Knowledge Discovery in Databases II

Winter Term 2015/2016

Lecture 3: Volume: High-Dimensional Data: Dimensionality reduction

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http://www.dbs.ifi.lmu.de/cms/Knowledge_Discovery_in_Databases_II_(KDD_II)

Outline

1. Introduction and challenges of high dimensionality
2. Feature Selection
3. Feature Reduction and Metric Learning
4. Clustering in High-Dimensional Data

Introduction

Idea: Instead of removing features, try to find a *low dimensional feature space* generating the original space as accurate as possible:

- Redundant features are summarized
- Irrelevant features are weighted by small values

Methods being discussed in the course:

- Reference point embedding
- Principal component analysis (PCA)
- Singular value decomposition(SVD)
- Fischer-Faces (FF) and Relevant Component Analysis(RCA)
- Large Margin Nearest Neighbor (LMNN)

Reference Point Embedding 1/2

Idea: Describe the position of each object by their *distances* to a set of *reference points.*

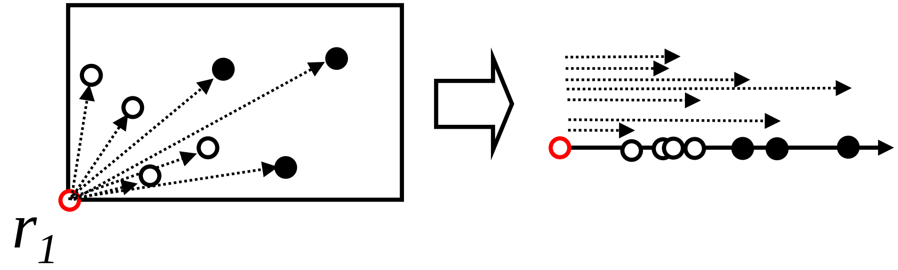
Given: Vector space $F = D_1 \times .. \times D_n$ where $D = \{D_1, .., D_n\}$.

Target: A *k*-dimensional space *R* which yields optimal solutions to given data mining task.

Method: For each reference point $R = \{r_1, .., r_k\}$ and a distance measure $d(\bullet, \bullet)$:

Transform vector $x \in F$:

$$r_R(x) = \begin{pmatrix} d(r_1, x) \\ \vdots \\ d(r_k, x) \end{pmatrix}$$



Reference Point Embedding 2/2

- Distance measure is usually determined by the application.
- Selection of reference points:
  - use centroids of the classes or cluster-centroids
  - using points on the margin of the data space

Advantages :

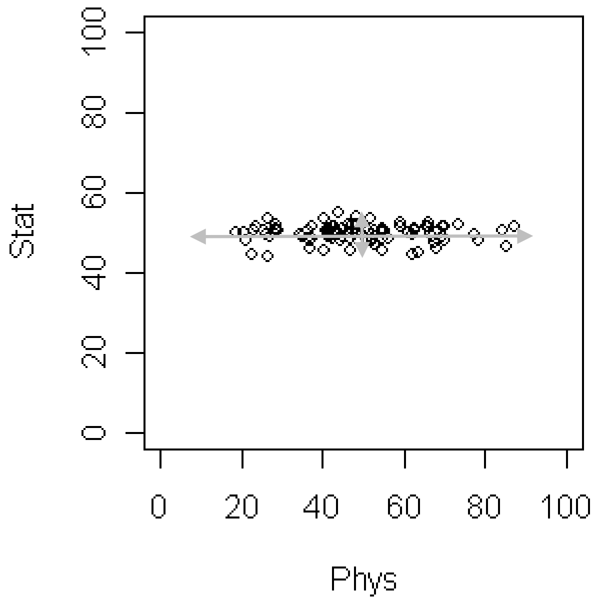
- Simple approach which is easy to implement
- The transformed vectors yields lower and upper bounds of the exact distances

Disadvantages:

- Even using *d* reference points does not reproduce a *d*-dimensional feature space
- Selecting good reference points is relevant and difficult

Principal Component Analysis (PCA): A simple example 1/3

- Consider the grades of students in Physics and Statistics.
- If we want to compare among the students, which grade should be more discriminative? Statistics or Physics?

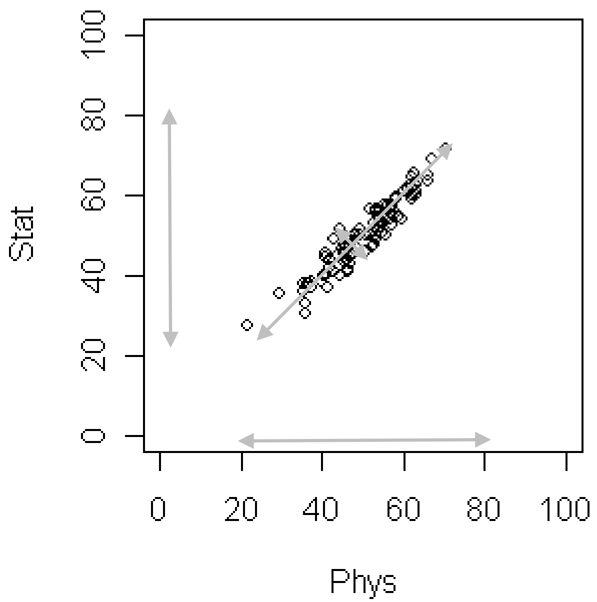


Physics since the variation along that axis is larger.

Based on:
http://astrostatistics.psu.edu/su09/lecturenotes/pca.html

Principal Component Analysis (PCA): A simple example 2/3

- Suppose now the plot looks as below.
- What is the best way to compare students now?



We should take linear combination of the two grades to get the best results.

