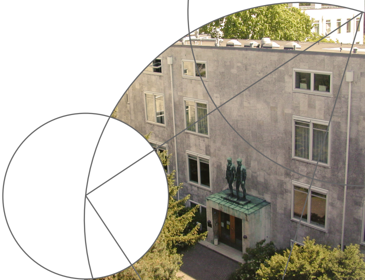
Faculty of Science

Principal Component Analysis

Machine Learning

Christian Igel
Department of Computer Science



Basic questions

- Principal component analysis (PCA, Karhunen-Loève transform) is arguably the most fundamental *unsupervised learning* algorithm.
- It is frequently used for (linear) reduction, (lossy) data compression, feature extraction, and data visualization.
- Let's consider $S = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ with $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathcal{X} = \mathbb{R}^d$.
- We ask how
  - to reduce the length of the description to $k < d$ variables such that as much information as possible is preserved?
  - many dimensions are needed to capture a certain percentage of the variability of the data?
  - to visualize the data in two or three dimensions preserving as much of its variability as possible?

Outline

1. Warmup: Basis and Coordinate System

2. More Warmup: Matrix Decomposition

3. Principal Component Analysis

4. Summary

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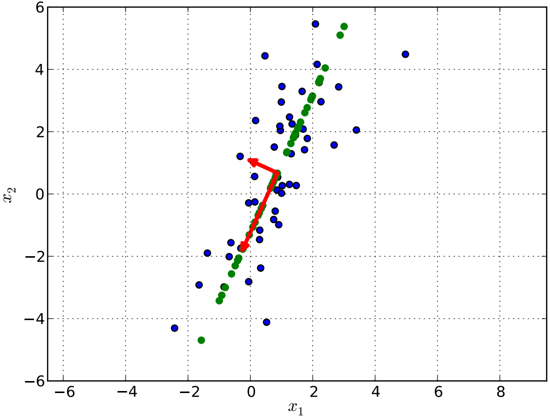
Basis vectors

- *Basis*: Set of linearly independent *basis vectors* $\boldsymbol{u}_1, \ldots$ that, in a linear combination, can represent every vector in given vector space
- Ortho*normal* basis: Basis vectors are orthogonal (i.e., $\boldsymbol{u}_i^\mathsf{T}\boldsymbol{u}_j = 0$ for $i \neq j$) and have unit length, $\|\boldsymbol{u}_i\| = \sqrt{\boldsymbol{u}_i^\mathsf{T}\boldsymbol{u}_1} = 1$
- Example: $\boldsymbol{x} \in \mathbb{R}^2$, orthonormal basis

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} , \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

  $\boldsymbol{x} = (1,0)^\mathsf{T} x_1 + (0,1)^\mathsf{T} x_2$
- Example can be read as "way from $\mathbf{0}$ to $\boldsymbol{x}$: First go x_1 units in the direction $(1,0)^\mathsf{T}$ and then x_2 units in direction $(1,0)^\mathsf{T}$"

2-dimensional example



Changing basis

- Changing basis means "expressing the way using two other, non-parallel directions $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$: First go z_1 units in the direction $\boldsymbol{u}_1$ and then z_2 units in direction $\boldsymbol{u}_2$" :

$$\boldsymbol{x} = \sum_{i=1}^{d} z_i \boldsymbol{u}_i = \sum_{i=1}^{d} (\boldsymbol{x}^{\mathsf{T}} \boldsymbol{u}_i) \boldsymbol{u}_i$$

- A lower dimensional representation uses "fewer directions" and a (different) origin/starting point.

Orthogonal matrix

- Gather basis vectors in $d \times d$ matrix $\boldsymbol{U}$ such that the columns of $\boldsymbol{U}$ correspond to the basis vectors.
- ith column of $\boldsymbol{U}$ is given by $\boldsymbol{u}_i$.
- Square matrix composed of an orthonormal basis is an *orthogonal* matrix having the property $\boldsymbol{U}^\mathsf{T} = \boldsymbol{U}^{-1}$.
- Define $d \times k$ matrix $\boldsymbol{U}_k$ as the first k basis vectors.
- ith column of $\boldsymbol{U}_k$ is given by $\boldsymbol{u}_i$ and the ith row of $\boldsymbol{U}^\mathsf{T}$ by $\boldsymbol{u}_i^\mathsf{T}$.

