Outline

1. Introduction and challenges of high dimensionality

2. Feature Selection

3. **Feature Reduction and Metric Learning**

4. Clustering in High-Dimensional Data

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

Some sample methods (among lots of others):

- 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.*

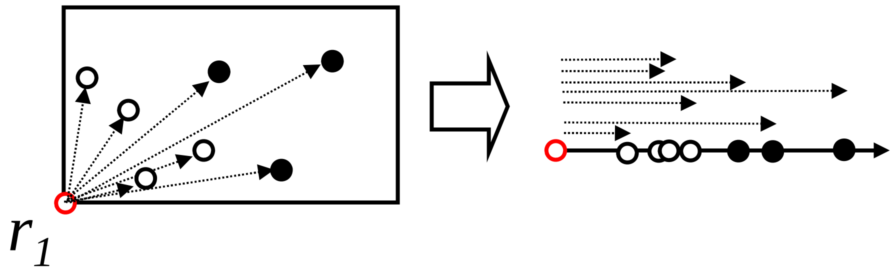
Given: Vector space F $=D_1\times..\times D_n$ where D $=\{D_1,..,D_n\}$.

Target: A *k*-dimensional space *R* which yields optimal solutions for a 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
  - use random sample

Advantages :

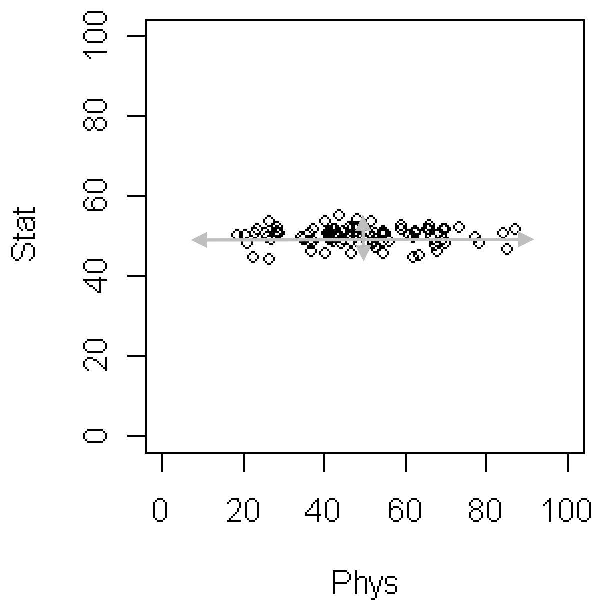
- Simple approach which is easy to implement
- The transformed vectors yields lower and upper bounds of the exact distances (What is that good for???)

Disadvantages:

- Even using *d* reference points does not reproduce a *d*-dimensional feature space
- Selecting good reference points is relevant but very 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?

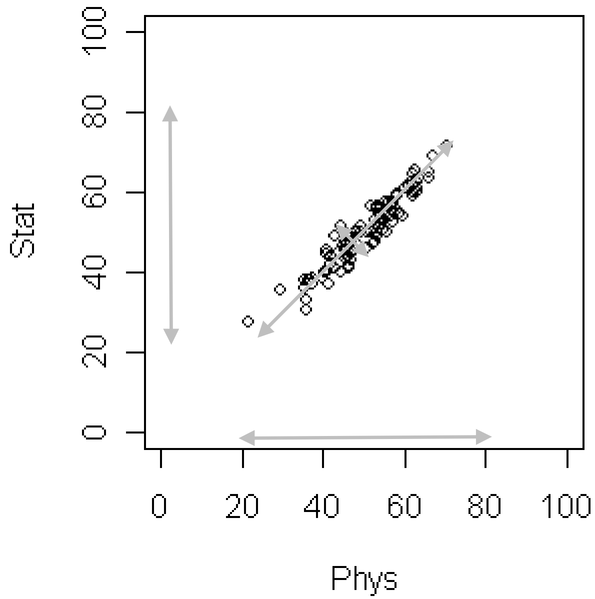


Physics since the variation along that axis is larger.

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 a linear combination of the two grades to get the best results.

