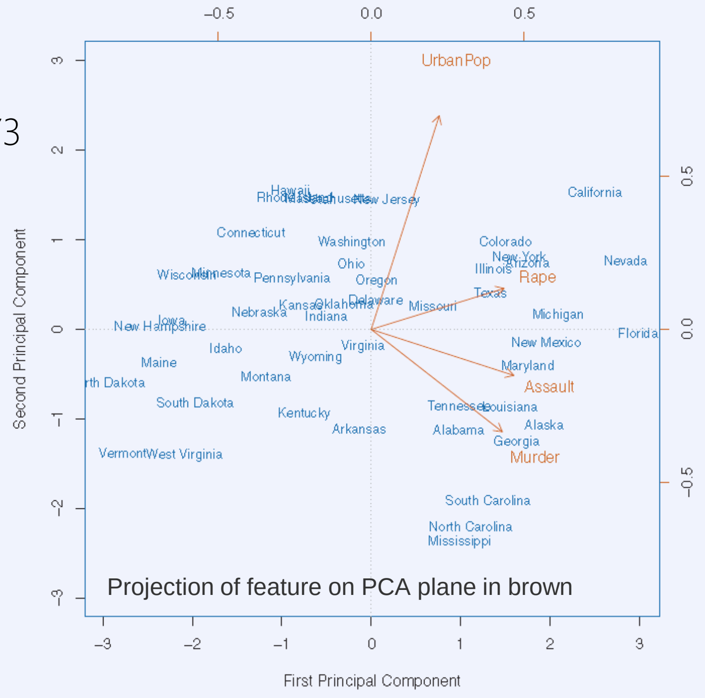
Principal Component Analysis

PCA of the **USArrests** dataset

- statistics in arrests per 100,000 residents in the US in 1973
- 50 observations, 1 per state, 4 inputs
  - **Murder** numeric murder arrests
  - **Assault**: numeric assault arrests
  - **UrbanPop**: percent urban population
  - **Rape**: numeric rape arrests

	PC1	PC2
Murder	**0.5358995**	**-0.4181809**
Assault	**0.5831836**	**-0.1879856**
UrbanPop	**0.2781909**	**0.8728062**
Rape	**0.5434321**	**0.1673186**

PCA "loading vector"
direction of the principal component



(ISLR 10.2)

Principal Component Analysis

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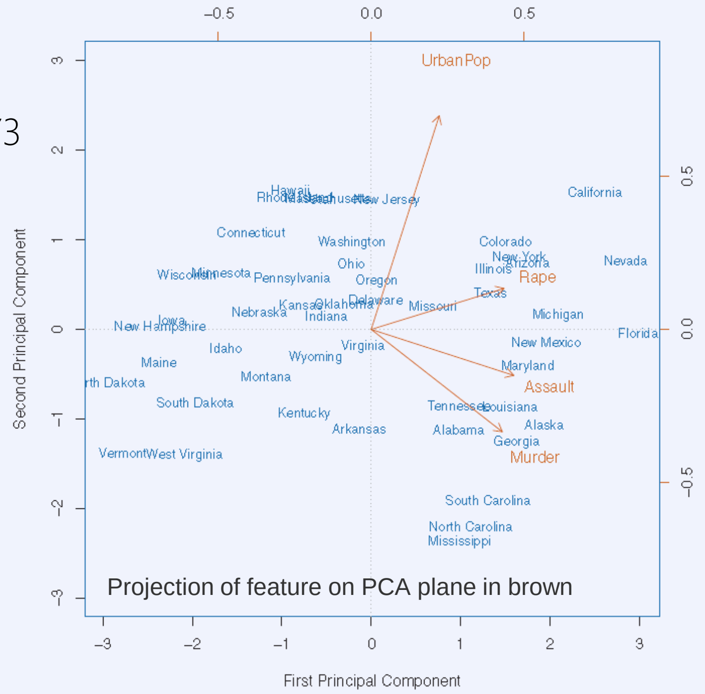
projection of feature vectors on principal component surface



Principal Component Analysis

Interpretation

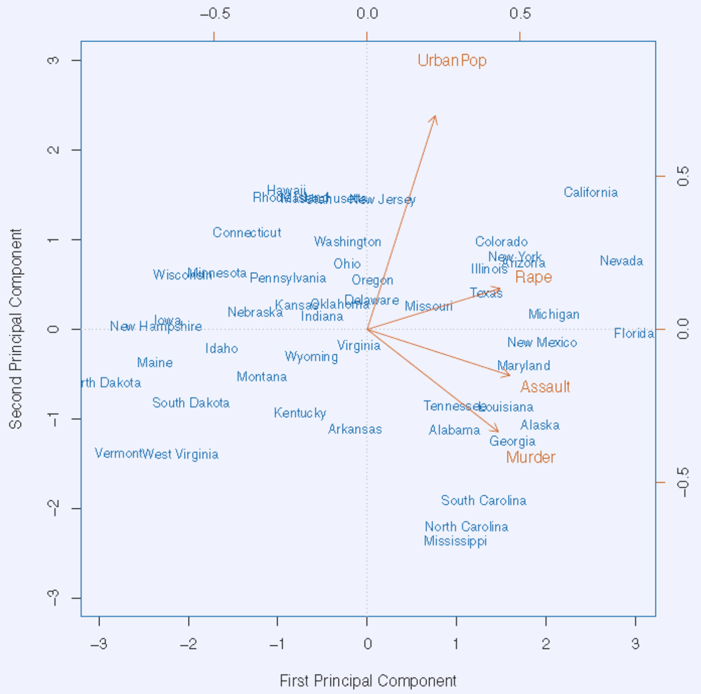
- crime variables are highly correlated:
  - projection vectors point in about same direction
- less correlation with **`UrbanPop`**

PC1 reflects crime rate

- high in California, Nevada, Florida
- low in W.-Virginia, the Dakotas etc.

PC2 reflects urbanization

- high in California
- low in the Carolinas and Mississippi



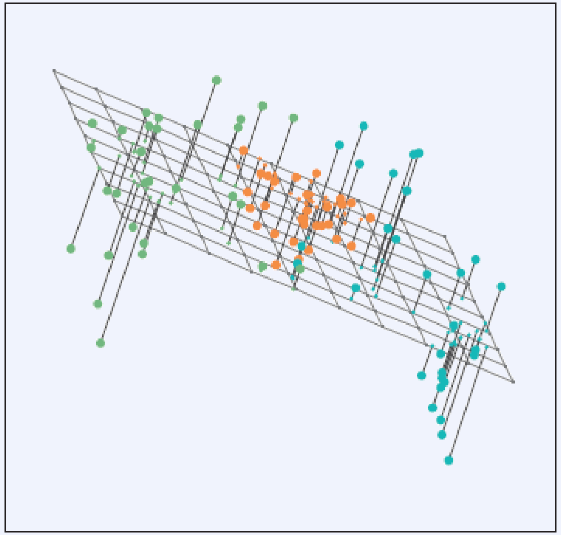
Principal Component Analysis

Interpretation 1

- PCs are directions of highest variance of the data
- PC score of an input is its projection onto the PC loading vector

Interpretation 2

- first PC minimizes the total sum of square distances
- second PC is the first PC of the residual, i.e. the direction in which the variance of the residual is maximized / distance is minimized
- the PC hyperplane is the affine subspace such that the total sum of square distances from the subspace is minimal


3D simulated dataset with the first two PCs

Interpretation 3

- PCA finds a a linear transformation into a new coordinate system where the data is linearly uncorrelated

Principal Component Analysis

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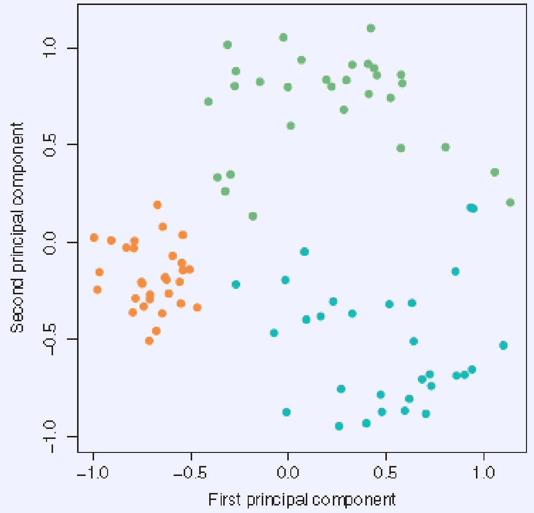


3D simulated dataset with the first two PCs

Interpretation 3

- PCA finds a a linear transformation into a new coordinate system where the data is linearly uncorrelated

How to choose the number of PCs

If the goal is to use PCA for visualization the we can only select 2 or 3

If the goal is to preprocess the data before another method (e.g. before running regression)

- select #PCs such that a target proportion of the total variance is explained (PVE)
  - total variance is $\sum_{j=1}^{p} \mathrm{Var}(X_j)$
  - variance explained by the m-th principal component $\mathbf{Var}(Z_m)$
- if we select k componets we explain $\frac{\sum_{i=1}^{k} \mathrm{Var}(Z_m)}{\sum_{j=1}^{p} \mathrm{Var}(X_j)}$
  - select k such that the above fraction equals e.g. 90%
  - look for an elbow in the PVE plot

