Lecture 5: Linear Subspace Projections: Principal Component Analysis

Machine Learning, Summer Term 2019

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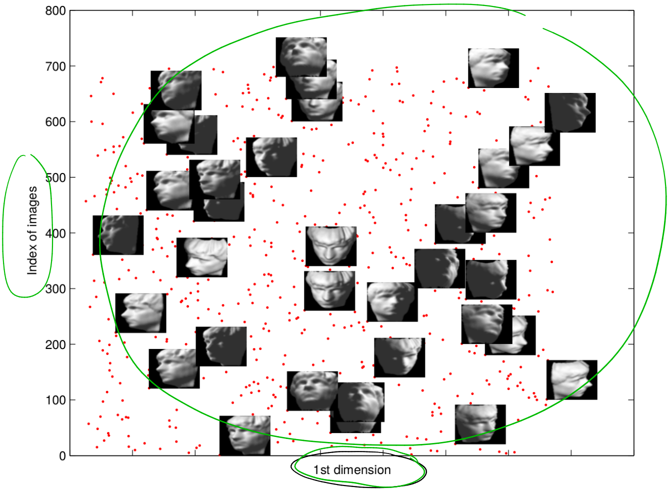
Lecture Overview

1. Motivation
2. The PCA Transformation
3. Wrapup: Related Topics, Summary, Preview

Lecture Overview

Example: Images of Faces

(Plots by Ali Ghodsi, "Dimensionality Reduction, A Short Tutorial", 2006)



Varying pose and and lighting conditions, 698 images (64x64 pixels) of the same face were generated. Dimensionality $D = 4096$

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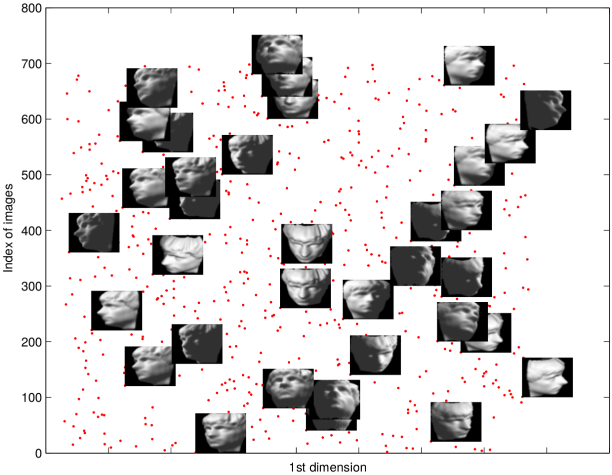

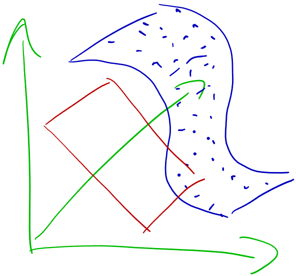

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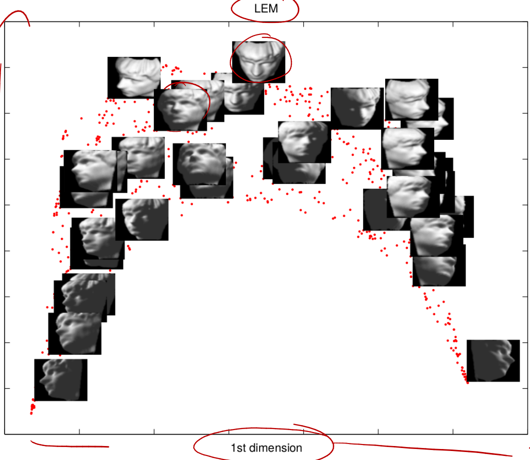
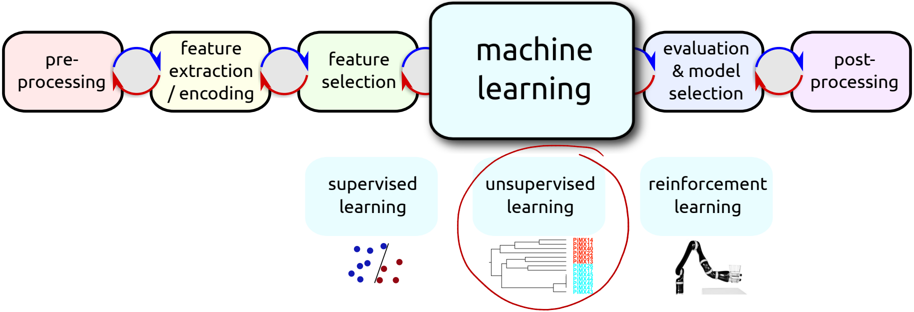


