TUTORIAL ON PRINCIPAL COMPONENT ANALYSIS, WITH APPLICATIONS IN R

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Abstract

This tutorial reviews the main steps of the principal component analysis of a multivariate data set and its subsequent dimensional reduction on the grounds of identified dominant principal components. The underlying computations are demonstrated and performed by means of a script written in the statistical software package R.

In Memoriam: Gisela Ernst (geb.: Freiberg) (1939 to 2020)

1 Introduction

This tutorial demonstrates the main theoretical and practical steps of the principal component analysis of a metrically scaled multivariate data set, and a subsequently performed dimensional reduction of the data set considered. The tutorial is based on a transparent exposition of all relevant computations by means of a script written with the statistical software package R distributed by the R Core Team (2020) [15] free of charge for many different operating systems via the website cran.r-project.org.

The methodological foundations of the principal component analysis and an associated dimensional reduction were laid in particular in the works by Pearson (1901) [14], Hotelling (1933) [8] and Kaiser (1960) [12]; see also Hatzinger et al (2014) [7], Hair et al (2010) [6] or Jolliffe (2002) [11].

The discussion to follow is divided into three parts. First, in Secs. 2 to 5, a trivariate example data set with measured values for three metrically scaled variables is loaded and then characterised and visualised with standard methods of Descriptive Statistics; cf. Ref. [4]. Then, in Secs. 6 to 10, the central tool from Linear Algebra needed to perform a principal component analysis is reviewed: this is the eigenvalue analysis of symmetrical quadratic matrixes and their diagonalisation by means of rotational transformations constructed from the matrixes’ eigenvectors. In Analytic Geometry this method is also known as principal axes transformation; cf. Bronstein et al (2005) [2]. Lastly, in Sec. 11, the procedure of a dimensional reduction of a multivariate data set based on an eigenvalue analysis of its sample correlation matrix is outlined in the context of the given trivariate example data set. The tutorial ends with a conclusion in Sec. 12.

The results to be presented have been generated with R Version 4.1.2.

2 Loading of required R packages

The following R packages and self-written script are loaded into an R session in order to perform all the calculations involved in this tutorial and to generate helpful visualisations of the distributions observed in the analysed data:

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library(tidyverse)

## - Attaching packages --------------------------------- tidyverse
1.3.1 -
## v ggplot2 3.3.5 v purrr 0.3.4
## v tibble 3.1.6 v dplyr 1.0.7
## v tidyr 1.1.4 v stringr 1.4.0
## v readr 2.1.1 v forcats 0.5.1
## - Conflicts -----------------------------------
tidyverse_conflicts() -
## x dplyr::filter() masks stats::filter()
## x dplyr::lag() masks stats::lag()

library(plotly)

##
## Attache Paket: 'plotly'
## Das folgende Objekt ist maskiert 'package:ggplot2':
##
##   last_plot
## Das folgende Objekt ist maskiert 'package:stats':
##
##   filter
## Das folgende Objekt ist maskiert 'package:graphics':
##
##   layout

library(psych)

##
## Attache Paket: 'psych'
## Die folgenden Objekte sind maskiert von 'package:ggplot2':
##
##   %+%, alpha

library(REdaS)

## Lade nötiges Paket: grid

library(e1071)

library(GGally)

## Registered S3 method overwritten by 'GGally':
## method from
##   +.gg ggplot2

source(file = "descripStats.R")

3 Loading of trivariate example data set (matrix $X$)

The example employed in this tutorial for illustrative purposes is given by a trivariate data set that contains measured values for the three metrically scaled variables height [cm], mass [kg] and age [yr] from a sample of $n = 187$ adult women. This trivariate data set is part of a larger data set analysed in
Howell (2001) [9], which needs to be loaded into the R session.

```r
load(file = "testData.RData")
str(object = testData)
## 'data.frame': 544 obs. of 4 variables:
##$ height: num 152 140 137 157 145 ...
##$ weight: num 47.8 36.5 31.9 53 41.3 ...
##$ age : num 63 63 65 41 51 35 32 27 19 54 ...
##$ male : int 1 0 0 1 0 1 0 1 0 1 ...
```

