Lecture 11: PCA vs CFA

Lecturer: Ksenia Kasianova
xeniakasianova@gmail.com

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Plan

1) PCA

2) PCA vs CFA

3) CFA

Intro

Multivariate Statistics

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PCA, **for Principal Component Analysis**, and **CFA, Common Factor Analysis**, are two statistical methods that are often covered together in classes on Multivariate Statistics.

PCA — Principal Component Analysis

Goal: Reducing the number of dimensions of a data set

Idea:

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=> "regrouping" the variables into a smaller number of variables, called components based on variation common to multiple variables:

– the first (newly created) component contains a maximum of variation

– the second component contains the second-largest amount of variation, etc.

– the last component logically contains the smallest amount of variation.

Choose only few of the newly created components rather than the original variables, while still retaining a maximum amount of variation.

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Use:

– data exploration, finding patterns in data of high dimension

– face recognition and image compression

PCA — Principal Component Analysis

Mathematical Model - Maximize variance of the new components

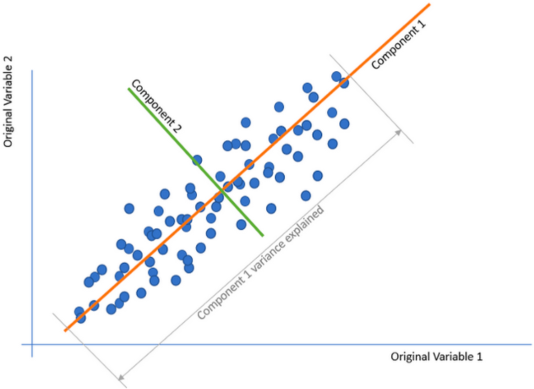

Figure: Schematic model of PCA

Mathematical definition of the PCA problem: find a linear combination of the original variables with maximum variance.

Mathematical Model - Maximize variance of the new components

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z is going to be computed based on our original variables $(\mathrm{X}_1, \mathrm{X}_2, \dots)$ multiplied by a weight for each of our variables $(u_1, u_2, ...)$.

This can be written as $\mathbf{z} = \mathbf{Xu}$.

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Solution:

– This problem is mathematically called **a constrained optimization using Lagrange Multiplier**

– In practice, sequential numerical optimization.

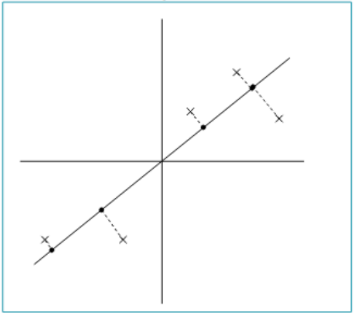
– Can be described as applying matrix decomposition to the correlation matrix of the original variables.

Goal: Maximizing the Variance

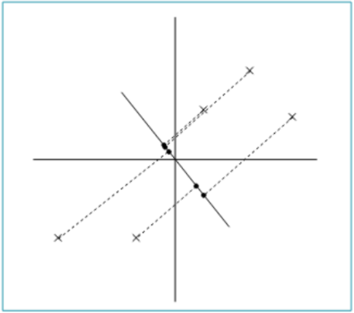
- Consider the two projections below

- Which maximizes the variance?

Option A



Option B



1) **PCA algorithm I (sequential)**

Given the centered data $\{\mathrm{x}_1, \ldots, \mathrm{x}_m\}$, compute the principal vectors:

$$\mathbf{w}_1 = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \left\{ \left(\mathbf{w}^T \mathbf{x}_\mathrm{i} \right)^2 \right\} \quad 1^{\text{st}} \text{ PCA vector}$$

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$$\mathbf{w}_k = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \left\{ \left[\mathbf{w}^T \left(\mathbf{x}_i - \sum_{j=1}^{k-1} \mathbf{w}_j \mathbf{w}_j^T \mathbf{x}_i \right) \right]^2 \right\} \quad k^{\mathrm{th}} \text{ PCA vector}$$