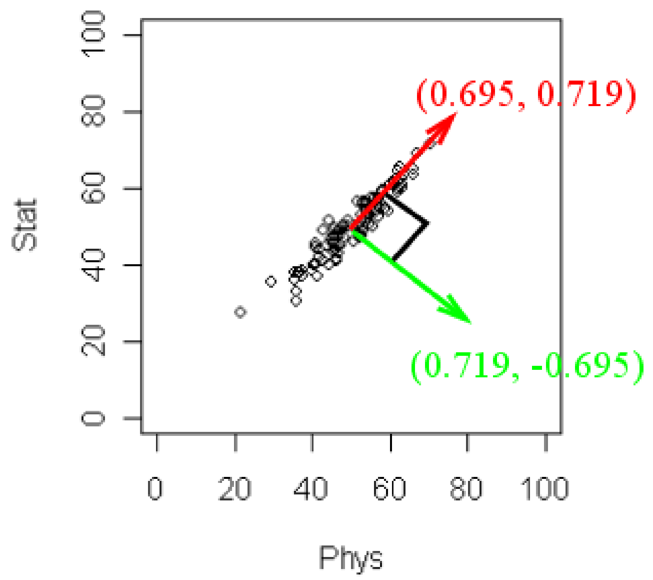
Here the direction of maximum variance is clear.

In general → PCA

Based on:
http://astrostatistics.psu.edu/su09/lecturenotes/pca.html

Principal Component Analysis (PCA): A simple example 3/3

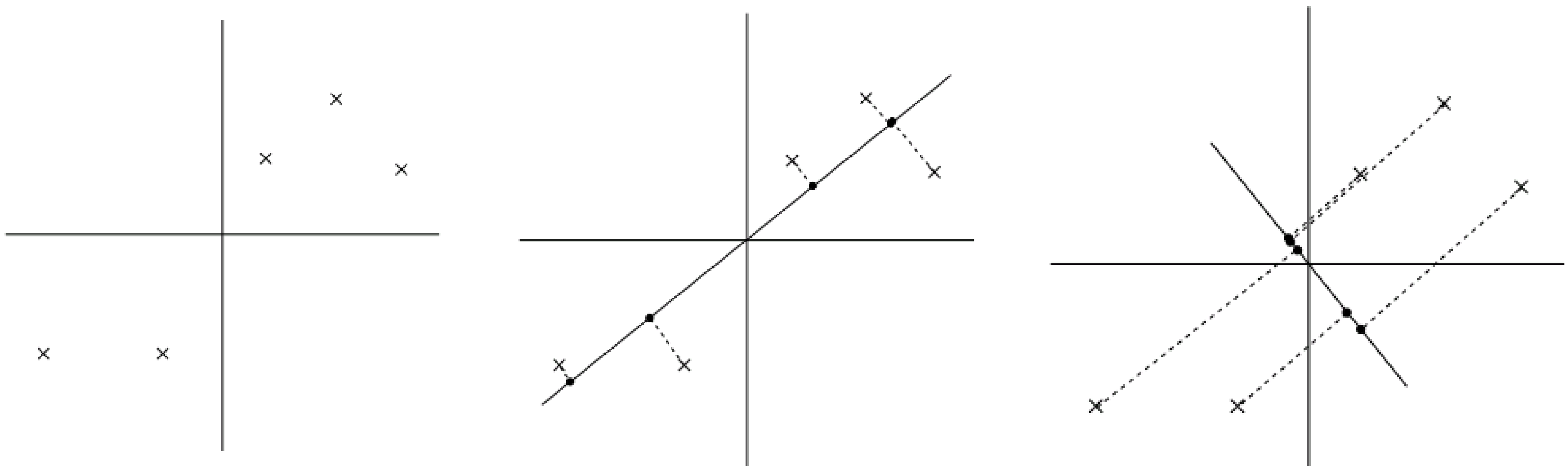
- PCA returns two principal components
  - The first gives the direction of the maximum spread of the data.
  - The second gives the direction of maximum spread perpendicular to the first



Based on:
http://astrostatistics.psu.edu/su09/lecturenotes/pca.html

Intuition

- The data starts off with some amount of variance/information in it. We would like to choose a direction *u* so that if we were to approximate the data as lying in the direction/subspace corresponding to *u*, as much as possible of this variance is still retained.



Initial data | Direction 1 | Direction 2

Idea: Choose the direction that maximizes the variance of the projected data

Principal Component Analysis (PCA)

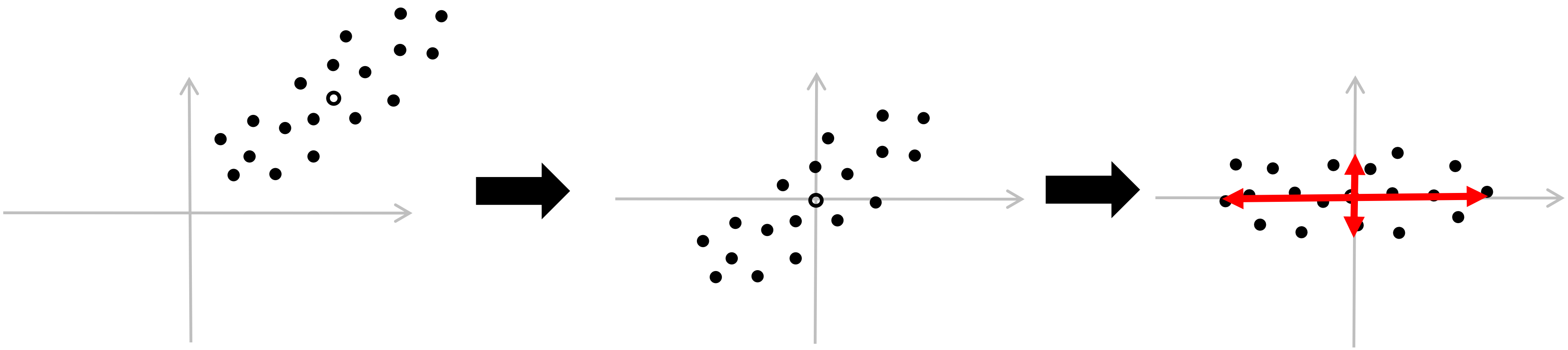
- PCA computes the most meaningful basis to re-express a noisy, garbled data set.
- Think of PCA as choosing a new coordinate system for the data, the principal components being the unit vectors along the axes
- PCA asks: *Is there another basis, which is a linear combination of the original basis, that best expresses our dataset?*
- General form: $PX=Y$

where P is a linear transformation, X is the original dataset and Y the re-representation of this dataset.

