Unsupervised Learning
& naïve bayes

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Outline

1. Naïve Bayes
2. Unsupervised learning
    a. Maniflod assumption
    b. Multidimensional Scaling (MDS)
    c. Isomap
    d. Locally linear embedding (LLE)
    e. t-SNE
    f. DBSCAN

Naïve Bayes

Naïve Bayes

Naive assumption
of features independence
leads to simple
and easy to calculate result

$$P(y|x_1,\dots,x_n) = P(y)\cdot\frac{P(x_1,\dots,x_n|y)}{P(x_1,\dots,x_n)}$$

$$\boxed{P(x_i|y,x_1,\dots,x_{i-1},x_{i+1},\dots,x_n) = P(x_i|y)}$$

$$P(y|x_1,\dots,x_n) = P(y)\cdot\frac{\prod_i P(x_i|y)}{P(x_1,\dots,x_n)}$$

$$\boxed{P(x_1,\dots,x_n) \equiv const}$$

$$\hat{y} = \arg\max_y P(y)\cdot\prod_i P(x_i|y)$$

What $P(x_i|y)$ really is?

Typical likelihood of the features

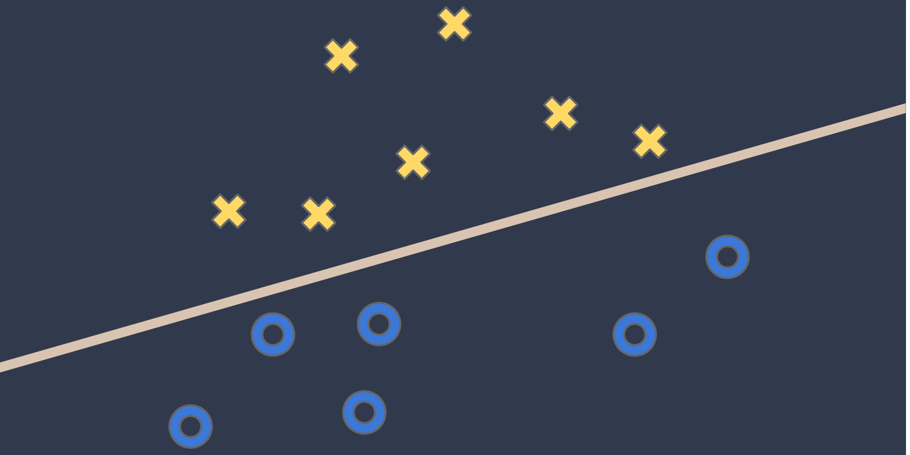
1. Gaussian
2. Multinomial
3. Bernoulli

$$P(x_i \mid y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x_i - \mu_y)^2}{2\sigma_y^2}\right)$$

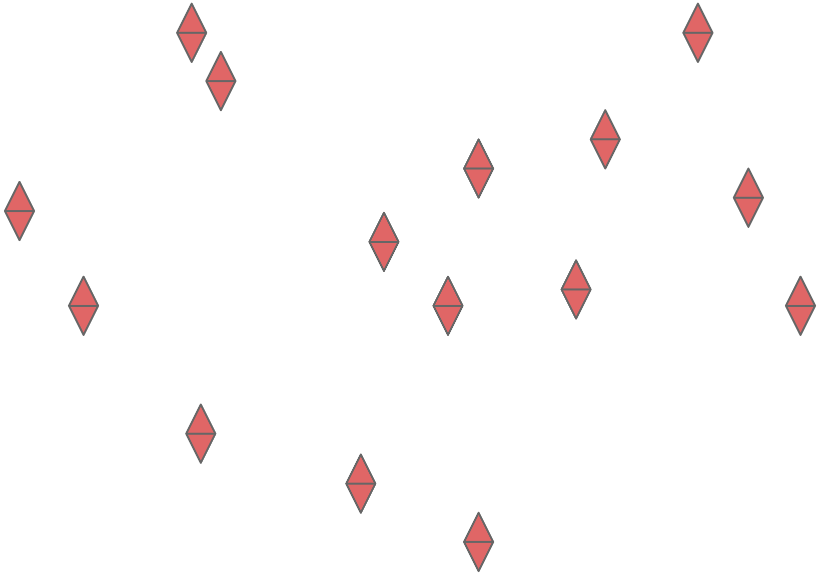
$$P(x_i \mid y) = P(i \mid y)x_i + (1 - P(i \mid y))(1 - x_i)$$