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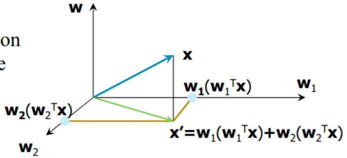
We maximize the variance of the projection in the residual subspace



Slide from Barnabas Poczos

2) **PCA algorithm II (sample covariance matrix)**

Given data $\{\mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{m}\}$, compute covariance matrix Σ

$$\Sigma = \frac{1}{m}\sum_{i=1}^{m}(\mathbf{x}_i - \bar{\mathbf{x}})\,(\mathbf{x} - \bar{\mathbf{x}})^T \quad \text{where } \bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i$$

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Lecture 11

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Plan

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By finding the eigenvalues and eigenvectors of the covariance matrix, we find that

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– larger eigenvalue $\Rightarrow$ more important eigenvectors PCA

Power iteration (Von Mises iteration is a standard algorithm for this)

Why the Eigenvectors?

Maximise $\quad \mathbf{u}^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}$

s.t $\quad \mathbf{u}^\top \mathbf{u} = 1$

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Intro
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Vector of partial derivatives set to zero

$$\mathbf{x}\mathbf{x}^\top \mathbf{u} - \lambda \mathbf{u} = \left(\mathbf{x}\mathbf{x}^\top - \lambda \mathbf{I}\right) \mathbf{u} = 0$$

As $\mathbf{u} \neq \mathbf{0}$ then $\mathbf{u}$ must be an eigenvector of $\mathbf{X}\mathbf{X}^\top$ with eigenvalue λ

Eigenvalues & Eigenvectors

- For symmetric matrices, eigenvectors for distinct eigenvalues are **orthogonal**

$$Sv_{\{1,2\}} = \lambda_{\{1,2\}} v_{\{1,2\}}, \text{ and } \lambda_1 \neq \lambda_2 \Rightarrow v_1 \bullet v_2 = 0$$

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- All eigenvalues of a positive semidefinite matrix are **nonnegative**

$$\forall w \in \Re^n, w^T S w \geq 0, \text{ then if } \mathrm{Sv} = \lambda \mathrm{v} \Rightarrow \lambda \geq 0$$

Eigen/diagonal Decomposition

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- Columns of $\boldsymbol{U}$ are eigenvectors of S

- Diagonal elements of $\boldsymbol{\Lambda}$ are eigenvalues of $\mathbf{S}$

$$\boldsymbol{\Lambda} = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_m\right), \quad \lambda_i \geq \lambda_{i+1}$$

PCA: Two Interpretations

E.g., for the first component.

I. Maximum Variance Direction: 1^{st} PC a vector v such that projection on to this vector capture maximum variance in the data (out of all possible one dimensional projections)

$$\frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{v}^T\mathbf{x}_i\right)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

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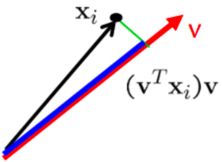
$$\frac{1}{n}\sum_{i=1}^{n}\left\|\mathbf{x}_i - \left(\mathbf{v}^T\mathbf{x}_i\right)\mathbf{v}\right\|^2$$

blue ^{2}+ green ^{2} $=$ black ^{2}

black ^{2} is fixed (it's just the data)

So, maximizing blue ^{2} is equivalent to minimizing green ^{2}



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Singular Value Decomposition of the centered data matrix **X**.

$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_m] \in \mathbb{R}^{N \times m}, \quad m: \text{ number of instances }, N: \text{ number of dimensions}$$

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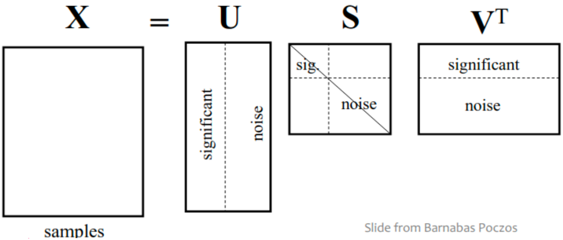
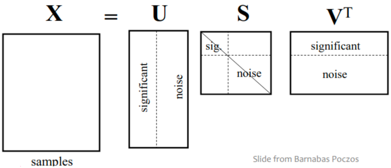