  - P is a matrix that transforms X into Y
  - Geometrically, P is a *rotation* and a *stretch* which again transforms X into Y
  - The eigenvectors are the rotations to the new axes
  - The eigenvalues are the amount of stretching that needs to be done
- The *p*'s are the principal components
  - Directions with the largest variance … those are the most important, most *principal*.

Principal Component Analysis (PCA)

Idea: Rotate the data space in a way that the principal components are placed along the main axis of the data space
=> Variance analysis based on principal components



- Rotate the data space in a way that the direction with the largest variance is placed on an axis of the data space
- Rotation is equivalent to a basis transformation by an orthonormal basis
  - Mapping is equal of angle and preserves distances:

$$x \cdot B = x\left(b_{*,1}, \ldots, b_{*,d}\right) = \left(\left\langle x, b_{*,1}\right\rangle, \ldots, \left\langle x, b_{*,d}\right\rangle\right) \quad mit \quad \underset{i \neq j}{\forall} \left\langle b_i, b_j \right\rangle = 0 \wedge \underset{1 \leq i \leq d}{\forall} \left\| b_i \right\| = 1$$

- B is built from the largest variant direction which is orthogonal to all previously selected vectors in B.

What do we need to know for PCA

- Basics of statistical measures:
  - variance
  - covariance
- Basics of linear algebra:
  - Matrices
  - Vector space
  - Basis
  - Eigenvectors, eigenvalues

Variance

- A measure of the spread of the data

$$VAR(X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

- Variance refers to a single dimension, e.g., height

Covariance

- A measure of how much two random variables vary together

$$COV(X,Y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_x)(y_i - \mu_y)$$

- What the values mean
  - Positive values: both dimensions move together (increase or decrease)
  - Negative values: while one dimension increases the other decreases
  - Zero value: the dimensions are independent of each other.

Covariance matrix

- Describes the variance of all features and the pairwise correlations between them

$$\Sigma_D = \begin{pmatrix} VAR(X_1) & \cdots & COV(X_1, X_d) \\ \vdots & \ddots & \vdots \\ COV(X_d, X_1) & \cdots & VAR(X_d) \end{pmatrix}$$

$$VAR(X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2 \qquad COV(X,Y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_x)(y_i - \mu_y)$$

- Properties:
  - For *d*-dimensional data, *d*x*d* covariance matrix
  - symmetric matrix as COV(X,Y)=COV(Y,X)

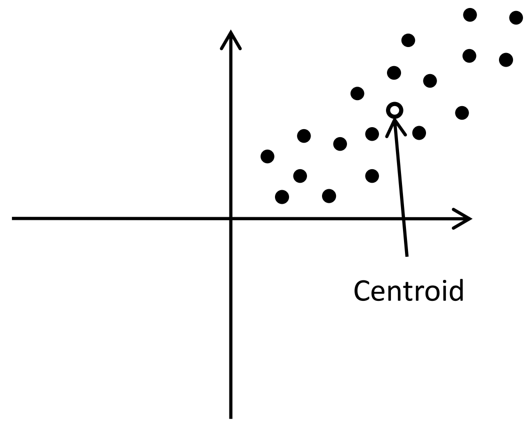
Data matrix

- Given n vectors $v_i \in IR^d$, $n \times d$ matrix

$$D = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} v_{1,1} & \cdots & v_{1,d} \\ \vdots & \ddots & \vdots \\ v_{n,1} & \cdots & v_{n,d} \end{pmatrix}$$ is called data matrix

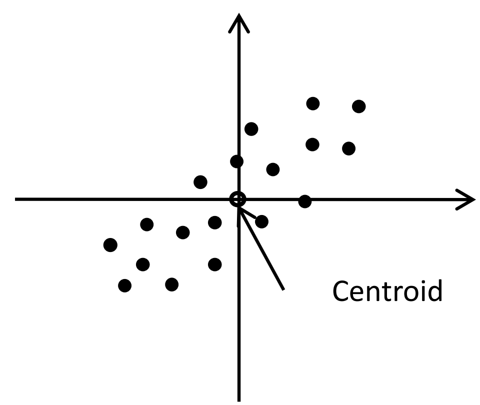
- Centroid/mean vector of D:

$$\vec{\mu} = \frac{1}{n} \cdot \sum_{i=1}^{n} v_i$$



- Centered data matrix:

$$D_{cent} = \begin{pmatrix} v_1 - \vec{\mu} \\ \vdots \\ v_d - \vec{\mu} \end{pmatrix}$$



DATABASE SYSTEMS GROUP

Covariance matrix and centered data matrix

- The covariance matrix can be expressed in terms of the centered data matrix as follows:

$$\Sigma_D = \begin{pmatrix} VAR(X_1) & \cdots & COV(X_1, X_d) \\ \vdots & \ddots & \vdots \\ COV(X_d, X_1) & \cdots & VAR(X_d) \end{pmatrix} = \frac{1}{n} D_{cent}^T D_{cent}$$

Vector/ Matrix basics

- Inner (dot) product of vectors x, y:

$$x \cdot y = x^T \cdot y = \begin{pmatrix} x_1 & \cdots & x_d \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ \vdots \\ y_d \end{pmatrix} = \langle x, y \rangle = \sum_{i=1}^{d} x_i \cdot y_i$$

- Outer product of vectors x, y:

$$x \otimes y = x \cdot y^T = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} \cdot \begin{pmatrix} y_1 & \cdots & y_d \end{pmatrix} = \begin{pmatrix} x_1 y_1 & \cdots & x_1 y_d \\ \vdots & \ddots & \vdots \\ x_d y_1 & \cdots & x_d y_d \end{pmatrix}$$

- Matrix multiplication:

$$A = [a_{ij}]_{m \times p};\ B = [b_{ij}]_{p \times n};$$

$$AB = C = [c_{ij}]_{m \times n}, where\ c_{ij} = row_i(A) \cdot col_j(B)$$

- Length of a vector
  - Unit vector: if $||a||=1$

$$\|a\| = \sqrt{a^T \cdot a} = \sqrt{\sum_{i=1}^{n} a_i^2}$$

Eigenvectors and eigenvalues

- Let D be dxd square matrix.
- A non zero vector v_i is called an *eigenvector* of D if and only if there exists a scalar λ_i such that: $Dv_i=\lambda_i v_i$.
  - λ_i is called an *eigenvalue* of D.