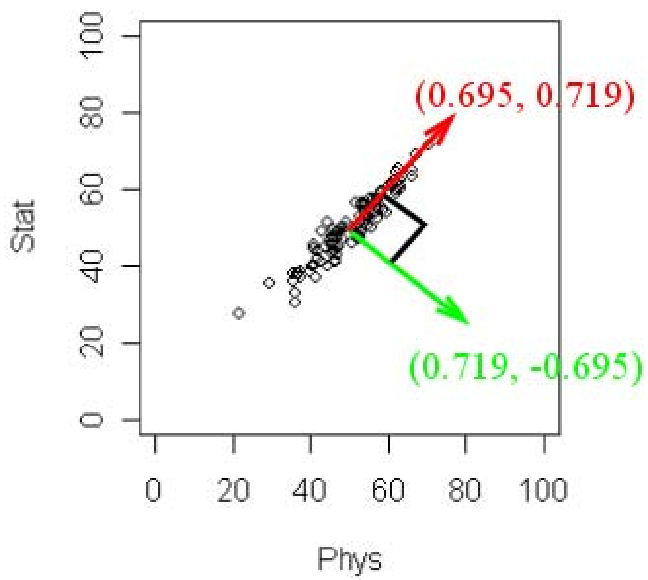
Here the direction of maximum variance is clear.

In general → PCA

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

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

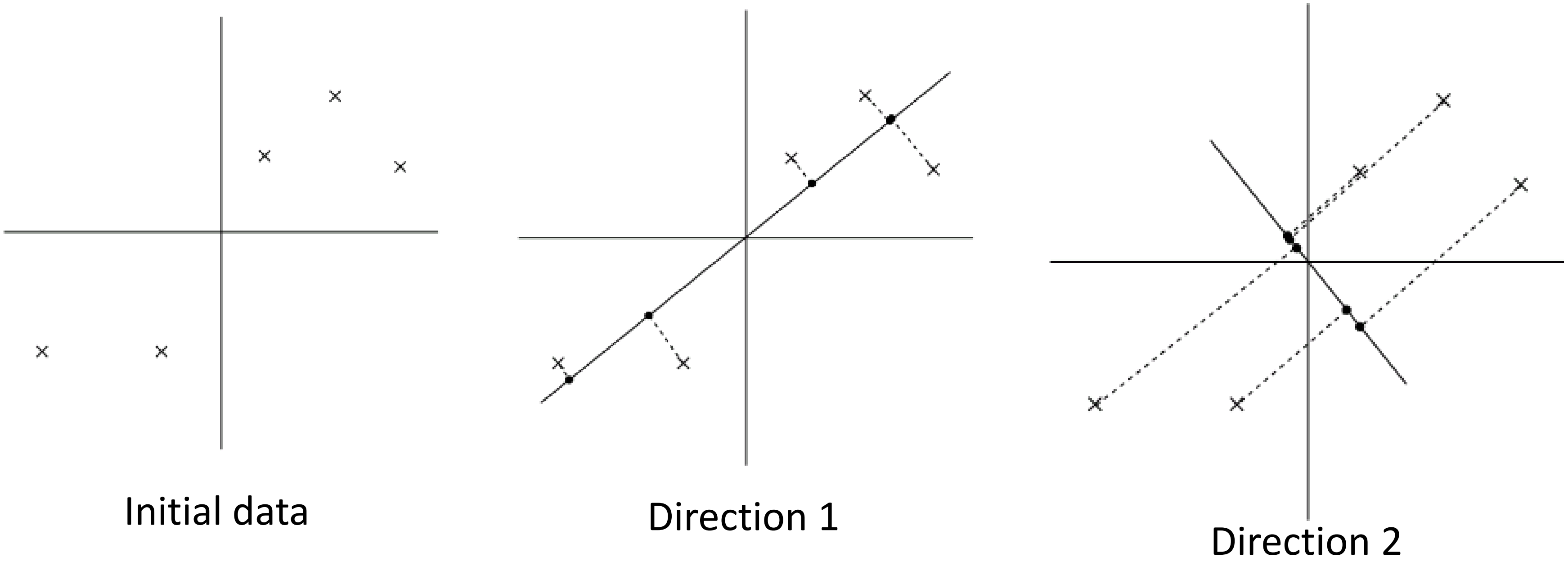
- PCA returns two principal components
  - The first gives the direction of the maximum spread of the data.
  - The second gives the direction of maximum spread perpendicular to the first



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.