Outline

Eigenvectors and eigenvalues

- For an eigenvector $\boldsymbol{u}_i \in \mathbb{R}^d$ of the $d \times d$ matrix $\boldsymbol{S}$ it holds by definition:

  $$\boldsymbol{S}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$$

  λ_i is the corresponding eigenvalue.

- We consider only consider eigenvectors of unit length and assume that the eigenvectors are sorted according to $i < j \Rightarrow \lambda_i \geq \lambda_j$.

Eigen decomposition of real symmetric matrix

Any *real symmetric* $d \times d$ matrix $\boldsymbol{M}$ can be decomposed as:

$$\boldsymbol{M} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{\mathsf{T}}$$

with

- $\boldsymbol{Q} \in \mathbb{R}^{d \times d}$ being orthogonal,
- $\boldsymbol{Q}^{\mathsf{T}} = \boldsymbol{Q}^{-1}$,
- $\boldsymbol{\Lambda} \in \mathbb{R}^{d \times d} = \mathrm{diag}(\lambda_1, \dots, \lambda_d)$ being diagonal, with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$ being the eigenvalues of $\boldsymbol{M}$, and
- the columns of $\boldsymbol{Q}$ being the corresponding eigenvectors.

Singular value decomposition (SVD)

Any real $N \times d$ matrix $\boldsymbol{X}$ can be decomposed (let's assume $N \geq d$) as:

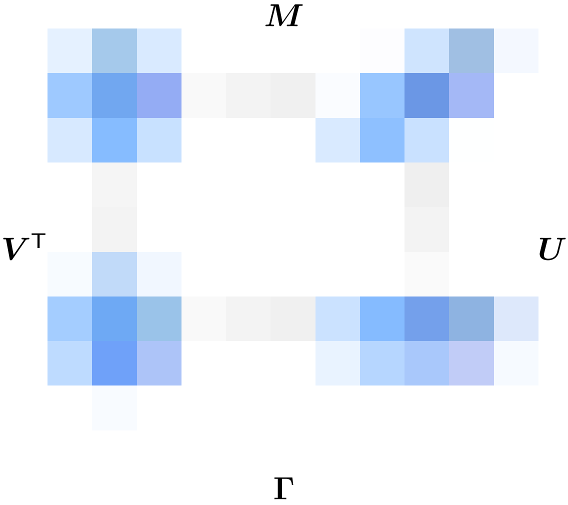
$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Gamma}\boldsymbol{V}^{\mathsf{T}}$$

with

- $\boldsymbol{U} \in \mathbb{R}^{N\times d}$ having orthonormal columns,
- $\boldsymbol{\Gamma} \in \mathbb{R}^{d\times d} = \operatorname{diag}(\gamma_1, \ldots, \gamma_d)$ being diagonal with $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_d$
- $\boldsymbol{V} \in \mathbb{R}^{d\times d}$ being orthogonal.

The columns of $\boldsymbol{V}$ are the *right singular vectors* of $\boldsymbol{X}$.

SVD example



drawing modified from Wikimedia Commons

SVD and eigen decomposition

- When $\boldsymbol{M}$ is positive semi-definite, its eigen decomposition is also a SVD.
- The right singular vectors of $\boldsymbol{X}$ are the eigenvectors of $\boldsymbol{X}^\mathsf{T}\boldsymbol{X}$.
- $\boldsymbol{X}^\mathsf{T}\boldsymbol{X}$ is positive (semi-) definite (i.e., all eigenvalues are non-negative), and the singular values of $\boldsymbol{X}$ are the square roots of the eigenvalues of $\boldsymbol{X}^\mathsf{T}\boldsymbol{X}$.

