CS6510
Applied Machine Learning

Dimensionality Reduction

4 Nov 2017

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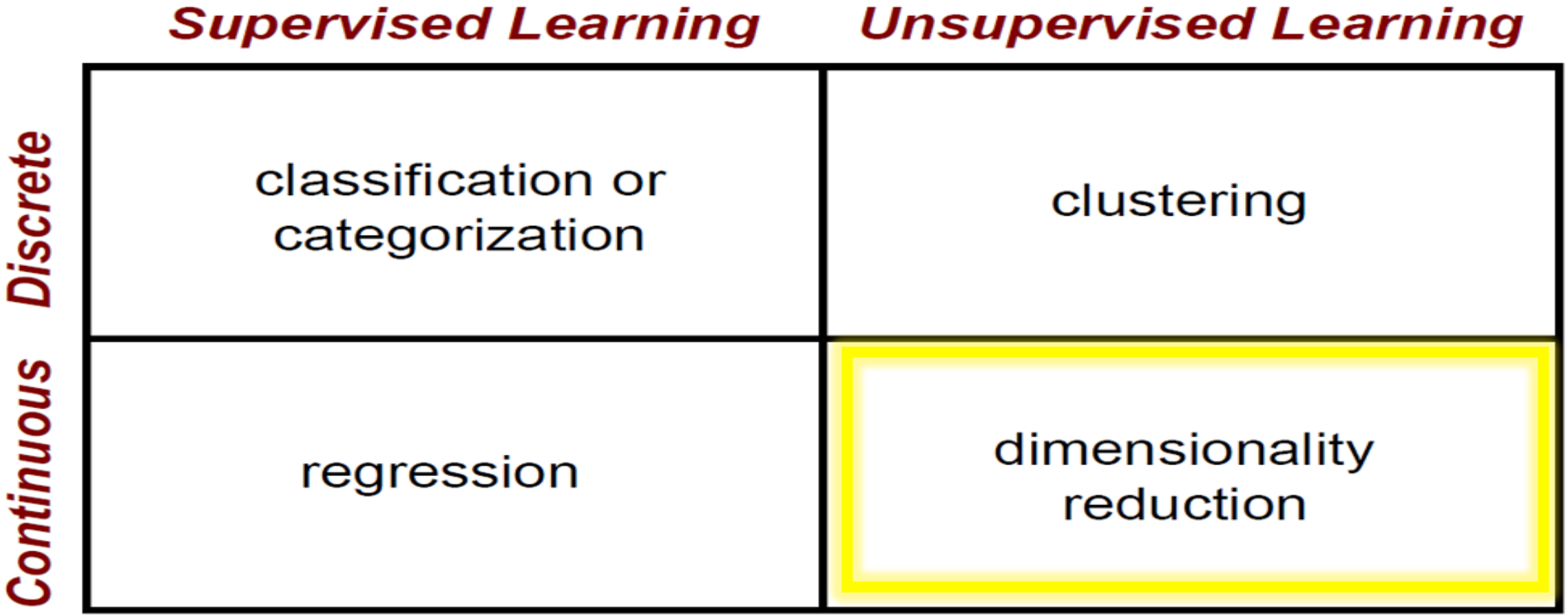
ML Problems


Supervised Learning
Unsupervised Learning
Discrete
Continuous
classification or categorization
clustering
regression
dimensionality reduction

Outline

- Linear Methods
  - Principal Component Analysis (PCA)
  - Fisher (Linear) Discriminant Analysis (LDA)
  - Multi-Dimensionality Scaling (MDS)
- Non-linear Methods
  - Kernel PCA
  - Manifold Learning methods: ISOMAP, LLE, Laplacian Eigenmaps
  - t-Stochastic Neighborhood Embedding (t-SNE)

How does the brain store these images?

What is Dimensionality Reduction

- Refers to the mapping of the original high-dimensional data onto a lower-dimensional space.
- Criterion for feature reduction can be different based on different problem settings.
  - Unsupervised setting: minimize the information loss
  - Supervised setting: maximize the class discrimination
- Given a set of data points of p variables $\{x_1, x_2, \cdots, x_n\}$

  Compute the linear transformation (projection)

$$G \in \Re^{p \times d} : x \in \Re^p \rightarrow y = G^T x \in \Re^d \ (d << p)$$

Linear DR

Dimensionality Reduction vs Feature Selection

- **Feature reduction**
  - All original features are used
  - The transformed features are linear combinations of the original features.

- **Feature selection**
  - Only a subset of the original features are used.

- Continuous versus discrete

Why DR?

- Most machine learning techniques may not be effective for high-dimensional data
  - Curse of Dimensionality
  - Query accuracy and efficiency degrade rapidly as the dimension increases
  - Lower space and time complexity
  - Visualization, Data compression, Noise/irrelevant feature removal
- The intrinsic dimension may be small
  - For example, the number of genes responsible for a certain type of disease may be small

High-dimensional data are strange

- Consider the hypersphere of radius r on a space of dimension d

$$\mathcal{S} = \left\{ \mathbf{x} | \sum_{i=1}^{d} x_i^2 \leq r^2 \right\}$$

- Its volume is

$$V_d(r) = \frac{r^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$$

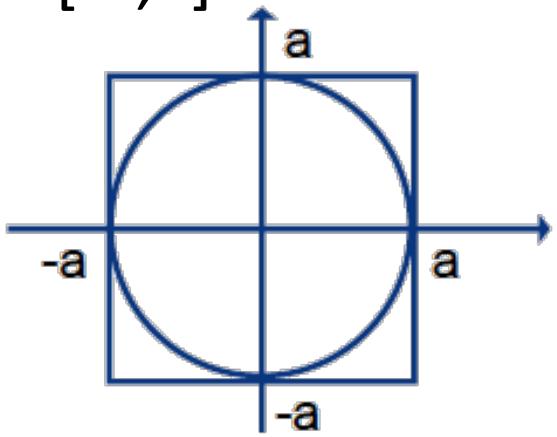
- Where Γ(n) is the Gamma function

$$\Gamma(n) = \int_0^\infty e^{-x} x^{n-1} dx$$

Source: N Vasconcelos

Hypercube vs Hypersphere

- Consider the hyper-cube $[-a,a]^d$ and the inscribed hyper-sphere, i.e.



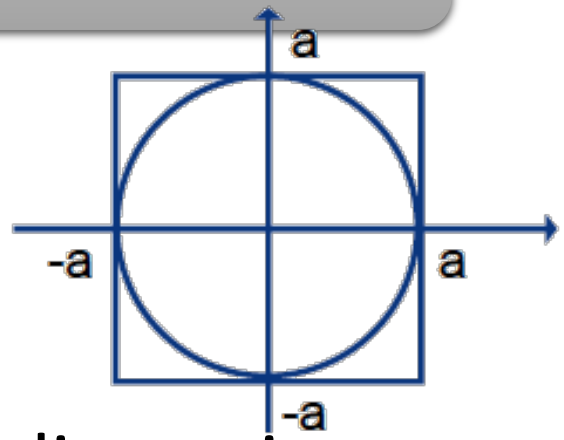
- What does your intuition tell you about the relative sizes of these two objects?
  - Volume of sphere ~= volume of cube
  - Volume of sphere >> volume of cube
  - Volume of sphere << volume of cube

Source: N Vasconcelos

Hypercube vs Hypersphere

- Let's compute the answer

$$f_d = \frac{Vol(sphere)}{Vol(cube)} = \frac{\frac{a^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}}{(2a)^d} = \frac{\pi^{\frac{d}{2}}}{2^d \Gamma\left(\frac{d}{2}+1\right)}$$



- Sequence that does not depend on a, just on the dimension d!

d	1	2	3	4	5	6	7
f_d	1	.785	.524	.308	.164	.08	.037

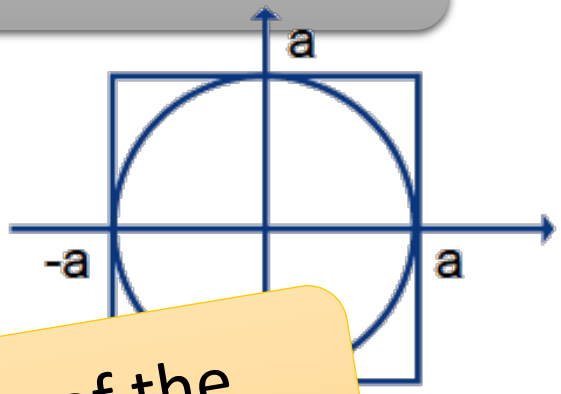
- It goes to zero, and goes to zero fast!

