Principal Component Analysis (PCA)

Konstantinos I. Bougioukas, MSc, PhD

School of Psychology
Faculty of Philosophy
Aristotle University of Thessaloniki

Principal Component Analysis (PCA) is a statistical technique used to **reduce the dimensionality of a dataset** while preserving as much of its original variability as possible.

PCA computes new variables, called **principal components,** which are obtained as **linear combinations** of the original variables.

$$PC1 : Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

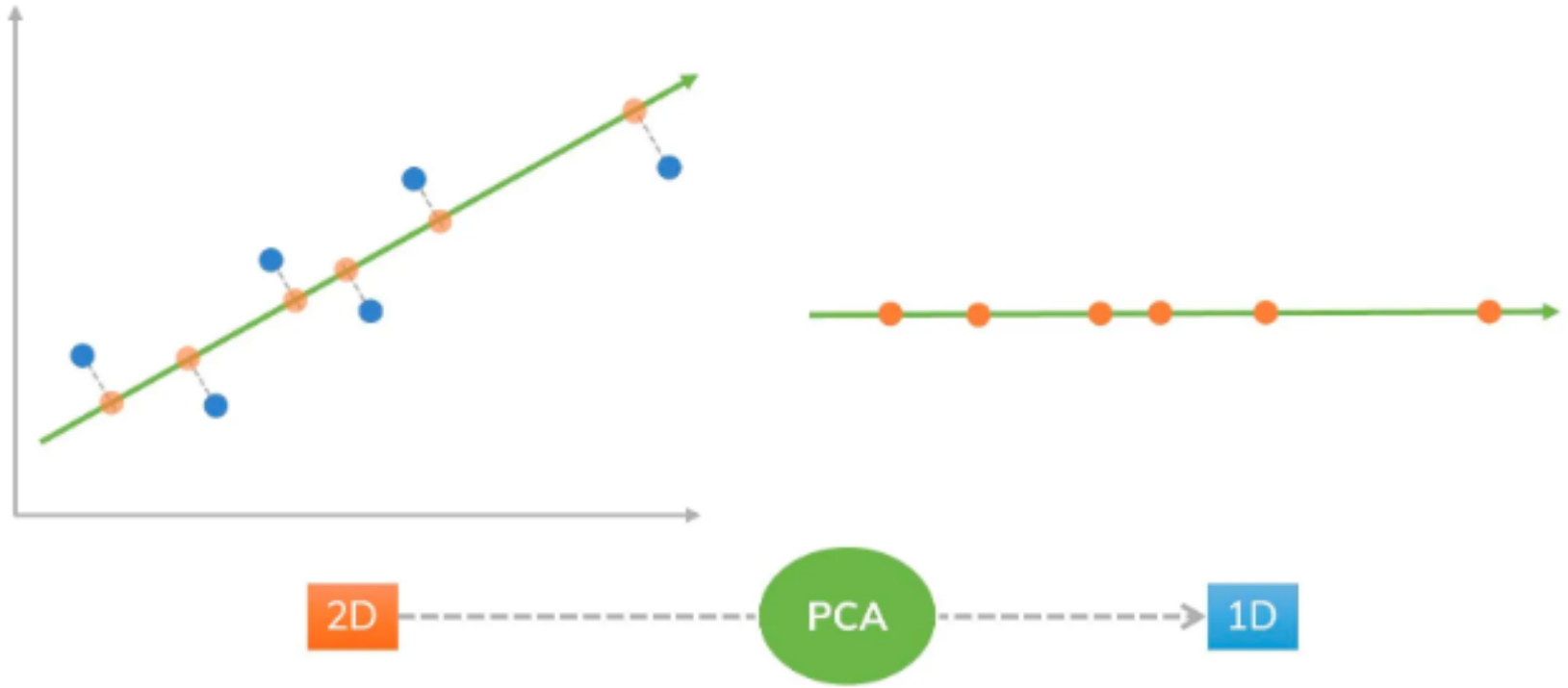
$$PC2 : Z_2 = \phi_{12}X_1 + \phi_{22}X_2 + \ldots + \phi_{p2}X_p$$

...

...