- How to find the eigenvalues/eigenvectors of D?
  - By solving the equation: $\det(D-\lambda I_{dxd})=0$ we get the eigenvalues
    - I_{dxd} is the identity matrix
  - For each eigenvalue λ_i, we find its eigenvector by solving $(D-\lambda_i)v_i=0$

Example

$$A = \begin{pmatrix} 2 & 7 \\ -1 & -6 \end{pmatrix}$$

$$A - \lambda I = \begin{pmatrix} 2 & 7 \\ -1 & -6 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2-\lambda & 7 \\ -1 & -6-\lambda \end{pmatrix}$$

$$\det(A - \lambda I) = (2-\lambda)(-6-\lambda) + 7 = \lambda^2 + 4\lambda - 5 = (\lambda+5)(\lambda-1)$$

2 eigenvalues: $\lambda_1 = -5 \quad \lambda_2 = 1$

Find the eigenvector of λ_1

$$(A - \lambda I_n)\vec{\eta} = \vec{0} \qquad \begin{pmatrix} 7 & 7 \\ -1 & -1 \end{pmatrix}\vec{\eta} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Find the eigenvector of λ_2

$$\begin{pmatrix} 1 & 7 \\ -1 & -7 \end{pmatrix}\vec{\eta} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\lambda_1 = -5 \qquad \vec{\eta}^{(1)} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\lambda_2 = 1 \qquad \vec{\eta}^{(1)} = \begin{pmatrix} -7 \\ 1 \end{pmatrix}$$

Eigenvectors decomposition

- Let D be *dxd* square matrix.
- Eigenvalue decomposition of the data matrix

$$D = V \Lambda V^T$$

$$V = (v_1, \cdots, v_d) \quad mit \underbrace{\forall_{i \neq j} \langle v_i, v_j \rangle = 0}_{\text{The eigenvectors are linearly independent}} \quad und \; \underbrace{\forall_{i=1}^{d} \| v_i \| = 1}_{\text{Every eigenvector is a unit vector}}$$

$$\Lambda = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_d \end{pmatrix}$$

Every eigenvector is a unit vector

The eigenvectors are linearly independent

The corresponding eigenvalues

- The columns of V are the eigenvectors of D
- The diagonal elements of Λ are the eigenvalues of D

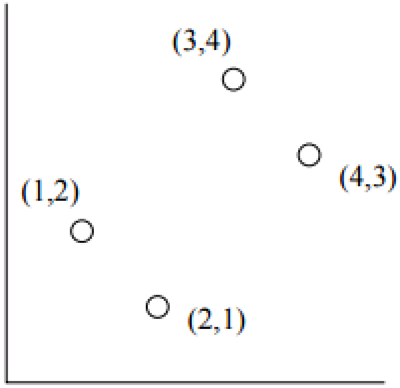
Feature reduction using PCA

1. Compute the covariance matrix Σ
2. Compute the eigenvalues and the corresponding eigenvectors of Σ
3. Select the *k* biggest eigenvalues and their eigenvectors (V‘)
4. The *k* selected eigenvectors represent an orthogonal basis
5. Transform the original $n \times d$ data matrix D with the $d \times k$ basis V‘:

$$D \cdot \mathrm{V}' = \begin{pmatrix} \mathrm{x}_1 \\ \vdots \\ \mathrm{x}_\mathrm{n} \end{pmatrix} \left(v_1', \cdots, v_k' \right) = \begin{pmatrix} \langle \mathrm{x}_1, v_1' \rangle & \cdots & \langle \mathrm{x}_1, v_k' \rangle \\ \vdots & \ddots & \vdots \\ \langle \mathrm{x}_\mathrm{n}, v_1' \rangle & \cdots & \langle \mathrm{x}_\mathrm{n}, v_k' \rangle \end{pmatrix}$$

Example of transformation

- Original



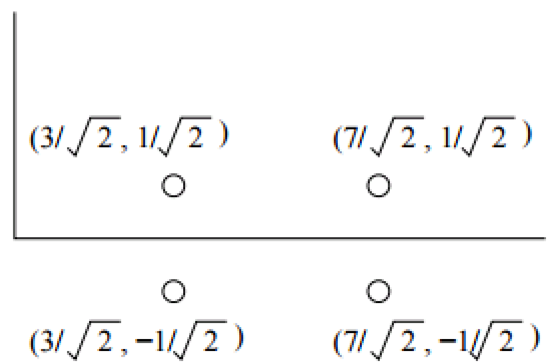
Eigenvectors

$$\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \qquad \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

- Transformed data

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{2} & 1/\sqrt{2} \\ 3/\sqrt{2} & -1/\sqrt{2} \\ 7/\sqrt{2} & 1/\sqrt{2} \\ 7/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

In the rotated coordinate system



Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

Percentage of variance explained by PCA

- Let *k* be the number of top eigenvalues out of *d* (*d* is the number of dimensions in our dataset)
- The percentage of variance in the dataset explained by the *k* selected eigenvalues is:

$$\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

- Similarly, you can find the variance explained by each principal component
- Rule of thumb: keep enough to explain **85%** of the variation

PCA results interpretation

- Example: iris dataset (d=4), results from R
- 4 principal components

	PC1	PC2	PC3	PC4
Sepal.Length	0.5038236	-0.45499872	0.7088547	0.19147575
Sepal.Width	-0.3023682	-0.88914419	-0.3311628	-0.09125405
Petal.Length	0.5767881	-0.03378802	-0.2192793	-0.78618732
Petal.Width	0.5674952	-0.03545628	-0.5829003	0.58044745

Importance of components:

	PC1	PC2	PC3	PC4
Proportion of Variance	0.7331	0.2268	0.03325	0.00686
Cumulative Proportion	0.7331	0.9599	0.99314	1.00000

Singular Value Decomposition (SVD)

Generalization of the eigenvalue decomposition

Let D_{nxn} be the data matrix and let k be its rank (max number of independent rows/ columns).