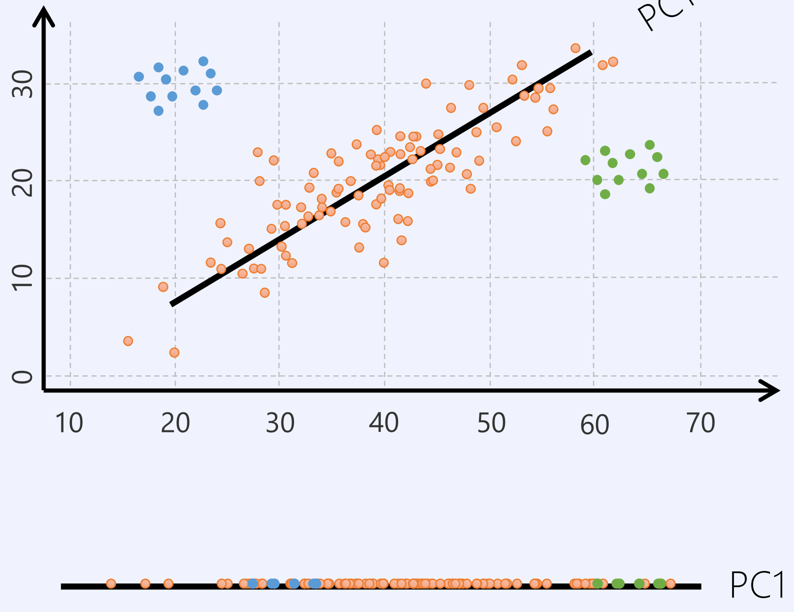
We can also just use cross-validation on the final dowstream error

Principal Component Analysis

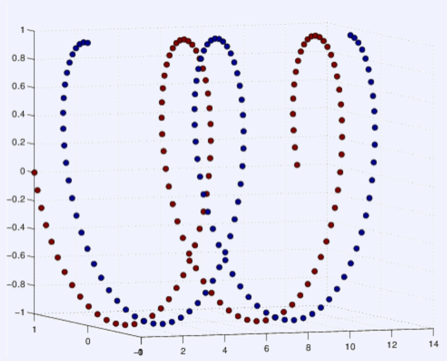
PCA finds the global (linear) structure in the data

- can lead to local inconsistencies
- far away points can become nearest neighbors
- depending on the application this is a problem

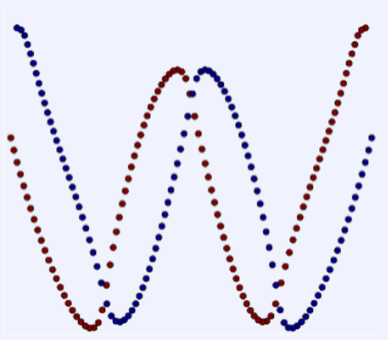
Idea: Preserve local structure (distances) instead



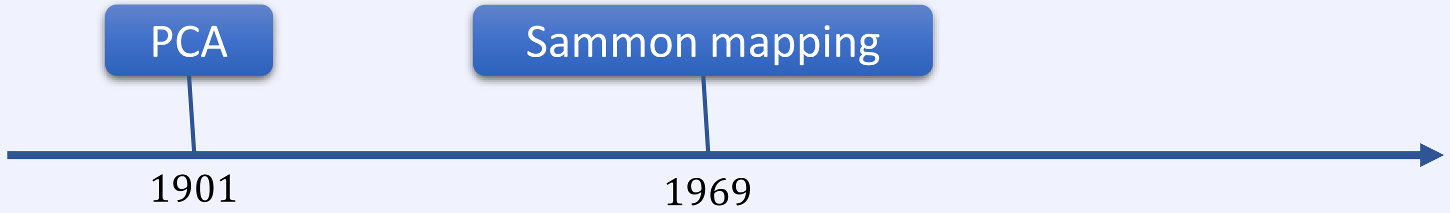
Sammon Mapping (MDS)



original 3D data



2D reduction with Sammon mapping



MDS: Multidimensional Scaling

Project high-dimensional distances onto low-dimensional space $\mathbb{R}^k$

- let data points be $x_1, \ldots, x_N \in \mathbb{R}^p$
- project onto $z_1, \ldots, z_N \in \mathbb{R}^k$
- minimize a stress function S

Kruskal-Shepard (least-squares): $S_M(z_1, \ldots, z_N) = \sum_{i \neq i'} (d_{ii'} - \|z_i - z_{i'}\|)^2$

Sammon mapping: $S_{S_m}(z_1, \ldots, z_N) = \sum_{i \neq i'} \frac{(d_{ii'} - \|z_i - z_{i'}\|)^2}{d_{ii'}}$

- emphasizes preserving smaller distances

Multidimensional Scaling & PCA

Minimization by gradient descent

- classic scaling for similarities $s_{ii'}$
- often we use the centered inner product $s_{ii'} = \langle x_i - \bar{x}, x_{i'} - \bar{x} \rangle$
- we then minimize

$$S_C(z_1, \dots, z_N) = \sum_{i,i'} (s_{ii'} - \langle z_i - \bar{z}, z_{i'} - \bar{z} \rangle)^2$$

by choosing $z_1, \dots, z_N \in \mathbb{R}^k$

- this has a solution in terms of eigenvectors
- if the similarities are centered inner products then in fact this is exactly principal components

Multidimensional Scaling

MDS only needs the similarities or dissimilarities, not the point coordinates

Non-metric version of Shepard-Kruskal scaling only uses ranks

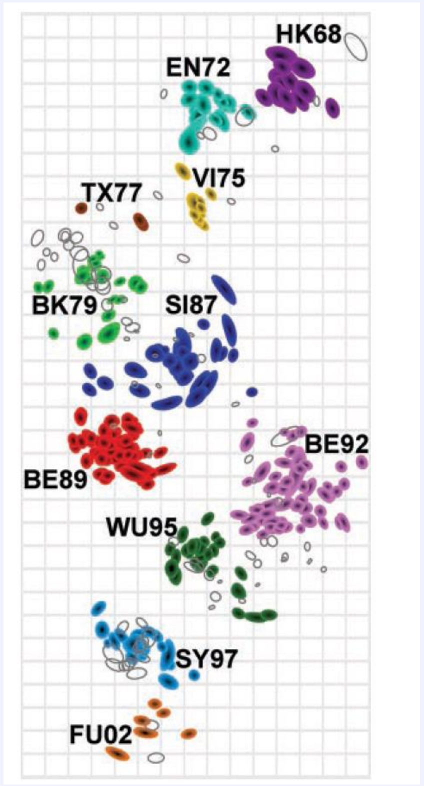
$$S_{NM}(z_1, \dots, z_N) = \frac{\sum_{i \neq i'} [\|z_i - z_{i'}\| - \theta(d_{ii'})]^2}{\sum_{i \neq i'} \|z_i - z_{i'}\|^2}$$

- θ is an arbitrary increasing function
- with θ fixed we minimize over z_i by gradient descent
- with z_i fixed the best monotonic θ is found by “isotonic regression” (version of quadratic programming)

Multidimensional Scaling

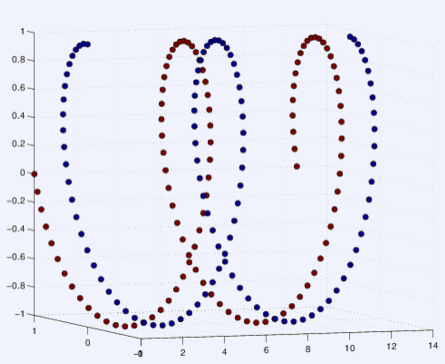
Example: Antigenic shift of influenza virus

- original space has 79 dimensions
- multiple runs of gradient descent with random starting solutions
- level of increase of stress function with decreasing $\boldsymbol{k}$
  can point to “dimensionality” of the data
- here results do not change significantly
  if one projects to 2, 3, 4, or 5 dimensions

