*** Applied Machine Learning Fundamentals ***
Principal Component Analysis

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SAP SE

October 31, 2019

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Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	**Dimensionality Reduction**

Agenda October 31, 2019

Section:

Introduction

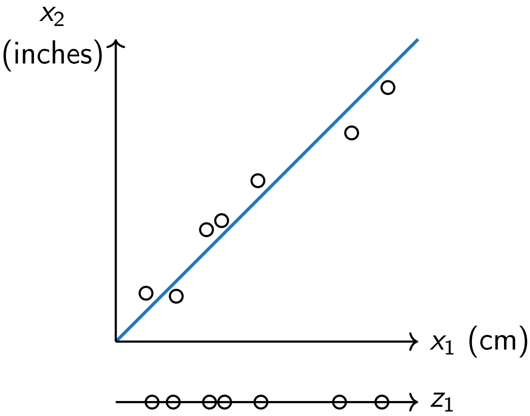
Why Dimensionality Reduction?

- Most data is high-dimensional
- Dimensionality reduction can be used for:
  - **Lossy (!)** data compression
  - Feature extraction
  - Data visualization

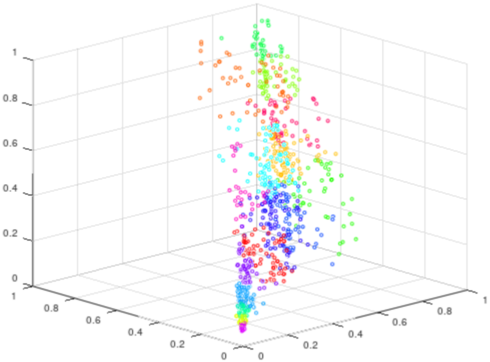
Dimensionality reduction can help to **speed up** learning algorithms substantially. Too many (correlated) features usually **decrease the performance** of the learning algorithm (cf. curse of dimensionality).

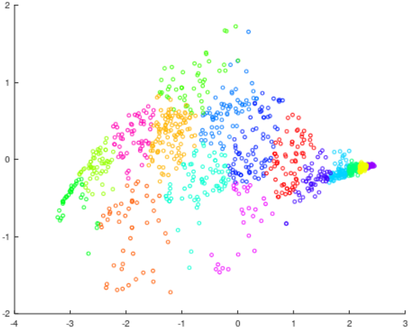
Use Case I: Data Compression / Feature Extraction

- The features *inches* and *cm* are closely related
- **Problems**:
  - Redundancy
  - More memory needed
  - Algorithms become slow
- **Solution**: Convert x_1 and x_2 into a new feature z_1 ($\mathbb{R}^2 \to \mathbb{R}$)



Use Case II: Data Visualization

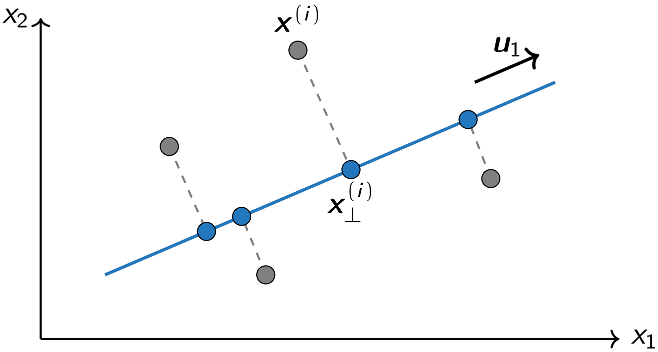




PCA: Principal Component Analysis

- PCA is an **unsupervised** algorithm
- It is known as the *Karhunen-Loève* transform
- PCA can be defined as the **orthogonal projection** of the data onto a lower dimensional **linear space** (*principal subspace*)
- Consider a data set of n observations $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}\}$
  - $\boldsymbol{x}^{(i)}$ is a real-valued vector in $\mathbb{R}^m$ (m-dimensional)
  - We want to project the data onto a space having dimensionality $k \ll m$, while **maximizing the variance of the projected data** ($\mathbb{R}^m \rightarrow \mathbb{R}^k$)
- Remove dimensions which are the least informative of the data

Orthogonal Projections



- $\boldsymbol{x}^{(i)}$ denote the original data points
- $\boldsymbol{x}_{\perp}^{(i)}$ is the orthogonal projection of $\boldsymbol{x}^{(i)}$ onto vector $\boldsymbol{u}_1$

Section:

Maximum Variance Formulation

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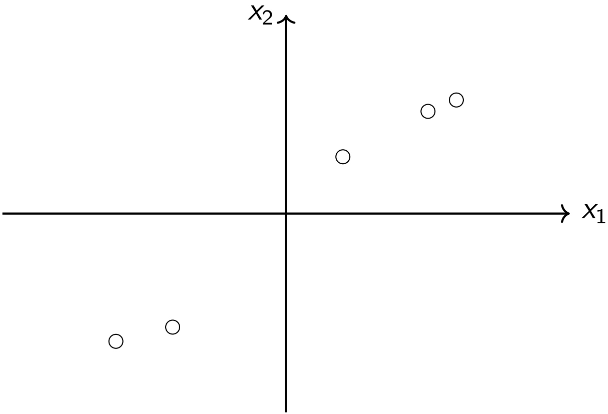
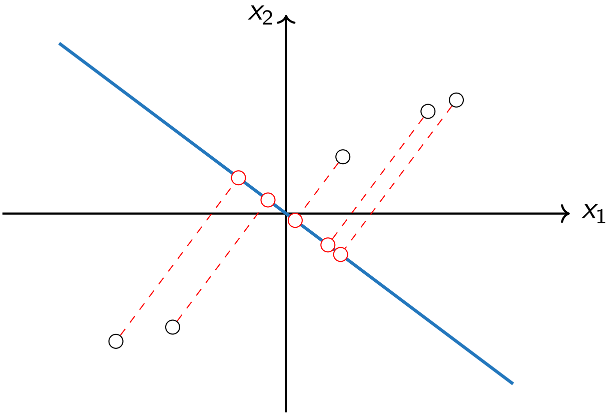
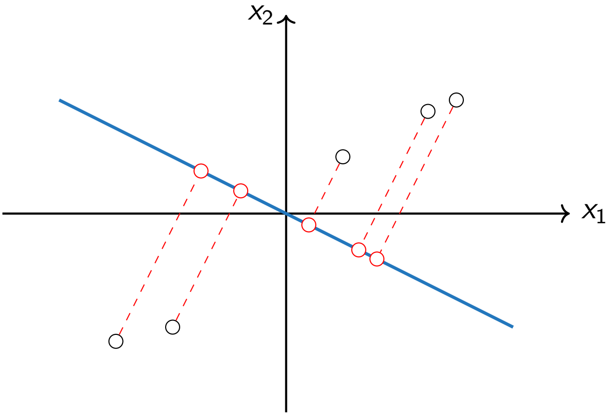
Maximum Variance Formulation