The trivariate data set that comprises measured values for the three variables height [cm], mass [kg] and age [yr] for a sample of women aged 18 yr or more is obtained via adequate filtering.

```r
X <-
testData %>%
dplyr::filter(.data = ., age >= 18 & male == 0) %>%
magrittr::set_colnames(x = .,
   value = c("height [cm]", "mass [kg]", "age [yr]", "male"))
str(object = X)
## 'data.frame': 187 obs. of 4 variables:
##$ height [cm]: num 140 137 145 149 148 ...
##$ mass [kg] : num 36.5 31.9 41.3 38.2 34.9 ...
##$ age [yr] : num 63 65 51 32 19 47 73 20 65.3 31 ...
##$ male : int 0 0 0 0 0 0 0 0 0 0 ...
```

The data matrix X constitutes the raw data matrix for the theoretical and practical considerations outlined in this tutorial.

3.1 Visualisation of data in X via 3D scatter plot

To begin with, the trivariate data set in X is first visualised by means of a 3D scatter plot. This is realised by using the function plot_ly() from the package plotly.

```r
fig1 <-
plotly::plot_ly(
   data = tibble::as_tibble(x = X),
   type = "scatter3d",
   x = X[, 1],
   y = X[, 2],
   z = X[, 3],
   mode = "markers",
   size = 1
) %>%
plotly::layout(title = paste0("Raw data in X ",
   "(original scales of measurement)")),
```

1The complete original data set may be obtained from the URL tspace.library.utoronto.ca/handle/1807/10395.

2Note that the orientation of the scale of measurement along the "x"-axis of this 3D scatter plot does not conform to the mathematical convention; the resultant reference frame does not constitute a right-handed oriented reference frame.
3.2 Visualisation of data in $X$ via scatter plot matrix

In addition, the trivariate data set in $X$ is now visualised by means of a scatter plot matrix, thus providing projections of the cloud of data points in the 3D scatter plot onto 2D horizontal and vertical slices. For this purpose the function `ggpairs()` from the R package GGally is used.

```r
GGally::ggpairs(data = tibble::as_tibble(X[, 1:3])) +
theme_bw()
```
Note that the plots of the univariate distributions of the three variables observed in the present sample, displayed along the diagonal of the scatter plot matrix, suggest qualitatively that the measured values for height [cm] and mass [kg] appear approximately normally distributed, whereas this property does not apply to age [yr].

### 3.3 Descriptive statistics for data in $X$

For the measured values of each of the three variables in the data matrix $X$, the following descriptive statistical measures are computed that characterise their respective observed univariate distributions:

1. **Mean and standard deviation**:

   ```r
   apply(X = X[, 1:3], MARGIN = 2, FUN = mean)
   ```

   ```
   ## height [cm] mass [kg] age [yr]
   ## 149.51352 41.81419 40.71230
   ```

   ```r
   apply(X = X[, 1:3], MARGIN = 2, FUN = sd)
   ```
2. **Standardised skewness** and **standardised excess kurtosis**: cf. Joanes and Gill (1998) [10] and van Elst (2019) [4]:

```r
standSkewness(X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## 0.0205191 1.7939789 3.3003240
```

```r
standKurtosis(X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## -0.6688236 -0.9719034 -1.3598265
```

As long as the computed values for *both* the standardised skewness and the standardised excess kurtosis range inside an interval with boundaries $Q_{0.025} = -1.96$ and $Q_{0.975} = +1.96$, corresponding to the central 95% probability interval for a standard normally distributed variable, one may assume according to statistical convention that one is dealing with **approximately normally distributed** univariate metrically scaled data; cf. Hair *et al* (2010) [6]. As the results obtained for the trivariate example data set in $X$ show, this property applies presently to the variables height [cm] and mass [kg], but not to the variable age [yr], the distribution of which classifies as right-skewed; cf. the scatter plot matrix discussed in Subsec. 3.2.