ML Design Cycle



Today's topic is how to project data to a useful subspace with unsupervised principal component analysis (PCA):

- Labels are not required

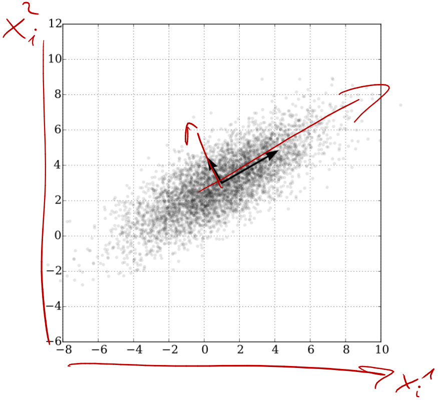
Typical Application of PCA: Dimensionality Reduction

Given:

- N high dimensional data points $\mathbf{x}_i \in \mathbb{R}^D$ with $i = 1 \ldots N$.
- Data is collected in matrix $\mathbf{X} \in \mathbb{R}^{N \times D}$

Scatter plot:

$D = 2$



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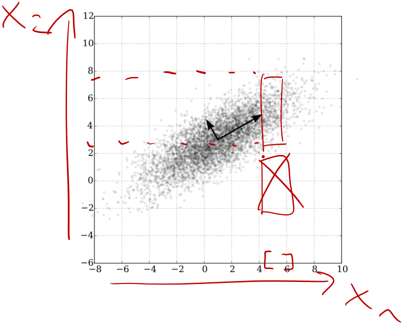

Let's assume, that

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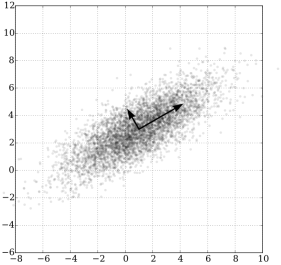
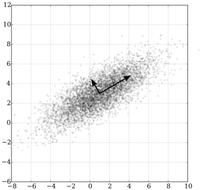


Let's assume, that

- the input dimensions are correlated
- some later method in the pipeline is *extremely* slow on high dimensional data...

What do you propose to do?

Simple Example: Dimensionality Reduction



Key ideas:

- Let's try to determine a subspace $\mathbb{R}^M$ of $\mathbb{R}^D$, with $M \leqslant D$.
- The subspace should contain the relevant part of our data.

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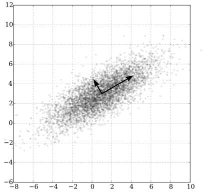

Key ideas:

- Let's try to determine a subspace $\mathbb{R}^M$ of $\mathbb{R}^D$, with $M < D$.
- The subspace should contain the relevant part of our data.
- Let's choose the new dimensions of this projected subspace such, that the data is uncorrelated.
- The subspace can be defined by a projection.

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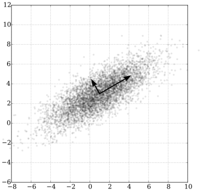

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 You have seen projections before - in which context?

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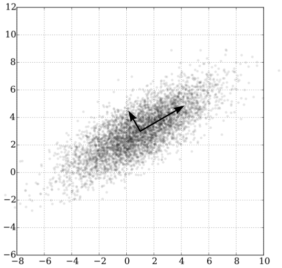

Principal component analysis (PCA) can be applied in such a scenario:

- PCA determines a linear subspace
- PCA makes the (somewhat strong!) assumption, that relevance is expressed by variance!