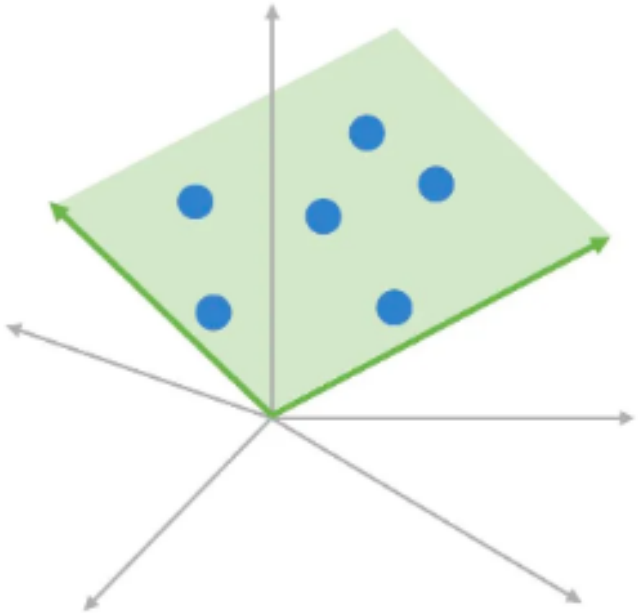
From 2D to 1D

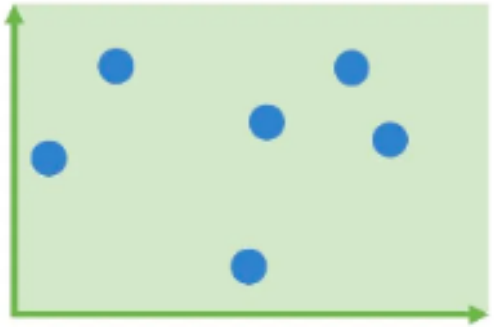
Minimize the orthogonal distance to the line.



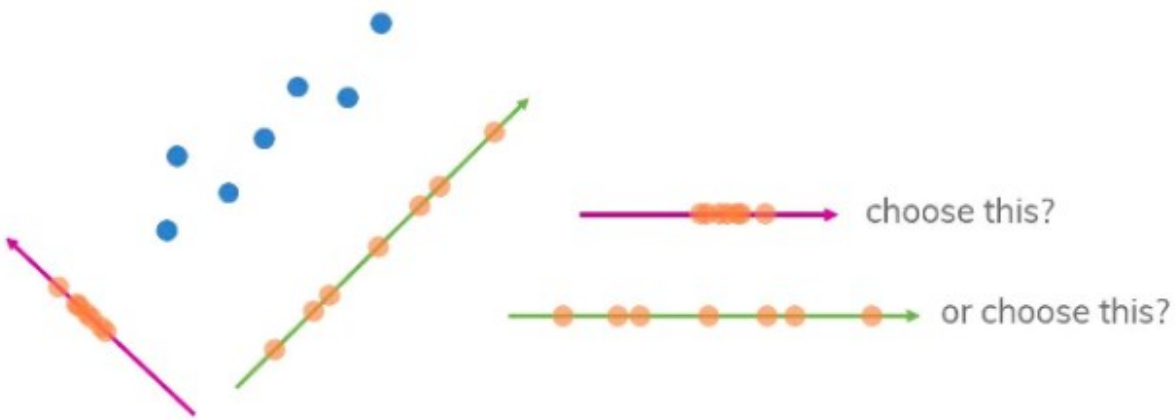
From 5D to 2D

How can we choose the green arrows (their directions and their magnitudes)?