Source: N Vasconcelos

Hypercube vs Hypersphere

- Let's compute the answer

$$f_d = \frac{Vol(sphere)}{Vol(cube)} = \frac{\frac{a^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}}{(2a)^d} = \frac{\pi^{\frac{d}{2}}}{2^d \Gamma\left(\frac{d}{2}+1\right)}$$



- Sequence that does not dep... d!

			5	6	7
	.524	.308	.164	.08	.037

As the dimension of the space increases, the volume of the sphere is much smaller (infinitesimal) than that of the cube!

- It goes to zero, and goes to zero fast!

Source: N Vasconcelos

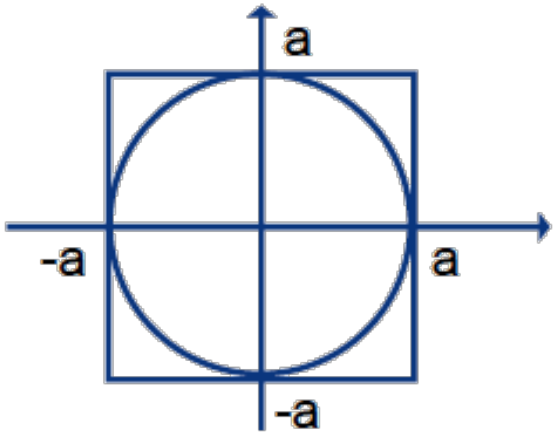
Hypercube vs Hypersphere

Actually not very surprising

1. d = 1

Volume is the same

2. d = 2

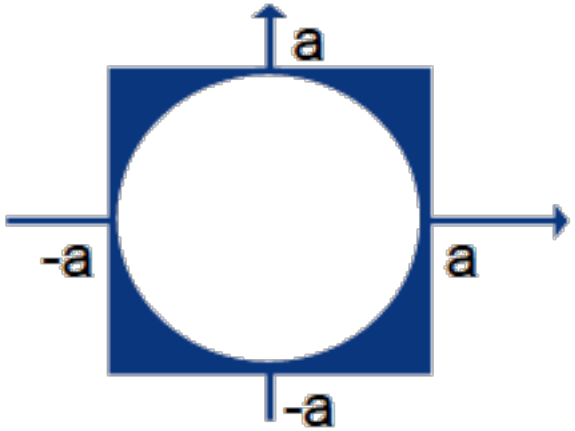


Volume of sphere is already smaller

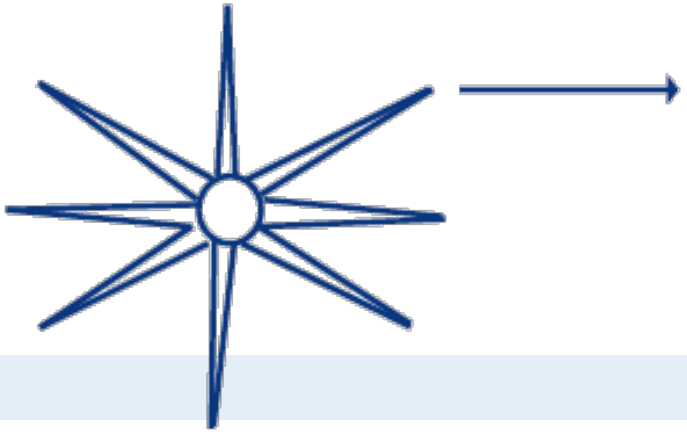
Source: N Vasconcelos

Hypercube vs Hypersphere

- As the dimension increases the volume of the shaded corners becomes larger



- In high dimensions the picture you should have in mind is

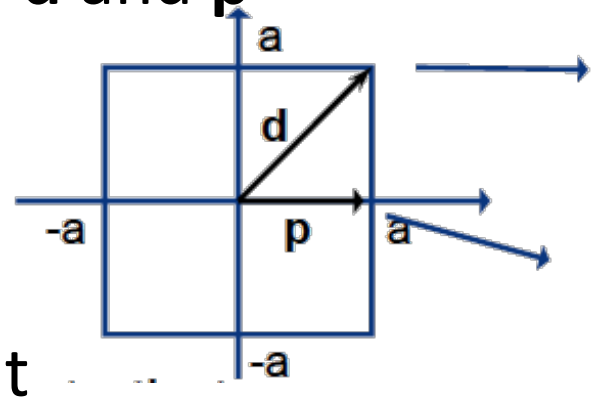


all the volume of the cube is in these spikes!

Source: N Vasconcelos

We can check mathematically

- Consider **d** and **p**



$$\mathbf{d} = (a, a, \ldots, a) \in \mathcal{R}^d$$

$$\mathbf{p} = (a, 0, \ldots, 0) \in \mathcal{R}^d$$

- Note that

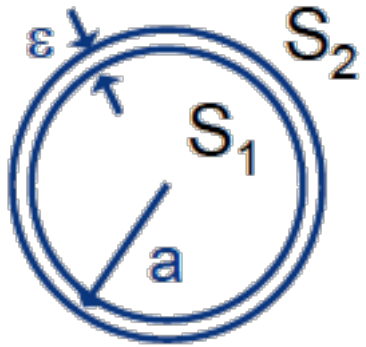
$$\frac{||d||^2}{||p||^2} = \frac{da^2}{a^2} = d \rightarrow \infty \qquad cos\theta = \frac{\mathbf{d}^T\mathbf{p}}{\sqrt{||d||^2||p||^2}} = \frac{a^2}{\sqrt{da^2a^2}} = \frac{1}{\sqrt{d}} \rightarrow 0$$

- **d** orthogonal to **p** as **d** increases and infinitely larger!!!

Source: N Vasconcelos

Wait, there is more!

- Consider the crust of unit hypersphere of thickness ε
- Let's compute the ratio of volumes



$$\frac{Vol(S_1)}{Vol(S_2)} = \frac{\frac{(a-\epsilon)^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}}{\frac{a^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}} = \frac{a^d\left(1-\frac{\epsilon}{a}\right)^d}{a^d} = \left(1-\frac{\epsilon}{a}\right)^d$$

- No matter how small ε is, ratio goes to zero as d increases
- i. e. **"all the volume is in the crust!"**

The Curse of Dimensionality

DR Methods: Categorization

- **Unsupervised**
  - Latent Semantic Indexing (LSI): truncated SVD
  - Independent Component Analysis (ICA)
  - Principal Component Analysis (PCA)
  - Canonical Correlation Analysis (CCA)

- **Supervised**
  - Linear Discriminant Analysis (LDA)

- **Semi-supervised**
  - Research topic

DR Methods

- **Linear**
  - Latent Semantic Indexing (LSI): truncated SVD
  - Principal Component Analysis (PCA)
  - Linear Discriminant Analysis (LDA)
  - Canonical Correlation Analysis (CCA)

- **Non-linear**
  - Nonlinear feature reduction using kernels
  - Manifold learning

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Principal Component Analysis (PCA)

- Find a low-dimensional space such that when $\boldsymbol{x}$ is projected there, information loss is minimized.
- The projection of $\boldsymbol{x}$ on the direction of $\boldsymbol{w}$ is: $z = \boldsymbol{w}^T\boldsymbol{x}$
- Find $\boldsymbol{w}$ such that Var(z) is maximized

$$\begin{aligned}\text{Var}(z) &= \text{Var}(\boldsymbol{w}^T\boldsymbol{x}) = E[(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})^2] \\ &= E[(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})] \\ &= E[\boldsymbol{w}^T(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T\boldsymbol{w}] \\ &= \boldsymbol{w}^T E[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T]\boldsymbol{w} = \boldsymbol{w}^T \sum \boldsymbol{w}\end{aligned}$$

where $\text{Var}(\boldsymbol{x}) = E[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T] = \sum$

PCA

- Maximize Var(z) subject to ||**w**||=1

$$\max_{\mathbf{w}_1} \mathbf{w}_1^T \Sigma \mathbf{w}_1 - \alpha\left(\mathbf{w}_1^T \mathbf{w}_1 - 1\right)$$

Using Lagrange multipliers, a la SVM

$\sum \mathbf{w}_1 = \alpha \mathbf{w}_1$ that is, $\mathbf{w}_1$ is an eigenvector of $\sum$

Choose the one with the largest eigenvalue for Var(z) to be max

- Second principal component: Max Var(z_2), s.t., $||\mathbf{w}_2||=1$ and orthogonal to $\mathbf{w}_1$

$$\max_{\mathbf{w}_2} \mathbf{w}_2^T \Sigma \mathbf{w}_2 - \alpha\left(\mathbf{w}_2^T \mathbf{w}_2 - 1\right) - \beta\left(\mathbf{w}_2^T \mathbf{w}_1 - 0\right)$$

How?

