Lecture 9

Dimensionality Reduction

ISLR 12, ESL 14, tSNE

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Supervised vs. Unsupervised Learning

We focused mostly on supervised learning, 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 are interested in finding something interesting about the data, such as hidden (latent) structure

- discover patterns, subgroups, or clusters among the variables or observations
- project the data from a high- to a low-dimensional space
- informative ways to visualize the data
- anomaly detection

There also exist other learning paradigms, but these are out of scope for the lecture

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

Unsupervised Learning

Unsupervised learning is exploratory and thus more challenging

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

There are also big advantages

- much easier to obtain large amounts of unlabeled data
- the most interesting tasks are unsupervised in nature, e.g. focused on discovery

Examples

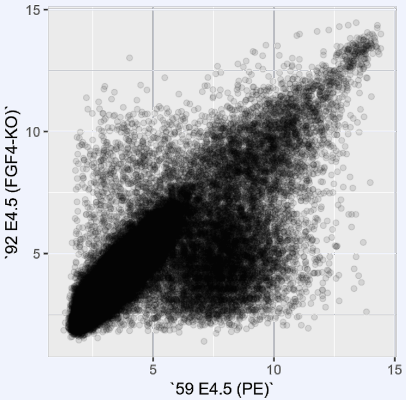
- grouping genomic signatures of cancer samples by subtype
- characterizing shoppers browsing and purchasing habits
- movies grouped by the ratings assigned by movie viewers

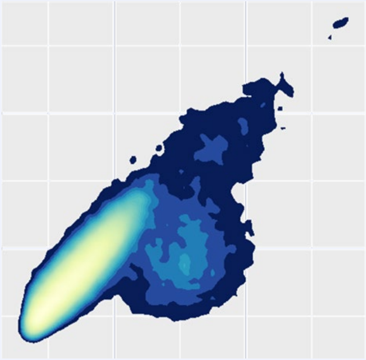
Visual Data Exploration

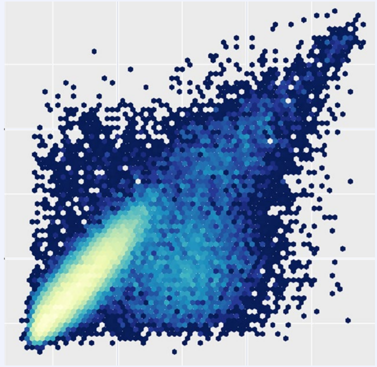
1D data: compute summary statistics: mean, mode, median, quartiles, box-whiskers plot

1D data distribution: histograms, dots and bee-swarm plot, kernel density estimation, violin plot

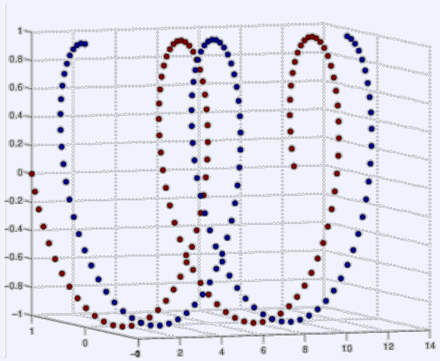
2D data: scatter plots, density plots, hexagon plots



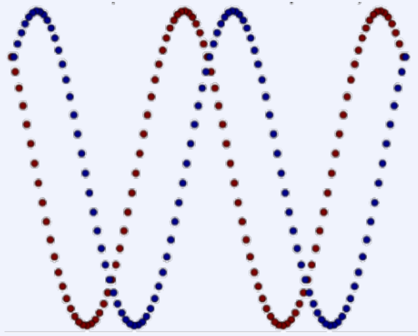




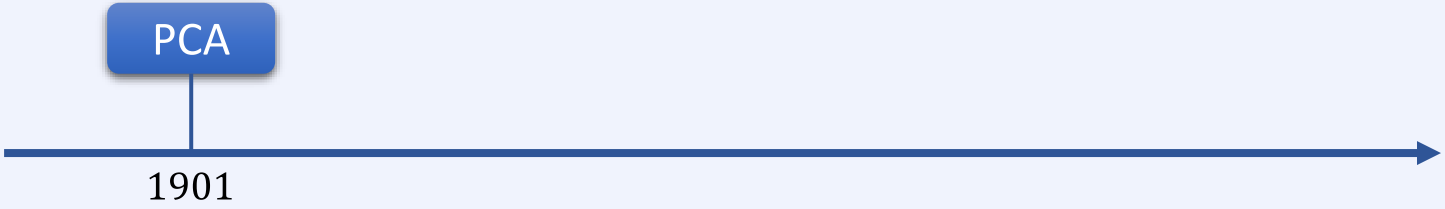
Visualizing more than two dimensions



original 3D data



2D reduction with PCA



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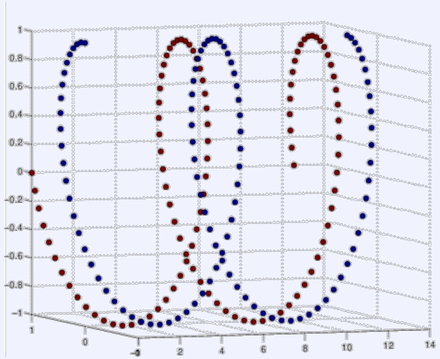

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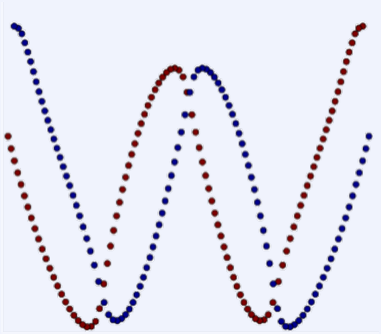
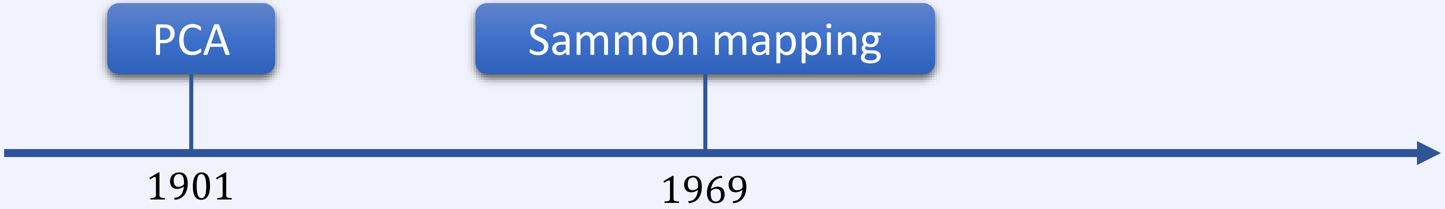
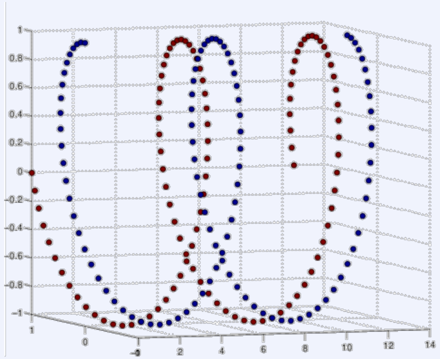


2D reduction with Sammon mapping



Visualizing more than two dimensions



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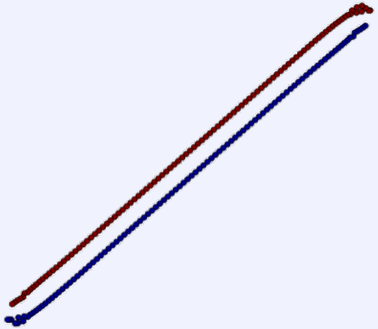
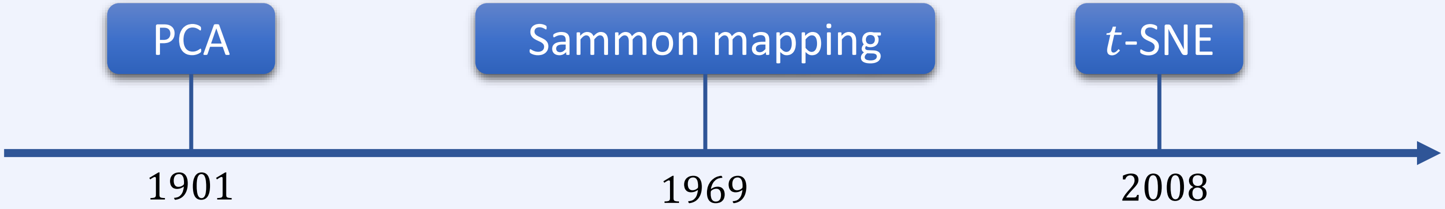


2D reduction with t-SNE



Dimensionality Reduction: Further Motivation

High-dimensional data is highly challenging

- hard to visualize high-dimensional data
- highly correlated dimension cause trouble for many algorithms
- computation is expensive because of high complexity of distance functions

As dimensionality goes up, we are struck by the curse of dimensionality

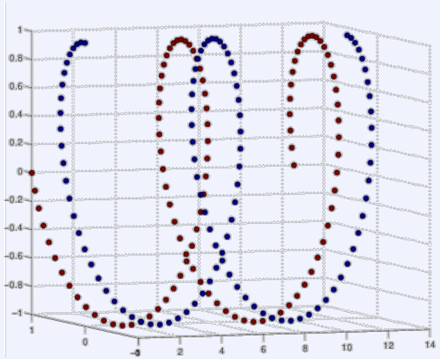
- we need exponential amounts of data to characterize the density
- distances between points become meaningless, they all tend to the same value