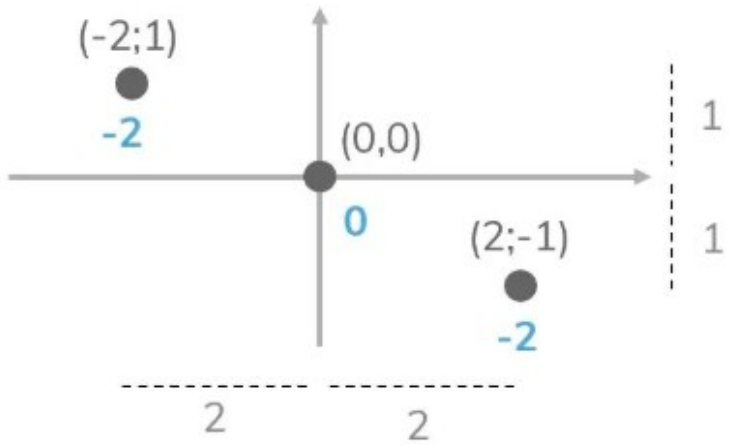
From a data points, there are many ways of projections, for example:

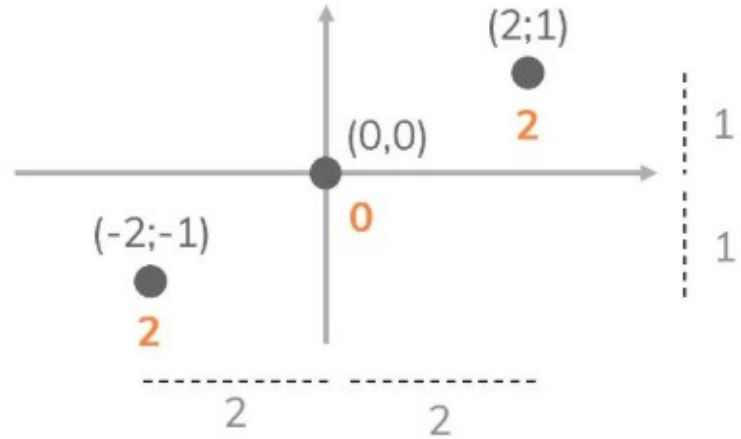


Maximize the Variance

Intuitively, the green line is better with more separated points. But how can we choose it "mathematically" (precisely)? We need to know about:

- Mean: finds the most balanced point in the data.
- Variance: measures the spread of data from the mean. However, variance is not enough. There are many different ways in that we get the same variance.
- Covariance: indicates the direction in that data are spreading.