We can decompose D into matrices O, S, A as follows

$$D = OSA^T$$

$$\begin{array}{cc} & \longleftarrow d \longrightarrow \\ n \updownarrow & \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \end{array} = \begin{array}{c} \longleftarrow k \longrightarrow \\ \begin{bmatrix} o_{1,1} & \cdots & o_{1,k} \\ \vdots & \ddots & \vdots \\ o_{n,1} & \cdots & t_{n,k} \end{bmatrix} \end{array} \cdot \begin{array}{c} \longleftarrow k \longrightarrow \\ \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k \end{bmatrix} \end{array} \cdot \begin{array}{cc} \longleftarrow d \longrightarrow & \\ \begin{bmatrix} a_{1,1} & \cdots & a_{1,d} \\ \vdots & \ddots & \vdots \\ a_{k,1} & \cdots & a_{k,d} \end{bmatrix} & \updownarrow k \end{array}$$

O is an $n \times k$ column-orthonormal matrix ; that is, each of its columns is a unit vector and the dot product of any two columns is 0.

S is a diagonal *k x k* matrix; that is, all elements not on the main diagonal are 0. The elements of S are called the *singular values* of D.

A is a *k x d* column-orthonormal matrix. Note that we always use *A* in its transposed form, so it is the rows of A^T that are orthonormal.

Decomposition based on numerical algorithms.

Example 1

- D: ratings of movies by users
- The corresponding SVD

	Matrix	Alien	Star Wars	Casablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	0	0	4	4
Jenny	0	0	0	5	5
Jane	0	0	0	2	2

Ratings of movies by users

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{bmatrix}}_{\mathbf{D}} = \underbrace{\begin{bmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .60 \\ 0 & .75 \\ 0 & .30 \end{bmatrix}}_{\mathbf{O}} \underbrace{\begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix}}_{\mathbf{S}} \underbrace{\begin{bmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{bmatrix}}_{\mathbf{A}^T}$$

- Interpretation of SVD
  - O shows two concepts “science fiction” and “romance”
  - S shows the strength of these concepts
  - A relates movies to concepts

Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

Example 2

- A slightly different D
- The corresponding SVD

	Matrix	Alien	Star Wars	Casablanca	Titanic
Joe	1	1	1	0	0
Jim	3	3	3	0	0
John	4	4	4	0	0
Jack	5	5	5	0	0
Jill	0	2	0	4	4
Jenny	0	0	0	5	5
Jane	0	1	0	2	2

$$\underbrace{\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}}_{\mathbf{D}} = \underbrace{\begin{bmatrix} .13 & .02 & -.01 \\ .41 & .07 & -.03 \\ .55 & .09 & -.04 \\ .68 & .11 & -.05 \\ .15 & -.59 & .65 \\ .07 & -.73 & -.67 \\ .07 & -.29 & .32 \end{bmatrix}}_{\mathbf{O}} \underbrace{\begin{bmatrix} 12.4 & 0 & 0 \\ 0 & 9.5 & 0 \\ 0 & 0 & 1.3 \end{bmatrix}}_{\mathbf{S}} \underbrace{\begin{bmatrix} .56 & .59 & .56 & .09 & .09 \\ .12 & -.02 & .12 & -.69 & -.69 \\ .40 & -.80 & .40 & .09 & .09 \end{bmatrix}}_{\mathbf{A}^T}$$

- Interpretation of SVD
  - O shows three concepts “science fiction” and “romance” and “”?
  - S shows the strength of these concepts
  - A relates movies to concepts

Source: http://infolab.stanford.edu/~ullman/mmds/ch11.pdf

Dimensionality reduction with SVD

- To reduce dimensionality, we can set the smallest singular values to 0 in S and eliminate the corresponding column in O and row in A^T
  - Check previous example
- How Many Singular Values Should We Retain?
  - Rule of thumb: retain enough singular values to make up 90% of the energy in Σ
  - Energy defined in terms of the singular values (matrix S)
  - In previous example, total energy is: $(12.4)^2 + (9.5)^2 + (1.3)^2 = 245.70$
  - The retained energy is: $(12.4)^2 + (9.5)^2 = 244.01$ >99%

Connection between SVD and PCA

Apply SVD to the covariance data:

$$\Sigma_D = \frac{1}{n} D_{cent}^T D_{cent}$$

$$D_{cent} = OSA^T$$

Recall O is orthonormal matrix, so $O^T O$ is the identity matrix

Recall S is a diagonal matrix, transposing has no effect

$$\Sigma_D = \left(OSA^T\right)^T OSA^T = AS^T\left(O^T O\right)SA^T = A\left(S^T S\right)A^T = A\begin{pmatrix} \lambda_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k^2 \end{pmatrix} A^T$$