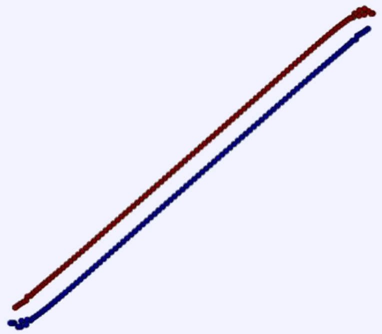


(Smith, Lapedes et al. Science 2004) 25

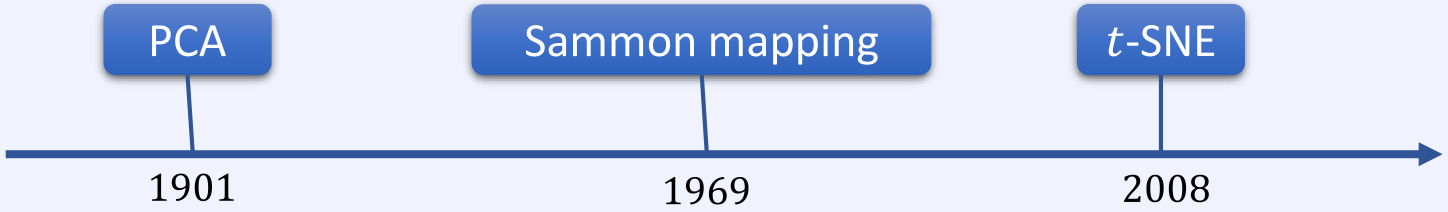
t-SNE



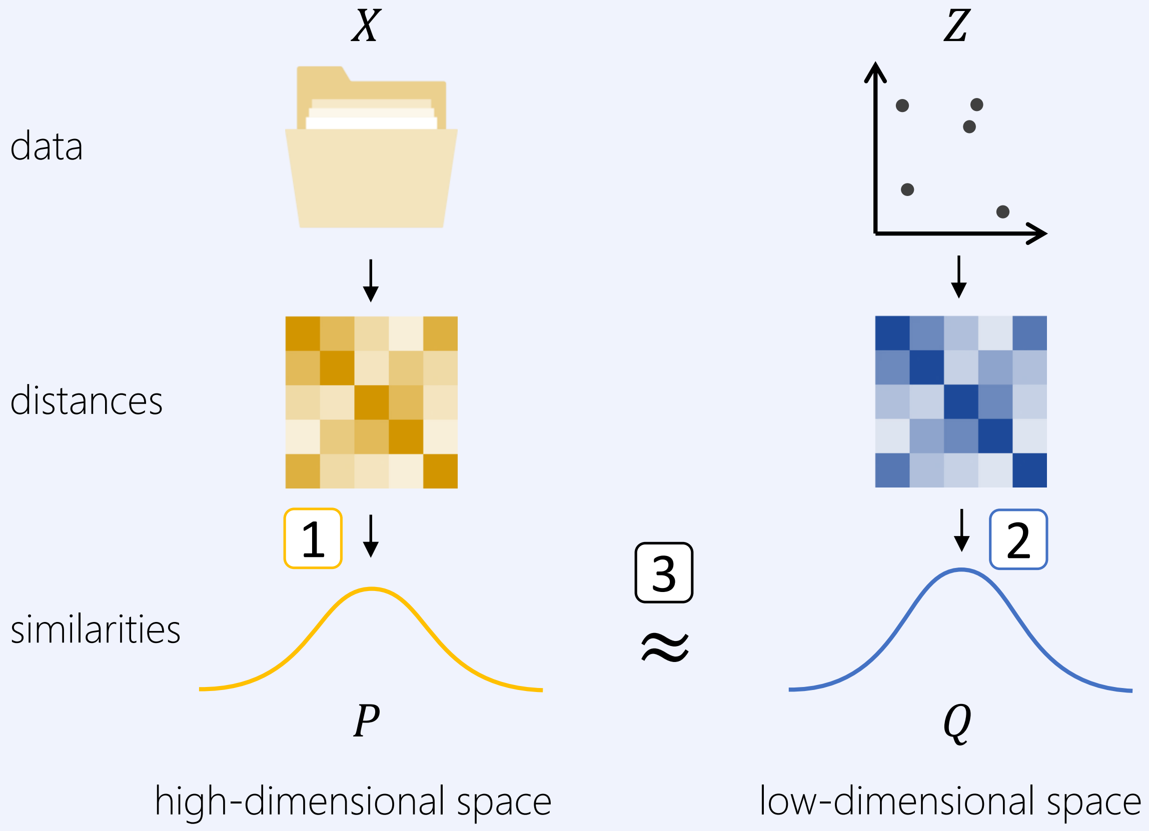
original 3D data



2D reduction with t-SNE

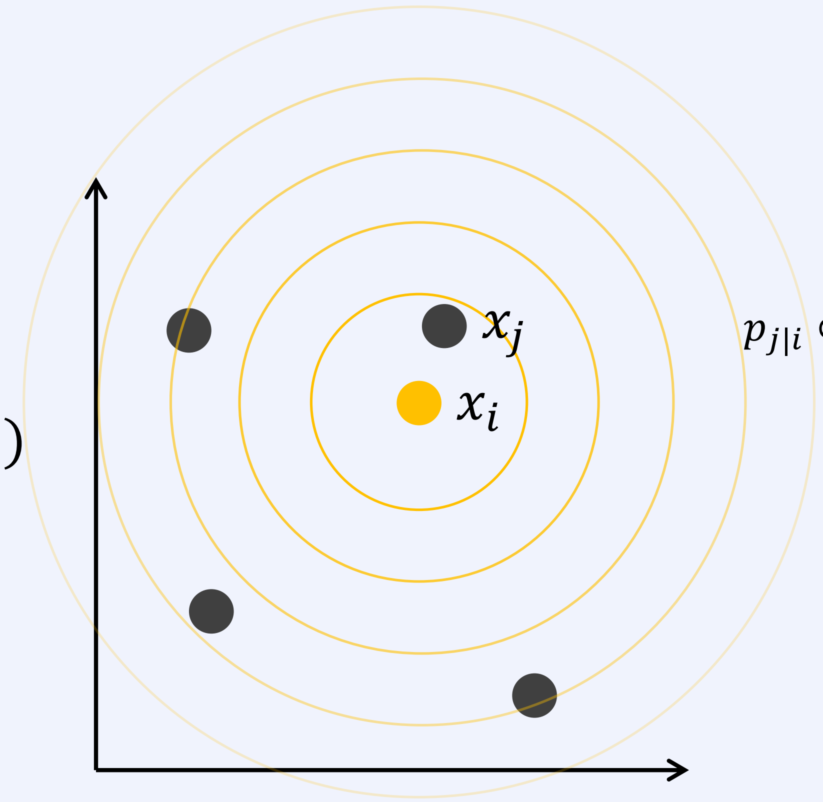


Stochastic Neighbor Embedding



1 High-Dimensional Similarities

$$P_i \propto N(x_i, \sigma_i)$$



$$p_{j|i} \propto \exp\left(-\frac{\left\|x_j - x_i\right\|^2}{2\sigma_i^2}\right)$$

1 High-Dimensional Similarities

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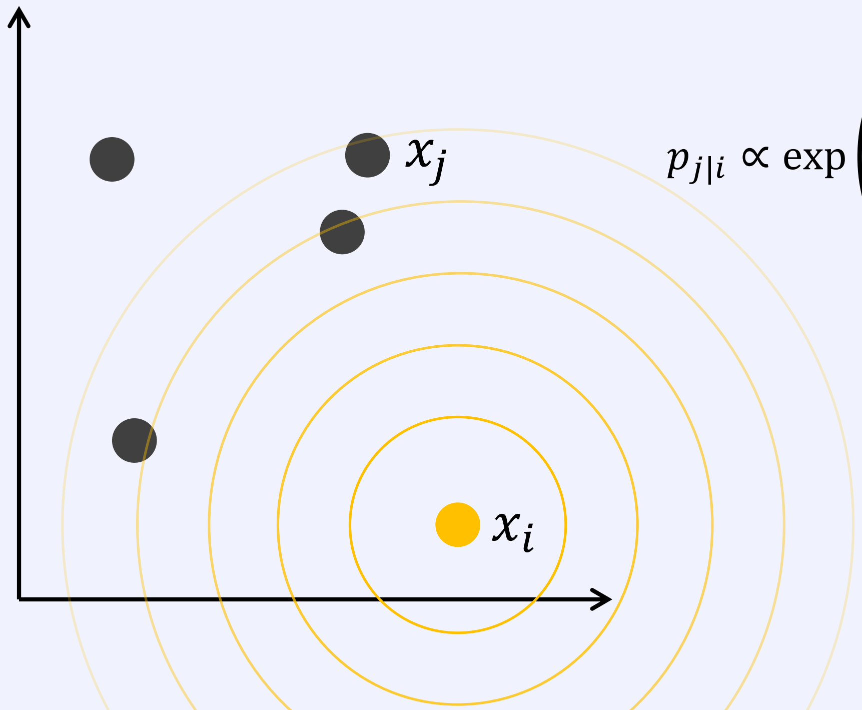