Idea: Choose the direction that maximizes the variance of the projected data (here: Dir. 1)

Principal Component Analysis (PCA)

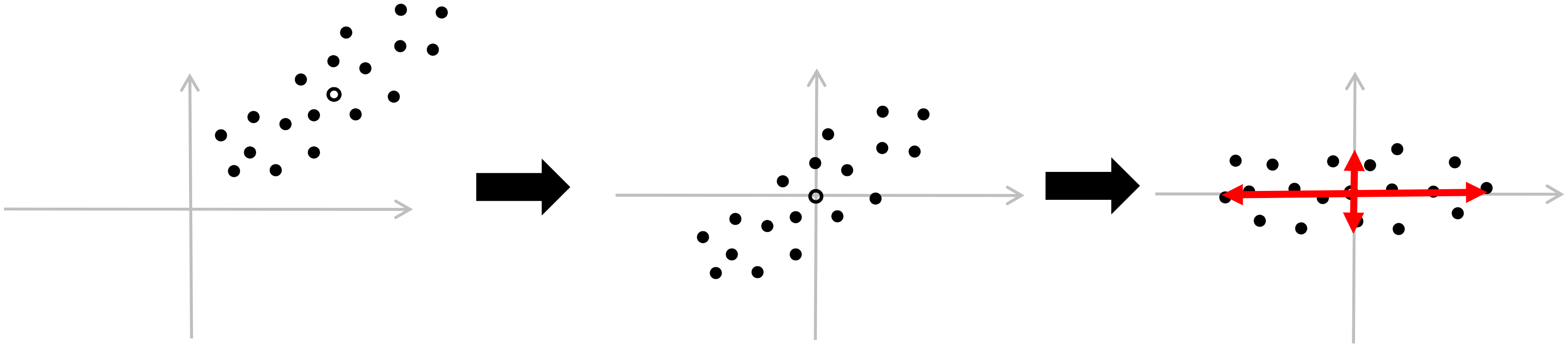
- PCA computes the most meaningful basis to re-express a noisy, garbled data set.
- Think of PCA as choosing a new coordinate system for the data, the principal components being the unit vectors along the axes
- PCA asks: *Is there another basis, which is a linear combination of the original basis, that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

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

- 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 (given the *n* data points)

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

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

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

Data matrix

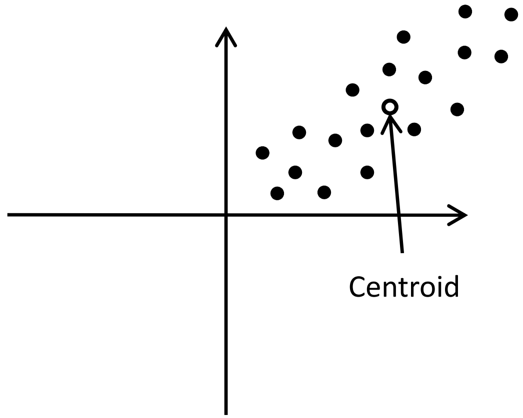
- Given n vectors $v_i \in IR^d$, the $n \times d$ matrix

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

is called data matrix

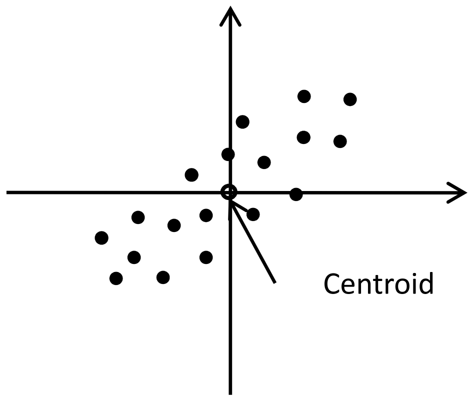
- Centroid/mean vector of D:

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



- Centered data matrix:

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



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

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

Mahalanobis Distance

- Quadratic forms or Mahalanobis distance:

$$d_A(x,y) = \left((x-y)A(x-y)^T\right)^{\frac{1}{2}} = \sqrt{(x-y)\begin{pmatrix} A_{1,1} & \cdots & A_{1,d} \\ \vdots & \ddots & \vdots \\ A_{d,1} & \cdots & A_{d,d} \end{pmatrix}(x-y)^T} = \sqrt{\sum_{i=1}^{d}\sum_{j=1}^{d}(x_i-y_i)A_{i,j}(x_j-y_j)}$$

Remark: If A is symmetric and positive definite then d_A is a metric.