Unsupervised learning

Supervised learning



Unsupervised learning

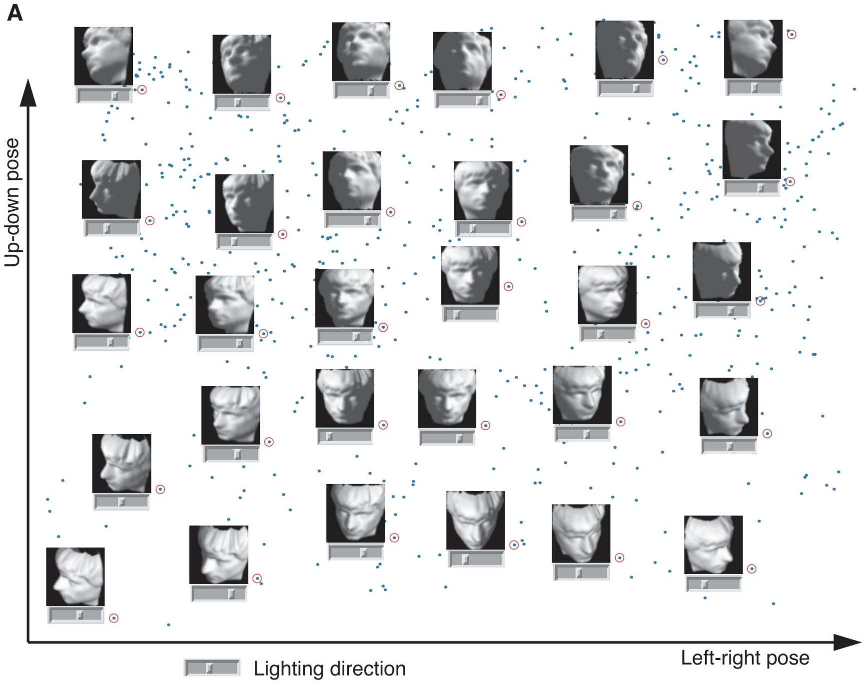


Manifold assumption

The data lie approximately
on a manifold of much lower dimension
than the input space

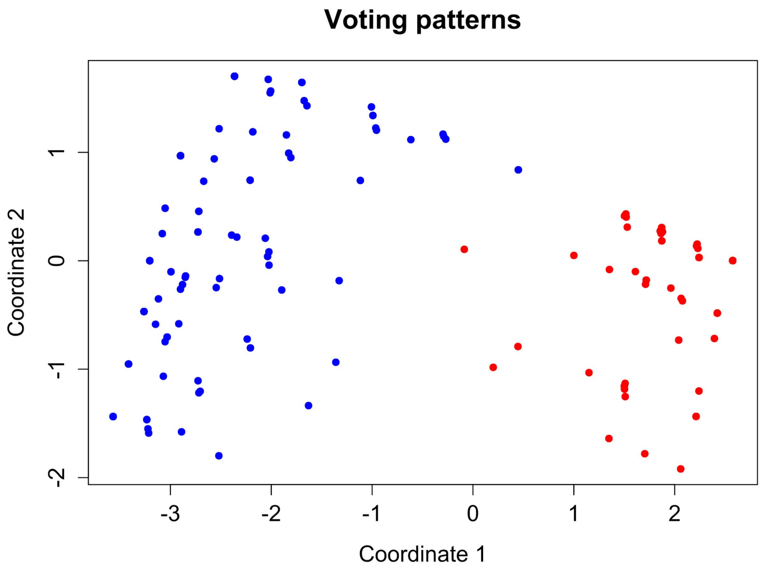
So problem dimensionality could be
(non-)linearly reduced

Approach doesn't require any labels



[Tenenbaum, de Silva, Langford
A Global Geometric Framework for Nonlinear Dimensionality Reduction]

Multidimensional Scaling (MDS)



Voting patterns in the United States House of Representatives

Goal:

Linearly embed to given lower space

Solution:

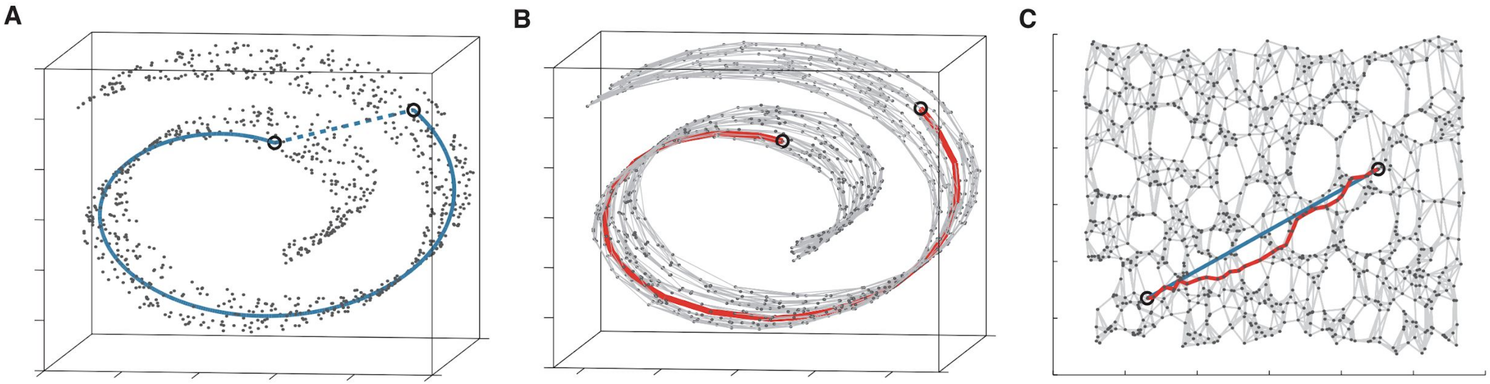
PCA

$$L = ||D_x - D_y||_2 \to \min_{y=Ax}$$

$$y = \Lambda^{1/2} V^T$$

Params: p - target dimensionality

Isomap



Now make distancies geodesic!
And measure distances on the produced graph

Params:

- n - number of neighbours to connect
- p - dimensionality of manifold

Original article

Isomap

Step		
1	Construct neighborhood graph	Define the graph G over all data points by connecting points i and j if [as measured by $d_X(i,j)$] they are closer than ϵ (ϵ-Isomap), or if i is one of the K nearest neighbors of j (K-Isomap). Set edge lengths equal to $d_X(i,j)$.
2	Compute shortest paths	Initialize $d_G(i,j) = d_X(i,j)$ if i,j are linked by an edge; $d_G(i,j) = \infty$ otherwise. Then for each value of $k = 1, 2, \ldots, N$ in turn, replace all entries $d_G(i,j)$ by $\min\{d_G(i,j), d_G(i,k) + d_G(k,j)\}$. The matrix of final values $D_G = \{d_G(i,j)\}$ will contain the shortest path distances between all pairs of points in G (*16*, *19*).
3	Construct d-dimensional embedding	Let λ_p be the p-th eigenvalue (in decreasing order) of the matrix $\tau(D_G)$ (*17*), and v_p^i be the i-th component of the p-th eigenvector. Then set the p-th component of the d-dimensional coordinate vector $\mathbf{y}_i$ equal to $\sqrt{\lambda_p} v_p^i$.

Floyd–Warshall algorithm

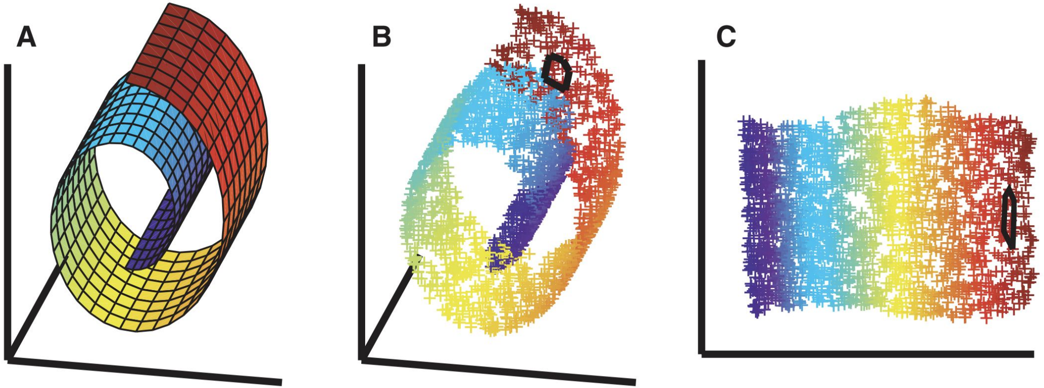
17. The operator τ is defined by $\tau(D) = -HSH/2$, where S is the matrix of squared distances $\{S_{ij} = D_{ij}^2\}$, and H is the "centering matrix" $\{H_{ij} = \delta_{ij} - 1/N\}$ (*13*).