Mean = 0

$$\text{x-variance} = \frac{2^2+0^2+2^2}{3} = \frac{8}{3}$$

$$\text{y-variance} = \frac{1^2+0^2+1^2}{3} = \frac{2}{3}$$

$$\text{Covariance} = \frac{(-2)+0+(-2)}{3} = -\frac{4}{3}$$

Mean = 0

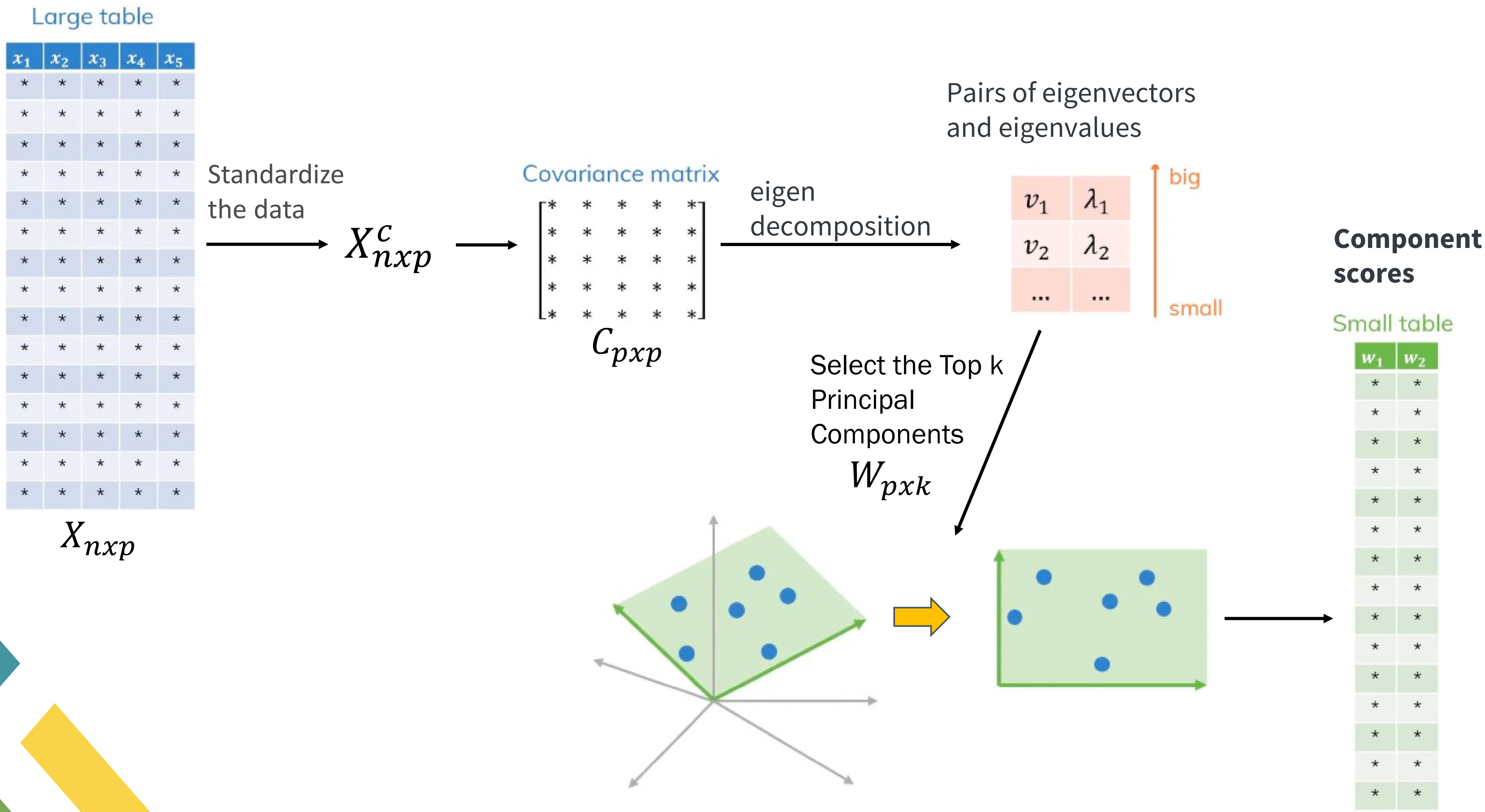
$$\text{x-variance} = \frac{2^2+0^2+2^2}{3} = \frac{8}{3}$$

$$\text{y-variance} = \frac{1^2+0^2+1^2}{3} = \frac{2}{3}$$

$$\text{Covariance} = \frac{2+0+2}{3} = \frac{4}{3}$$

PCA algorithm

1. Standardize the data
2. From the original data (a lot of features $x_1, x_2 \ldots, x_p$), we construct a covariance matrix C.
3. Compute the eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_p$ and correspondent eigenvectors $v_1, v_2, \ldots v_p$ of that matrix.
4. Select the top $k<p$ couples λ and v (the highest eigenvalues) and we get a reduced projection matrix W_k (k eigenvectors as its columns; loadings, if scaled by $\sqrt{\lambda}$).
5. Projection original data points to the k-dimensional plane. This step creates new data points on a new dimensional space (k).



Large table
x1 x2 x3 x4 x5
X_{nxp}
Standardize the data
X^{c}_{nxp}
Covariance matrix
C_{pxp}
eigen decomposition
Pairs of eigenvectors and eigenvalues
v_1 λ_1
v_2 λ_2
big
small
Select the Top k Principal Components
W_{pxk}
Component scores
Small table
w1 w2

Eigenvectors and Eigenvalues

Eigenvectors matrix: V_{pxp}

$$\mathbf{V} = \begin{bmatrix} | & | & & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1p} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{p1} & \alpha_{p2} & \cdots & \alpha_{pp} \end{bmatrix}$$

Eigenvalue matrix: Λ_{pxp}

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p \end{bmatrix}$$

Loadings of first principal component: PC1

$$\phi_{i1} = \alpha_{i1}\sqrt{\lambda_1} \qquad \text{i = 1, 2,..., p}$$

$$\phi_{11}, \phi_{21}, \ldots, \phi_{p1}$$

$$PC1 : Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

Proportion of variance explained

To determine the proportion of total variance explained by the first principal component (i.e., direction by that component), we use the following formula:

$$\frac{\lambda_1}{\lambda_1 + \lambda_2 + \lambda_3 + \ldots + \lambda_p}$$

Component rotation (not a part of classical PCA)

Additional step

Rotation in PCA redistributes the variance between components, making the **loadings more distinct and interpretable**. In other words, rotation typically causes each observed variable to load highly on precisely one component. This clarifies the grouping of variables and makes the underlying dimensions easier to understand.