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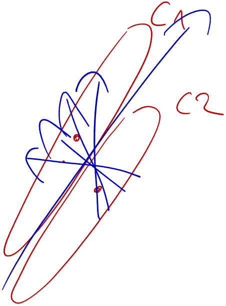

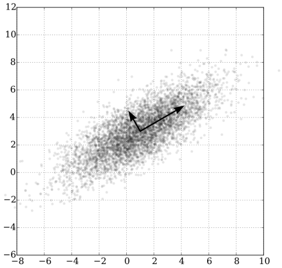

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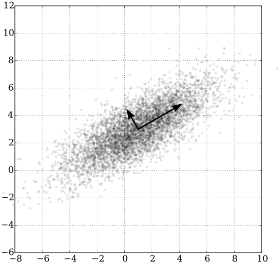

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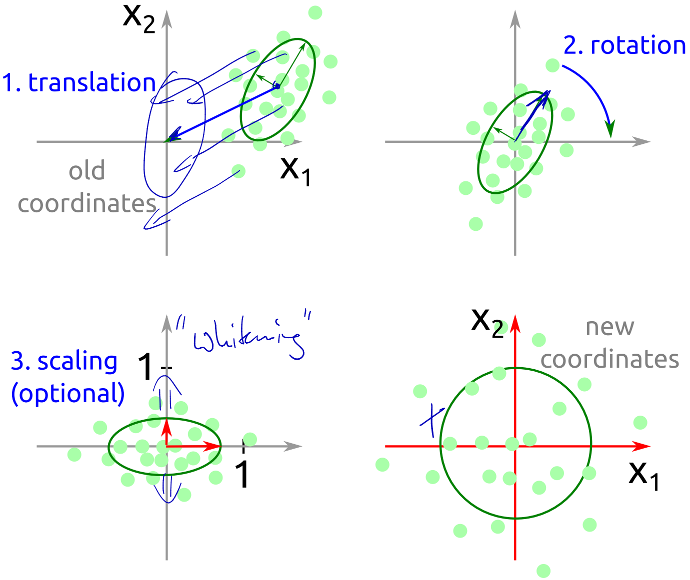
- PCA determines a linear subspace
- PCA makes the (somewhat strong!) assumption, that relevance is expressed by variance! (**Problematic?** 🖐🏾🖐🏼)
- → Can we reduce our data to the subspace with highest variance?

Intuition of PCA



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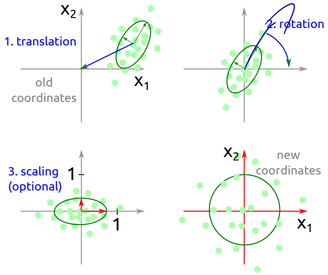
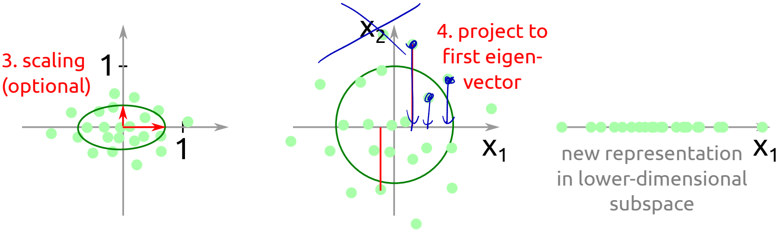
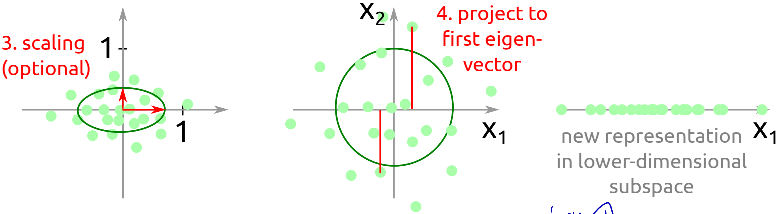


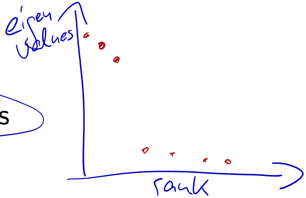
Principal component analysis (PCA) performs the following steps:

- Translation of data $\mathbf{X}$ to the origin
- Rotation, such that eigenvectors of $\mathbf{X}$ form the new axes
- (optional:) Scale the projected data according to the eigenvalues

Intuition of PCA for Dimensionality Reduction







Dimensionality reduction with PCA:

- Project data only to the first M eigenvectors (sorted by strongest eigenvalues)

Assume we have found a lower-dimensional representation with PCA.