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- Let's consider $S = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ with $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathcal{X} = \mathbb{R}^d$.
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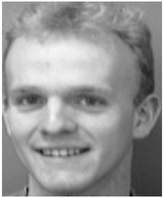
Example: Cambridge face database








Basic idea

- Find k-dimensional affine linear model $f : \mathbb{R}^k \to \mathbb{R}^d$ of the d-dimensional data representing S as accurately as possible:

$$f(\boldsymbol{z}) = \boldsymbol{b} + \boldsymbol{U}_k \boldsymbol{z} \ ,$$

  where $\boldsymbol{z} \in \mathbb{R}^k$, $\boldsymbol{b} \in \mathbb{R}^d$, and $\boldsymbol{U}_k \in \mathbb{R}^{d \times k}$.

- Vectors $\boldsymbol{u}_1, \dots, \boldsymbol{u}_k \in \mathbb{R}^d$ are the columns of $\boldsymbol{U}_k$ and we require them to be pairwise orthogonal and of unit length.

- Model represents data in $\mathbb{R}^d$ by k-dimensional parameters $\boldsymbol{z}$.

Reconstruction error

- We measure model quality by sum-of-squares *reconstruction error*

$$J = \frac{1}{N}\sum_{i=1}^{N} \|\boldsymbol{x}_i - f(\boldsymbol{z}_i)\|^2 \ .$$

- Formal goal of PCA

$$\min_{\boldsymbol{b},\boldsymbol{U}_k,\{\boldsymbol{z}_1,\dots,\boldsymbol{z}_N\}} \frac{1}{N}\sum_{i=1}^{N} \|\boldsymbol{x}_i - f(\boldsymbol{z}_i)\|^2$$

subject to the constraints on $\boldsymbol{U}_k$.

Solution

- The choice for $\boldsymbol{b}$ is the empirical mean:

$$\overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{x}_i$$

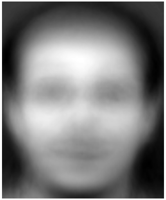
- Data points should be encode by

$$\boldsymbol{z}_i = \boldsymbol{U}_k^{\mathsf{T}}(\boldsymbol{x}_i - \overline{\boldsymbol{x}}) \quad .$$

- k columns of $\boldsymbol{U}_k$ should correspond to the first k eigenvectors of the *data covariance matrix* or *empirical covariance matrix*

$$\boldsymbol{S} = \frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{x}_i - \overline{\boldsymbol{x}})(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^{\mathsf{T}} \quad .$$

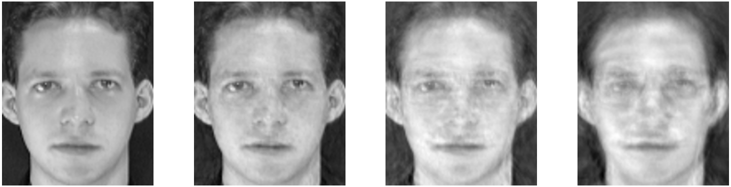
Mean face



$$\overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{x}_i$$

Eigenfaces

Reconstruction using eigenfaces



using all, 300, 200, 100 eigenfaces

PCA algorithm

Algorithm 1: dimensionality reduction using PCA

Input: data $S = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$, number of dimensions k

1 compute the empirical mean $\overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i$

2 compute empirical covariance matrix
$\boldsymbol{S} = \frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{x}_i - \overline{\boldsymbol{x}})(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^{\mathsf{T}}$

3 compute the $d \times k$ matrix $\boldsymbol{U}_k$ composed of the first k eigenvectors of $\boldsymbol{S}$, where the eigenvectors are ordered by decreasing eigenvalue

4 compute $\boldsymbol{z}_i = \boldsymbol{U}_k^{\mathsf{T}}(\boldsymbol{x}_i - \overline{\boldsymbol{x}})$ for $i = 1, \dots, N$

Output: mean $\overline{\boldsymbol{x}}$, principal components $\boldsymbol{U}_k$, projected data $\{\boldsymbol{z}_1, \dots, \boldsymbol{z}_N\}$, model $f(\boldsymbol{z}) = \overline{\boldsymbol{x}} + \boldsymbol{U}_k\boldsymbol{z}$