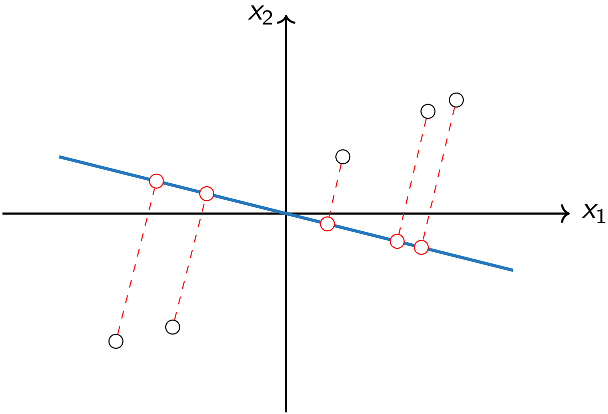
Maximum Variance Formulation



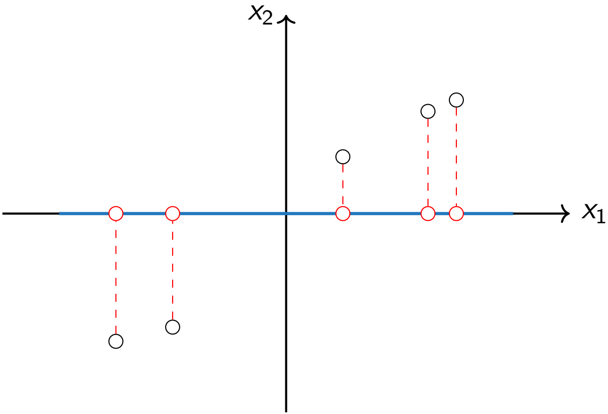
Maximum Variance Formulation



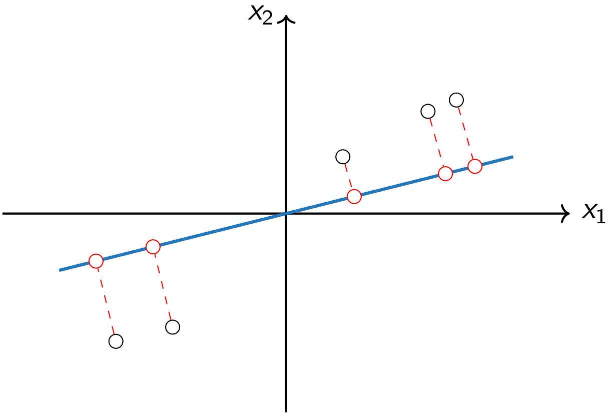
Maximum Variance Formulation



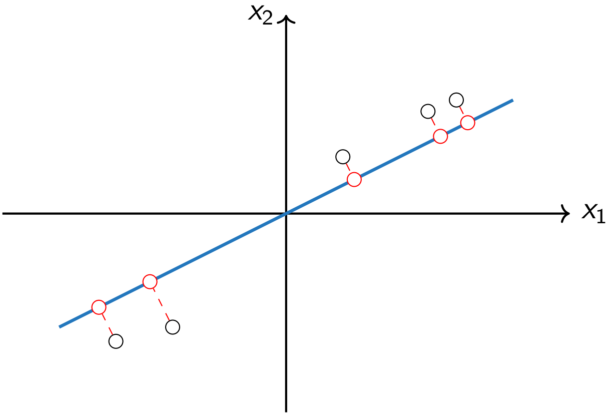
Maximum Variance Formulation



Maximum Variance Formulation



Maximum Variance Formulation



Maximum Variance Formulation (Ctd.)

- In the following we assume $k = 1$ (projection onto a line defined by a unit vector $\boldsymbol{u}_1$)
- Each data point $\boldsymbol{x}^{(i)}$ is projected onto a scalar value $\boldsymbol{u}_1^\intercal \boldsymbol{x}^{(i)}$
- The mean of the projected data is $\boldsymbol{u}_1^\intercal \overline{\boldsymbol{x}}$, where $\overline{\boldsymbol{x}}$ is the sample set mean:

$$\overline{\boldsymbol{x}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}^{(i)} \tag{1}$$

- The variance of the projected data is given by:

$$\frac{1}{n} \sum_{i=1}^{n} \left(\boldsymbol{u}_1^\intercal \boldsymbol{x}^{(i)} - \boldsymbol{u}_1^\intercal \overline{\boldsymbol{x}} \right)^2 = \boldsymbol{u}_1^\intercal \boldsymbol{\Sigma} \boldsymbol{u}_1 \tag{2}$$

Maximum Variance Formulation (Ctd.)

- $\boldsymbol{\Sigma}$ is the covariance matrix defined by:

$$\boldsymbol{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} \overbrace{(\boldsymbol{x}^{(i)} - \overline{\boldsymbol{x}})(\boldsymbol{x}^{(i)} - \overline{\boldsymbol{x}})^{\intercal}}^{\textbf{Outer product} \rightarrow \textbf{matrix}} \tag{3}$$

- The projected variance $\boldsymbol{u}_1^{\intercal} \boldsymbol{\Sigma} \boldsymbol{u}_1$ is maximized with respect to $\boldsymbol{u}_1$
- Constraint: $\|\boldsymbol{u}_1\| = 1$, otherwise $\boldsymbol{u}_1$ grows unboundedly
- We have to solve the following optimization problem:

$$\max_{\boldsymbol{u}_1} \{\boldsymbol{u}_1^{\intercal} \boldsymbol{\Sigma} \boldsymbol{u}_1 + \lambda_1 (1 - \boldsymbol{u}_1^{\intercal} \boldsymbol{u}_1)\} \tag{4}$$

Maximum Variance Formulation (Ctd.)

- $\nabla_{\boldsymbol{u}_1}\{\boldsymbol{u}_1^\mathsf{T}\boldsymbol{\Sigma}\boldsymbol{u}_1 + \lambda_1(1 - \boldsymbol{u}_1^\mathsf{T}\boldsymbol{u}_1)\} \overset{!}{=} 0 \qquad \Longrightarrow \boldsymbol{\Sigma}\boldsymbol{u}_1 = \lambda_1\boldsymbol{u}_1$
- This is an **eigenvalue problem**
- The equation tells us that $\boldsymbol{u}_1$ must be an eigenvector of $\boldsymbol{\Sigma}$
- If we left-multiply by $\boldsymbol{u}_1^\mathsf{T}$ and use $\boldsymbol{u}_1^\mathsf{T}\boldsymbol{u}_1 = 1$, we see: $\boldsymbol{u}_1^\mathsf{T}\boldsymbol{\Sigma}\boldsymbol{u}_1 = \lambda_1$

The variance reaches a maximum if we set $\boldsymbol{u}_1$ equal to the eigenvector having the largest eigenvalue λ_1. This eigenvector is the first principal component.