- Weighted Euclidian Distance: A is a diagonal matrix with $A_i > 0$:

$$d_A(x,y) = \sqrt{(x-y)\begin{pmatrix} A_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & A_d \end{pmatrix}(x-y)^T} = \sqrt{\sum_{i=1}^{d} A_i (x_i-y_i)^2}$$

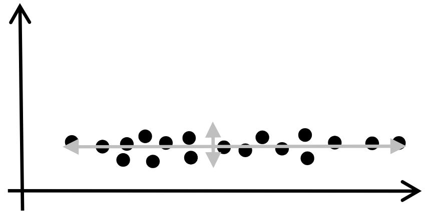
- **Connection to basis transformation** :

  If there is a symmetric decomposition $A = B \cdot B^T$ then the Mahalanobis distance is equivalent to the Euclidian distance under basis transformation B:

$$d_M(x,y) = \left((x-y)B \cdot B^T (x-y)^T\right)^{\frac{1}{2}} = \left((xB-yB)\cdot(xB-yB)^T\right)^{\frac{1}{2}} = d_{eucl}(xB, yB)$$

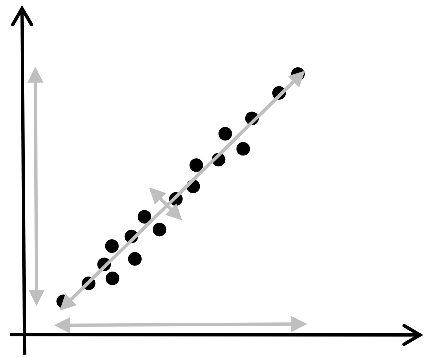
Variance Analysis for feature selection

- Which attributes are the most important to the distance ?
  => attributes with strongly varying value differences $|x_i\text{-}y_i|$
  => distance to the mean value is large $|x_i\text{-}\mu_i|$
  => variance is large: $\frac{1}{n}\sum_{i=1}^{n}(x_i-\mu_i)^2$



Idea: Variance Analysis (= unsupervised feature selection)

- Attributes with large variance allow strong distinction between objects
- Attributes with small variance: difference between objects are negligible
- Method:
  - Determine the variance between the values in each dimension
  - Sort all features w.r.t. to the variance
  - Select *k* features having the strongest variance



Beware: Even linear correlation can distribute one strong feature over arbitrarily many other dimension!!!

Eigenvectors and eigenvalues

- Let D be d x d 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
    - o I_{dxd} is the identity matrix
  - For each eigenvalue λ_i, we find its eigenvector by solving $(D - \lambda_i)v_i=0$

Eigenvectors decomposition

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

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

$$V = (v_1, \cdots, v_d) \text{ such that } \underset{i \neq j}{\forall} \langle v_i, v_j \rangle = 0 \text{ and } \underset{i=1}{\overset{d}{\forall}} \|v_i\| = 1$$

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

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

Eigenvalue decomposition of the covariance matrix

- Applying the eigenvalue decomposition to the covariance matrix:

$$\Sigma_D = V\Lambda V^T = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_d \end{pmatrix} (v_1, \cdots, v_d)$$

- v_i: Orthogonal principal components (eigenvectors)
- λ_i: Variance along each direction (eigenvalues)

Beware: λ_i=0 means that the corresponding direction is a linear combination of other principal components.

=> Depending on the algorithm completely redundant dimension cause (numerical) problems

Workaround: Add a diagonal matrix with very small values δ_i to Σ_D.