Often, however, 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

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

PCA



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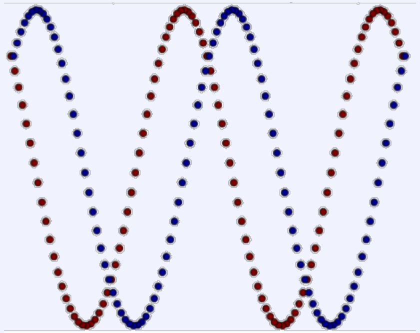
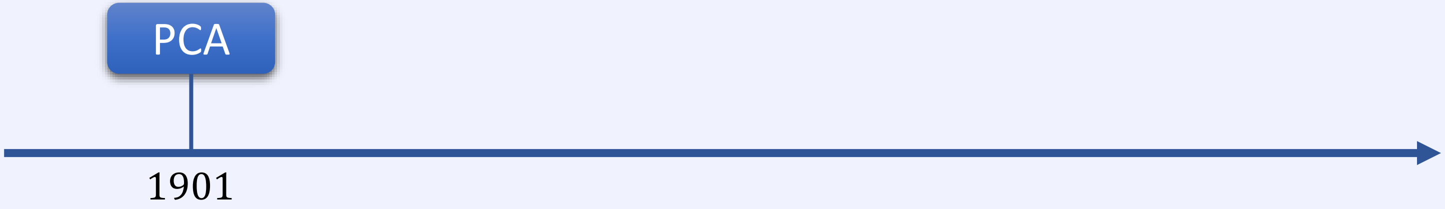


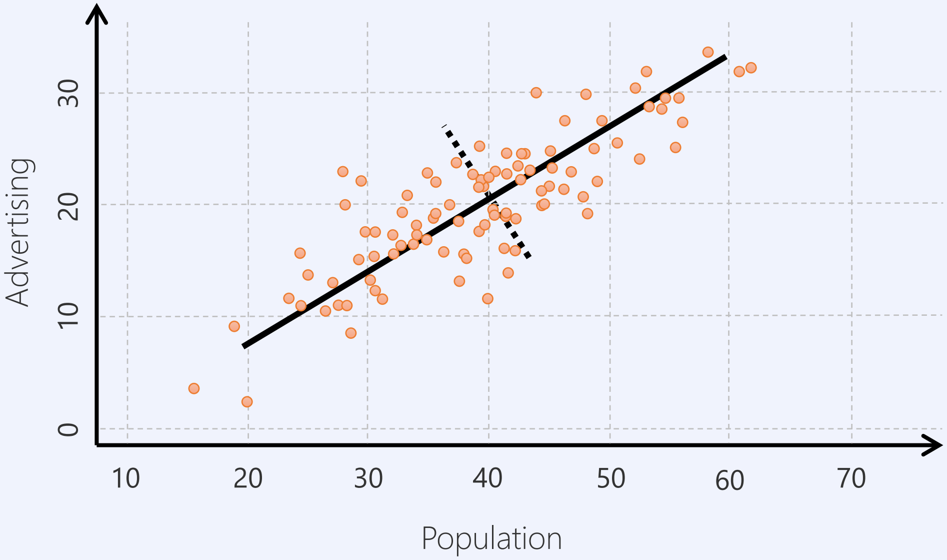
2D reduction with PCA



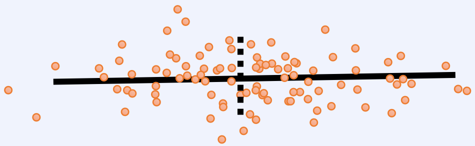
Principal Component Analysis

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

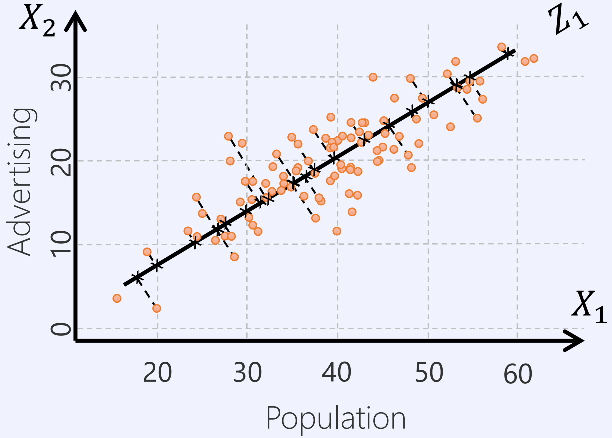
Principal Component Analysis

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 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

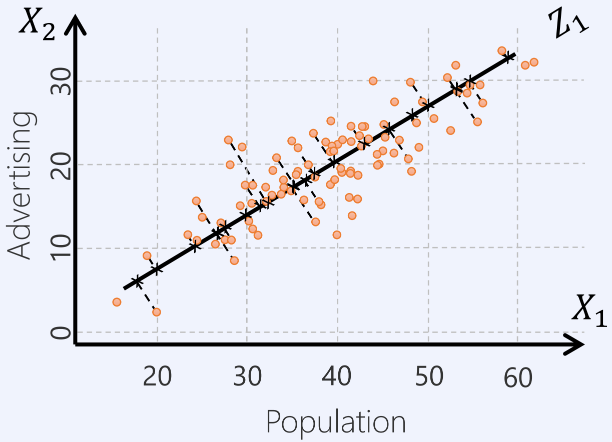
Formally we define the first PC Z_1 as a **linear combination** of mean-centered X_j

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

- 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**

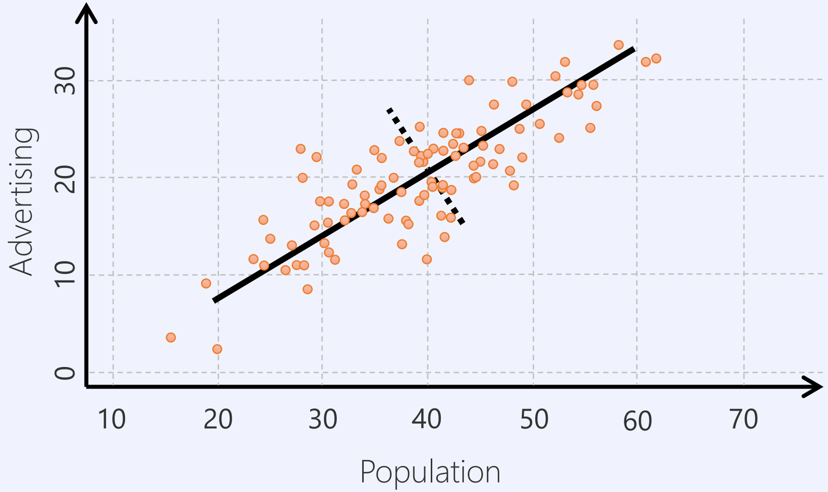
- Solve the following problem subject to the scaling constraint

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



Example Principal Component Analysis

- first PC $Z_1 = 0.839(\textbf{pop} - \overline{\textbf{pop}}) + 0.544(\textbf{ad} - \overline{\textbf{ad}})$
- we call the coefficients $\phi_{11} = 0.839, \phi_{21} = 0.544$ the component loadings



Facts

- 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. $Var(\phi_{11}(\textbf{pop} - \overline{\textbf{pop}}) + \phi_{21}(\textbf{ad} - \overline{\textbf{ad}}))$ is maximum
- at the same time first PC is the closest line to the data

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

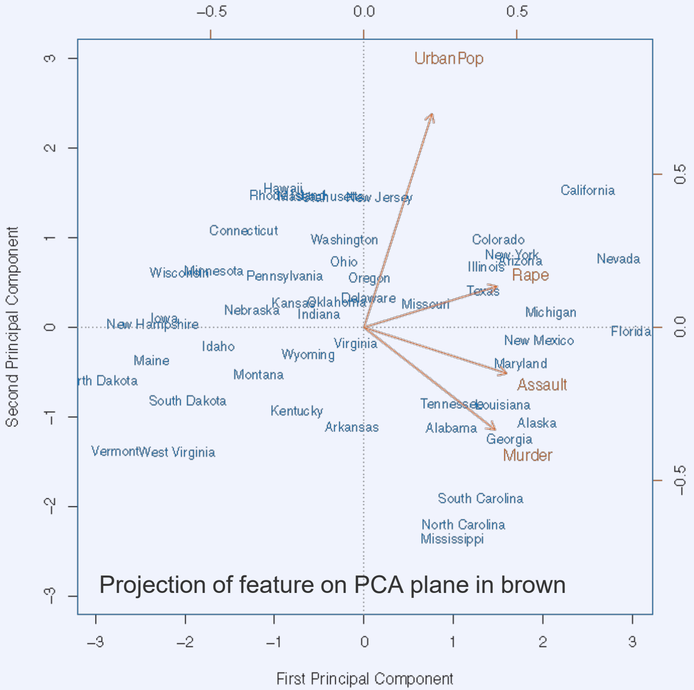
Example Principal Component Analysis

PCA of the **USArrests** dataset

- statistics in arrests per 100,000 residents in the US (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