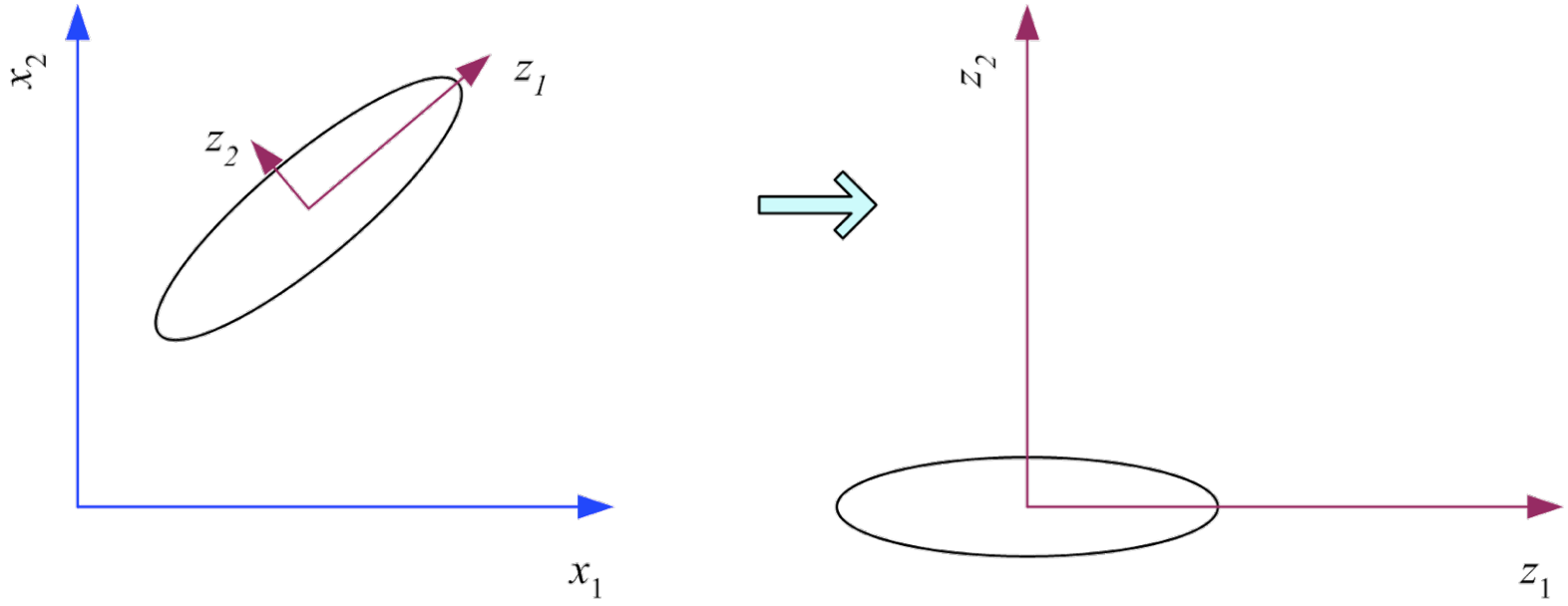
$\sum \mathbf{w}_2 = \alpha \mathbf{w}_2$ that is, $\mathbf{w}_2$ is another eigenvector of $\sum$

and so on.

PCA

$$\mathbf{z} = \mathbf{W}^T(\boldsymbol{x} - \boldsymbol{m})$$

where the columns of $\mathbf{W}$ are the eigenvectors of $\sum$, and $\boldsymbol{m}$ is sample mean; Centers the data at the origin and rotates the axes



How to choose k

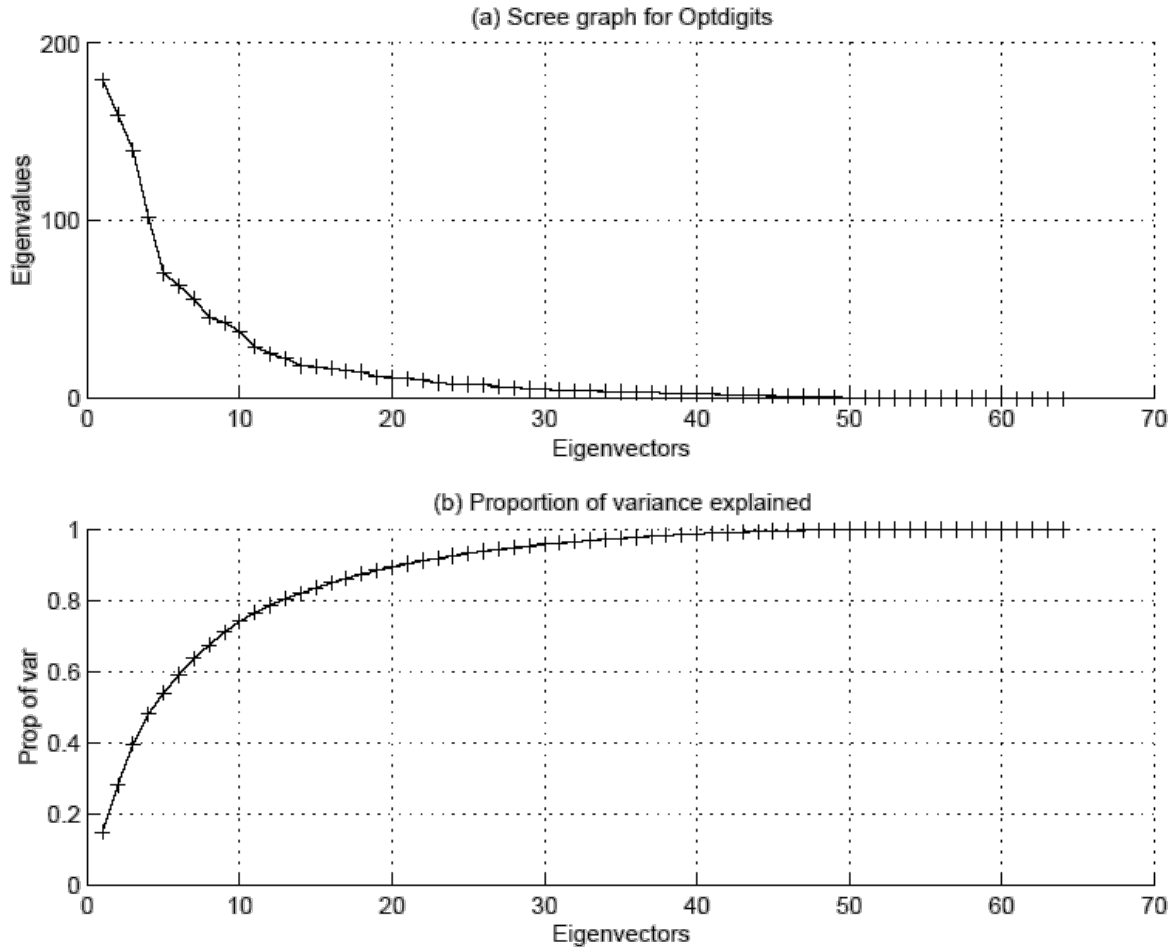
- Proportion of Variance (PoV) explained