Maximum Variance Formulation (Ctd.)

- Additional principal components can be defined in an **incremental fashion**
- Choose each new component such that it **maximizes the remaining projected variance**
- All principal components are **orthogonal to each other**
- Projection onto k dimensions:
  - The lower-dimensional space is defined by the k eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k$ of the covariance matrix $\boldsymbol{\Sigma}$
  - These correspond to the k largest eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$

Section:

PCA Algorithm

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Algorithm 1: PCA Algorithm

Input: Input data $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}\} \in \mathbb{R}^{n \times m}$, number of dimensions k

Output: Projected data $\boldsymbol{Z} \in \mathbb{R}^{n \times k}$

$\overline{\boldsymbol{x}} \longleftarrow \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}^{(i)}$ `// sample set mean`

$\boldsymbol{\Sigma} \longleftarrow \frac{1}{n} \sum_{i=1}^{n} (\boldsymbol{x}^{(i)} - \overline{\boldsymbol{x}})(\boldsymbol{x}^{(i)} - \overline{\boldsymbol{x}})^{\intercal}$ `// covariance matrix`

Perform **s**ingular **v**alue **d**ecomposition to find the eigenvectors of matrix $\boldsymbol{\Sigma}$:

$$[\boldsymbol{U}, \boldsymbol{S}, \boldsymbol{V}] = SVD(\boldsymbol{\Sigma})$$

Select first k eigenvectors: $\boldsymbol{U}_k \longleftarrow \boldsymbol{U}_{(:,:k)}$ `// eig.vecs with largest eig.vals.`

$\boldsymbol{Z} \longleftarrow \boldsymbol{U}_k^{\intercal} \boldsymbol{X}$

Projection of the Data

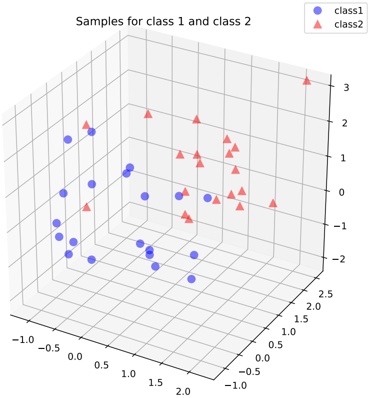
- Matrix $\boldsymbol{U}$ is obtained by applying **singular value decomposition** to $\boldsymbol{\Sigma}$

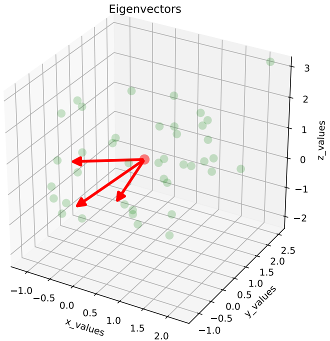
$$\boldsymbol{U} = \begin{bmatrix} | & | & & | \\ \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_m \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{m \times m} \tag{5}$$

- The projection $\mathbb{R}^m \to \mathbb{R}^k (k \ll m)$ is performed as follows:

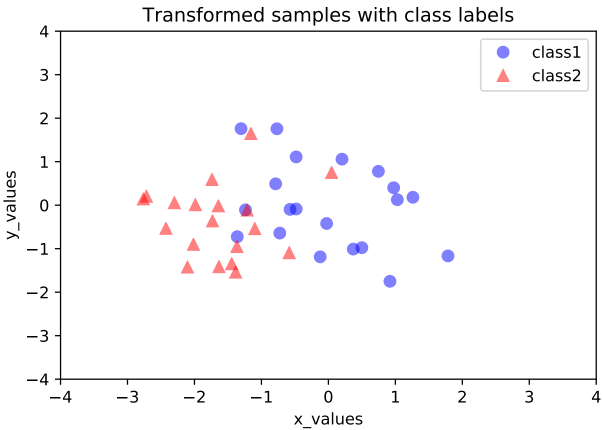
$$\begin{bmatrix} z_1^{(i)} \\ \vdots \\ z_k^{(i)} \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_k \\ | & | & & | \end{bmatrix}^{\intercal} \begin{bmatrix} x_1^{(i)} \\ \vdots \\ x_m^{(i)} \end{bmatrix} \tag{6}$$