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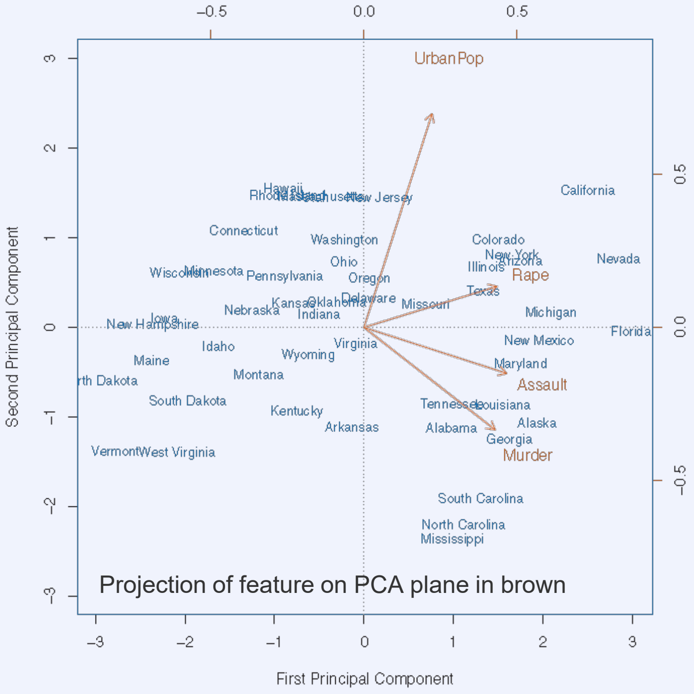
projection of feature vectors on principal component surface



(ISLR 10.2)

Example Principal Component Analysis

Interpretation

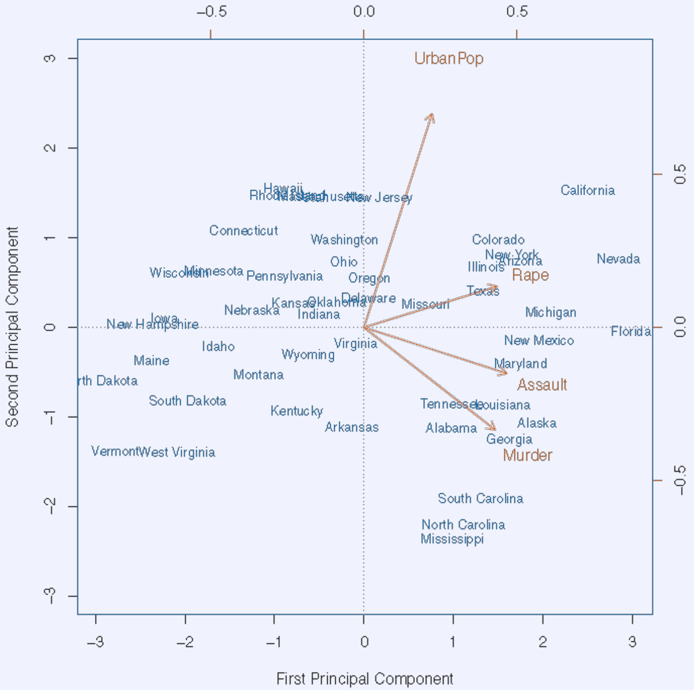
- crime variables are highly correlated
  - projection vectors point in about same direction
- less correlation with **`UrbanPop`**

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



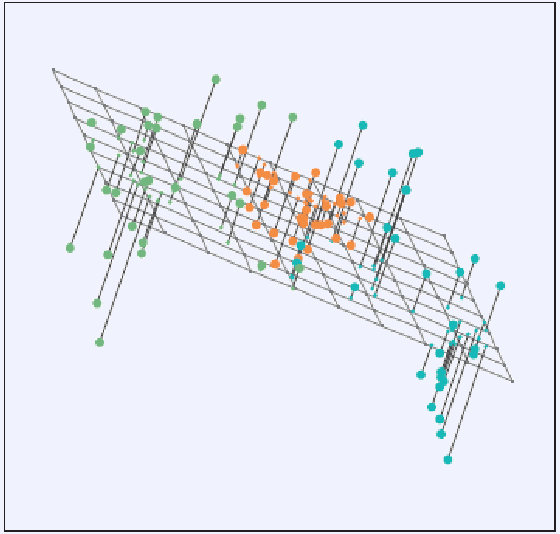
Principal Component Analysis

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

Principal Component Analysis

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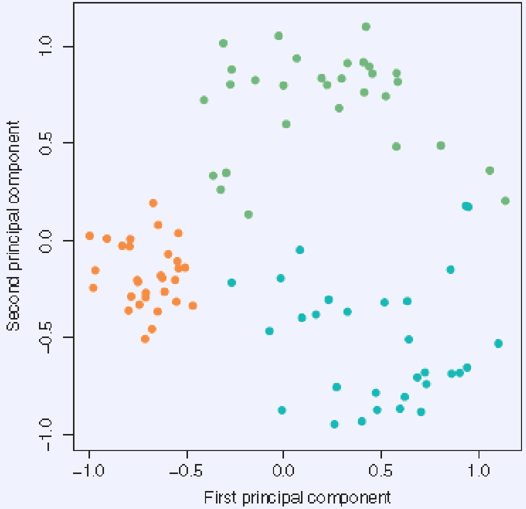


3D simulated dataset with the first two PCs

Interpretation 3

- PCA finds a 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 then 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 $\mathrm{Var}(Z_m)$
- if we select k components, 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

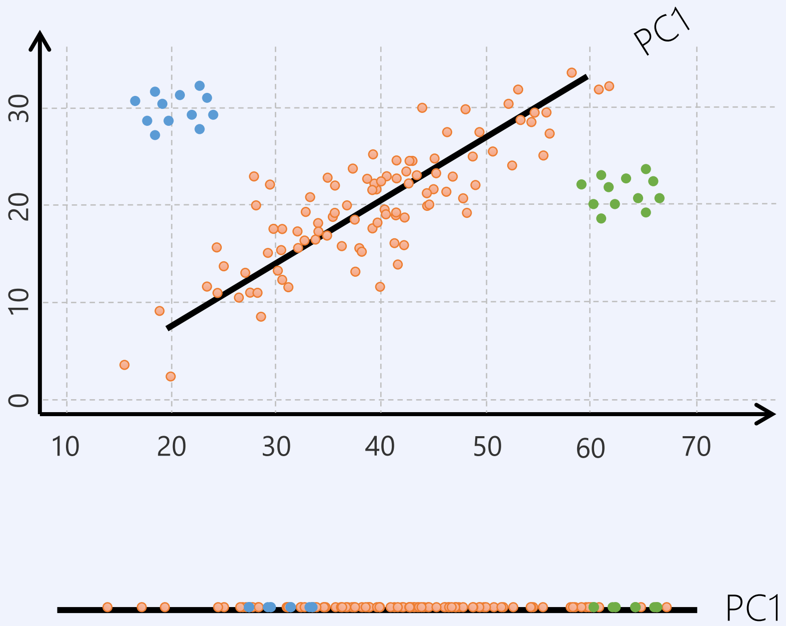
- but only if such an error exists for our actual task…

Principal Component Analysis

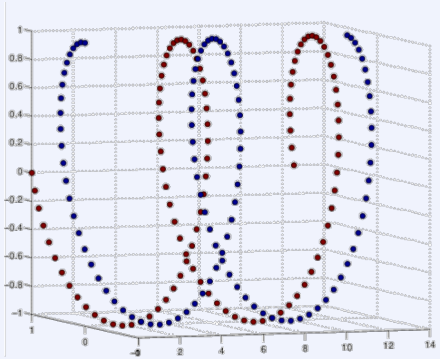
PCA finds the global (linear) structure in the data

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

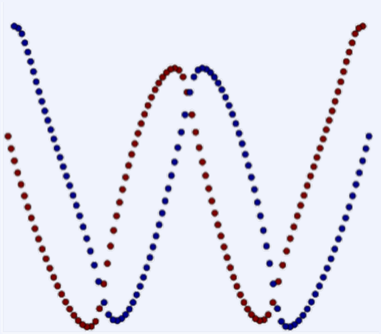
Idea: Preserve local structure (distances) instead



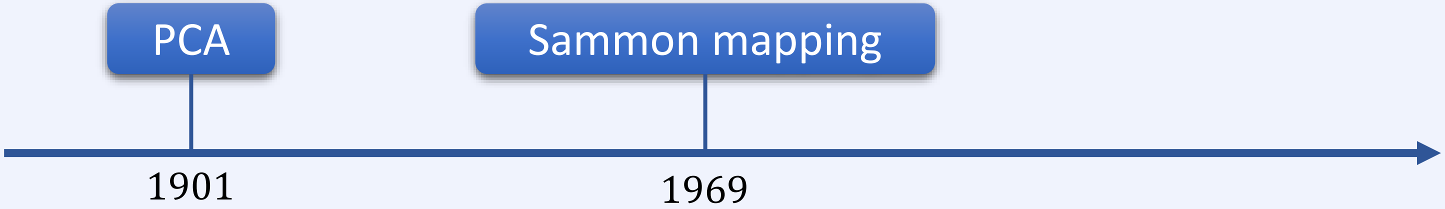
Sammon Mapping (MDS)



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 $x_1, \dots, x_N \in \mathbb{R}^p$
- project onto $z_1, \dots, z_N \in \mathbb{R}^k$
- minimize a stress function S