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$

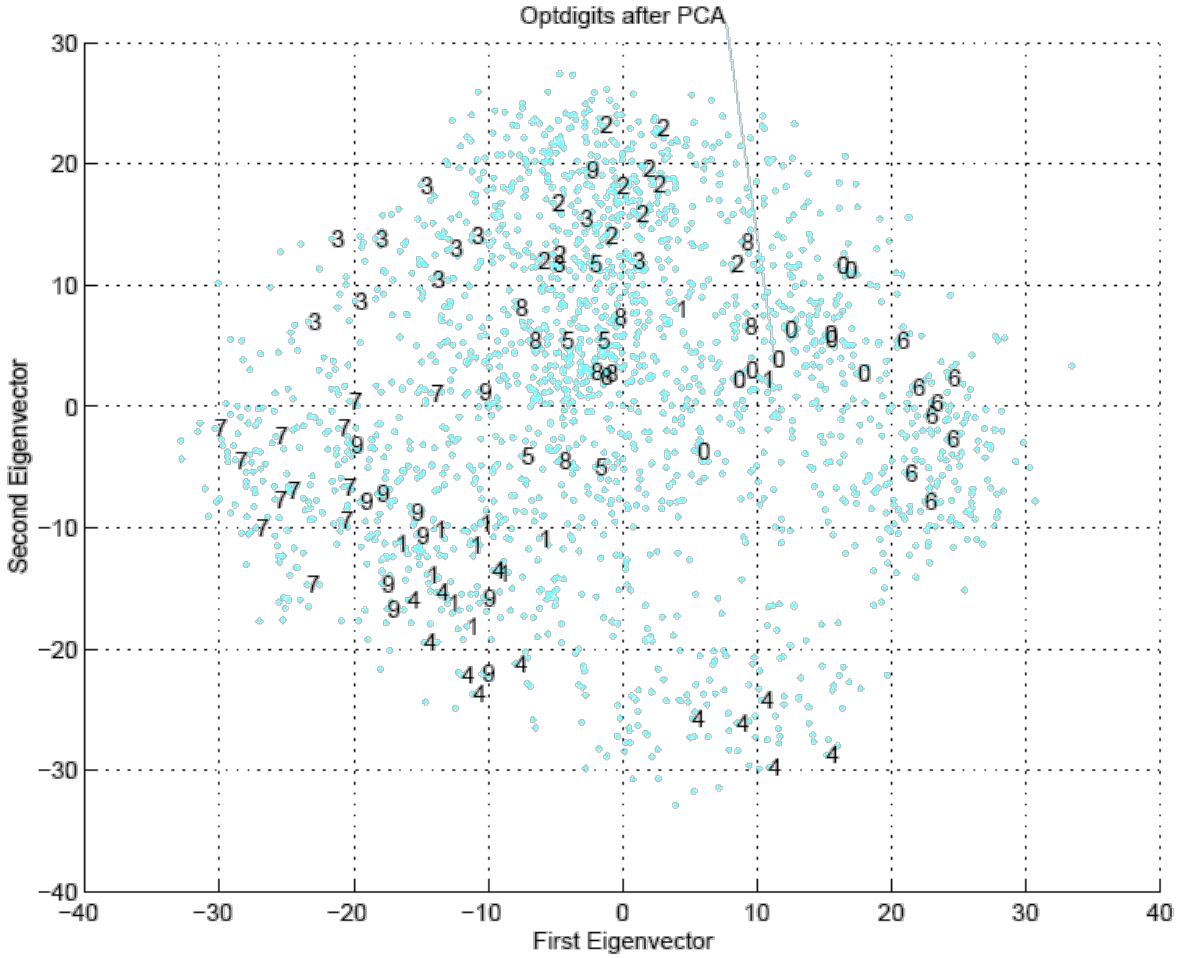
when λ_i are sorted in descending order

- Typically, stop at PoV>0.9
- See graph plots of PoV vs *k*, stop at "elbow"

Illustration



Example


Optdigits after PCA
Second Eigenvector
First Eigenvector
30
20
10
0
−10
−20
−30
−40
−40
−30
−20
−10
0
10
20
30
40

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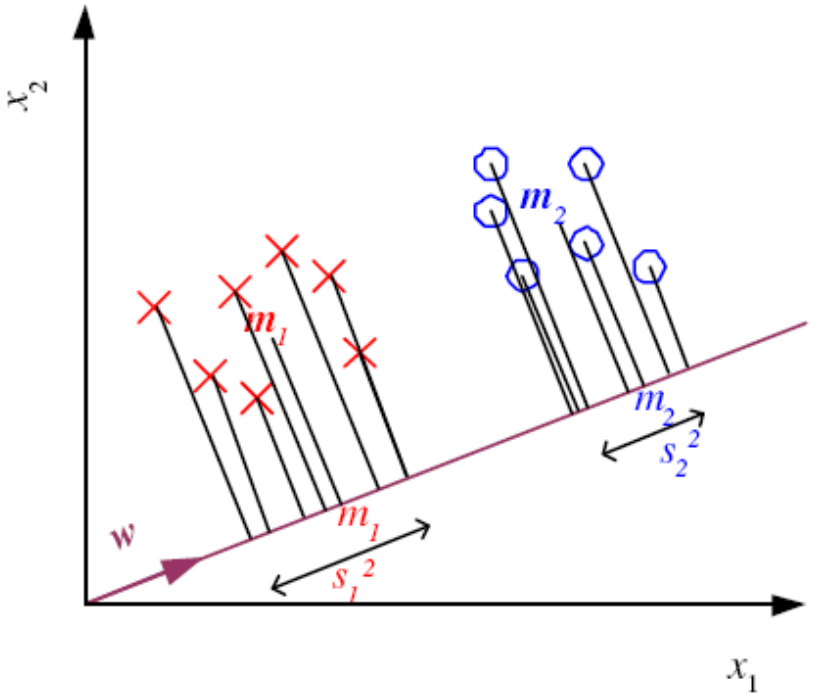
Linear Discriminant Analysis

- Supervised linear DR method
- Find a low-dimensional space such that when ***x*** is projected, classes are well-separated.
- Find ***w*** that maximizes

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

$$m_1 = \frac{\sum_t \mathbf{w}^T \mathbf{x}^t r^t}{\sum_t r^t} \qquad s_1^2 = \sum_t \left(\mathbf{w}^T \mathbf{x}^t - m_1\right)^2 r^t$$



Linear Discriminant Analysis

- Between-class scatter:

$$\begin{aligned}(m_1 - m_2)^2 &= \left(\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2\right)^2 \\ &= \mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\mathbf{w} \\ &= \mathbf{w}^T\mathbf{S}_B\mathbf{w} \text{ where } \mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\end{aligned}$$

- Within-class scatter:

$$\begin{aligned}s_1^2 &= \sum_t \left(\mathbf{w}^T\mathbf{x}^t - m_1\right)^2 r^t \\ &= \sum_t \mathbf{w}^T(\mathbf{x}^t - \mathbf{m}_1)(\mathbf{x}^t - \mathbf{m}_1)^T\mathbf{w}r^t = \mathbf{w}^T\mathbf{S}_1\mathbf{w} \\ \text{where } \mathbf{S}_1 &= \sum_t (\mathbf{x}^t - \mathbf{m}_1)(\mathbf{x}^t - \mathbf{m}_1)^T r^t \\ s_1^2 + s_2^2 &= \mathbf{w}^T\mathbf{S}_W\mathbf{w} \text{ where } \mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2\end{aligned}$$

Fisher's Linear Discriminant

- Find ***w*** that max

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{\left|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w}\right|}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- LDA soln:

$$\mathbf{w} = c \cdot \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- Alternative parametric soln:

$$\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$$

when $p(\mathbf{x}|C_i) \sim \mathcal{N}(\mu_i, \Sigma)$

Fisher's Linear Discriminant

- Within-class scatter:

$$\mathbf{S}_W = \sum_{i=1}^{K} \mathbf{S}_i \qquad \mathbf{S}_i = \sum_t r_i^t \left(\mathbf{x}^t - \mathbf{m}_i\right)\left(\mathbf{x}^t - \mathbf{m}_i\right)^T$$

- Between-class scatter:

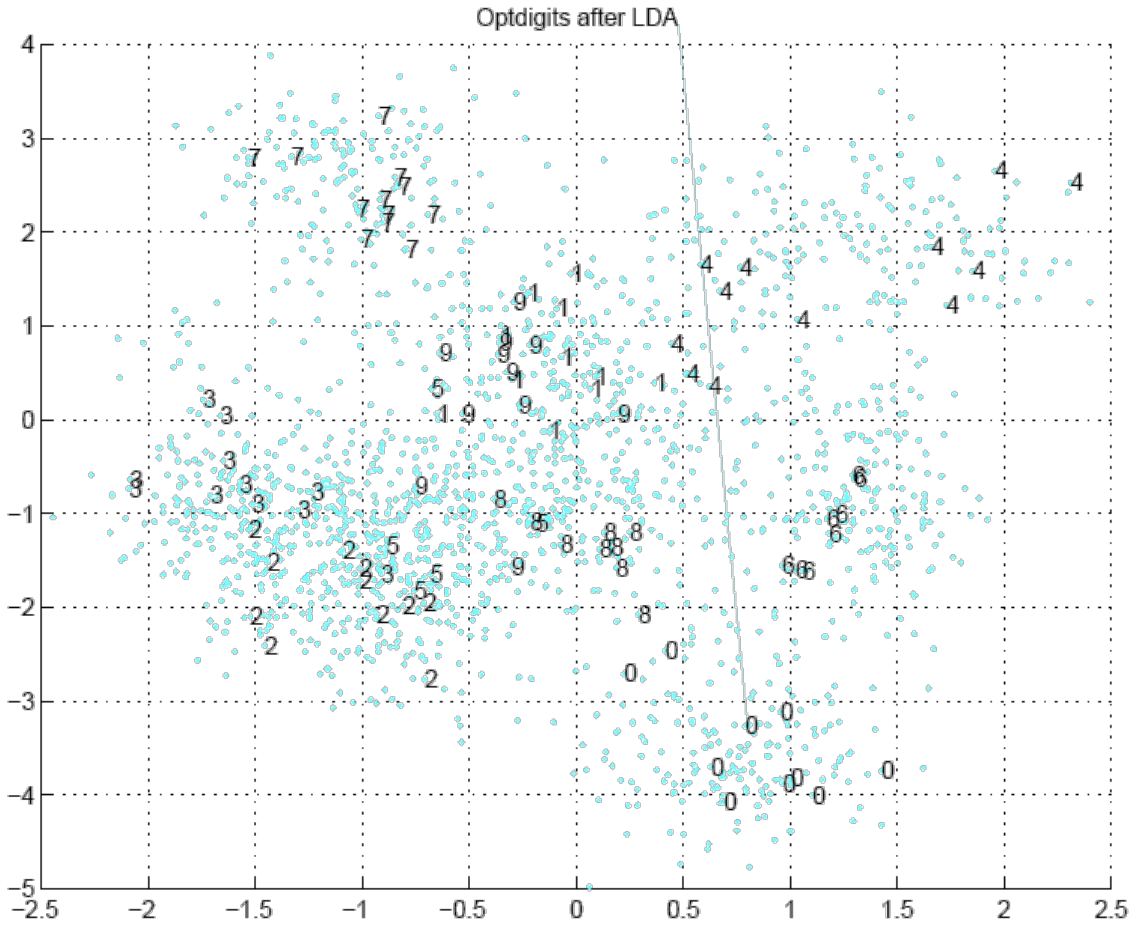
$$\mathbf{S}_B = \sum_{i=1}^{K} N_i \left(\mathbf{m}_i - \mathbf{m}\right)\left(\mathbf{m}_i - \mathbf{m}\right)^T \qquad \mathbf{m} = \frac{1}{K}\sum_{i=1}^{K} \mathbf{m}_i$$

- Find $\mathbf{W}$ that max

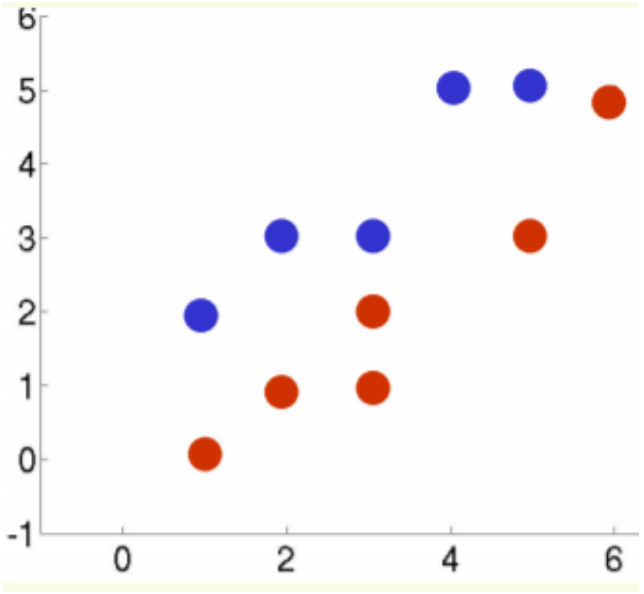
$$J(\mathbf{W}) = \frac{\left|\mathbf{W}^T \mathbf{S}_B \mathbf{W}\right|}{\left|\mathbf{W}^T \mathbf{S}_W \mathbf{W}\right|}$$

The largest eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$

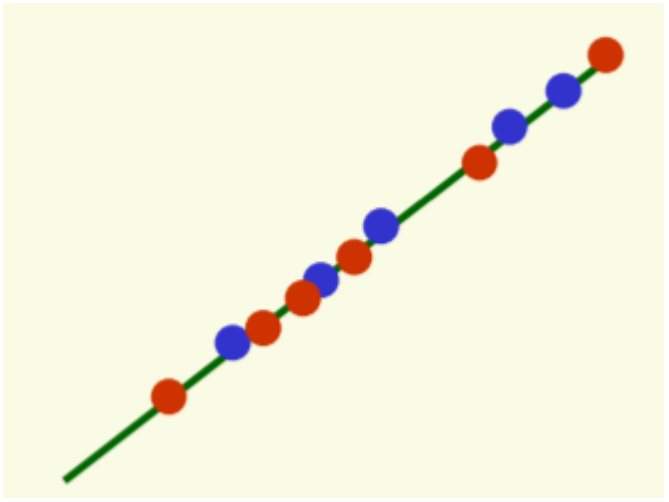
LDA: Illustration



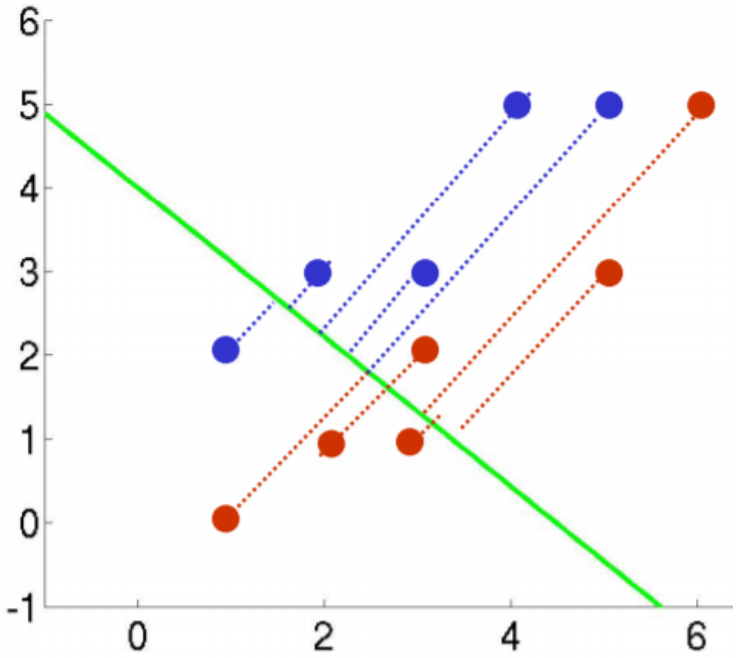
LDA: Illustration



Data



PCA projection



LDA projection

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Multi-Dimensional Scaling

- History: T. Cox and M. Cox, 2001
- Attempts to preserve pairwise distances
- Different formulation of PCA, but yields similar result form

$$\min_{Y} \sum_{i=1}^{N}\sum_{j=1}^{N}(d_{ij}^{(X)} - d_{ij}^{(Y)})^2 \qquad \text{where } d_{ij}^{(X)} = \|x_i - x_j\|^2 \text{ and } d_{ij}^{(Y)} = \|y_i - y_j\|^2.$$