PCA Result


Samples for class 1 and class 2
class1
class2
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3
2
1
0
−1
−2


Eigenvectors
x_values
y_values
z_values
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3
2
1
0
−1
−2

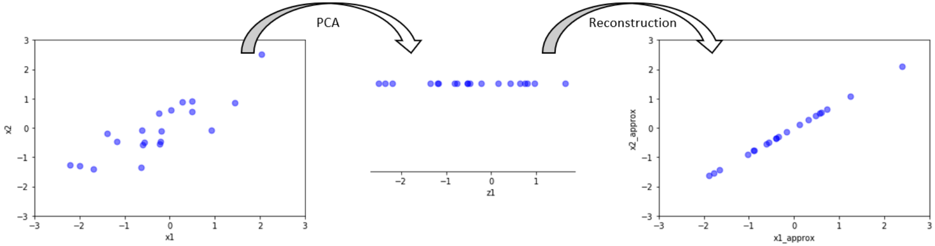
PCA Result (Ctd.)



Reconstruction from compressed Representation

It is possible to compute an approximate reconstruction of the data after having applied PCA ($\mathbb{R}^k \rightarrow \mathbb{R}^m$):

$$\boldsymbol{x}_{\approx}^{(i)} = \boldsymbol{U}_k \boldsymbol{z}^{(i)} \tag{7}$$



Choosing the Number of Components

- The goal is to preserve as much variance as possible
- Minimize the **average projection error** given by:

$$\frac{1}{n}\sum_{i=1}^{n}\|\boldsymbol{x}^{(i)} - \boldsymbol{x}_{\approx}^{(i)}\|^2 \tag{8}$$

- **Total variation** in the data is computed as follows:

$$\frac{1}{n}\sum_{i=1}^{n}\|\boldsymbol{x}^{(i)}\|^2 \tag{9}$$

Choosing the Number of Components (Ctd.)

- Typically, k is chosen to be the smallest value such that:

$$\frac{\overbrace{{}^{1}\!/_{n} \sum_{i=1}^{n} \|\boldsymbol{x}^{(i)} - \boldsymbol{x}_{\approx}^{(i)}\|^2}^{\text{average projection error}}}{\underbrace{{}^{1}\!/_{n} \sum_{i=1}^{n} \|\boldsymbol{x}^{(i)}\|^2}_{\text{total variation}}} \leqslant \gamma \tag{10}$$

- This means that $(1 - \gamma) \cdot 100\,\%$ of the variance is retained

You can be more efficient...

- The above algorithm is computationally very expensive
- The same result can be computed much more efficient, remember:

$$[\boldsymbol{U}, \boldsymbol{S}, \boldsymbol{V}] = SVD(\boldsymbol{\Sigma}) \tag{11}$$

- We can use the $(m \times m)$-matrix $\boldsymbol{S}$ (eigenvalues on the main diagonal):

$$\boldsymbol{S} = \begin{bmatrix} S_{11} & 0 & \dots & 0 \\ 0 & S_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & S_{mm} \end{bmatrix} \tag{12}$$

You can be more efficient... (Ctd.)

- For a given k, the fraction of variance retained can be computed as follows:

$$1 - \frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{m} S_{ii}} \leqslant 1 - \gamma \tag{13}$$

- The matrix has to be computed only once and can be reused for all k

Simplification:

$$\frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{m} S_{ii}} \geqslant 1 - \gamma$$

Section:

PCA Applications

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Application of PCA to Images: Eigenfaces

Figure: 100 images of faces

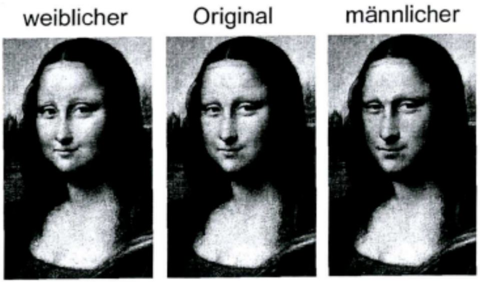
Figure: First 36 principal components

Application of PCA to Images: Eigenfaces (Ctd.)

Figure: Original images

Figure: Reconstructed images

Application of PCA to Images: Face Morphing



Section:

Wrap-Up

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Summary

Self-Test Questions

What's next...?

☠ The Exam ☠

Just kidding... (maybe)

Recommended Literature and further Reading

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Principal Component Analysis
Date: October 31, 2019

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Do you have any questions?