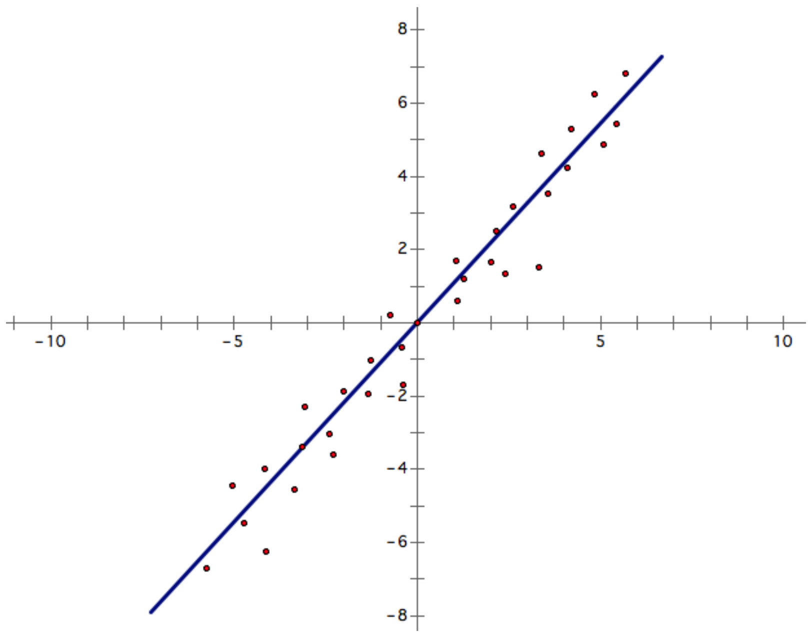
- Here: A is a matrix of eigenvectors
- Eigenvalues of the covariance matrix = squared singular values of D

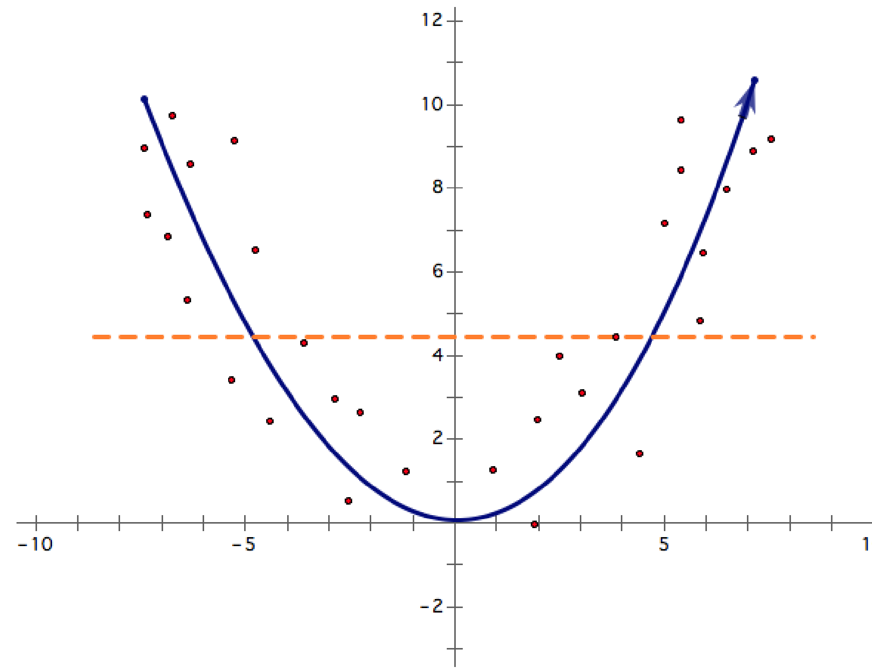
Conclusion: Eigenvalues and eigenvectors of the covariance matrix Σ can be determined by the SVD of the data matrix D.

$\Rightarrow$ SVD is sometimes a better way to perform PCA (Large dimensionalities e.g., text data)
$\Rightarrow$ SVD can cope is dependent dimensions (k<d is an ordinary case in SVD)

Kernel PCA

An extension of PCA using techniques of kernel methods.