- **Orthogonal Rotation:** Methods like Varimax keep the components uncorrelated (i.e., orthogonal). This preserves the core mathematical properties of PCA, ensuring that the components remain independent.
  (NOTE: the factor loadings can be interpreted as **correlation coefficients** between the original observed variables and the rotated components).

- **Oblique Rotation:** We don't use this type of rotation in PCA because the components are no longer orthogonal. Exploratory factor analysis (EFA) may be a more technically appropriate model.

PC Loadings and variance

Component Loadings

	Component				
	1	2	3	4	Uniqueness
Obj1	0.574				0.632
Obj2	0.581				0.613
Obj3	0.531				0.679
Obj4	0.604				0.596
Obj5	0.532				0.635
Obj6				0.428	0.576
Obj7					0.675
Obj8	0.572				0.531
Obj9	0.468				0.732
Obj10	0.545				0.674
Marg1		0.784			0.367
Marg2		0.615			0.499
Marg3		0.596			0.602
Marg4		0.559			0.614
Marg5		0.601			0.575
Marg6	0.368	0.403			0.671
Marg7		0.511			0.714
Str1			0.648		0.505
Str2			0.381		0.724

PC1 PC2 PC3 PC4

Loadings

Observed variables (features)

Jamovi includes a column named uniqueness to show how much of each variable's variance remains unexplained by the k components we kept.