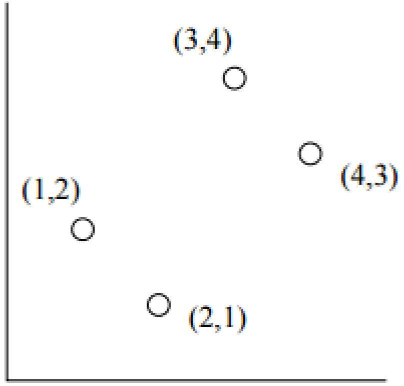
Feature reduction using PCA

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



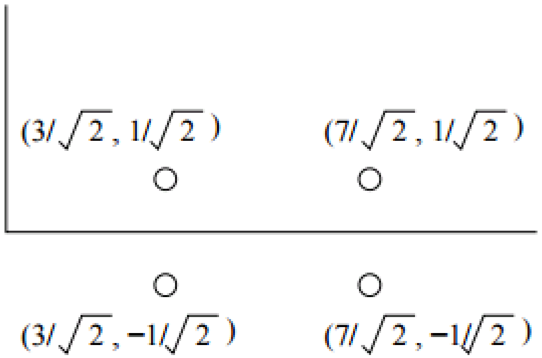
Eigenvectors

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

- 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 (at least) **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

=> Choose PC1 and PC2 explaining appr. 96% of the total variance

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

$$D = OSA^T$$

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

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

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

	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

- 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 S
  - 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

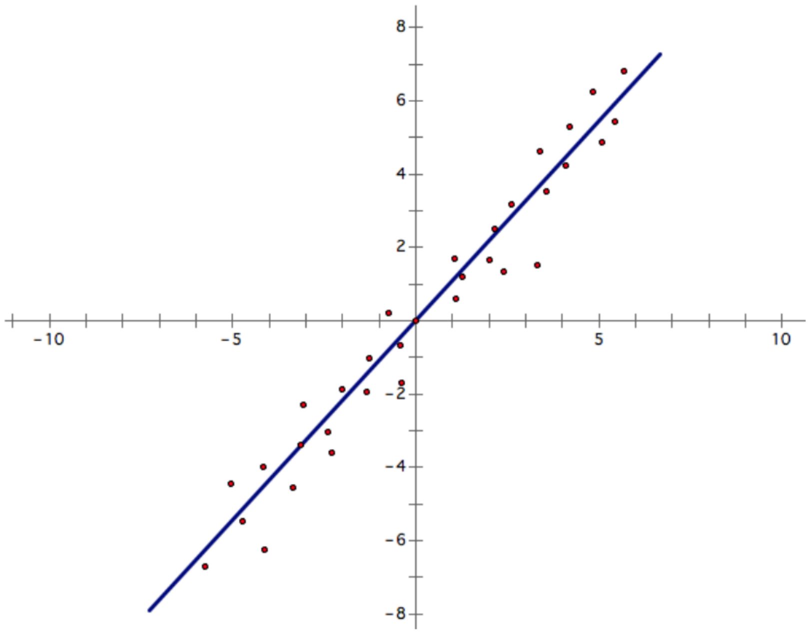
Conclusion: Eigenvalues and eigenvectors of the covariance matrix Σ can be determined by the SVD of the data matrix D.

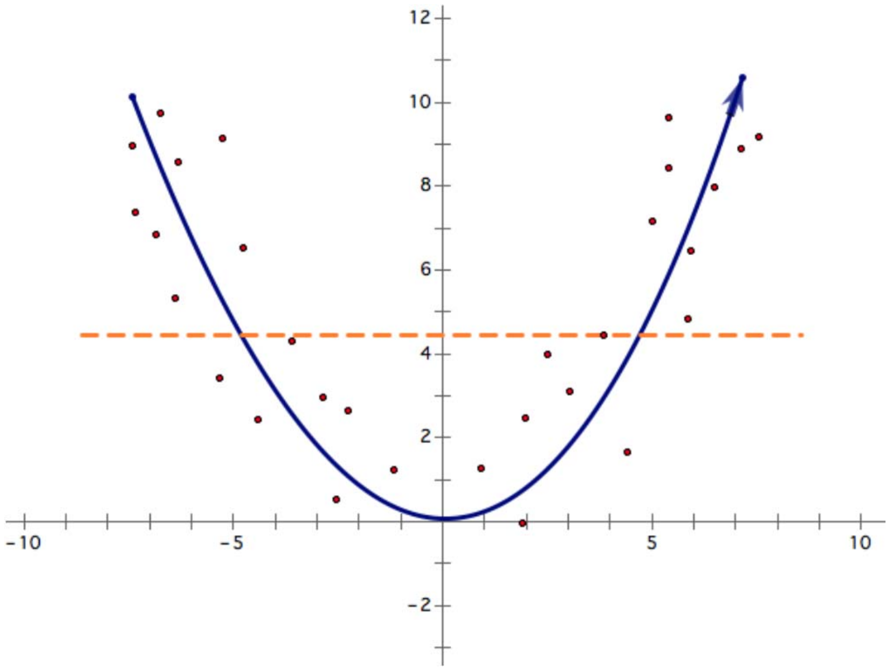
$\Rightarrow$ SVD is sometimes a better way to perform PCA (Large dimensionalities e.g., text data)