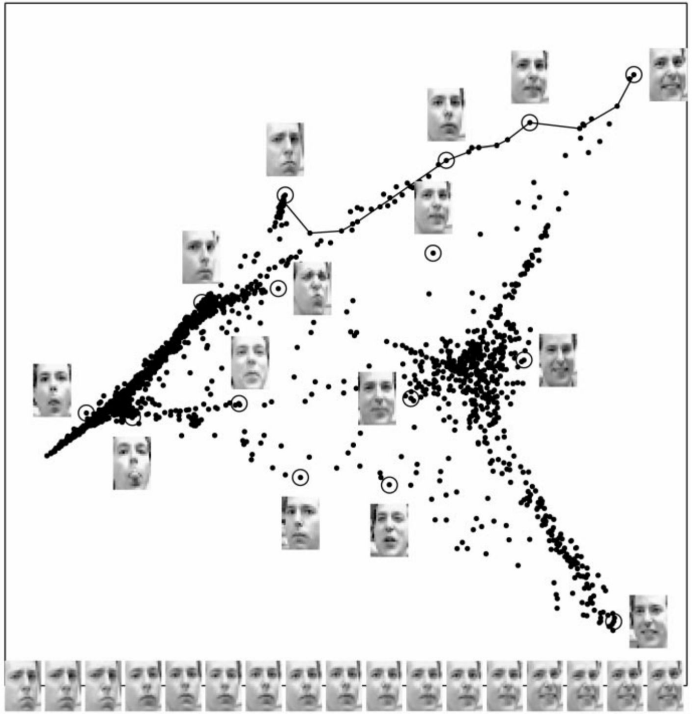
Locally linear embedding (LLE)

Idea:

Smooth manifold can be locally approximated linearly.
Linear peases can be flattened

Original article





Locally linear embedding (LLE)

Two steps of embedding and two objective functions:

1. estimate point by its K neighbours

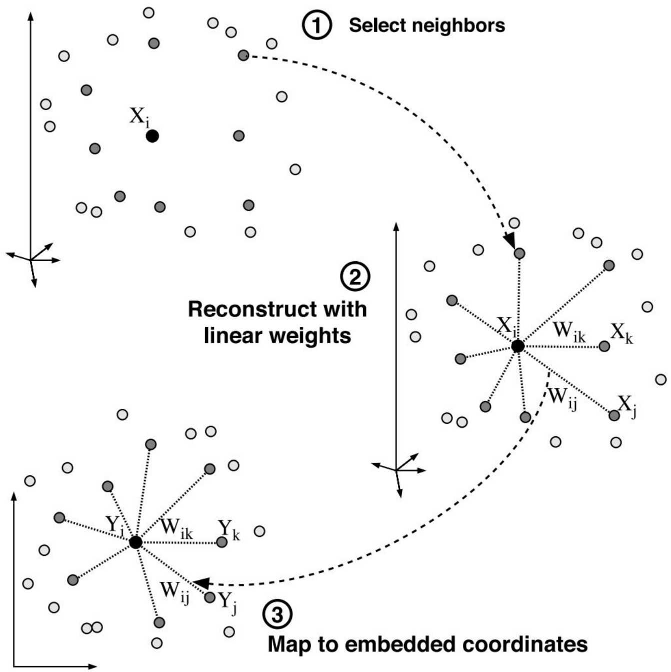
$$\varepsilon(W) = \sum_{i=1}^{n} ||x_i - \sum_{j=1}^{K} W_{ij} x_j||^2$$

2. Estimate new points based on known relations

$$\Phi(Y) = \sum_{i=1}^{n} ||y_i - \sum_{j=1}^{n} W_{ij} y_j||^2$$

Params:

n - number of neighbours to connect
p - dimensionality of manifold



Many more...

- Hessian Eigenmapping
- Spectral Embedding
- Local Tangent Space Alignment
- Riemannian Geometry
- ......

t-SNE

t-distributed $\underbrace{\text{Stochastic Neighbor Embedding}}_{\text{SNE}}$

original article

Stochastic Neighbor Embedding

Idea:

Convert pairwise distances to probabilities, preserve probabilities through the spaces

$$p_{j|i} = \frac{\exp(-\frac{||x_i - x_j||^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{||x_i - x_k||^2}{2\sigma_i^2})}$$

asymmetric probability
of object i chooses j as its neighbour

$$q_{j|i} = \frac{\exp(-||y_i - y_j||^2)}{\sum_{k \neq i} \exp(-||y_i - y_k||^2)}$$

the same in target space

Let’s construct embedding s.t. this distributions are close.
What are close distributions?