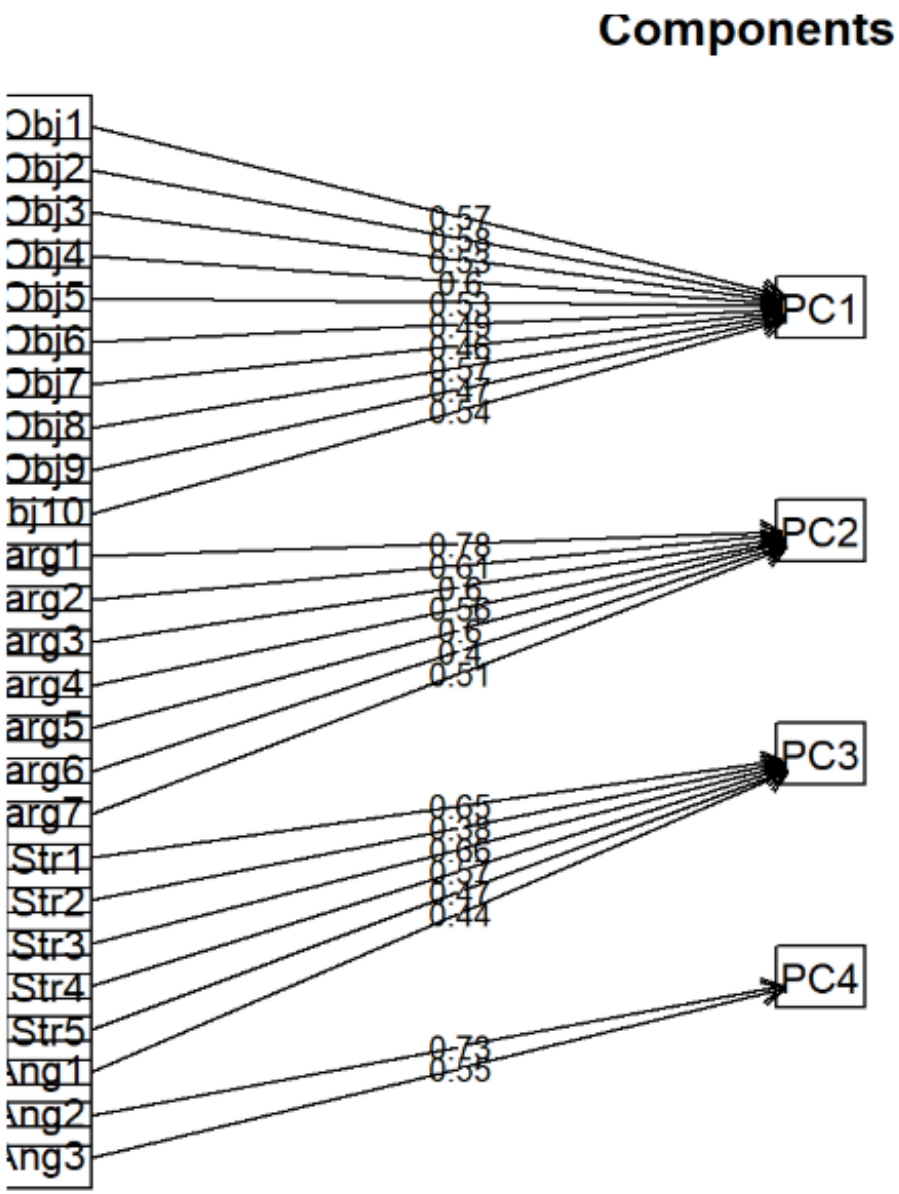
Summary

Component	SS Loadings	% of Variance	Cumulative %
1	3.31	13.23	13.23
2	2.92	11.66	24.90
3	2.05	8.19	33.09
4	1.56	6.24	39.32

The SS Loadings column represents the **eigenvalues λ** for each component

Component Analysis diagram-Varimax rotation

Orthogonal rotation



PCA Assumptions

Identity matrix

$$I_5 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

- **Bartlett's test of sphericity**

A significant result ($p < 0.05$) indicates that the correlation matrix significantly differs from an identity matrix. This suggests that the variables share enough correlation to justify the use of principal component analysis (PCA).

- **Kaiser-Meyer-Olkin (MKO) index of Sampling Adequacy**

(bare minimum of 0.5, values between 0.5 and 0.7 as mediocre, values between 0.7 and 0.8 as good, values between 0.8 and 0.9 as great, values above 0.9 are superb)

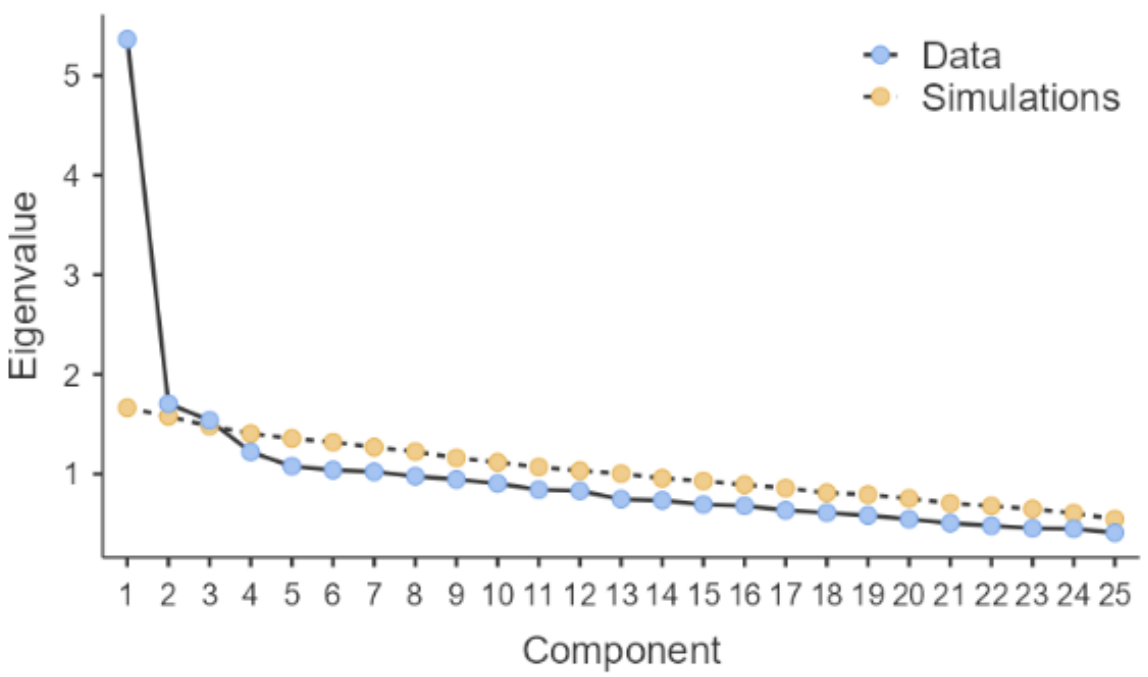
- **Address outliers.**

How do we specify the Number of Components?