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

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

- 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

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

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

- 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 actual point coordinates

The non-metric version of Shepard-Kruskal scaling only needs ranks

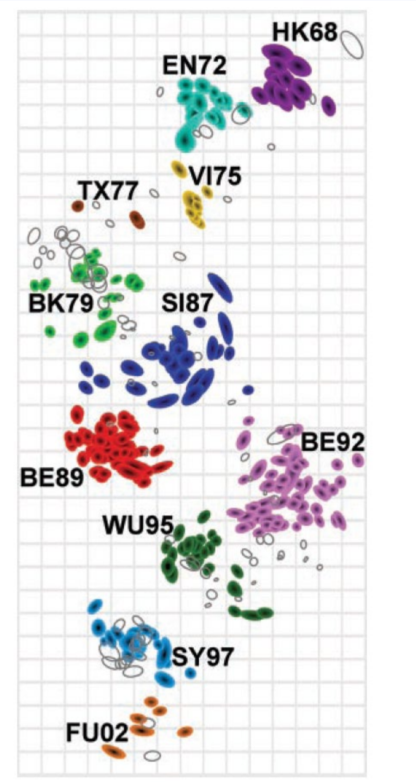
$$S_{NM}(z_1, \ldots, z_N) = \frac{\sum_{i \neq i'} [\|z_i - z_{i'}\| - \theta(d_{ii'})]^2}{\sum_{i \neq i'} \|z_i - z_{i'}\|^2}$$

- 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)

Example Multidimensional Scaling

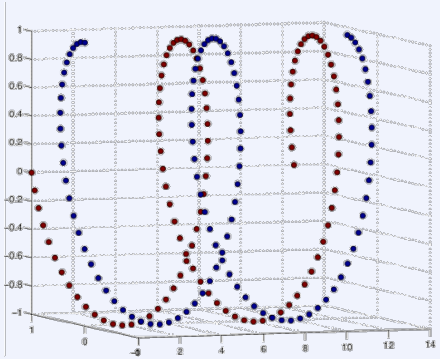
Antigenic shift of influenza virus

- original space has 79 dimensions
- multiple runs of gradient descent with random starting solutions
- level of increase of stress function with decreasing 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)

t-SNE



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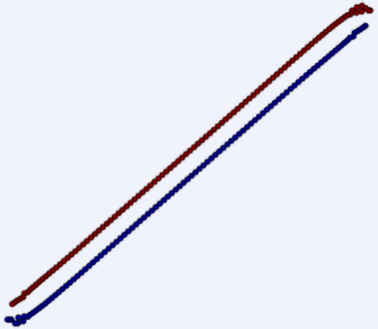
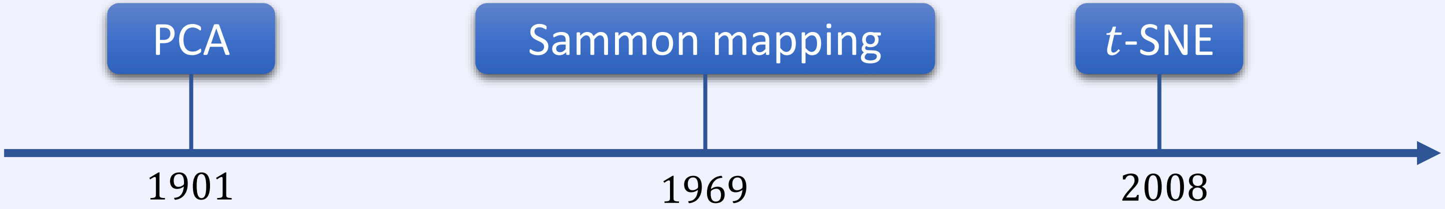
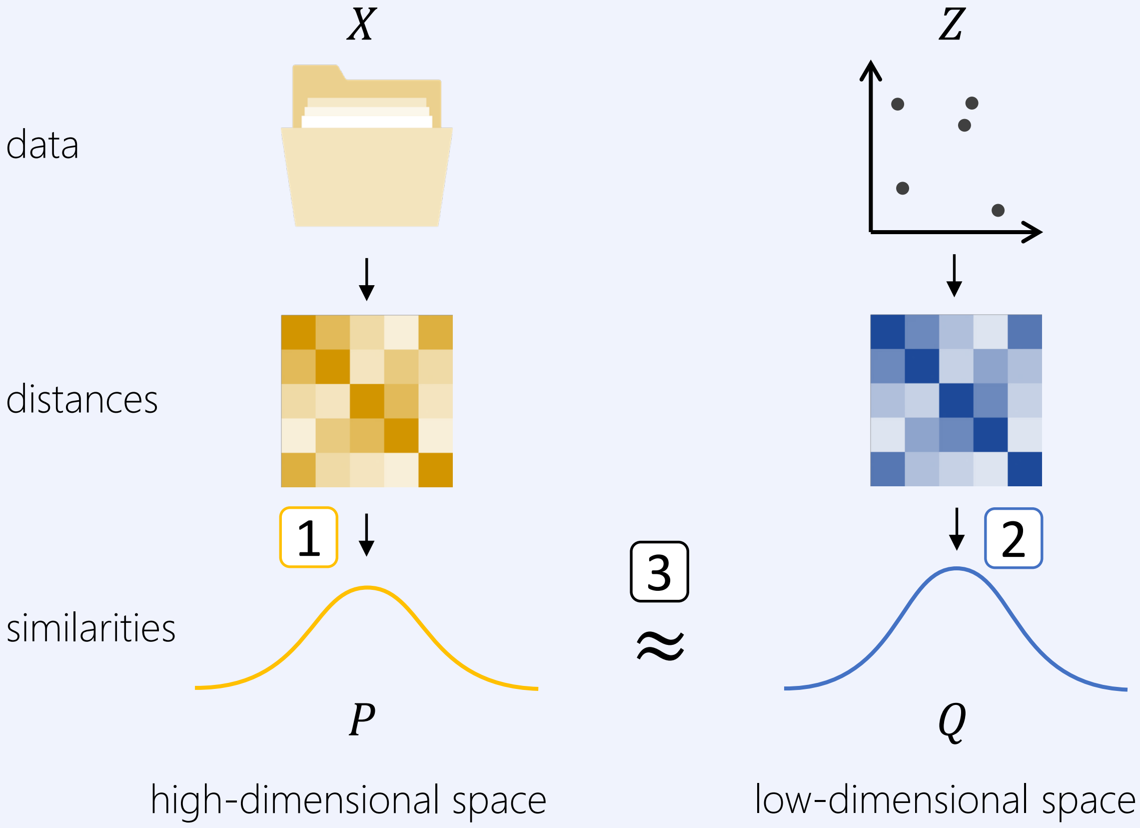