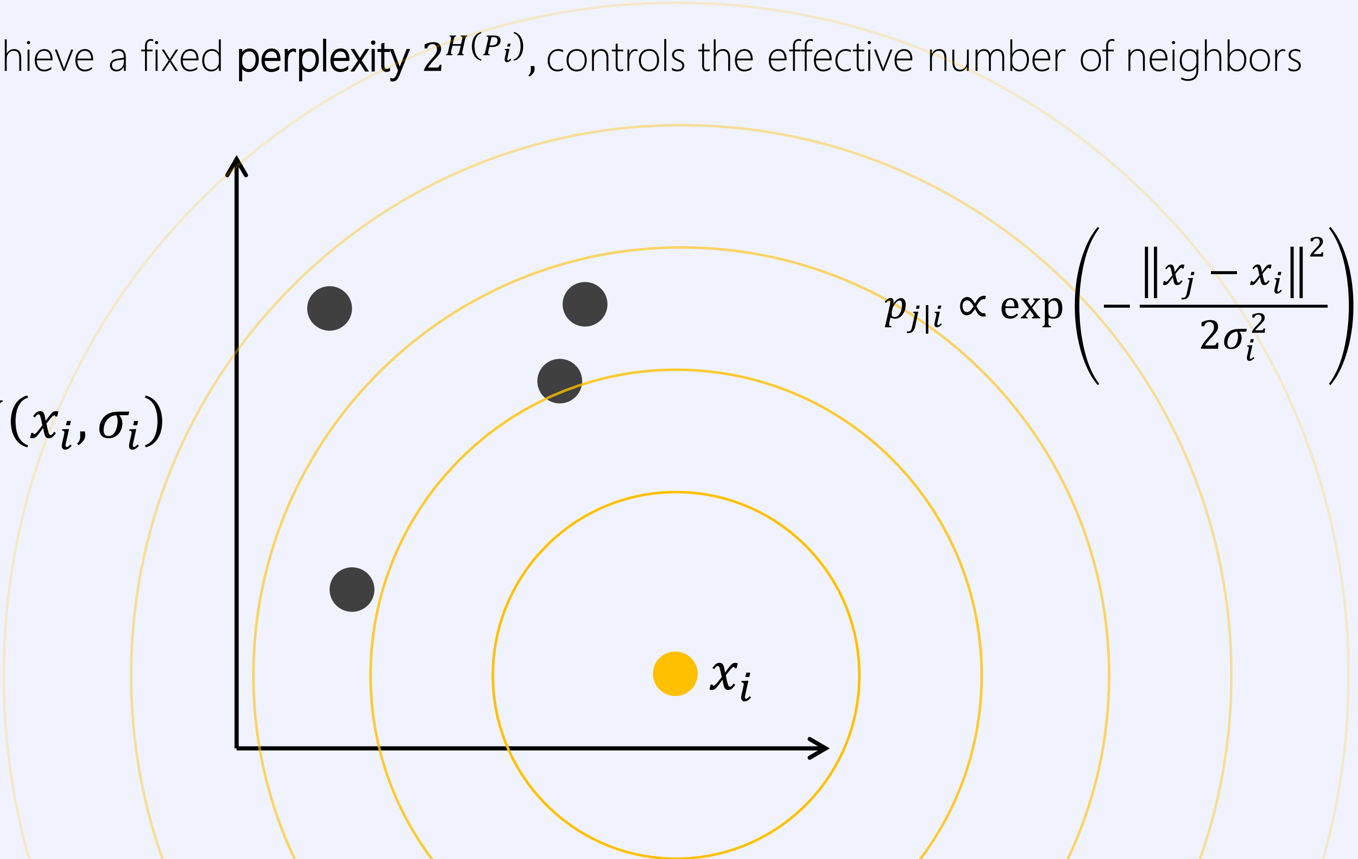
$$p_{j|i} \propto \exp\left(-\frac{\left\|x_j - x_i\right\|^2}{2\sigma_i^2}\right)$$

1 High-Dimensional Similarities

Choose σ_i to achieve a fixed **perplexity** $2^{H(P_i)}$, controls the effective number of neighbors

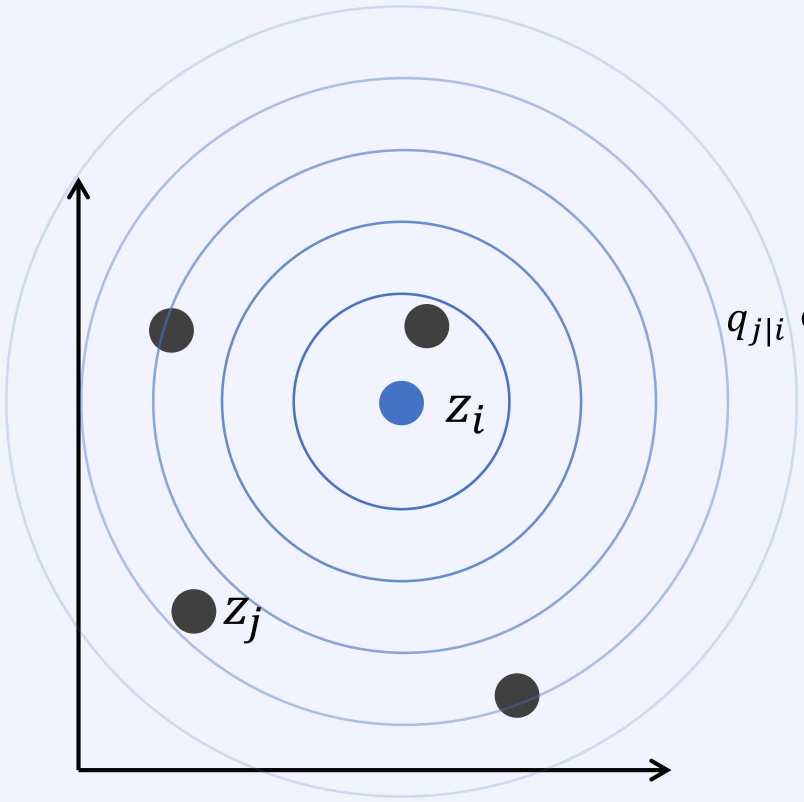
$$P_i \propto N(x_i, \sigma_i)$$

$$p_{j|i} \propto \exp\left(-\frac{\left\|x_j - x_i\right\|^2}{2\sigma_i^2}\right)$$