$\Rightarrow$ SVD can cope with dependent dimensions (k<d is an ordinary case in SVD)

Kernel PCA

An extension of PCA using techniques of kernel methods.

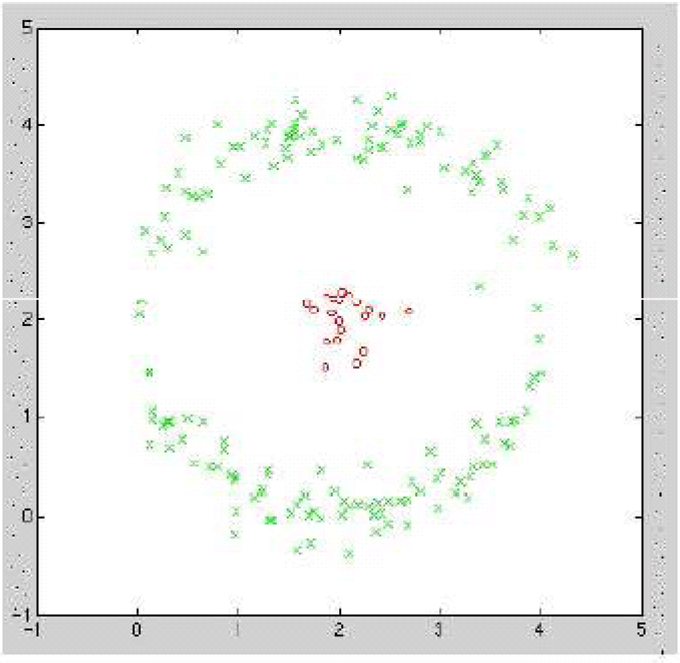




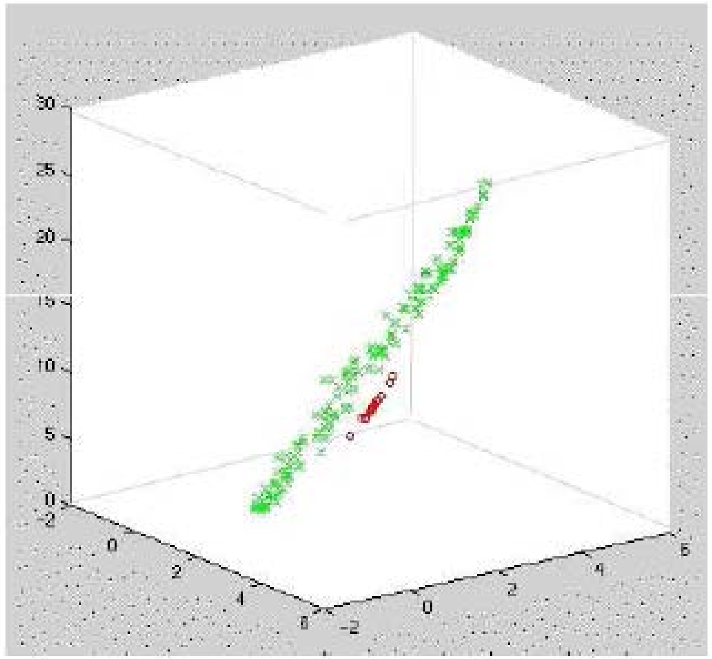
Left figure displays a 2D example in which PCA is effective because data lie near a linear subspace.
In the right figure though, PCA is ineffective, because data the data lie near a parabola.
In this case, the PCA compression of the data might project all points onto the orange line, which is far from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

Basic idea (see Kernels and SVMs)

- 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

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

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

Basic idea (see Kernels and SVMs)

- Wait a minute! Seriously? You suggest to pump up the feature space to get a better discriminability of points?