2D reduction with t-SNE

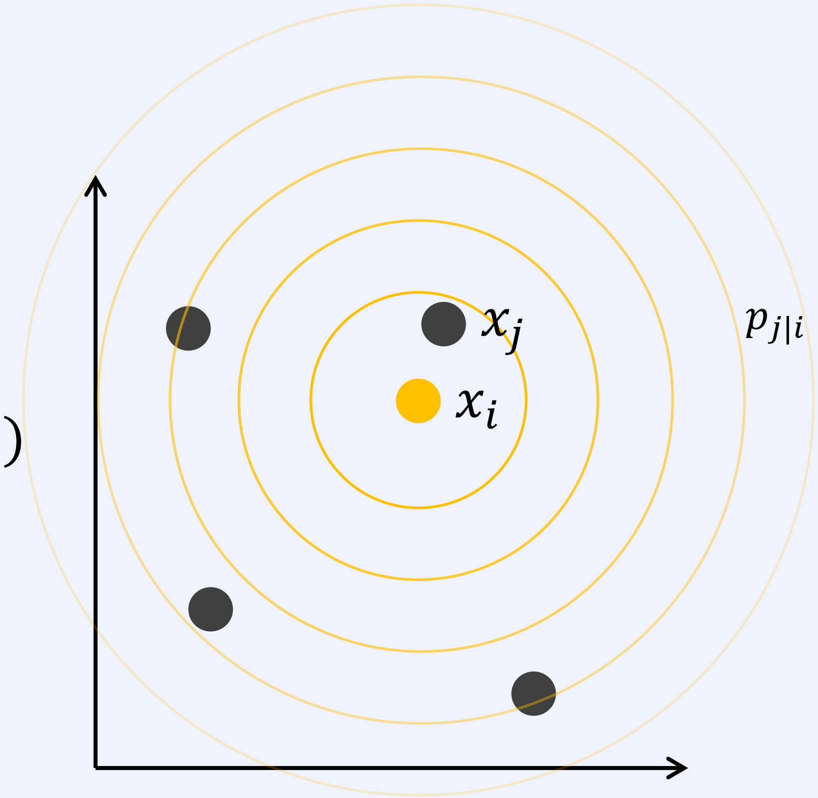


Stochastic Neighbor Embedding



1 High-Dimensional Similarities

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



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

1 High-Dimensional Similarities

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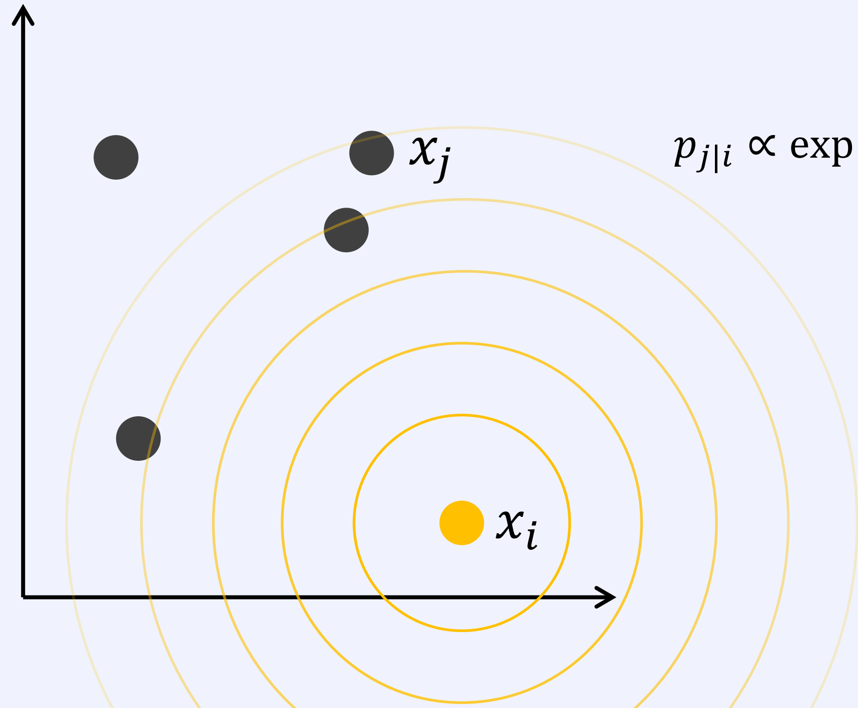
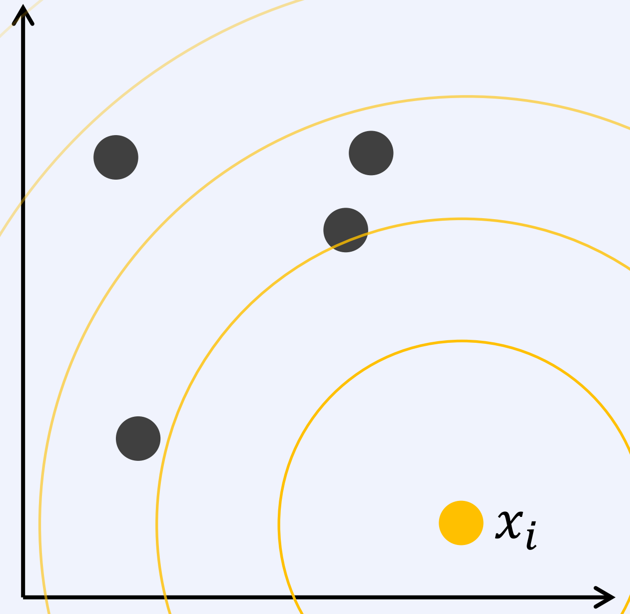


$$p_{j|i} \propto \exp\left(-\frac{\left\|x_j - x_i\right\|^2}{2\sigma_i^2}\right)$$

1 High-Dimensional Similarities

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

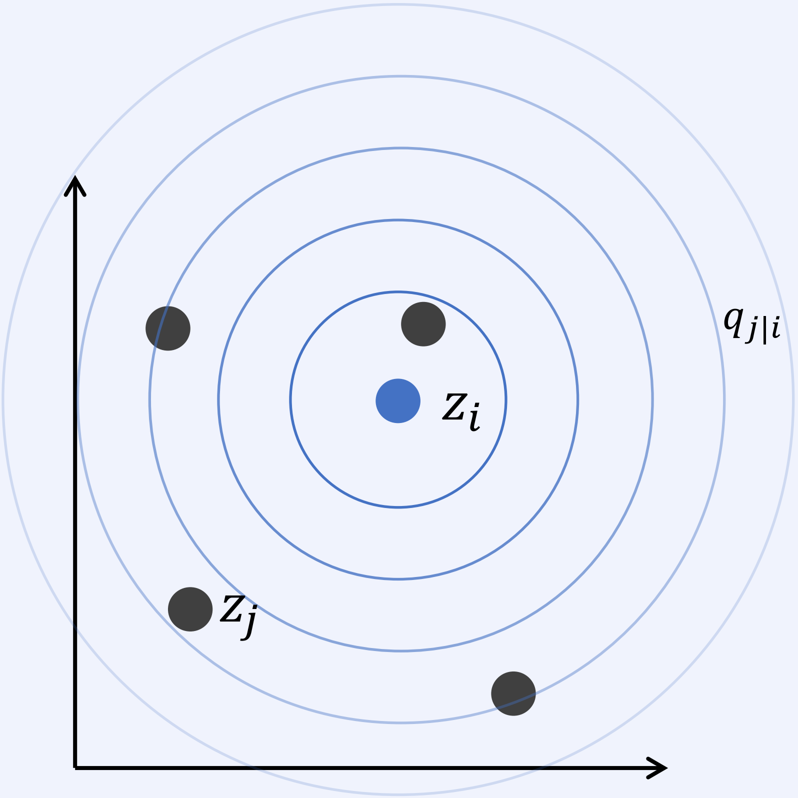
$$P_i \propto N(x_i, \sigma_i)$$



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

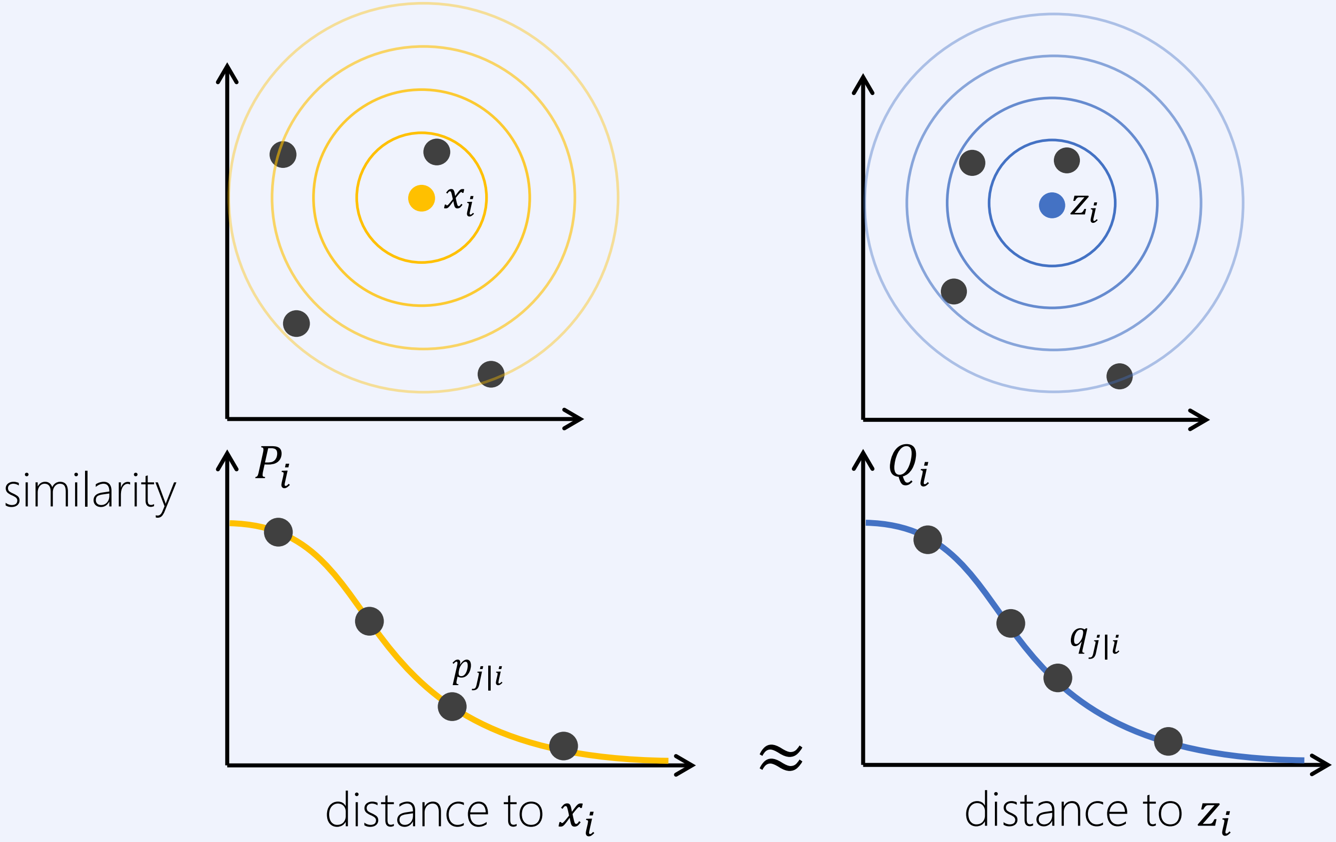
2 Low-Dimensional Similarities

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



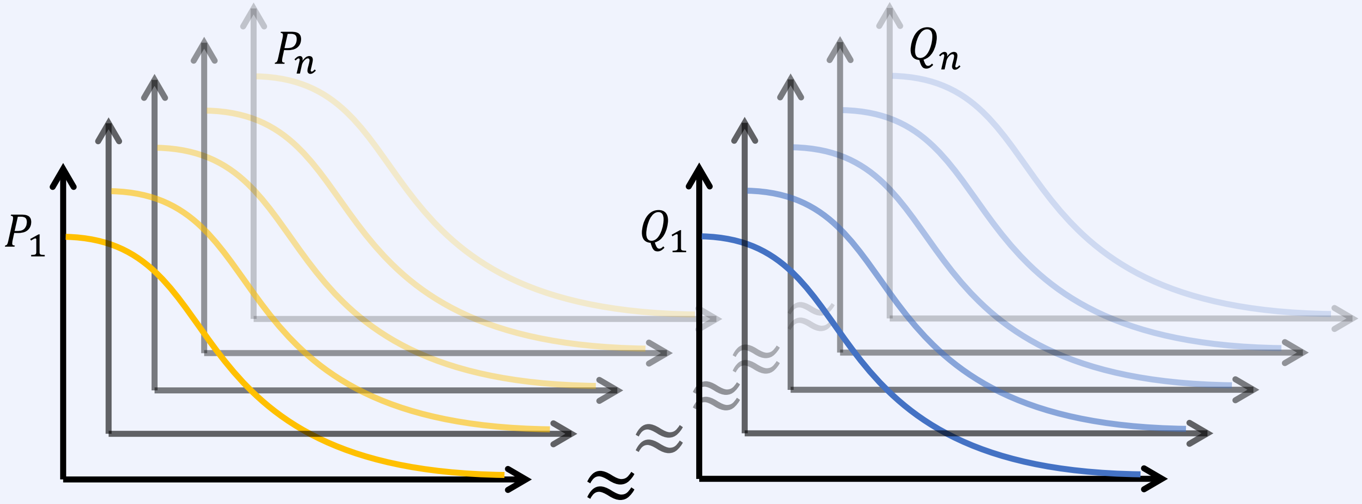
$$q_{j|i} \propto \exp\left(-\frac{\|z_j - z_i\|^2}{2}\right)$$