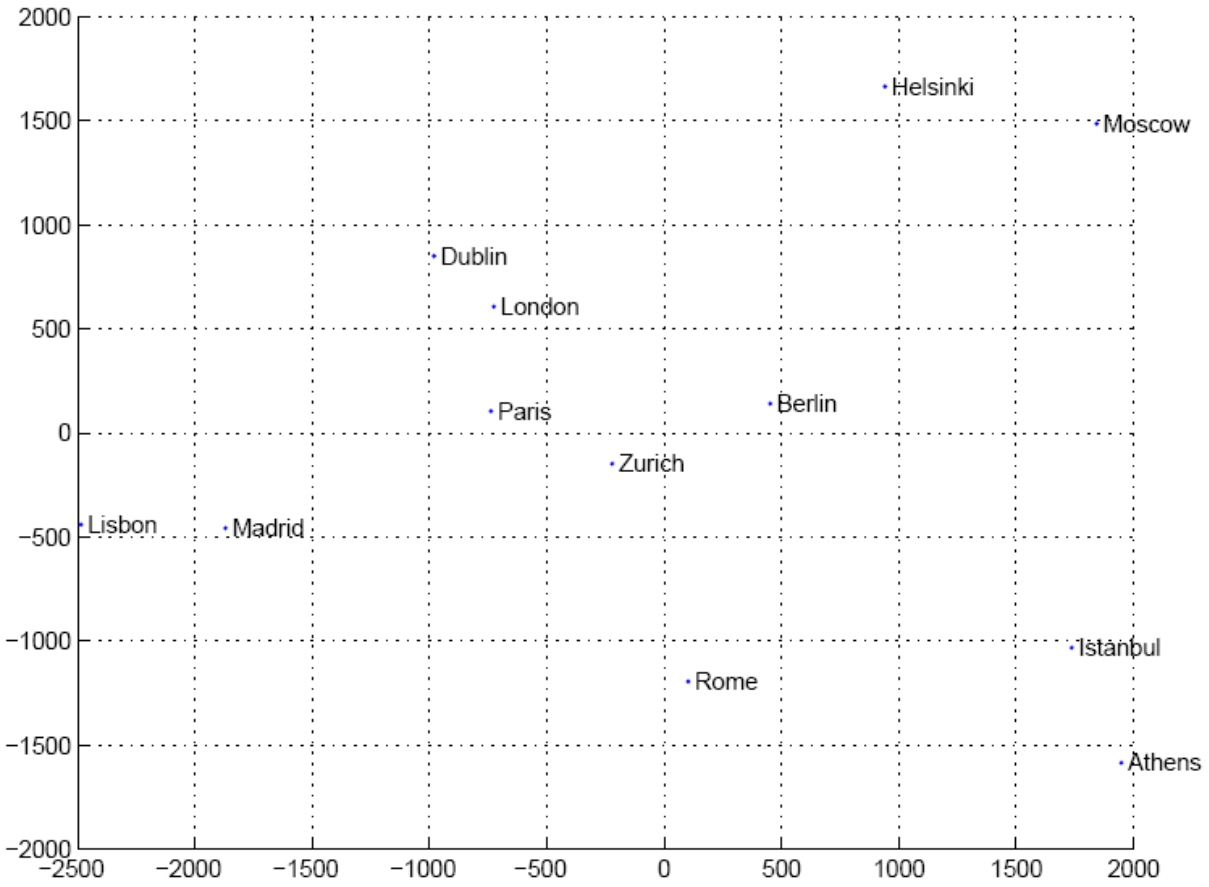
- Transformation

$$X^\top X = -\frac{1}{2} H D^{(X)} H \quad \text{where } H = I - \tfrac{1}{N}\mathbf{1}\mathbf{1}^\top.$$

$$\min_{Y} \sum_{i=1}^{N}\sum_{j=1}^{N}(x_i^\top x_j - y_i^\top y_j)^2$$

Source: Haiqin Yang

MDS: Illustration



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Kernel PCA

- History: S. Mika et al, NIPS, 1999
- Data may lie on or near a nonlinear manifold, not a linear subspace
- Find principal components that are nonlinearly to the input space via nonlinear mapping $x \mapsto \Phi(x)$

- Objective $\min_{U_k} \sum_{i=1}^{N} \left\| \Phi(\mathbf{x}_i) - U_k U_k^T \Phi(\mathbf{x}_i) \right\|^2$

- Solution found by SVD: $\Phi(X) = U \Sigma V^T$

  U contains the eigenvectors of $\Phi(X)\Phi(X)^T$

Source: Haiqin Yang

Kernel PCA

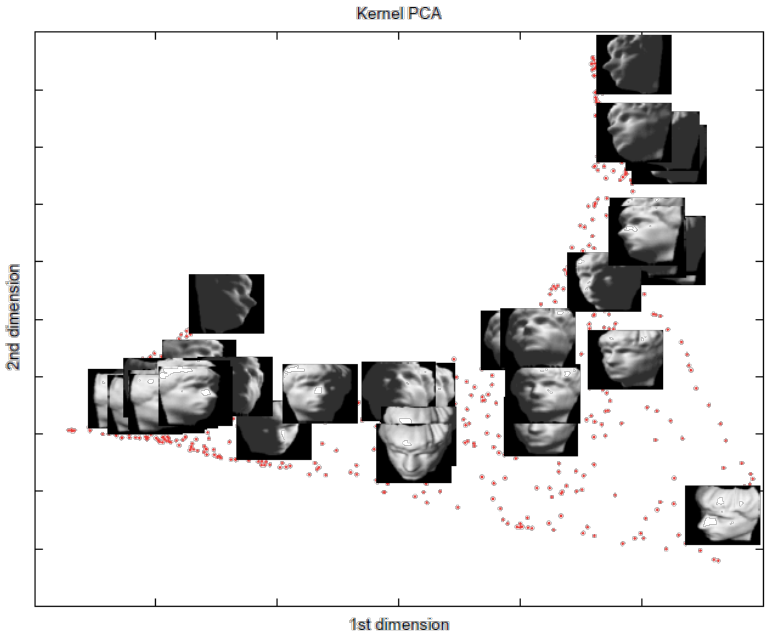
- Centering

$$\tilde{\Phi}(X) = \Phi(X) - E_x[\Phi(X)] \qquad \tilde{K}(x,y) = \tilde{\Phi}(x)\tilde{\Phi(y)}$$

$$\tilde{K}(x,y) = (\Phi(x) - E_x[\Phi(x)]).(\Phi(y) - E_y[\Phi(y)])$$

$$= K(x,y) - E_x[K(x,y)] - E_y[K(x,y)] + E_x[E_y[K(x,y)]]$$

- Issue: Difficult to reconstruct



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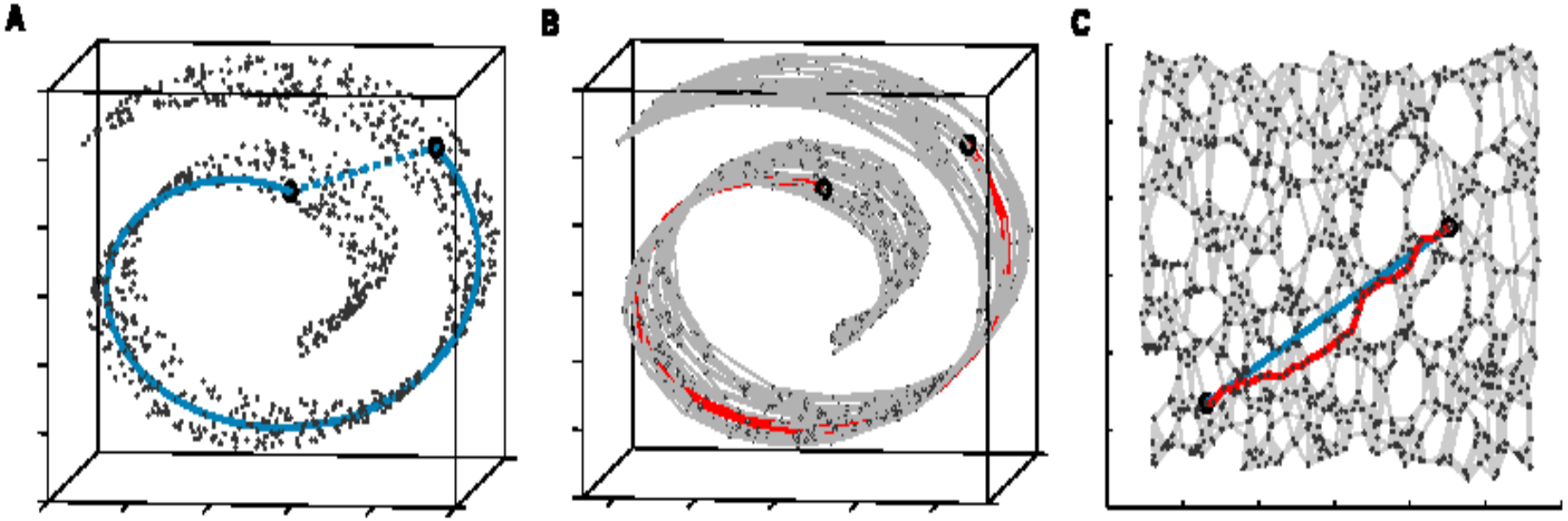
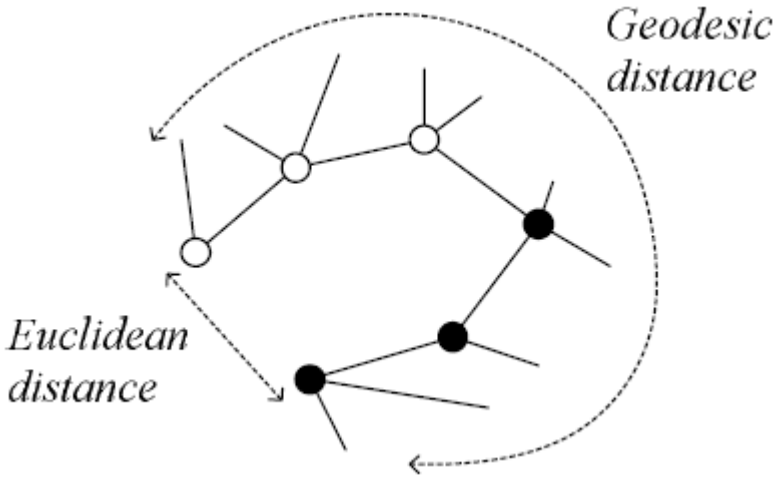
Manifold Learning



A manifold is a topological space which is locally Euclidean.