Will we be able to save measuring time in the future, as we don't need to measure all variables?

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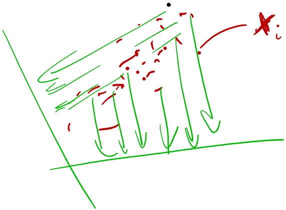

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We want $\mathbf{u}_1$ to maximize the variance of the projected data:

$$\underset{\mathbf{u}_1}{\operatorname{argmax}} \sum_{n=1}^{N} \{\mathbf{u}_1^T \mathbf{x}_n - \mathbf{u}_1^T \overline{\mathbf{x}}\}^2 = \underset{\mathbf{u}_1}{\operatorname{argmax}} \; \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1$$

with $\mathbf{S}$ being the data covariance matrix.

The Principal Component Transformation

Attention: maximizing $\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1$ with respect to $\mathbf{u}_1$ requires a constraint, otherwise $\mathbf{u}_1$ would simply grow to infinity...:

$u_1^T S u_1$

$100 \cdot u_1^T S \, 100 \cdot u_1$

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Setting the derivative with respect to $\mathbf{u}_1$ to zero, we obtain

$$0 = \underline{\mathbf{S} \mathbf{u}_1} - \underline{\lambda_1 \mathbf{u}_1}$$

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linear transform

Let's re-write this to

$$\mathbf{S}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

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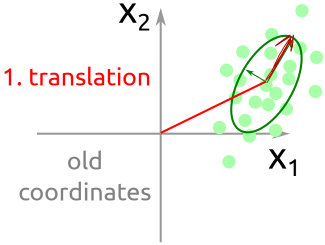
This meets our intuition, compare



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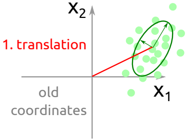
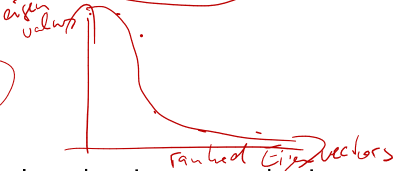


$$\mathbf{S}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

Multiplying with $\mathbf{u}_1^T$ from the left and making use of $\mathbf{u}_1^T\mathbf{u}_1 = 1$, variance is given by:



$$\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1 = \lambda_1$$

Observe:

- Variance is maximized, if we set $\mathbf{u}_1$ equal to the eigenvector having the largest eigenvalue λ_1.

Obtaining More Than One Projection Direction

We have seen how to obtain the first projection direction via $\mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 = \lambda_1$.

Any idea how to find the next one(s)?

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Further projection directions can be obtained by iterating the procedure, making sure that the following eigenvector is orthogonal to the ones obtained so far.

- Delivers a set of M eigen~~values~~ vectors $\mathbf{u}_1, \ldots, \mathbf{u}_M$
- Eigenvalues can be sorted according to the eigenvalues $\lambda_1, \ldots, \lambda_m$

Comment:
consider the spectrum of eigenvalues
to determine a suitable value of M

Lecture Overview

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- Data compression / dimensionality reduction (if you think, that variance matters!)