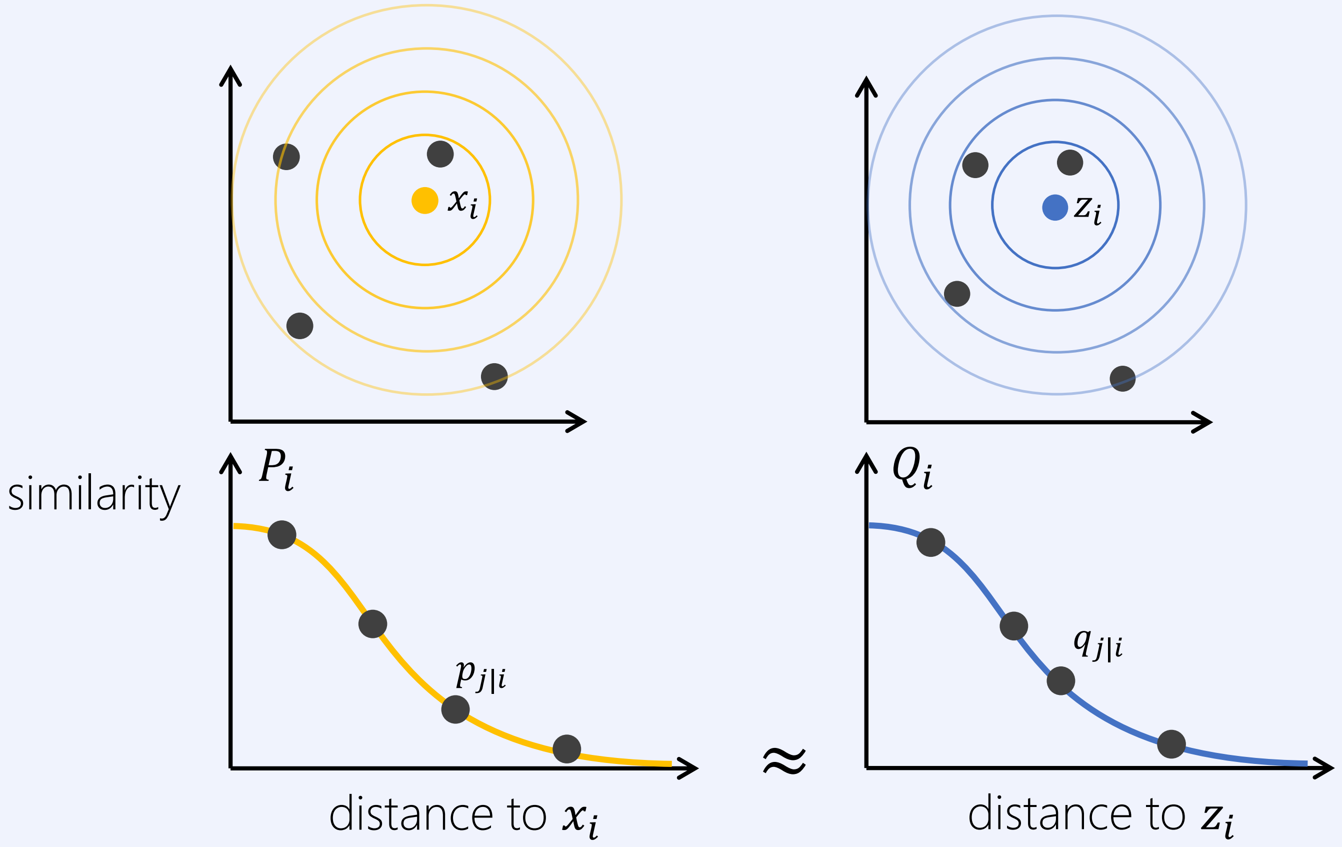
2 Low-Dimensional Similarities

$$Q_{j|i} \propto N\left(z_i, \frac{1}{\sqrt{2}}\right)$$



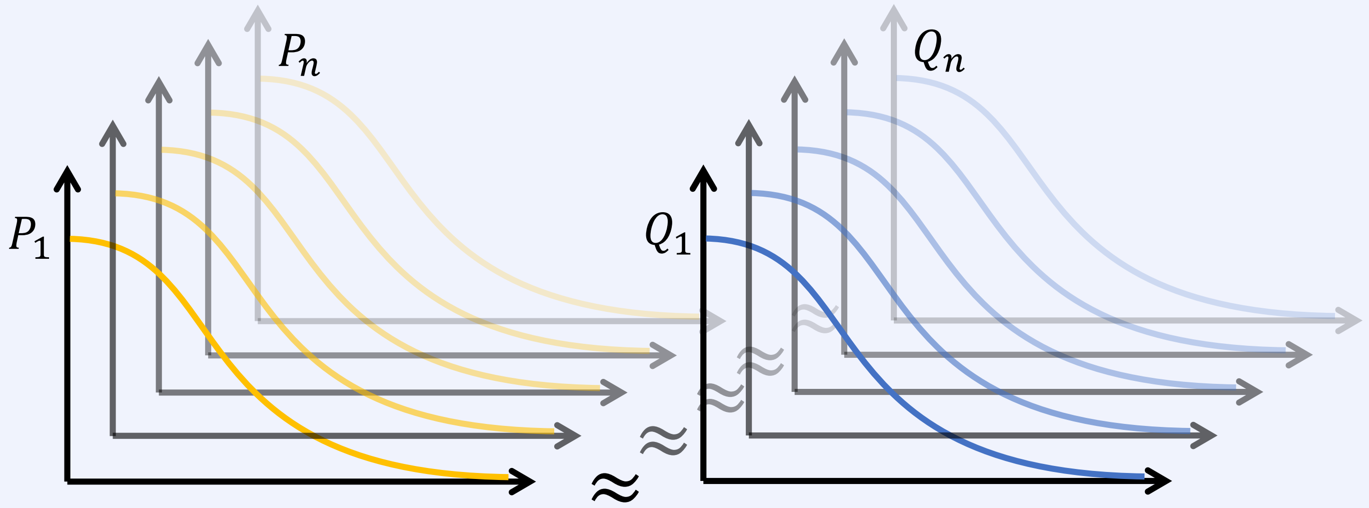
$$q_{j|i} \propto \exp\left(-\frac{\left\|z_j - z_i\right\|^2}{2}\right)$$

3 Comparing Distributions


x_i
z_i
similarity
P_i
Q_i
$p_{j|i}$
$q_{j|i}$
$\approx$
distance to $\boldsymbol{x_i}$
distance to $\boldsymbol{z_i}$

3 Comparing Distributions

Find an embedding $\boldsymbol{Z}$ minimizing the difference between all P_i, Q_i distributions



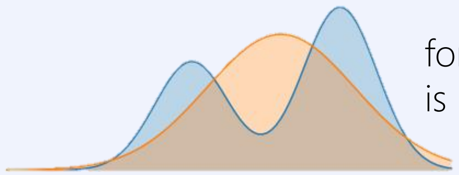
3 Comparing Distributions with KL divergence

The KL divergence is a principled way to measure the “distance” between distributions

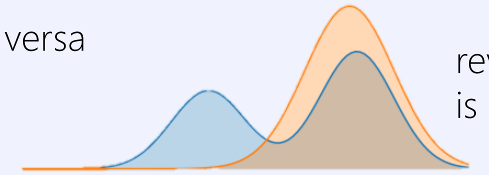
$$C_i = KL(P_i \parallel Q_i) = H(P_i, Q_i) - H(P_i) = \sum_{i \neq j} p_{j|i} \cdot \log \frac{p_{j|i}}{q_{j|i}}$$

expected #bits to encode P_i using Q_i expected #bits to encode P_i

example: given P optimize Q



forward $KL(P_i||Q_i)$
is **mean**-seeking



reverse $KL(Q_i||P_i)$
is **mode**-seeking

Properties of KL

- $KL(P_i \parallel Q_i) \geq 0$ for any P_i and Q_i
- $KL(P_i \parallel Q_i) = 0$ iff $P_i = Q_i$
- is asymmetric $KL(P_i \parallel Q_i) = KL(Q_i \parallel P_i)$
- large penalty when small $q_{j|i}$ for a large $p_{j|i}$ but not vice versa

Stochastic Neighbor Embedding (SNE) Summary

Go from distances in high-dimensional space to conditional probabilities

- $p_{j|i}$ is the probability that data point $\boldsymbol{x}_i$ "wants" data point $\boldsymbol{x}_j$ as its neighbour
- $q_{j|i}$ is the probability that transformed point $\boldsymbol{z}_i$ "wants" point $\boldsymbol{z}_j$ to be its neighbour
- variances $\boldsymbol{\sigma}_i$ are picked such that each point has "approximately the same number of neighbors"

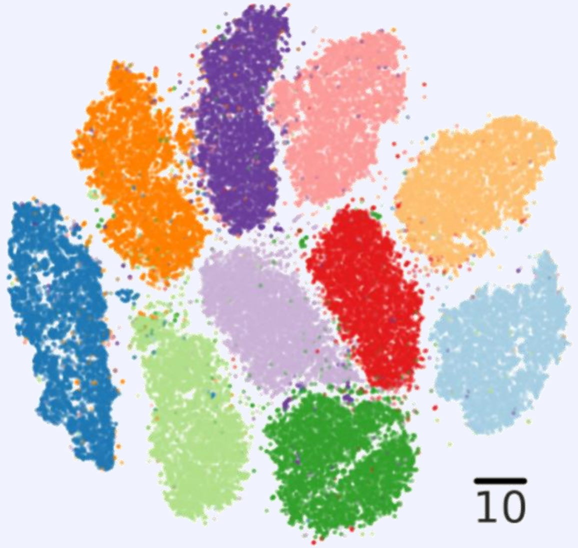
Find $\boldsymbol{z}_i$'s such that neighborhood probabilities are similar to those in original space

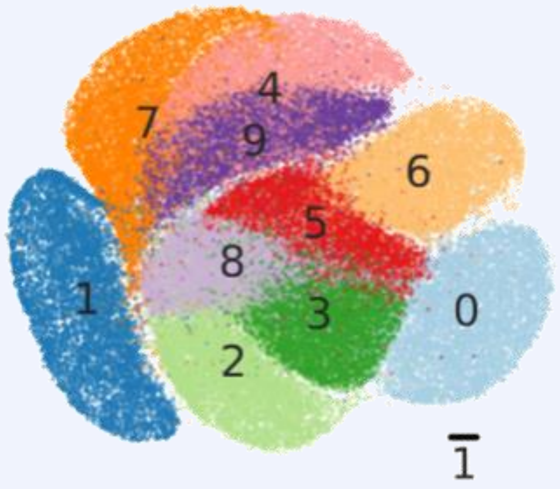
Use KL divergence to measure the "distance" between neighborhood probabilities

Use gradient descent to find z_i, $\frac{\partial C_i}{\partial z_i} = 2\sum_j \left(p_{j|i} - q_{j|i} + p_{i|j} - q_{i|j}\right)(z_i - z_j)$

- can be interpreted as force based layout

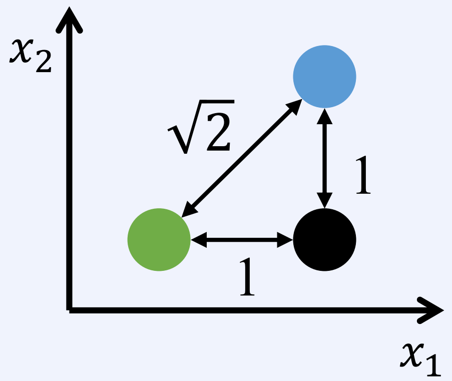
The Crowding Problem

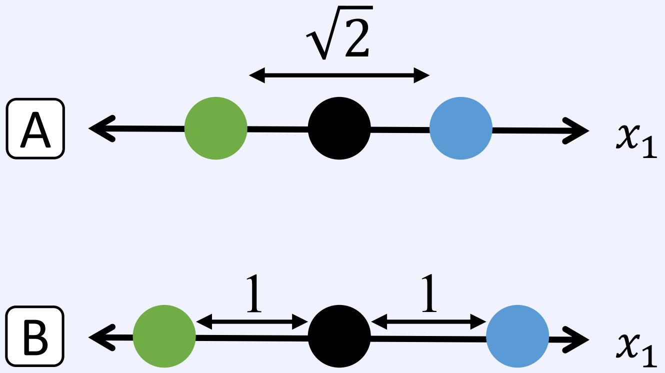




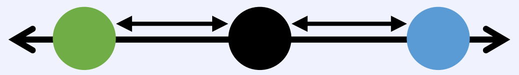
(Kobak et al. "Heavy-tailed kernels reveal a finer cluster structure in t-SNE visualisations", 2019) 36