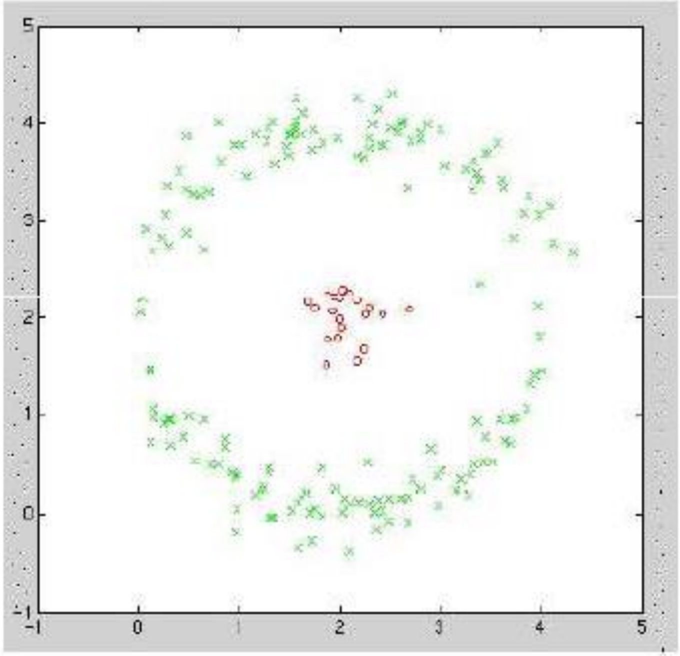




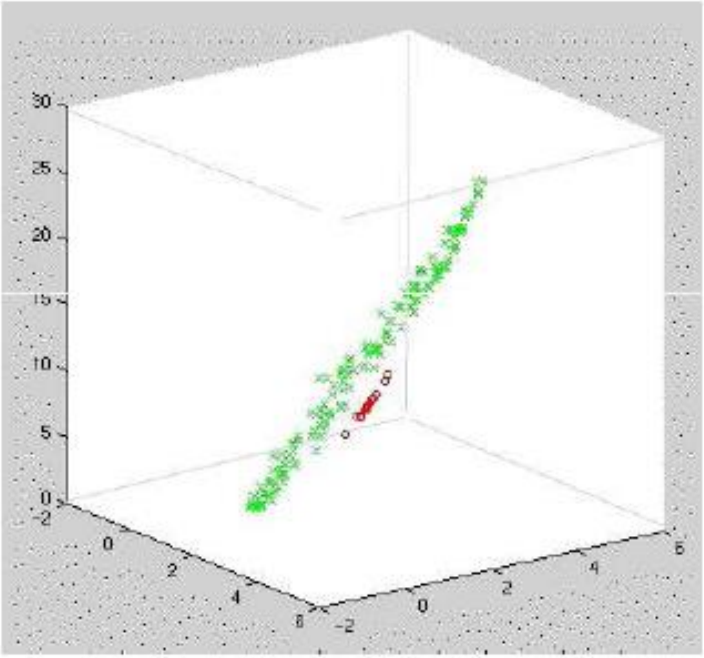
Left figure displays a 2D example in which PCA is effective because data lie near a linear subspace.
In the right figure though, PCA is ineffective, because data the data lie near a parabola. In this case, the PCA compression of the data might project all points onto the orange line, which is far from ideal.

Basic idea

- Project the data into a higher dimensional space



These classes are linearly inseparable in the input space



We can make the problem linearly separable by a simple mapping

$$\Phi : \mathbf{R}^2 \rightarrow \mathbf{R}^3$$

$$(x_1, x_2) \mapsto (x_1, x_2, x_1^2 + x_2^2)$$

Kernel trick

- High-dimensional mapping can seriously increase computation time.
- Can we get around this problem and still get the benefit of high dimensions?
- Yes! Kernel Trick

$$K\left(x_i, x_j\right) = \phi(x_i)^T \phi(x_j)$$

- Different types of kernels
  - Polynomial
  - Gaussian
  - …

Example: Polynomial kernel

- For degree-*d* polynomials, the polynomial kernel is defined as

$$K(x,y) = (x^{\mathsf{T}} y + c)^d$$

- Example:

$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{(2)}x_1 x_2, x_2^2)$$

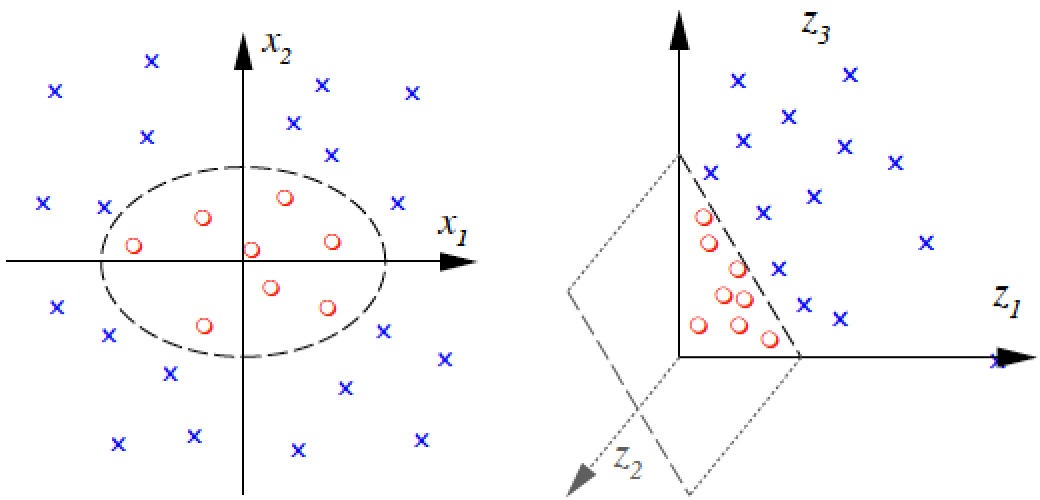


Image from: http://i.stack.imgur.com/qZV3s.png

Kernel PCA

Connection between the orthonormal busies O und A: $D = OSA^T$

- A is a k-dimensional basis of eigenvectors of $D^T \cdot D$
  (cf. previous slide)
- *Analogously: O is a* k-dimension basis of Eigenvectors $D \cdot D^T$
  - $D \cdot D^T$ is a kernel matrix for the linear kernell <x,y> (cf. SVMs in KDD I)
  - The vectors of A and O are connected in the following way:

$$D_{cent} = OSA^T \Rightarrow O^T D_{cent} = O^T OSA^T = SA^T \Rightarrow S^{-1} O^T D_{cent} = A^T$$

$$\Rightarrow a_j = \sum_{i=1}^{n} o_{i,j} x_i$$

The j^{th} *d*-dimensional eigenvector in A is a linear combination of the vectors in D based on k-dimensional j^{th} eigenvectors as weighting vector (the i^{th} values is the weight for vector d_i)

$\Rightarrow$ A basis in vector space corresponds to a basis in the kernel space

$\Rightarrow$ A PCA can be computed for any kernel space based on the kernel matrix (Kernel PCA allows PCA in a non-linear transformation of the original data)

Kernel PCA

Let $K(x,y) = \langle \Phi(x), \Phi(y) \rangle$ be a kernel for the non-linear transformation Φ(x).

Assume: *K(x,y)* is known, but Φ(x) is not explicitly given.

- Let K be the kernel matrix of D w.r.t. *K(x,y)* :

$$K = \begin{pmatrix} K(x_1, x_1) & \cdots & K(x_i, x_n) \\ \vdots & \ddots & \vdots \\ K(x_n, x_1) & \cdots & K(x_n, x_n) \end{pmatrix}$$

- The eigenvalue decomposition of K : $K = VSV^T$
  where V is a n-dimensional basis from eigenvectors of K
- To map *D* w.r.t. *V* the principal components in the target space the vectors x_i in *D must be transformed using* the kernel *K(x,y)*.

$$y' = \begin{pmatrix} \left\langle \Phi(y), \sum_{i=1}^{n} v_{i,1} \Phi(x_i) \right\rangle \\ \vdots \\ \left\langle \Phi(y), \sum_{i=1}^{n} v_{i,k} \Phi(x_i) \right\rangle \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} v_{i,1} \langle \Phi(y), \Phi(x_i) \rangle \\ \vdots \\ \sum_{i=1}^{n} v_{i,k} \langle \Phi(y), \Phi(x_i) \rangle \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} v_{i,1} K(y, x_i) \\ \vdots \\ \sum_{i=1}^{n} v_{i,k} K(y, x_i) \end{pmatrix}$$

Matrix factorization as an Optimization Task

SVD and PCA are standard problems in Algebra.