3. **Counts of outliers, extremal values** and **6-sigma-events**: cf. Toutenburg (2004) [16]:

```r
outliers(X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## 0 1 0
```

```r
extremalValues(X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## 0 0 0
```

```r
sixSigmaEvents(X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## 0 0 0
```

4 **Standardisation of trivariate data set (matrix $Z$)**

In a next step, the raw data in $X$ needs to be transformed onto a common **dimensionless scale of measurement**, with respect to which **measured values** for univariate metrically scaled **variables** are expressed as **deviations from the mean in multiples of the standard deviation**. This kind of transformation is referred to as **standardisation**.
In consequence of standardisation, the univariate data for each of the three variables in the resultant data matrix \(Z\) exhibit a mean of 0 and a standard deviation of 1. This property will be displayed shortly.

The data matrix \(Z\) of standardised measured values ("z-scores") constitutes the basis of all subsequent steps of statistical data analysis.

### 4.1 Visualisation of data in \(Z\) via 3D scatter plot

```r
fig2 <-
  plotly::plot_ly(
    data = tibble::as_tibble(x = Z),
    type = "scatter3d",
    x = Z[, 1],
    y = Z[, 2],
    z = Z[, 3],
    mode = "markers",
    size = 1
  ) %>%
  plotly::layout(title = paste0("Standardised data in Z ",
                              "(unit scale of measurement)"),
                scene = list(  
                  xaxis = list(title = "height std [1]"),
                  yaxis = list(title = "mass std [1]",
                                zaxis = list(title = "age std [1]"
                                ))
  )
fig2
```
4.2 Visualisation of data in $Z$ via scatter plot matrix

\[ GGally::ggpairs(data = tibble::as_tibble(x = Z)) + theme_bw() \]
As the comparison of this scatter plot matrix with the one given in Subsec. 4.2 for the original measured values shows qualitatively, standardisation has preserved the observed uni- and bivariate (and trivariate) distributional properties of the trivariate data set. Otherwise, a transformation of this type would have to be rejected as an illegitimate procedure.

4.3 Visualisation of data in $Z$ via parallel box plots

```r
Z %>%
tibble::as_tibble(x = .) %>%
tidyr::pivot_longer(
  data = .,
  cols = c(`height_std [1]`, `mass_std [1]`, `age_std [1]`),
  names_to = "dimension",
  values_to = "zscore"
) %>%
dplyr::mutate(
  dimension = forcats::fct_relevel(}
```
The parallel box plots point to the existence of a heterogeneity of variances between the univariate data for each of the three variables in the data matrix $Z$.

The preservation of the distributional properties of the data under standardisation is demonstrated from the univariate perspective by the next step of statistical data analysis.

### 4.4 Descriptive statistics for data in $Z$

Again, descriptive statistical measures are computed that characterise observed univariate distributions, this time for the data in $Z$ ("z-scores"): 

\[
\begin{align*}
.f \text{ = dimension,} \\
c \text{("height\_std \([1]\)"}, "mass\_std \([1]\)"}, "age\_std \([1]\)"))
\end{align*}
\]

\[
\text{%>
 ggplot(data = ., mapping = aes(x = dimension, y = zscore)) + geom_boxplot() + xlab(label = "dimension") + ylab(label = "zscore \([1]\)"} + theme_bw()
\]

The parallel box plots point to the existence of a heterogeneity of variances between the univariate data for each of the three variables in the data matrix $Z$. 

The preservation of the distributional properties of the data under standardisation is demonstrated from the univariate perspective by the next step of statistical data analysis.
1. **Mean** and **standard deviation**: 

```r
apply(X = Z, MARGIN = 2, FUN = mean) %>%
  round(x = ., digits = 4)
```

```r
## height_std [1] mass_std [1] age_std [1]
## 0 0 0
```

```r
apply(X = Z, MARGIN = 2, FUN = sd)
```

```r
## height_std [1] mass_std [1] age_std [1]
## 1 1 1
```