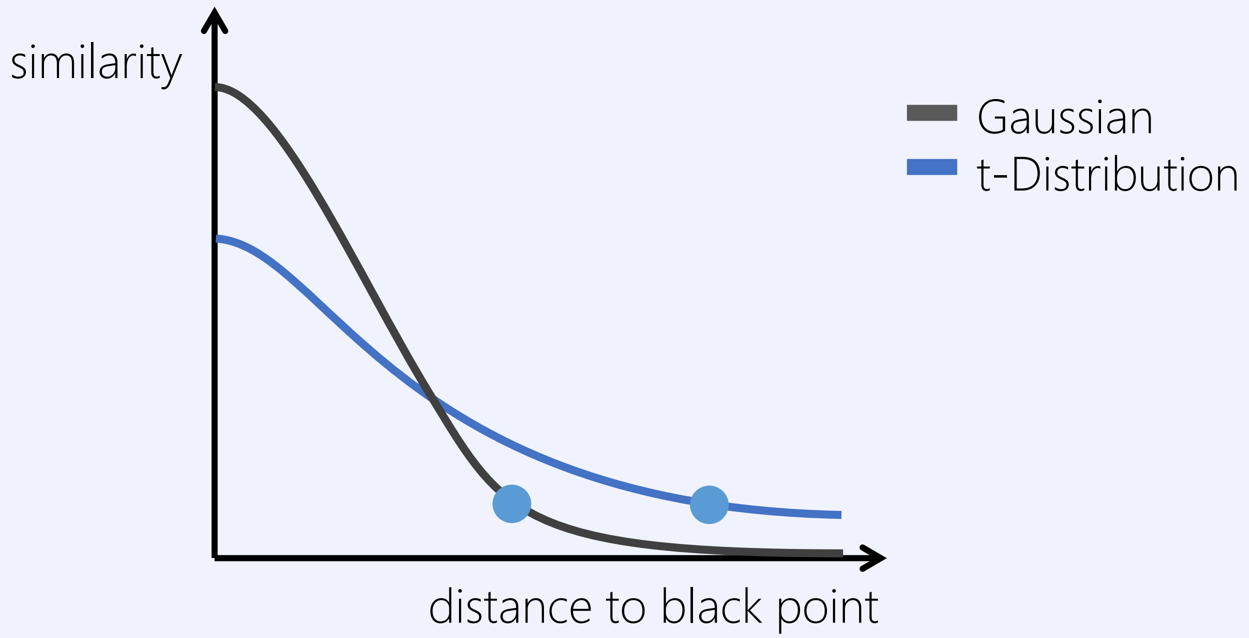
The Crowding Problem



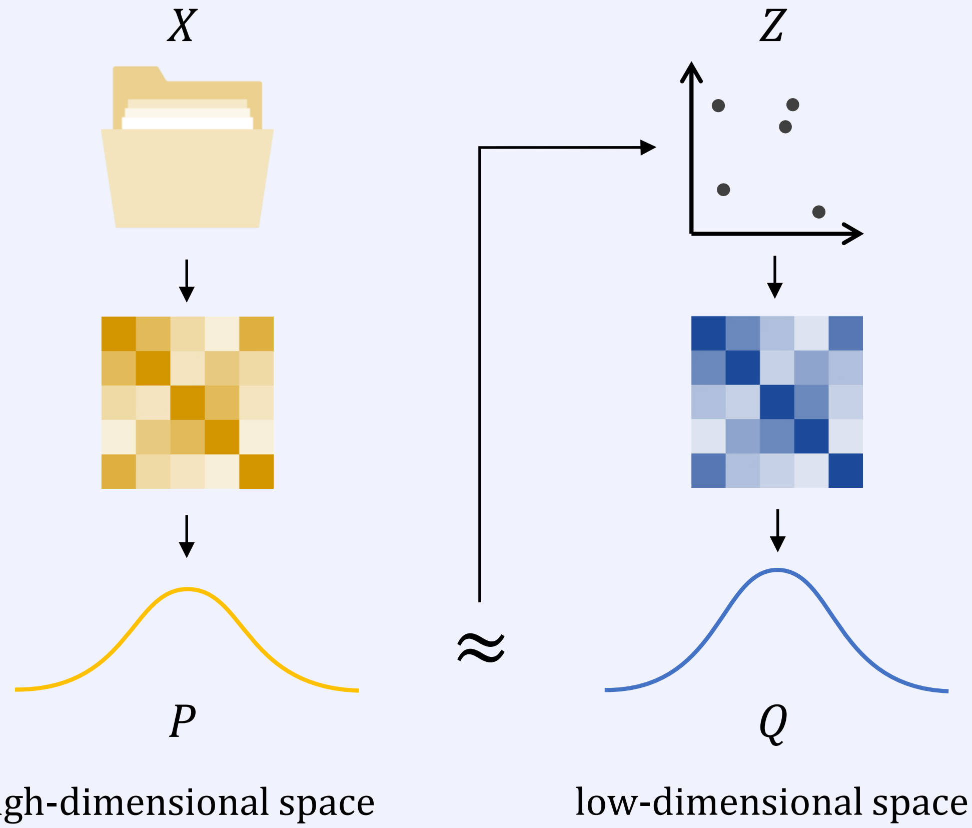


Solving the Crowding Problem



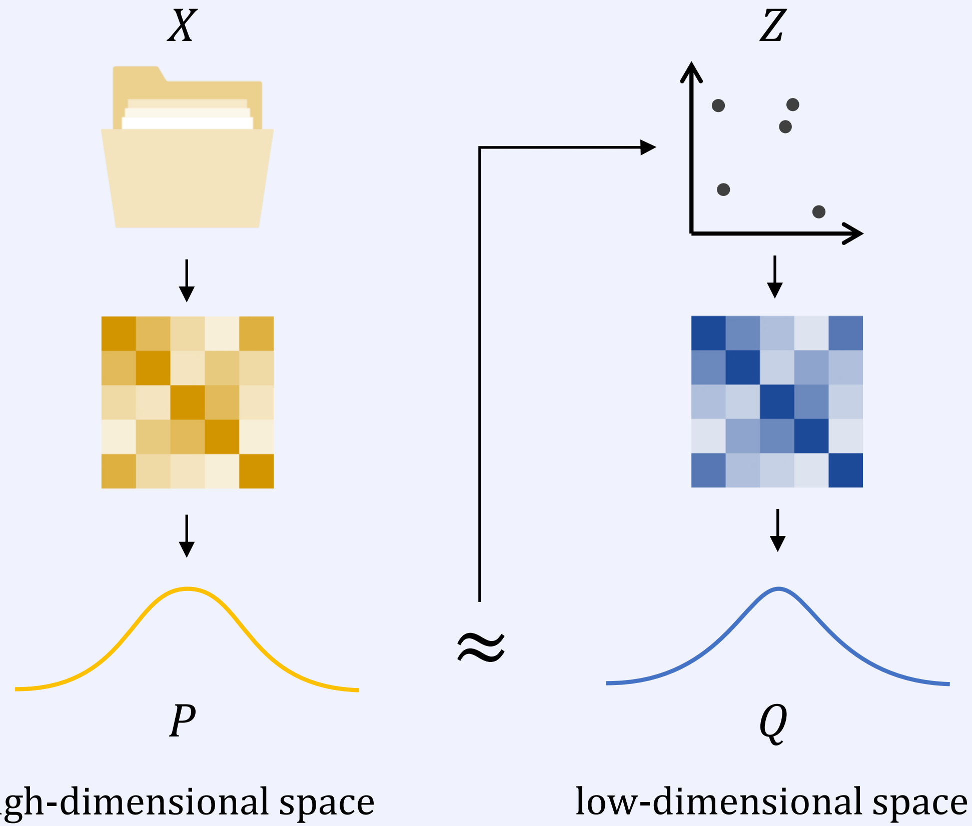


Stochastic Neighbor Embedding



(Hinton & Roweis, 2002)

t-distributed Stochastic Neighbor Embedding



(van der Maarten & Hinton, 2008)

From SNE to t-SNE

Use a **symmetric** distance function and **joint** instead of conditional probabilities

- One main P and Q by symmetrizing and normalizing $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2n}$ and set $p_{ii} = 0$
- $C = KL(P \| Q) = \sum_{i,j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$
- makes the optimization problem easier to solve

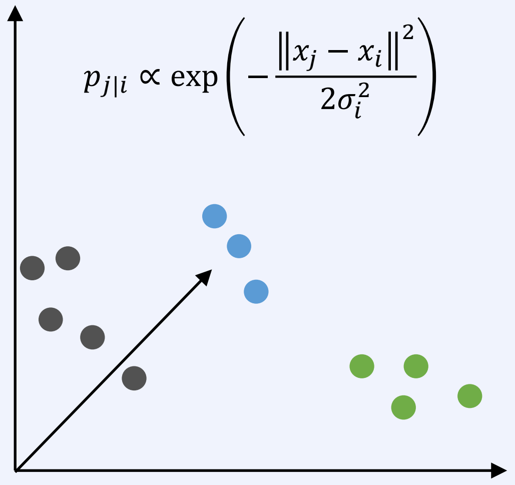
Use t-distributions for the (lower dimensional) map space $q_{ij} = \frac{(1+\|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l}(1+\|y_k - y_l\|^2)^{-1}}$