Slide from Barnabas Poczos



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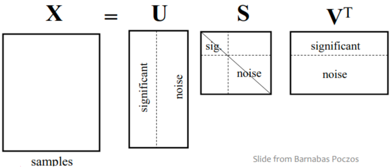
PCA — Principal Component Analysis



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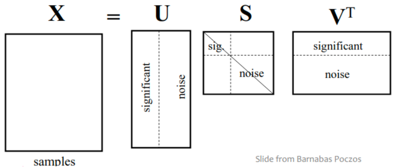

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Columns of $\mathbf{V}^\top$

- The coefficients for reconstructing the samples

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Sometimes, however, we are not purely interested in maximizating variance, but to get the most useful **interpretations** to our newly defined dimensions.

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- PCA is a type of factor analysis. PCA is observational whereas FA is a modeling technique.

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The principle:

– there a certain number of factors in a data set

– each of the measured variables captures a part of one or more of those factors.

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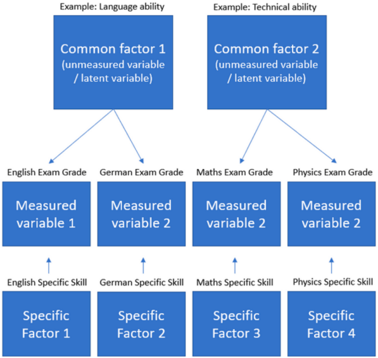
In this case, we could try to find a latent variable for language ability and a second latent variable for technical ability.



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Mathematically, CFA is similar to multiple regression analysis in that each variable is expressed as a linear combination of underlying factors.

The covariation among the variables consists of two terms (not overtly observed)

– a small number of common factors

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If the variables are standardised, the factor model may be represented as:

$$X_i = A_{i1}F_1 + A_{i2}F_2 + A_{i3}F_3 + \ldots + A_{im}F_m + V_iU_i$$

where $X_i = i$ th standardised variable

$A_{ij} =$ standardised multiple regression coefficient of variable i on common factor j

$F =$ common factor

$V_i =$ standardised regression coefficient of variable i on unique factor i

$U_i =$ the unique factor for variable i

$m =$ number of common factors.

Def.: Communality – the amount of variance a variable shares with all other variables included in the analysis

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The common factors themselves can be expressed as linear combinations of the observed variables:

$$F_i = W_{i1}X_1 + W_{i2}X_2 + W_{i3}X_3 + \ldots + W_{ik}W_k$$

where $\quad F_i =$ estimate of i th factor

$W_i =$ weight or factor score coefficient

$k =$ number of variables.

CFA – Common Factor Analysis

The factor model:

$$X_i = A_{i1}F_1 + A_{i2}F_2 + A_{i3}F_3 + \ldots + A_{im}F_m + V_iU_i$$

where $X_i = i$ th standardised variable

The unique factors U_i are correlated with each other and with the common factors F.

The common factors themselves can be expressed as linear combinations of the observed variables:

$$F_i = W_{i1}X_1 + W_{i2}X_2 + W_{i3}X_3 + \ldots + W_{ik}W_k$$

where $F_i =$ estimate of i th factor

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It is possible to select weights or factor score coefficients so that:

– the first factor explains the largest portion of the total variance

– the second factor accounts for most of the residual variance, subject to being uncorrelated with the first factor (the second highest variance), etc.

Example (cont.):

Consider latent variables: the general ability of a student for Language and Technical subjects.

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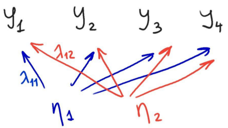

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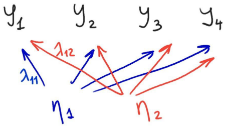

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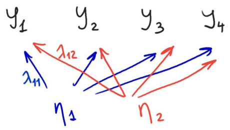

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$$\vdots$$

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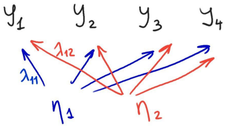

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common unique

– λ_{ij} shows "Ability for learning German while taking into account the general ability for learning languages".