Isomap

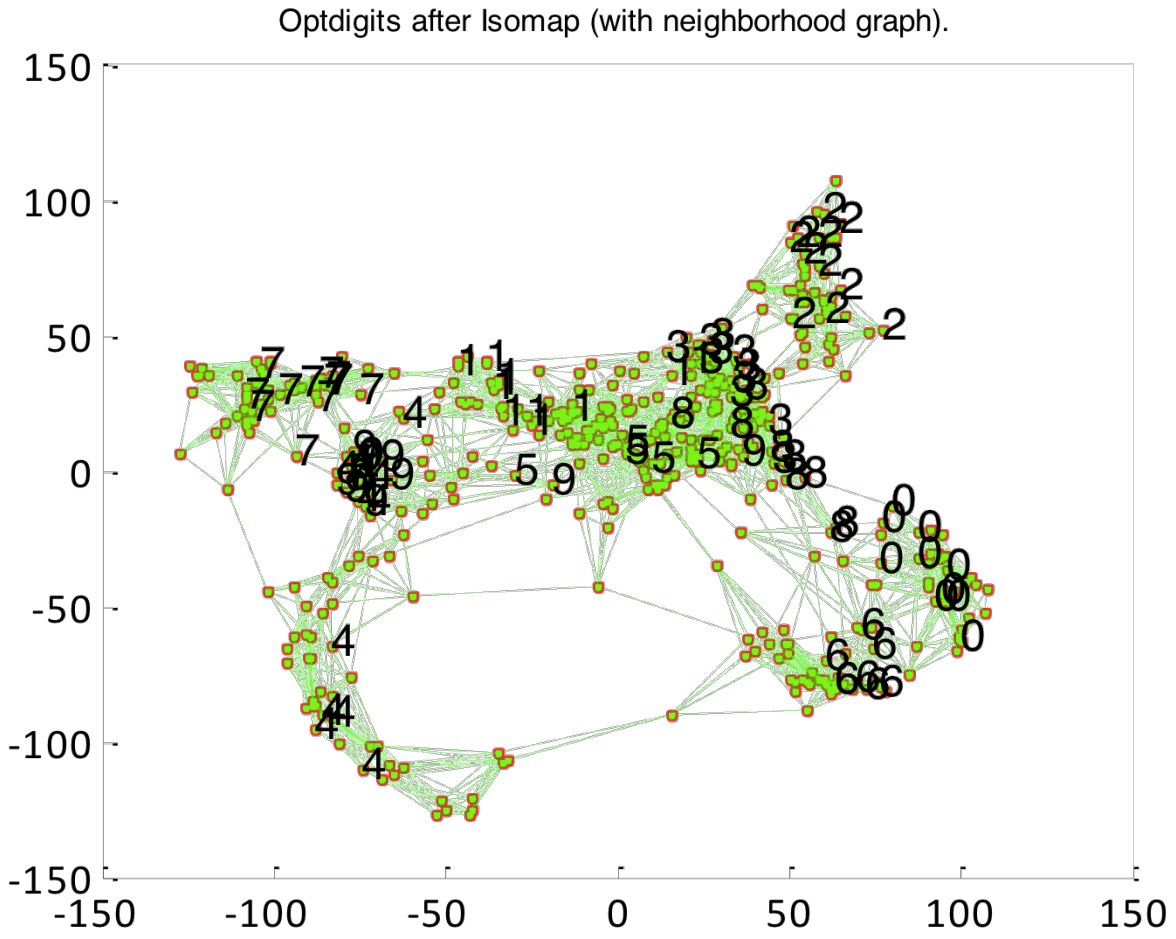
- Geodesic distance is the distance along the manifold that the data lies in, as opposed to the Euclidean distance in the input space



Isomap

- Instances r and s are connected in the graph if $||\boldsymbol{x}^r-\boldsymbol{x}^s||<e$ or if $\boldsymbol{x}^s$ is one of the *k* neighbors of $\boldsymbol{x}^r$ .The edge length is $||\boldsymbol{x}^r-\boldsymbol{x}^s||$
- For two nodes r and s not connected, the distance is equal to the shortest path between them
- Once the *N*x*N* distance matrix is thus formed, use MDS to find a lower-dimensional mapping

Isomap: Illustration



Locally Linear Embedding (LLE)

- History: S. Roweis and L. Saul, Science, 2000
- Procedure
  1. Identify the neighbors of each data point
  2. Compute weights that best linearly reconstruct the point from its neighbors

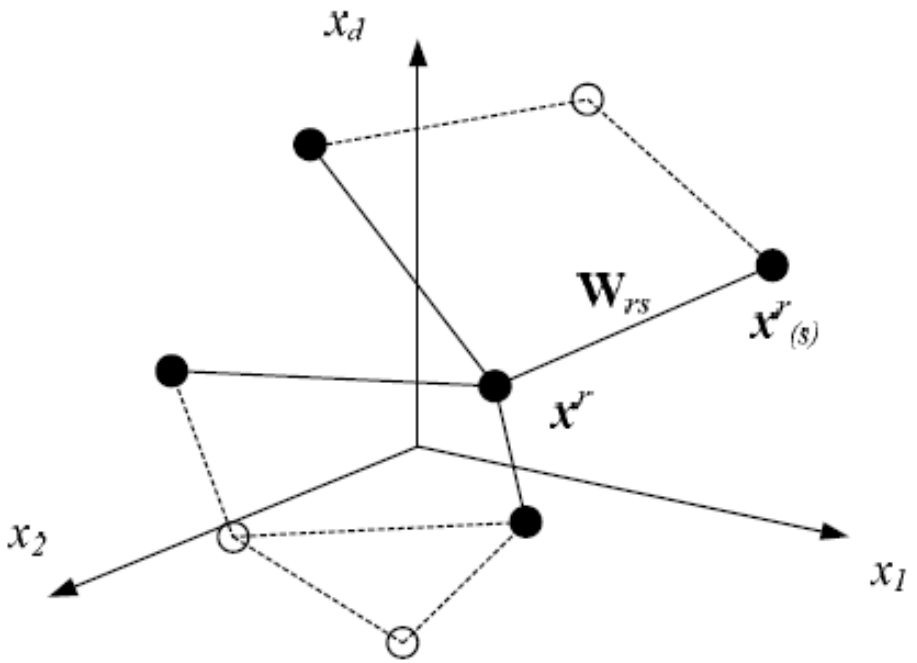
$$\min_{\mathbf{w}} \sum_{i=1}^{N} \|\mathbf{x}_i - \sum_{j=1}^{k} w_{ij}\mathbf{x}_{N_i(j)}\|^2$$

  3. Find the low-dimensional embedding vector which is best reconstructed by the weights determined in Step 2

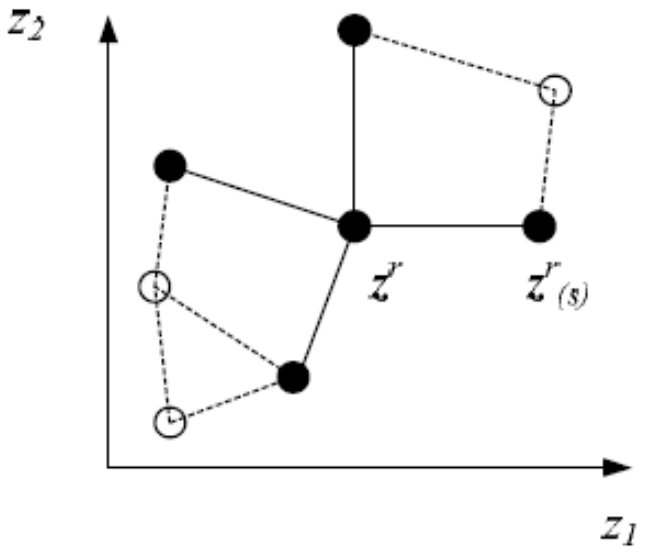
$$\min_{Y} \sum_{i=1}^{N} \|\mathbf{y}_i - \sum_{j=1}^{k} w_{ij}\mathbf{y}_{N_i(j)}\|^2 \Leftrightarrow \min_{Y} \operatorname{tr}(Y^\top Y L)$$