- heavier (compared to Gaussian) tail of t-distribution compensates for less space in lower dimensions
- volume of a ball scales with r^d so discrepancy in available space gets more pronounced as r grows.
- helps to avoid "crowding" effect and more faithfully reflect longer range structure

(van der Maarten & Hinton, 2008)

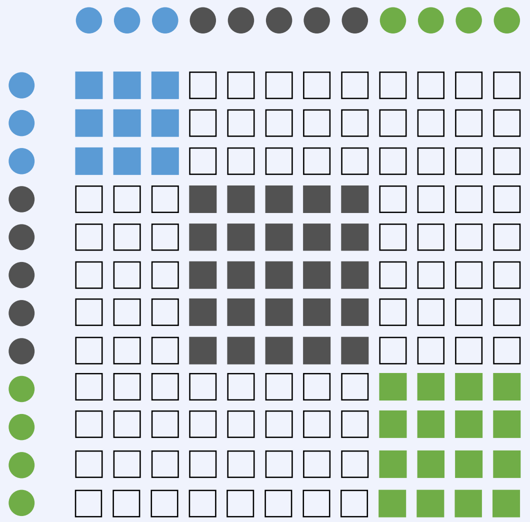
Another interpretation of SNE and t-SNE

Preserve **neighborhood** graph: low. dim neighbors as similar as possible to original neighbors



$$p_{j|i} \propto \exp\left(-\frac{\|x_j - x_i\|^2}{2\sigma_i^2}\right)$$

high dimensional data



neighbor / similarity graph

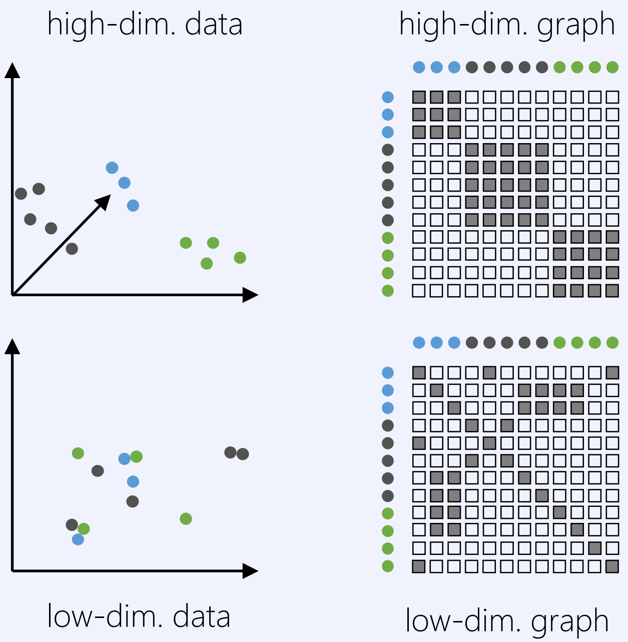
Another interpretation of SNE and t-SNE

Preserve **neighborhood** graph: low. dim neighbors as similar as possible to original neighbors

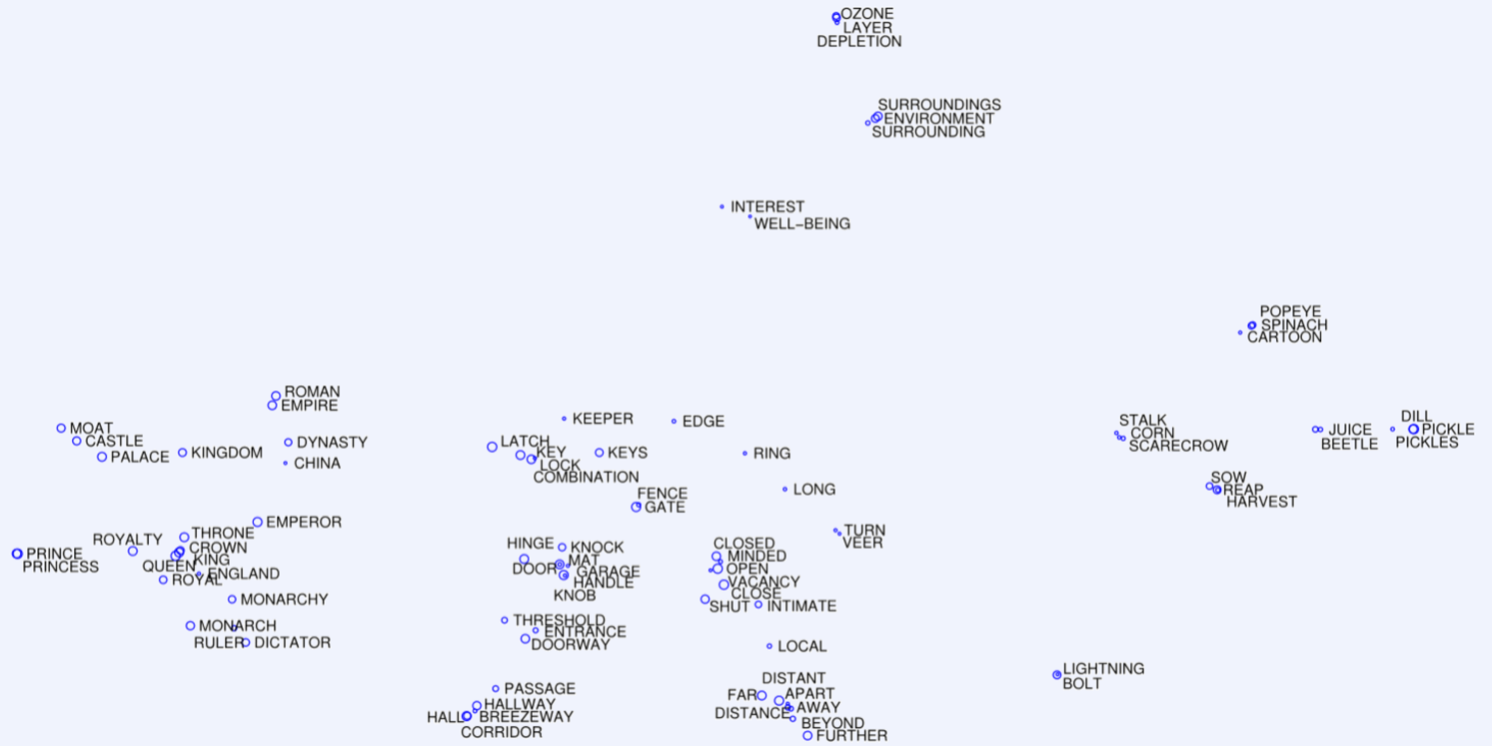
- construct neighborhood graph in high-dim. space
- initialize points in low-dim. Space
- construct neighborhood graph in low-dim space
- optimize coordinates so the two graphs look the same