3 Comparing Distributions



3 Comparing Distributions

Find an embedding Z minimizing the difference between all P_i, Q_i distributions



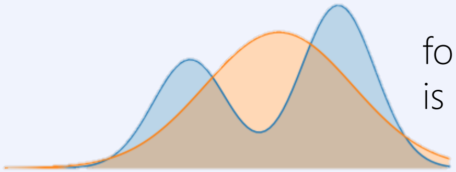
3 Comparing Distributions with KL divergence

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

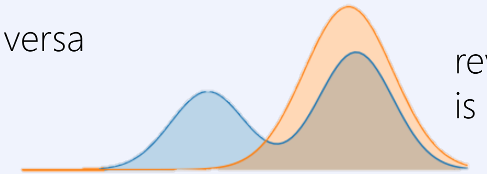
$$C_i = KL(P_i \parallel Q_i) = H(P_i, Q_i) - H(P_i) = \sum_{i \neq j} p_{j|i} \cdot \log \frac{p_{j|i}}{q_{j|i}}$$

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

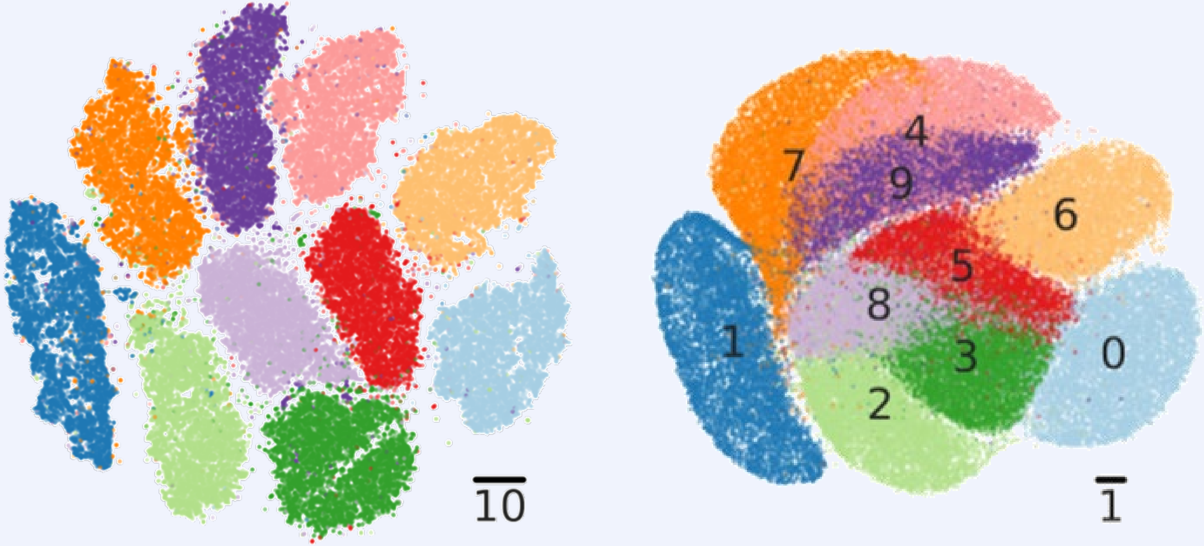
Use KL divergence to measure the "distance" between neighborhood probabilities

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

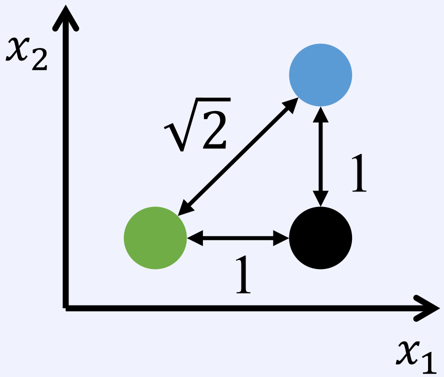
(Hinton & Roweis, 2002)

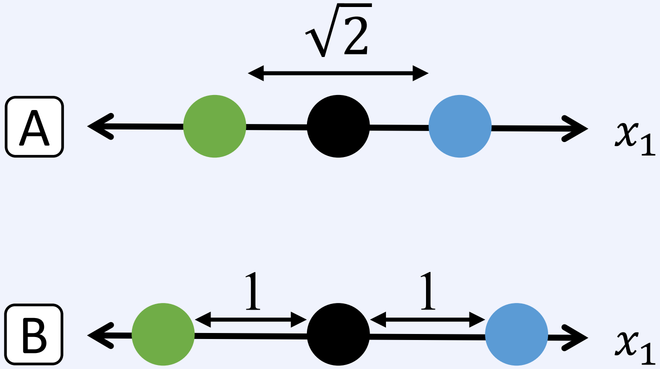
The Crowding Problem



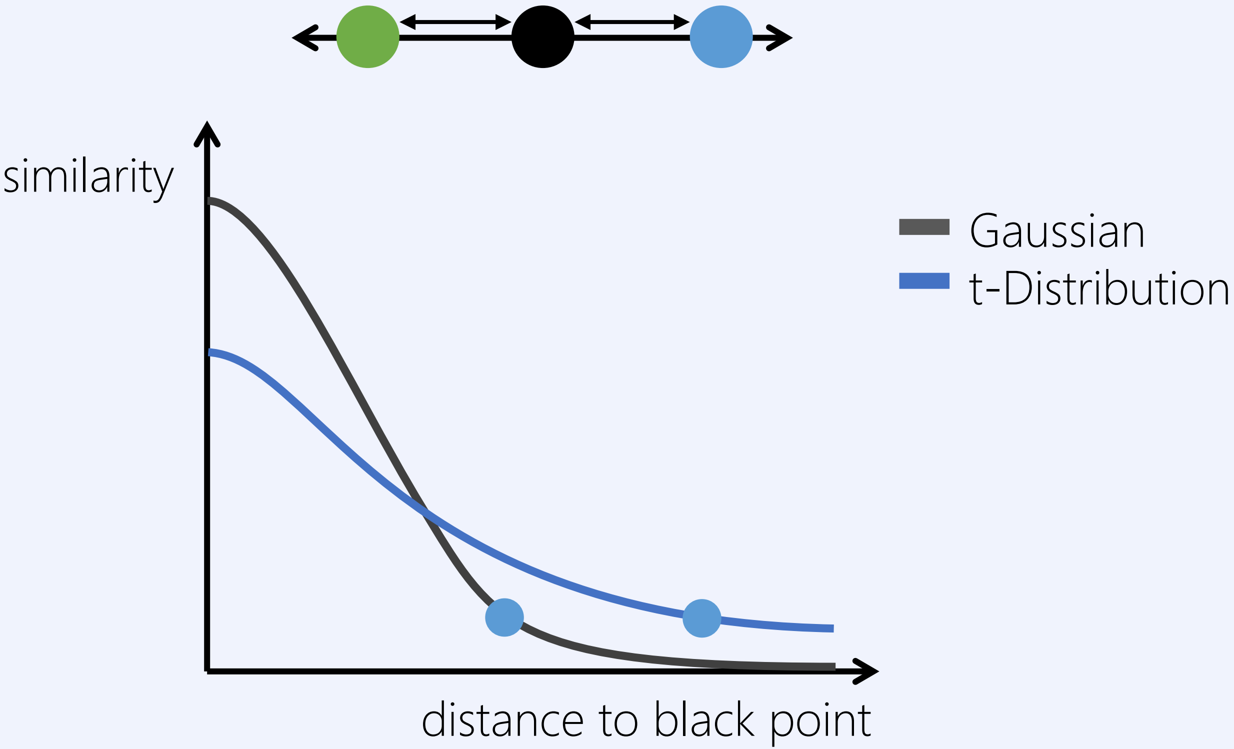
(Kobak et al. "Heavy-tailed kernels reveal a finer cluster structure in t-SNE visualisations", 2019)