Kullback–Leibler divergence

$$D_{KL}(P \parallel Q) = \sum_{i,j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Suspiciously similar to Shannon entropy

Learn more

Stochastic Neighbor Embedding

$$p_{j|i} = \frac{\exp(-\frac{||x_i - x_j||^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{||x_i - x_k||^2}{2\sigma_i^2})}$$

$$q_{j|i} = \frac{\exp(-||y_i - y_j||^2)}{\sum_{k \neq i} \exp(-||y_i - y_k||^2)}$$

$$D_{KL}(P \,||\, Q) \to \min_{Y}$$

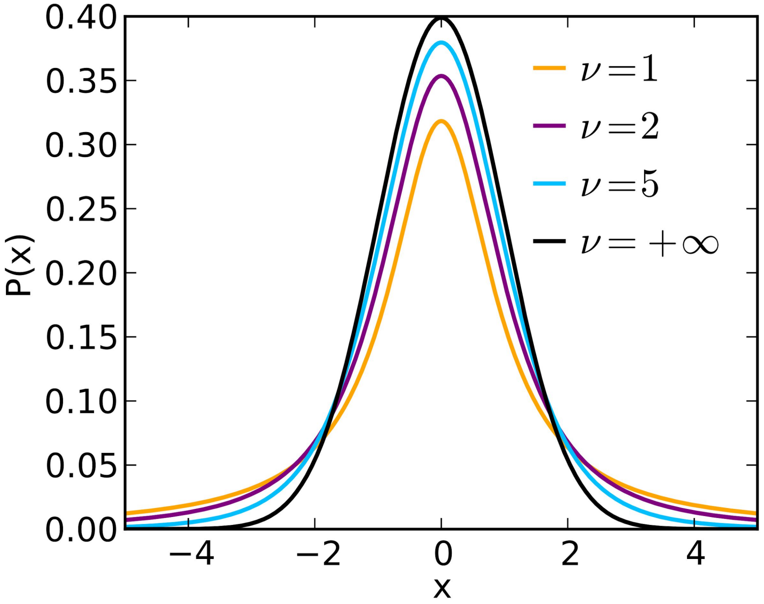
t-distributed Stochastic Neighbor Embedding

Patches over SNE:

1. make distribution symmetric
2. make it decrease faster than Gaussian (use Student's t-distribution)

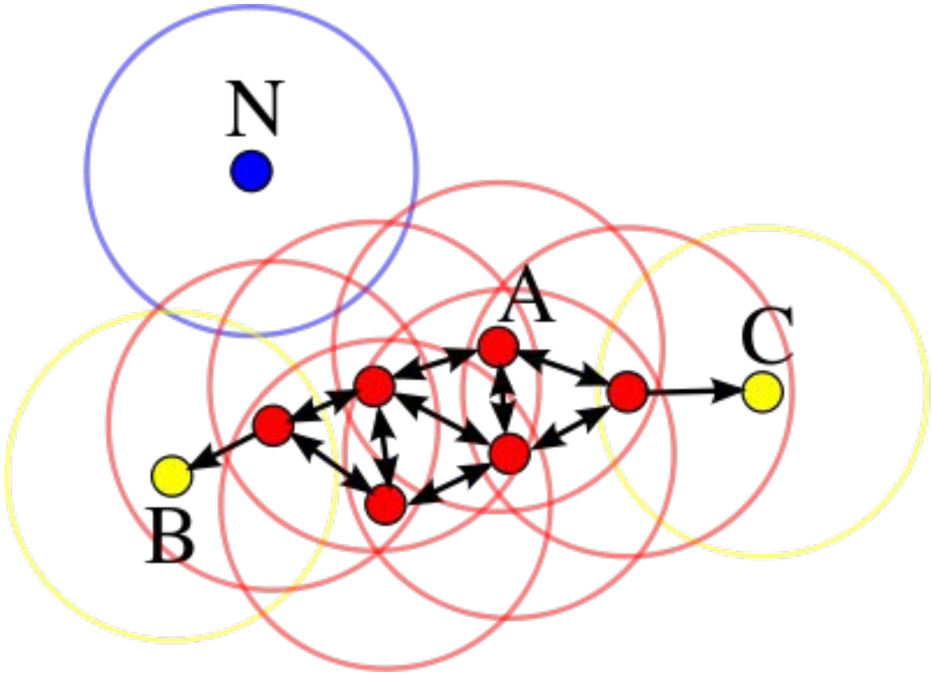
$$q_{ij} = \frac{\exp\left(-\|y_i - y_j\|^2\right)}{\sum_{k \neq l} \exp\left(-\|y_k - y_l\|^2\right)}$$

$$p_{ij} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma^2\right)}{\sum_{k \neq l} \exp\left(-\|x_k - x_l\|^2 / 2\sigma^2\right)}$$



Original article

DBSCAN



Links

1. Good lecture on MDS, Isomap, LLE
2. Lecture on t-SNE (this one is good too)
3. Slides about clusterization
4. Metrics in clusterization
5. Slides about ICA
6. More clustering methods (in russian)