Computing all pairwise distances can be very slow

Idea: (Approximately) compute only k nearest neighbors

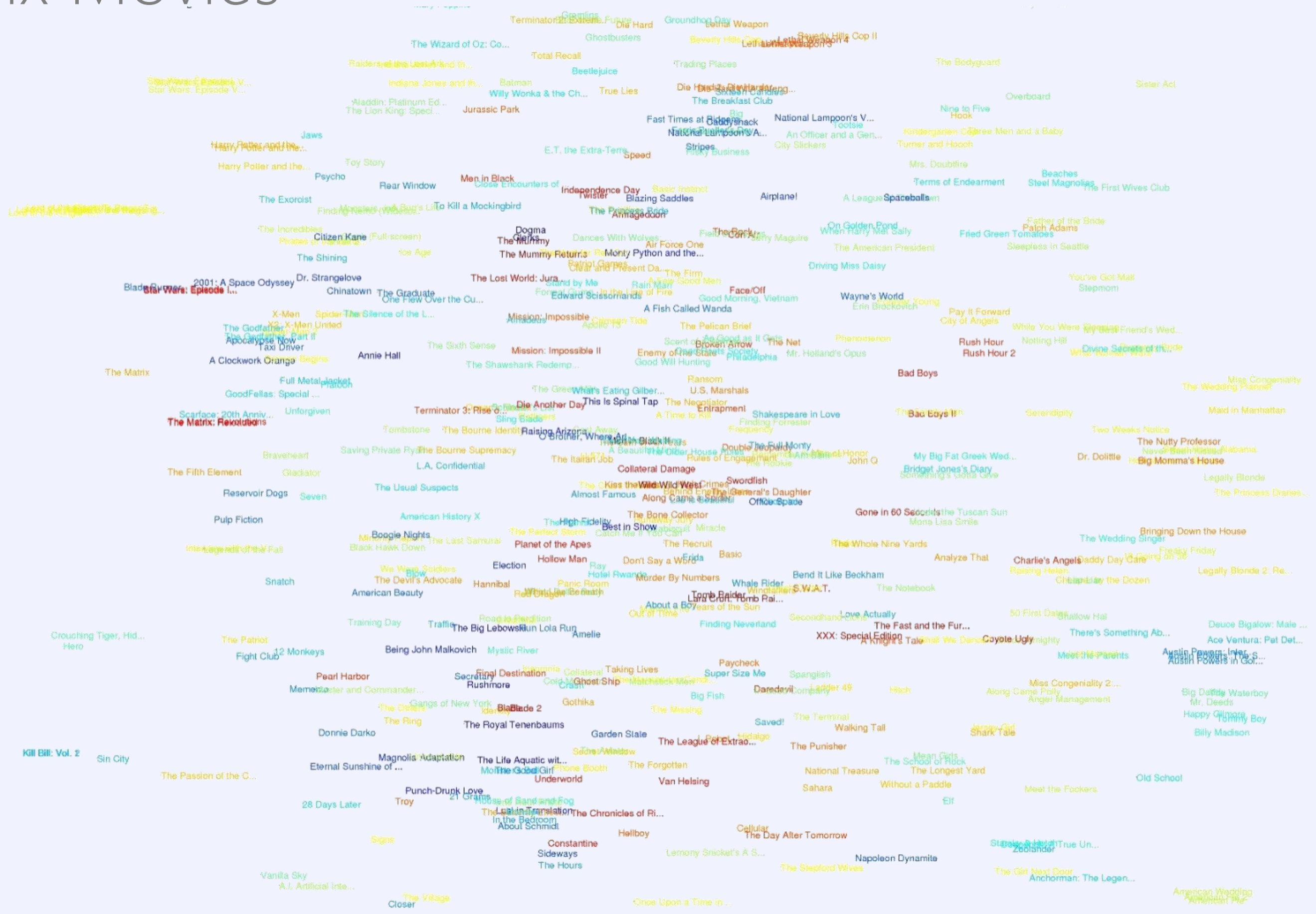


Word Association Data

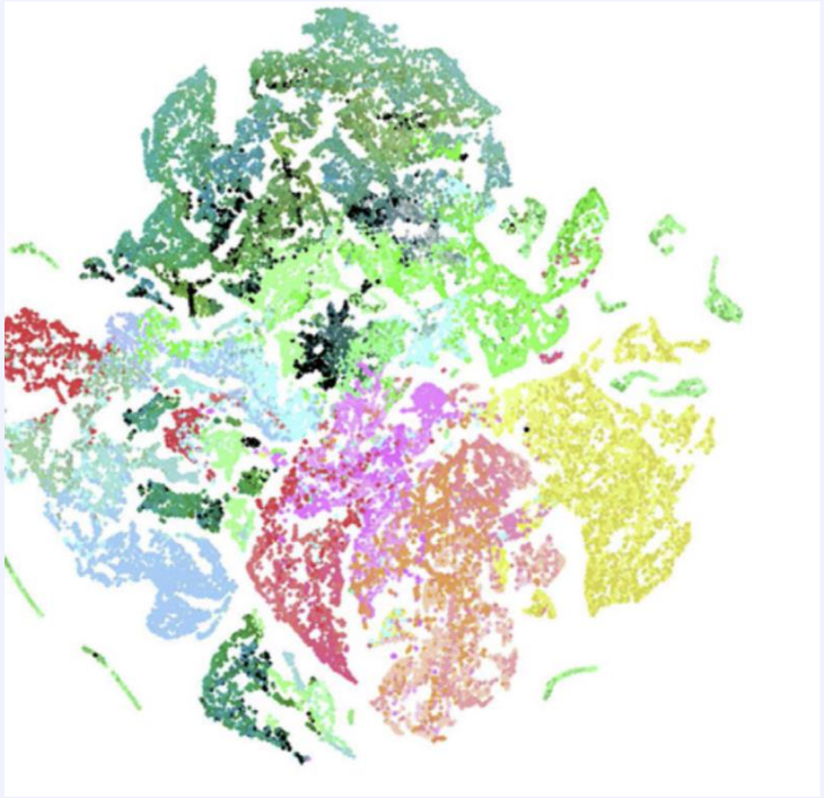


https://lvdmaaten.github.io/tsne/

Netflix Movies



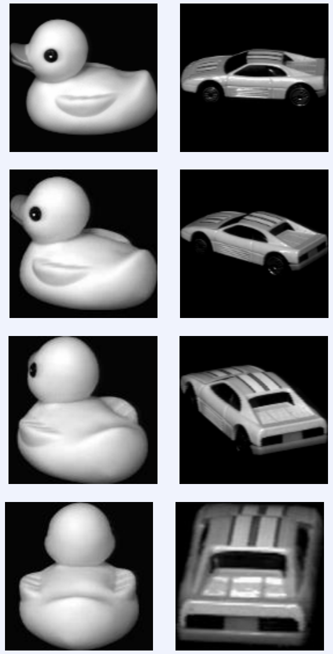
Mouse Brain Cells

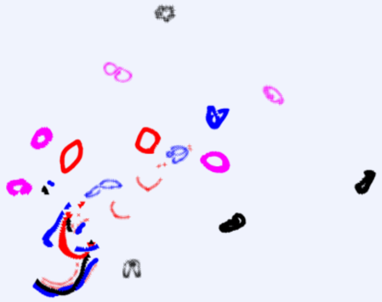


(Mahfouz et al. 2014) 46

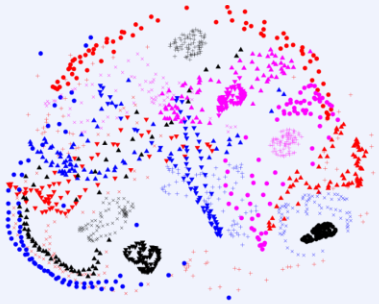
COIL-20 Object Data Set

Examples from COIL-20

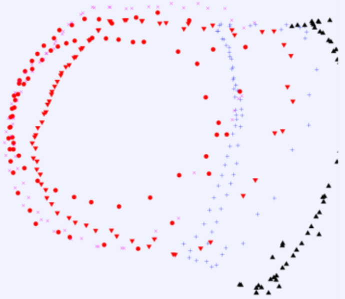




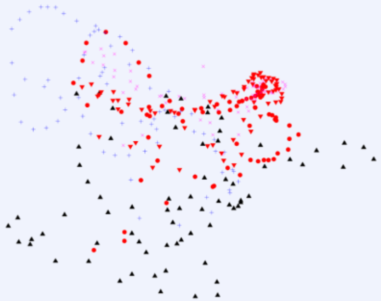
t-SNE



Sammon mapping



Isomap



LLE

Advantages and Disadvantages of t-SNE

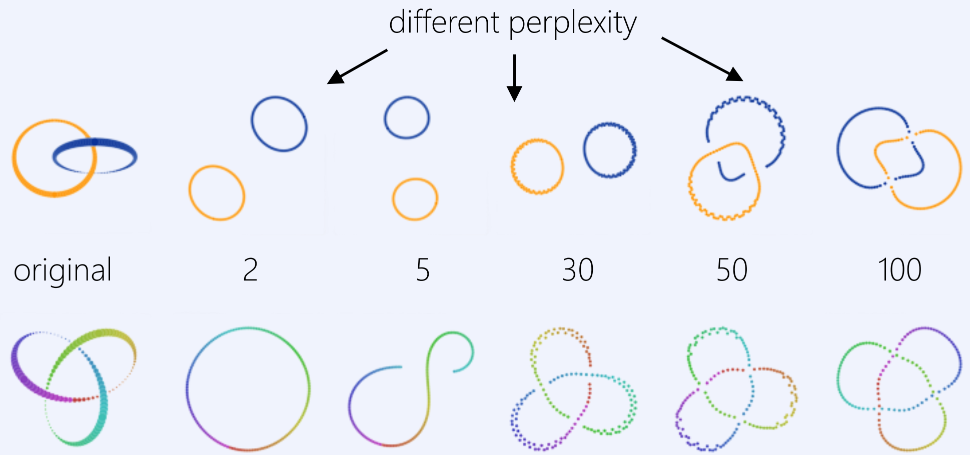
- current standard for visualizing high-dimensional data
- helps understand "black-box" algorithms like DNN
- reduced "crowding problem" with heavy tailed distribution

- t-SNE plots can sometimes be mysterious or misleading
  - Be careful with cluster sizes and cluster distances
- can be sensitive to hyperparameters
- random noise does not always look random
- no easy way to compute the embedding of new data
- not great for more than 3 dimensions

Popular alternative: **U**niform **M**anifold Approximation and **P**rojection (UMAP)

Interactive t-SNE

[Interactive widgets to better understand t-SNE.](#)



Summary

High-dimensional data is challenging in many ways

Goal of dimensionality reduction is to reduce the dimensions while preserving some structure

PCA is linear transformation that preserves the global structure
- finds the hyperplane that maximizes variance of the data / minimizes distance to projection

MDS directly preserves distances

t-SNE preserves similarity between datapoints defined by e.g. a Gaussian kernel