The Crowding Problem

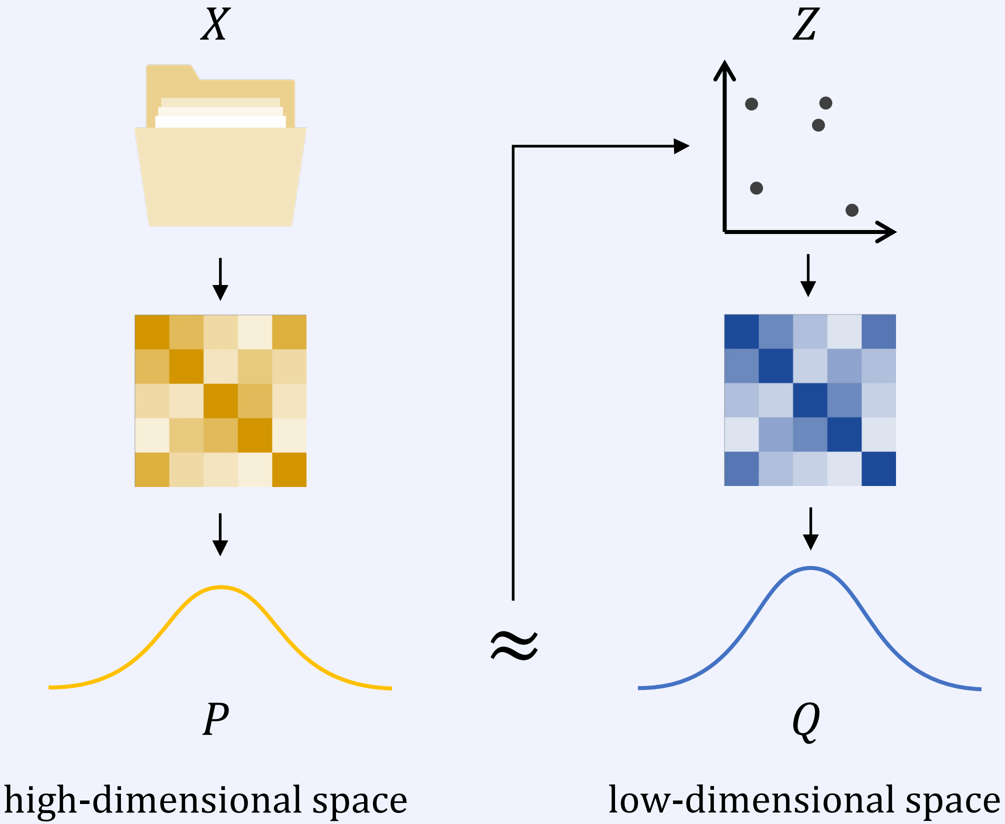




Solving the Crowding Problem

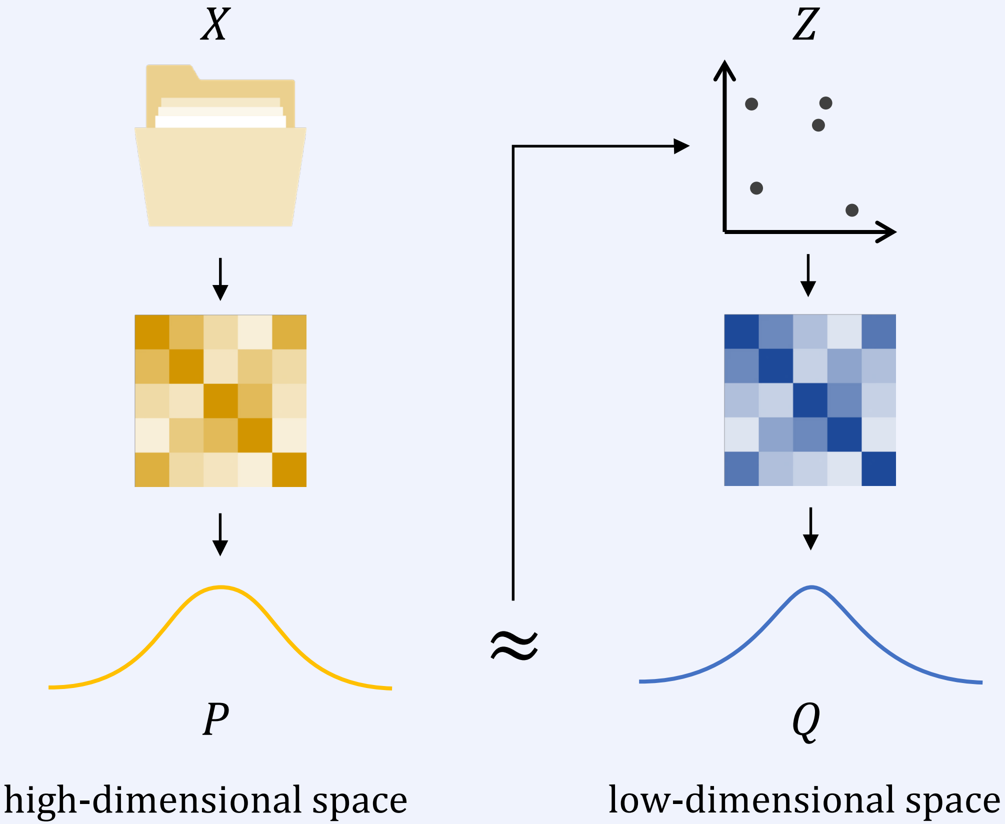


Stochastic Neighbor Embedding



(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 $q_{ij} = \frac{(1+\|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l}(1+\|y_k - y_l\|^2)^{-1}}$

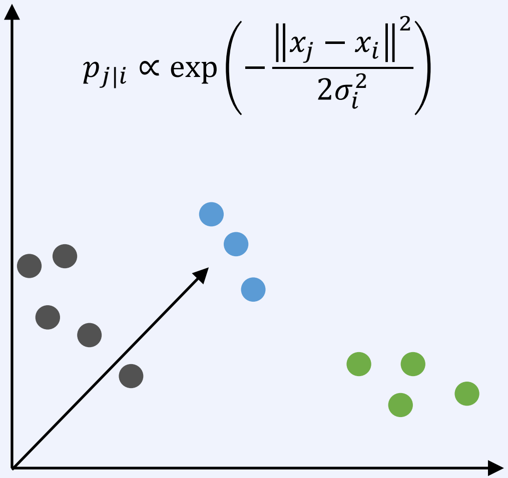
- heavier (compared to Gaussian) tail of the t-distribution compensates for less space in lower dimensions
- volume of a ball scales with r^d, so discrepancy in available space gets more pronounced as r grows
- helps to avoid “crowding” effect and more faithfully reflect longer range structure

(van der Maarten & Hinton, 2008)