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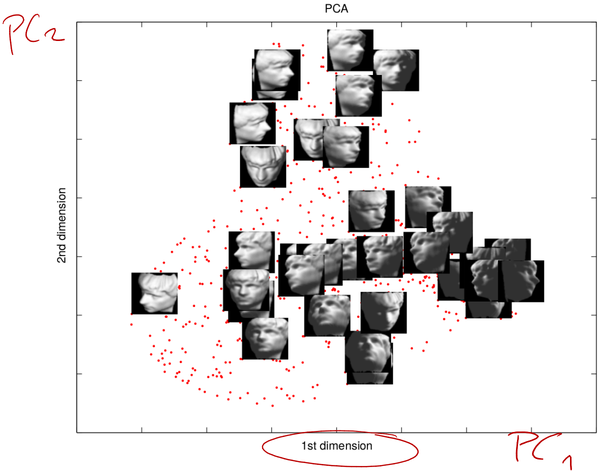

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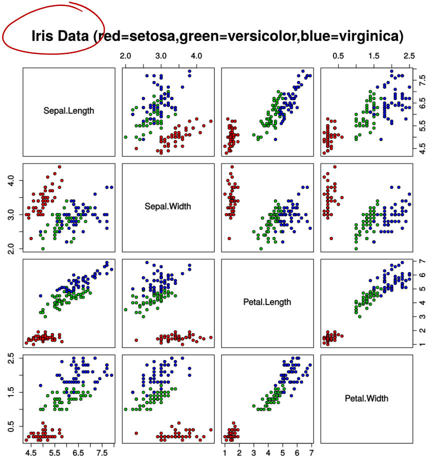
- Data visualization using a projection onto $M = 2$ or $M = 3$



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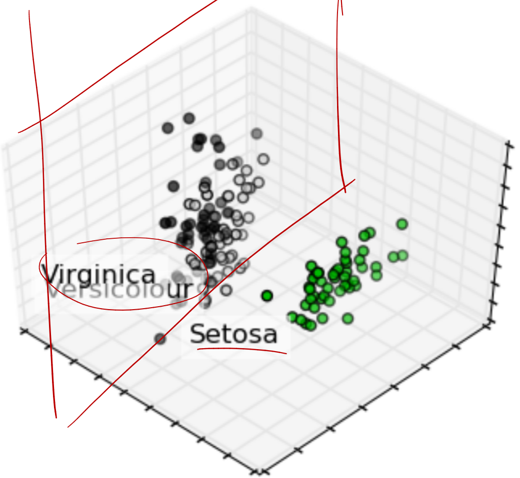

Alternative Names and Formulations for PCA

Depending on the context, principal component analysis is also referred to as

- Linear algebra: singular value decomposition SVD
- Linear algebra: eigenvalue decomposition EVD
- Image processing, control theory: Hotelling transform
- Karhunen-Loève transform
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Comments:

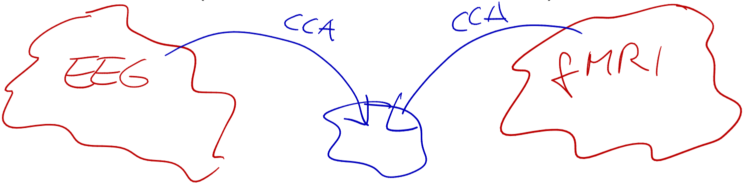
- There are many algorithmic approaches to derive projection directions (Raleigh coefficient, SVD, Bayesian PCA, iterative vs. analytical, ...)
- Using the covariance matrix has disadvantages, if dimensionality D is large.

Further Reading for PCA

- Section 12.1 of Bishop's book was mostly used for these slides
- Wikipedia.org on PCA for a great top-down overview!

Related Subspace Methods

- Whitening / sphereing: transform data to zero mean and unit covariance as a common preprocessing step
- Factor analysis FA (incorporate domain-specific assumptions)
- Canonical correlation analysis CCA (relate two data sources to a common subspace which maximizes cross-covariance)
- Kernel-PCA (non-linear extension of PCA)



Summary by learning goals

Having heard this lecture, you can now . . .

- explain, what PCA is doing
- explain, how the novel basis vectors are obtained
- program an iterative version of the algorithm
- formulate assumptions made by PCA (e.g. what happens, if we forget the translation to the origin?)
- name typical use cases of PCA
- (assignments) explain the role and benefits of whitening
- (assignments) explain typical pitfalls related to the use of PCA