- Matrix decomposition can be formulated as a optimization task.
- This allows a computation via numerical optimization algorithms
- In this formulation the diagonal matrix is often distributed to both basis matrixes

$$D = ASB^T = \left(A \begin{pmatrix} \sqrt{\lambda_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\lambda_k} \end{pmatrix} \right) \left(\begin{pmatrix} \sqrt{\lambda_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\lambda_k} \end{pmatrix} B^T \right) = UV^T$$

- As an optimization problem: $L(U,V) = \left\| D - UV^T \right\|_f^2$

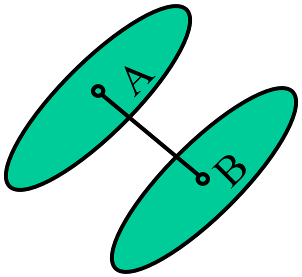
(squared Frobenius Norm of a matrix) $\left\| M \right\|_f^2 = \sum_{i=1}^{n} \sum_{j=1}^{m} \left| m_{i,j} \right|^2$

subject to: $\underset{i \neq j}{\forall} : \langle v_i, v_j \rangle = 0 \wedge \langle u_i, u_j \rangle = 0$

Fischer Faces

Idea: Use examples to increase the discriminative power of the target space.

$$\Sigma_b = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$



$$\Sigma_w = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Target:

- Minimize the similarity between objects from different classes.
  (between class scatter matrix: Σ_b)

  Σ_b: Covariance matrix of the class centroids

$$\bar{\mu} = \frac{1}{|C|} \sum_{c \in C} \mu_c$$

$$\Sigma_b = \frac{1}{|C|} \begin{bmatrix} \mu_1 - \bar{\mu} \\ .. \\ \mu_m - \bar{\mu} \end{bmatrix}^T \cdot \begin{bmatrix} \mu_1 - \bar{\mu} \\ .. \\ \mu_m - \bar{\mu} \end{bmatrix}$$

- Maximize similarity between objects belonging to the same class
  (within class scatter matrix Σ_w)

  Σ: Average covariance matrix of all classes.

$$\Sigma_w = \frac{\sum_{C_i \in C} \Sigma_{C_i}}{|C|}$$

Fischer Faces

Determine basis x_i *in a way that* $S = \frac{x_i^T \cdot \Sigma_b \cdot x_i}{x_i^T \cdot \Sigma_w \cdot x_i}$ is maximized subject to $i \neq j : \langle x_i, x_j \rangle = 0$

Computation: Determine a orthonormal basis with dimensionality d' < d. Reduction to the eigenvalue decomposition.

$$\lambda_i \cdot x_i = \lambda_i \cdot \Sigma_w^{-1} \cdot \Sigma_b$$

Remark: The vector having the largest eigenvalue corresponds to the normal vector of the separating hyper plane in linear discriminant analysis or Fisher's discriminant analysis. (cf. KDD I)

Relevant Component Analysis (RCA)

Fischer Faces are limited due to nature of Σ_b and Σ_w :

Assumption of mono-modal classes:
each class is assumed to follow a multivariate

=> distribution of class centroids Σ_b

=> within correlation in Σ_w

Conclusion: Multi-modal or non-Gaussian distribution are not modeled well

Relevant Component Analysis:

- Remove linear dependent features (e.g. with SVD)
- Given: chunks data which are known to consist of similar objects.
  => replace Σ_w with an within-chunk matrix: $$\Sigma_{wc} = \frac{1}{|C|} \sum_{C_i \in C} \frac{1}{|C_i|} C_i^T C_i$$
- The covariance of all data objects is dominated by dissimilarity $$\Sigma = \frac{1}{|D|} D^T D$$
  => replace Σ_b with the covariance matrix of D

Large Margin Nearest Neighbor (LMNN)

Observation: Objects in a class might vary rather strongly.

Idea: Define an optimization problem only considering the distances the most similar objects from the same and other classes.

Define: $y_{i,j}=1$ *if* x_i and x_j *are from the same class else* $y_{i,j}=0$

- *Target:* $L: IR^d \rightarrow IR^d$ linear transformation of the vector space: $D(x,y) = \|L(x) - L(y)\|^2$
- Target neighbors: T_x k-nearest neighbors from the same class

  $\eta_{i,j}=1$: x_j is a target neighbor of x_i *else* $\eta_{i,j}=0$
- Training by minimizing the following error function:

$$E(L) = \sum_{i=1}^{n}\sum_{j=1}^{n}\eta_{i,j}\|L(x_i) - L(x_j)\|^2 + c\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{l=1}^{n}\eta_{i,j}(1-y_{i,l})\left[1 + \|L(x_i) - L(x_j)\|^2 - \|L(x_i) - L(x_l)\|^2\right]_+$$

  where $[z]_+ = \max(z, o)$
- Problem is a ***semi-definite program***
  => Standard optimization problem where the optimization paramters must form a semi-definite matrix. Here the matrix is the basis transformation L(x).

Summary

- Linear basis transformation yield a rich framework to optimize feature spaces
- Unsupervised methods delete low variant dimensions (PCA und SVD)
- Kernel PCA allows to compute PCA in non-linear kernel spaces
- Supervised methods try to minimize the within class distances while maximizing between class distances
- Fischer Faces extend linear discriminant analysis based on the assumption that all classes follow Gaussian distributions
- Relevant Component Analysis(RCA) generalize this notion and only minimize the distances between chunks of similar objects
- Large Margin Nearest Neighbor(LMNN) minimizes the distances to the nearest target neighbors and punish small distances to non-target neighbors in other classes

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