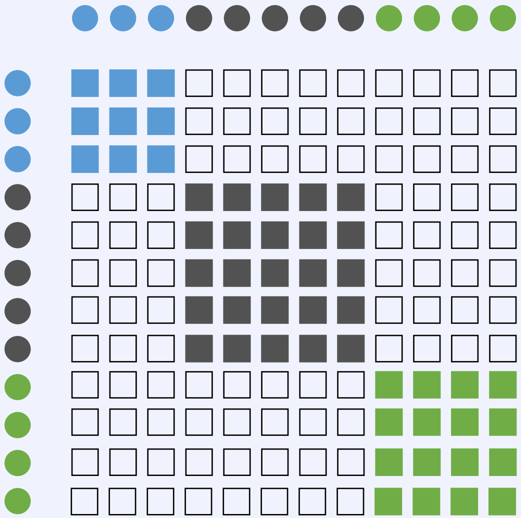
Another interpretation of SNE and t-SNE

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

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



high dimensional data

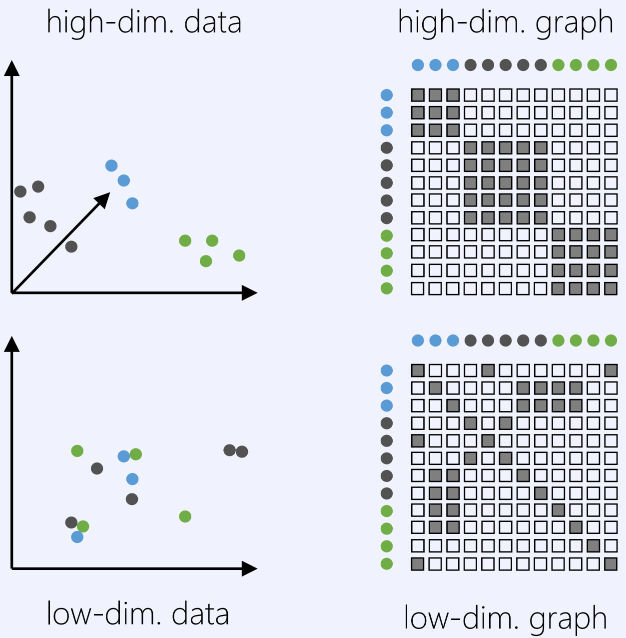


neighbor / similarity graph

Another interpretation of SNE and t-SNE

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

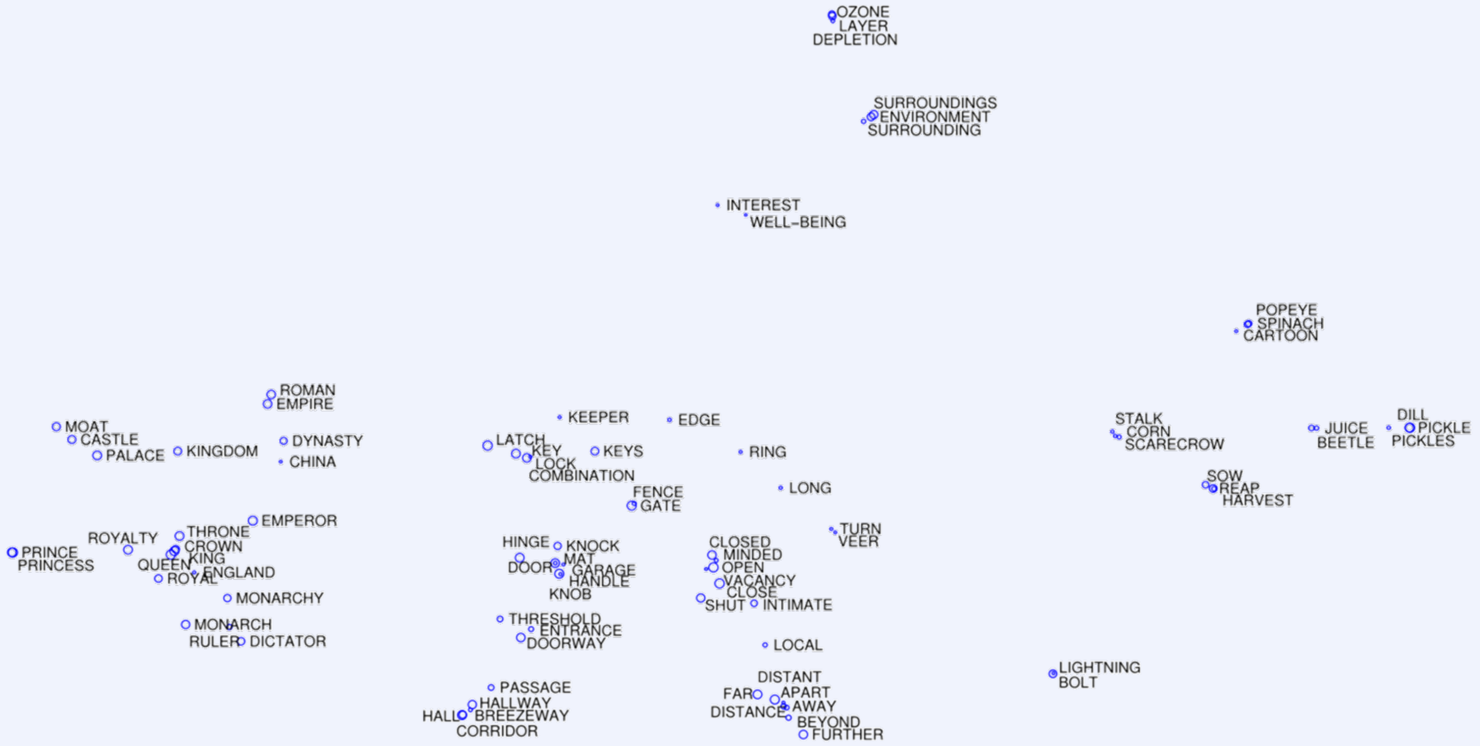
- construct neighborhood graph in high-dim. space
- initialize points in low-dim. space
- construct neighborhood graph in low-dim. space
- optimize coordinates so the two graphs look the same



Computing all pairwise distances can be very slow

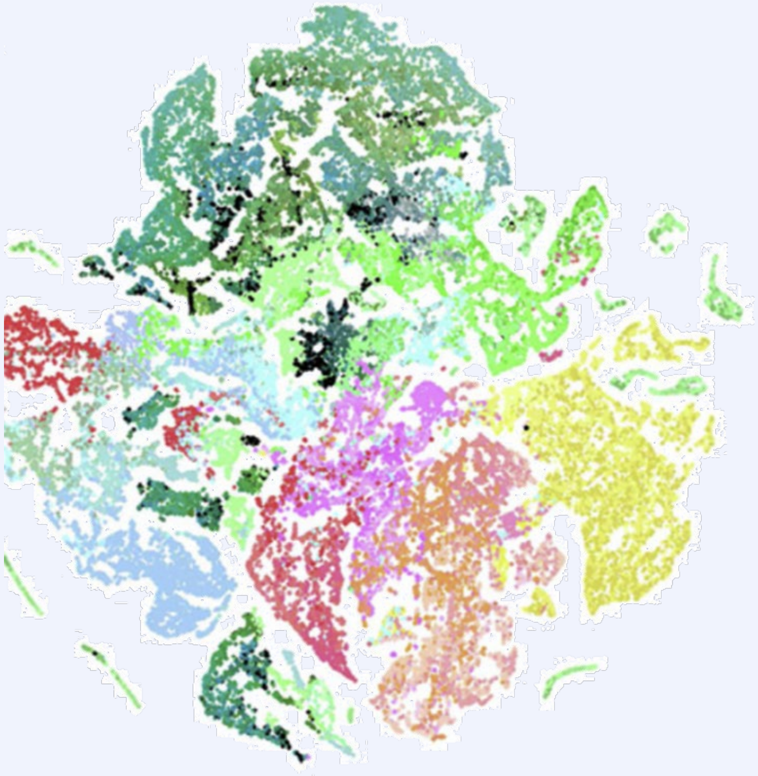
Idea: (Approximately) compute only k nearest neighbors

Word Association Data



Netflix Movies

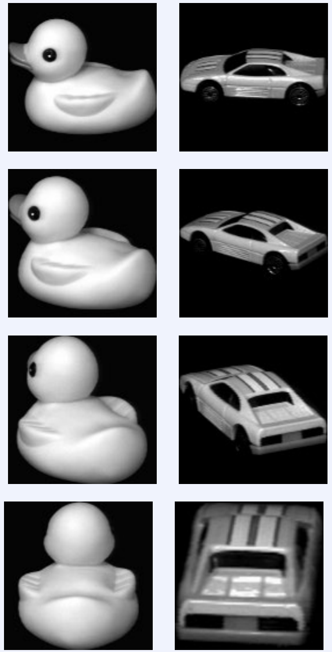
Mouse Brain Cells

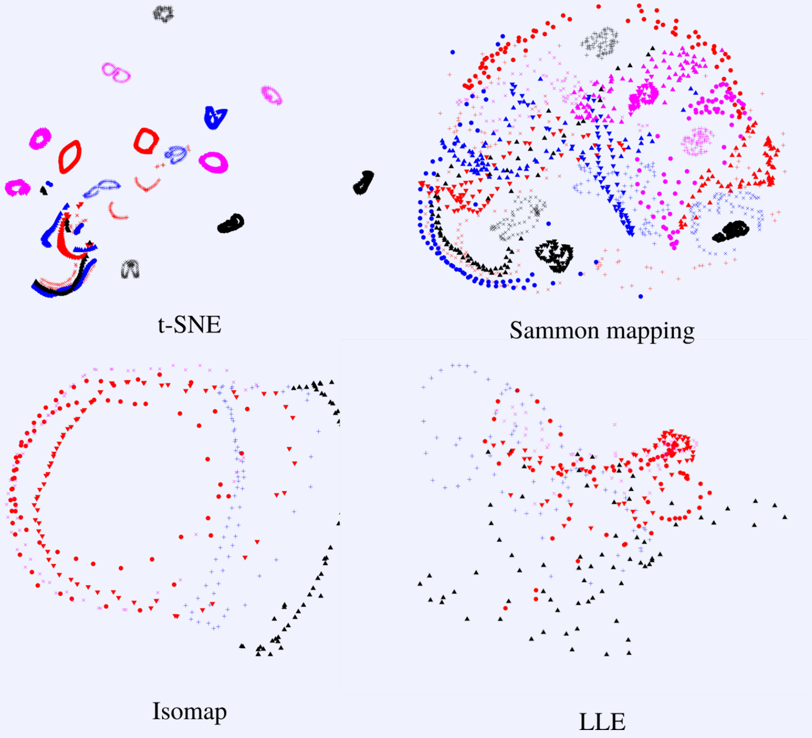


(Mahfouz et al. 2014)

COIL-20 Object Data Set

Examples from COIL-20





(van der Maarten & Hinton, 2008)

Advantages and Disadvantages of t-SNE

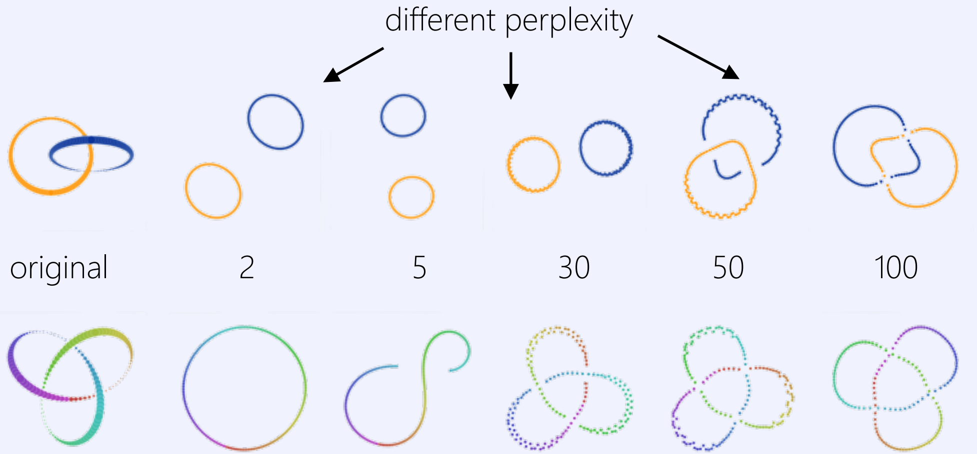
- current standard for visualizing high-dimensional data
- helps understand ”black-box” algorithms like DNN
- reduced ”crowding problem” with heavy tailed distribution

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

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