Eckart and Young theorem

The (squared) Frobenius norm of an $N \times d$ matrix $\boldsymbol{X}$ is

$$\|\boldsymbol{X}\|_F^2 = \sum_{n=1}^{N} \sum_{i=1}^{d} x_{ij}^2 \enspace .$$

The $N \times d$ matrix $\tilde{\boldsymbol{X}}$ with rank k approximating the $N \times d$ matrix $\boldsymbol{X}$ best in terms of the Frobenius norm $\|\boldsymbol{X} - \tilde{\boldsymbol{X}}\|_F^2$ is

$$\tilde{\boldsymbol{X}} = \boldsymbol{X}\boldsymbol{V}_k\boldsymbol{V}_k^{\mathsf{T}} \enspace ,$$

where $\boldsymbol{V}_k$ is the matrix of top-k right singular vectors of $\boldsymbol{X}$.

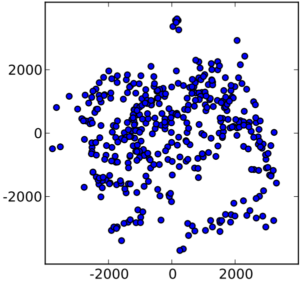
Maximizing variance

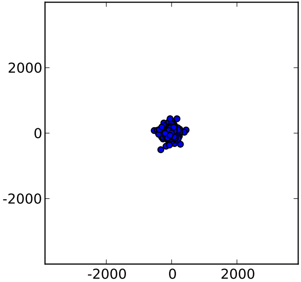
- We measure the variability of S by the trace $\mathrm{trace}\{\boldsymbol{S}\} = \sum_{i=1}^{d} s_{ii} = \sum_{i=1}^{d} \lambda_i = \sum_{j=1}^{d} \boldsymbol{u}_j^\mathsf{T} \boldsymbol{S} \boldsymbol{u}_j$. (Sum of the eigenvalues of a diagonalizable matrix is equal to its trace.)
- Accordingly the variability of $\boldsymbol{z}_1, \dots, \boldsymbol{z}_N$ is

$$\frac{1}{N} \sum_{i=1}^{N} \left[\boldsymbol{U}_k^\mathsf{T} \boldsymbol{x}_i - \boldsymbol{U}_k^\mathsf{T} \overline{\boldsymbol{x}}\right] \left[\boldsymbol{U}_k^\mathsf{T} \boldsymbol{x}_i - \boldsymbol{U}_k^\mathsf{T} \overline{\boldsymbol{x}}\right]^\mathsf{T} = \sum_{j=1}^{k} \boldsymbol{u}_j^\mathsf{T} \boldsymbol{S} \boldsymbol{u}_j \quad .$$

- Minimizing reconstruction error corresponds to maximizing variance.

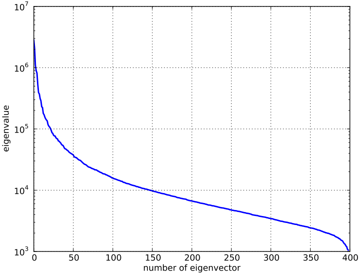
Variance of faces





first two eigenvalues vs. eigenvalues 99 and 100

"Explained variance"



We have:

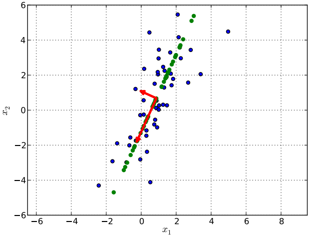
$$\mathrm{trace}\{\boldsymbol{S}\} = \sum_{j=1}^{d} \boldsymbol{u}_j^{\mathsf{T}} \boldsymbol{S} \boldsymbol{u}_j = \sum_{i=1}^{d} \lambda_i$$

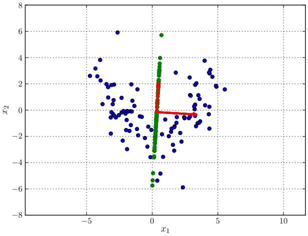
The quotient

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

measures the fraction of variance "explained" by the first k principal components.

Linear and non-linear example





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Summary

Principal component analysis (PCA) is frequently used for

- dimensionality reduction,
- noise reduction, and
- visualization.

It

- is an affine linear model of the data,
- is a change of basis, new basis vectors are orthogonal,
- minimizes reconstruction error, and
- maximizes variance.