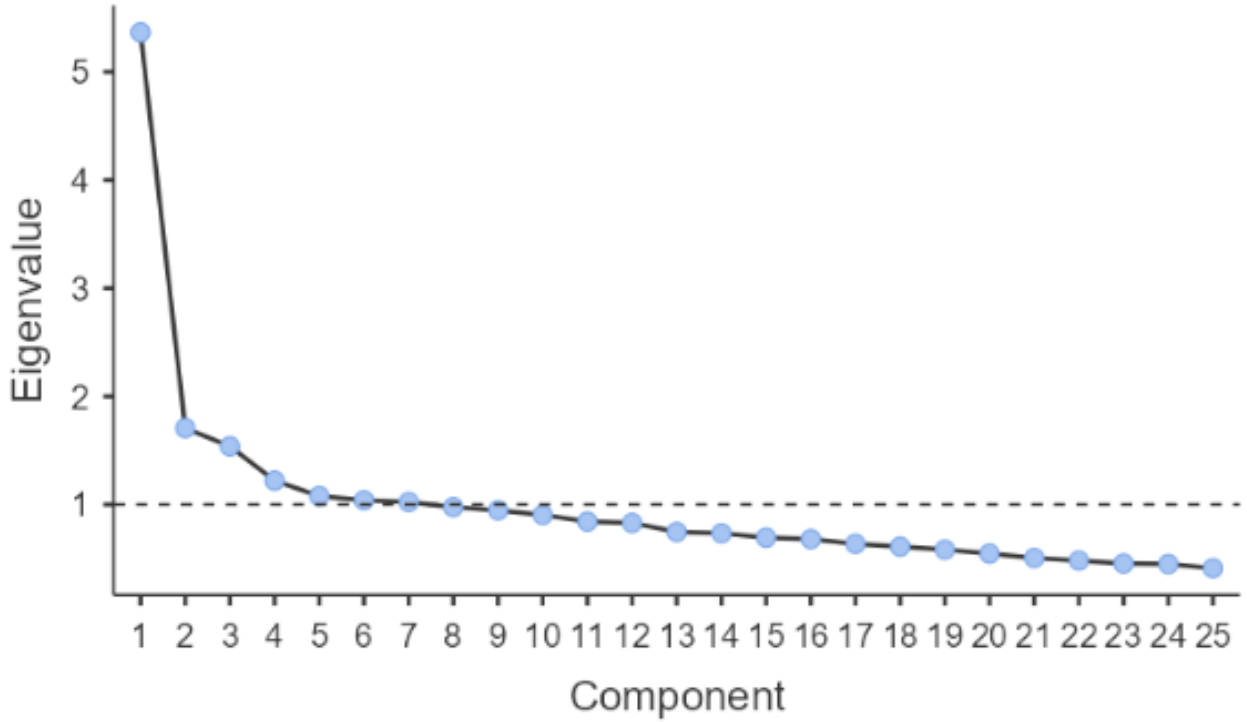
Our decisions on how many components to keep can be guided by several methods:

- **Cumulative variance explained** – Retain enough components to account for a desired proportion of total variance.
- **Parallel analysis** – Compare the observed eigenvalues with those obtained from randomly generated data to determine which components are meaningful.
- **Kaiser's criterion** – Retain components with **eigenvalues greater than 1**.
- **Theoretical justification** – Retain components that align with prior knowledge, conceptual frameworks, or hypotheses relevant to the domain of study (fixed number).

Scree Plot



Scree plot determining the number of components based on parallel analysis.



Scree plot determining the number of components based on Kaiser's criterion.