And how does that compare to the curse of dimensionality?

- Well: look at all that stuff we did a little closer.
- Results on (un)stability of distances and neighborhoods are based on the assumption that you add features that are
  - Independent
  - Randomly distributed
- Using a Kernel, you do a (completely) different thing
  - You add „relevant“ features that are combinations of others (i.e. not independent and probably not random)
  - ***In fact, there is a curse AND a blessing in high dimensions***

$$\Phi : \mathbf{R}^2 \to \mathbf{R}^3$$
$$(x_1, x_2) \mapsto (x_1, x_2, x_1^2 + x_2^2)$$

Kernel trick

- But: 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

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

- 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:

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

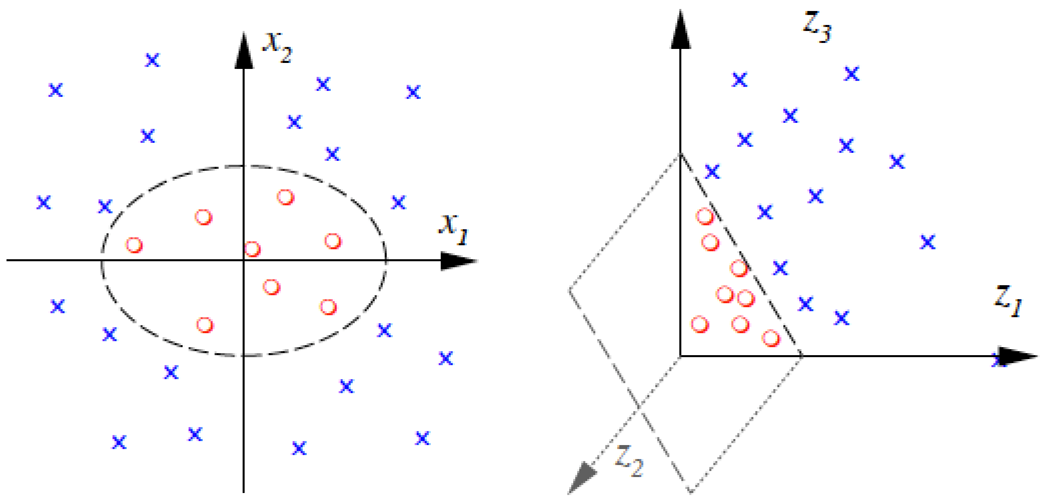


Image from: http://i.stack.imgur.com/qZV3s.png

Kernel PCA

Connection between the orthonormal basis 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 an 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: $L(U,V) = \left\| D - UV^T \right\|_f^2$

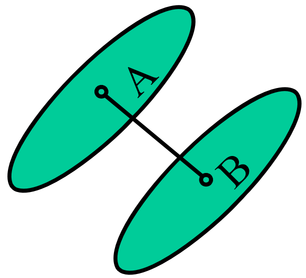
(squared Frobenius Norm of a matrix) $\|M\|_f^2 = \sum_{i=1}^{n} \sum_{j=1}^{m} \left| m_{i,j} \right|^2$

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

Fischer Faces

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

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



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

Target:

- Minimize the similarity between objects from different classes.
  (between class scatter matrix: Σ_b)
  Σ_b: Covariance matrix of the class centroids
- Maximize similarity between objects belonging to the same class
  (within class scatter matrix Σ_w)
  Σ_w: Average covariance matrix of all classes.

Solution:

- 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 $i \neq j : \langle x_i, x_j \rangle = 0$

Fischer Faces

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)

Discussion: Fischer Faces are limited due to the assumption of mono-modal classes: each class is assumed to follow a multivariate

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

RCA & LMNN

Relevant Component Analysis (RCA):

- Remove linear dependent features (e.g. with SVD).
- Given: chunks of data which are known to consist of similar objects.

  => replace Σ_w with an within-chunk matrix:
- The covariance of all data objects is dominated by dissimilarity
  => replace Σ_b with the covariance matrix of *D*

Large Margin Nearest Neighbor (LMNN):

- Objects in a class might vary rather strongly.
- Idea: Define an optimization problem only considering the distances of the most similar objects from the same and other classes.

LMNN

If you want to know the details …

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→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 parameters 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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