CFA – Common Factor Analysis

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– λ_{i1} attributes one part of its variation to first common latent variable (η_1)

– λ_{i2} attributes one part of its variation to first common latent variable (η_2)

– part of variation related to a specific factor (specific to this variable; ϵ).

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To solve this, the same mathematical solution as in PCA is used, except for a small difference.

– In PCA we apply matrix decomposition to the correlation matrix.

– In Factor Analysis, we apply matrix decomposition to a correlation matrix in which the diagonal entries are replaced by $1 - \text{var}(\mathbf{d})$, one minus the variance of the specific factor of the variable.

CFA – Common Factor Analysis

Assumptions:

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6. Factor analysis is designed for interval data, although it can also be used for ordinal data (e.g. scores assigned to Likert scales).

Terminology:

Factor – a latent (hidden, unobserved) variable which describes the association among the number of observed variables.

– The maximum number of factors are equal to a number of observed variables.

– Every factor explains a certain variance in observed variables.

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Factor Rotation – re-distributed the commonalities with a clear pattern of loadings.

– Rotation is a tool for better interpretation of factor analysis.

– Rotation can be orthogonal or oblique.

CFA – Common Factor Analysis

Factor loading – a matrix which shows

– the relationship of each variable to the underlying factor,

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Communalities – the sum of the squared loadings for each variable.

– represents the common variance

– ranges from $0 - 1$ and value close to 1 represents more variance.

CFA – Common Factor Analysis

There are three main steps in a factor analysis:

1. Calculate initial factor loadings.

– **Principal component method:** looks for a set of factors which can account for the total variability in the original variables.

– **Principal axis factoring:** tries to find the lowest number of factors which can account for the variability in the original variables that is associated with these factors

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Two methods will tend to give similar results if

- the variables are quite highly correlated

- the number of original variables is quite high.

Whichever method is used, the resulting factors at this stage will be uncorrelated.

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Types of rotation method:

– orthogonal rotation the rotated factors will remain uncorrelated (varimax rotation)

– in oblique rotation the resulting factors will be correlated.

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When calculating the final factor scores (the values of the m factors, $F_1, F_2, \ldots, F_m$, for each observation), a decision needs to be made as to how many factors to include.

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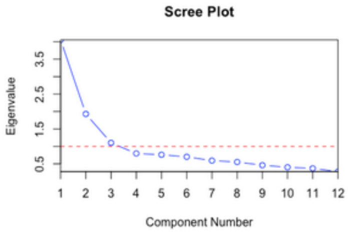
- Use the scree plot of the eigenvalues. This will indicate whether there is an obvious cut-off between large and small eigenvalues.



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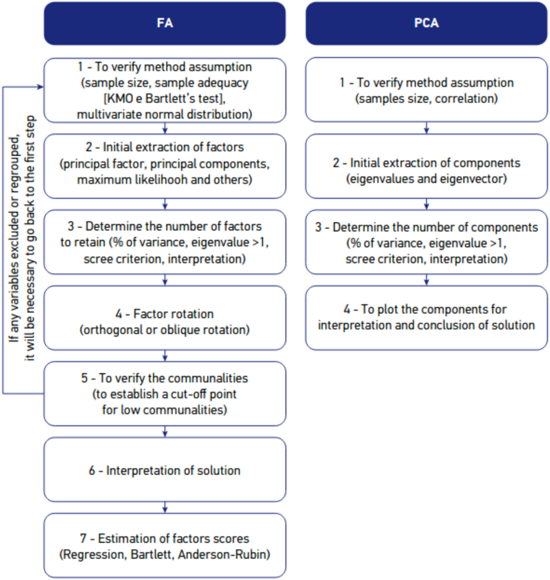

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- PCA does not estimate specific effects, so it simply finds the mathematical definition of the "best" components (components who maximize variance).

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Different Applications

– As Factor Analysis is more flexible for interpretation it is valuable in studies for marketing and psychology.

– PCA's allows for dimension reduction while keeping a maximum amount of information in a data set, hence, iused to simplify EDA or to preprocess data.