Centering Y with unit variance

LLE

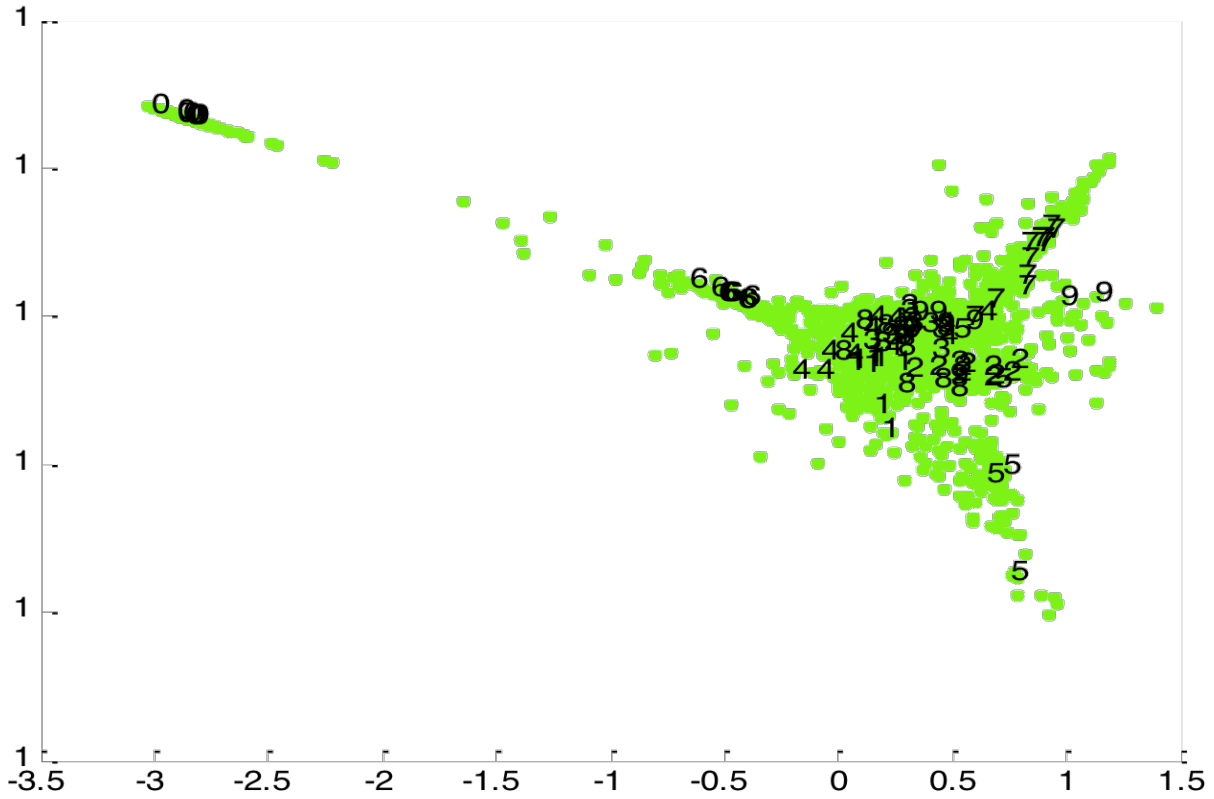


x space



z space

LLE: Illustration



Laplacian Eigenmaps

- History: M. Belkin and P. Niyogi, 2003
- Similar to locally linear embedding
- Different in weights setting and objective function
  - Weights

$$W_{ij} = \begin{cases} 1 & i, j \text{ are connected} \\ \exp\left(\frac{-\|x_i - x_j\|^2}{s}\right) & \text{otherwise} \end{cases}$$

  - Objective

$$\min_Y \sum_{i=1}^{N}\sum_{j=1}^{N}(\mathbf{y}_i - \mathbf{y}_j)W_{ij} \iff \min_Y \operatorname{tr}(YLY^\top)$$

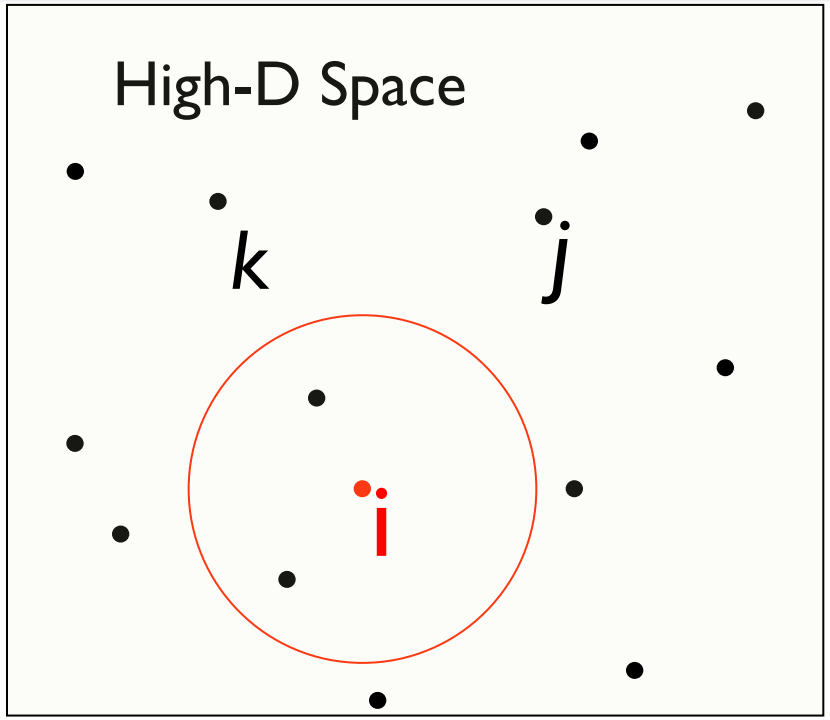
where $L = R - W$, R is diagonal and $R_{ii} = \sum_{j=1}^{N} W_{ij}$.

Outline

- Linear Methods
  - Principal Component Analysis (PCA)
  - Fisher (Linear) Discriminant Analysis (LDA)
  - Multi-Dimensionality Scaling (MDS)
- Non-linear Methods
  - Kernel PCA
  - Manifold Learning methods: ISOMAP, LLE, Laplacian Eigenmaps
  - t-Stochastic Neighborhood Embedding (t-SNE)

Stochastic Neighborhood Embedding

- First convert each high-dimensional similarity into the probability that one data point will pick the other data point as its neighbor.
- To evaluate a map:
  - Use the pairwise distances in the low-dimensional map to define the probability that a map point will pick another map point as its neighbor.
  - Compute the Kullback-Leibler divergence between the probabilities in the high-dimensional and low-dimensional spaces.



$$p_{j|i} = \frac{e^{-d_{ij}^2 / 2\sigma_i^2}}{\sum_k e^{-d_{ik}^2 / 2\sigma_i^2}}$$

probability of picking j given that you start at i

SNE

$$Cost = \sum_i KL(P_i \,||\, Q_i) = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Q is the probability of picking j when you start at I in low-D space

- For points where p_{ij} is large and q_{ij} is small we lose a lot.
  - Nearby points in high-D really want to be nearby in low-D
- For points where q_{ij} is large and p_{ij} is small we lose a little because we waste some of the probability mass in the Q_i distribution.
  - Widely separated points in high-D have a mild preference for being widely separated in low-D.

Readings

- "Introduction to Machine Learning" by Ethem Alpaydin, Chapter 6
- Additional
  - More about t-SNE: https://lvdmaaten.github.io/tsne/
  - Dimensionality Reduction: A Comparative Review (a very good read)
  - A toolbox for 34 dimensionality reduction methods: https://lvdmaaten.github.io/drtoolbox/ (Matlab)