2. **Standardised skewness** and **standardised excess kurtosis**; cf. Joanes and Gill (1998) [10] and van Elst (2019) [4]:

```r
standSkewness(Z)
```

```r
## height_std [1] mass_std [1] age_std [1]
## 0.0205191 1.7939789 3.3003240
```

```r
standKurtosis(Z)
```

```r
## height_std [1] mass_std [1] age_std [1]
## -0.6688236 -0.9719034 -1.3598265
```

## 5 Sampling adequacy of trivariate data set in Z for principal component analysis

The **sampling adequacy** for a **principal component analysis** of the present **trivariate data set** is evaluated by employing Bartlett’s (1951) [1] test of sphericity, as well as the standardised **KMO** and **MSA measures** according to Kaiser, Meyer und Olkin (KMO); cf. Kaiser (1970) [12], Guttman (1953) [5] and Hatzinger et al (2014) [7]. For this purpose, one may use the functions `bart_spher()` and `KMO()` from the R package REdaS.

Bartlett’s (1951) [1] frequentist **null hypothesis significance test** subjects the assumption of sphericity of the **envelope** of the **cloud of data points** (defined via the matrix $Z$) in, presently, Euclidian space $\mathbb{R}^3$ to an empirical check. For the given **trivariate data set** this yields

```r
REdaS::bart_spher(x = Z)
```

```r
## Bartlett's Test of Sphericity
##
## Call: REdaS::bart_spher(x = Z)
##
## X2 = 100.12
## df = 3
## p-value < 2.22e-16
```
In view of the calculated $p$-value, the null hypothesis can be rejected at a significance level of $\alpha = 0.01$. Most likely the empirically attested deformation of the envelope is not due to chance. Non-sphericity of the envelope may thus be assumed and so supports the intention of performing a principal component analysis on the trivariate data set in $Z$.\footnote{The non-sphericity of the envelope of the cloud of data points defined via $Z$ is conspicuous in the 3D scatter plot displayed in Subsec. 4.1.}

The standardised KMO and MSA measures, which both take values in the interval $[0; 1]$, assume for the trivariate data set in $Z$ the values

\begin{verbatim}
  kmoZ <- REdaS::KMOS(x = Z)
  print(x = kmoZ, stats = "KMO")
  
  print(
    x = kmoZ,
    stats = "MSA",
    sort = TRUE,
    digits = 7,
    show = 1:3
  )
\end{verbatim}

The KMO measure quantifies the sampling adequacy of the entire data set in $Z$, whereas, in contrast, the MSA measure individually quantifies the sampling adequacy of the measured values for every single variable. According to, e.g., Hatzinger et al (2014) \cite{Hatzinger2014} or Hair et al (2010) \cite{Hair2010}, a good sampling adequacy for the data set in $Z$ is given when both standardised measures range between 0.8 und 1.0. Of course, in this respect, the presently considered trivariate data set in $Z$ constitutes a negative example. However, as it proves very useful for demonstrating the main theoretical and practical steps of the principal component analysis of a metrically scaled multivariate data set, and is also accessible to the reader’s imagination, this tutorial continuous to employ it in the steps of statistical data analysis taken in the following sections.

6 Calculation of sample correlation matrix $R$ and its inverse $R^{-1}$

The sample correlation matrix $R$ of the considered trivariate data set in $X$ is defined in terms of algebraic projections of “$z$-scores” onto themselves by

\[ R := \frac{1}{n-1} Z^\top Z , \]
The sample correlation matrix $R$ exhibits a non-zero value for its determinant and therefore classifies as regular. It follows that there exists an inverse, $R^{-1}$, which is given here for completeness:

```
det(x = Rmat)
```

```
## [1] 0.5806328
```

```
RmatInv <- solve(Rmat)
```

```
## height_std [1] mass_std [1] age_std [1]
## height_std [1] 1.6304987  -0.9941702  0.0743531
## mass_std [1] -0.9941702  1.6624566  0.1984769
## age_std [1]  0.0743531  0.1984769  1.0596680
```

For the example considered, the trace of the sample correlation matrix $R$ amounts to

```
sum(diag(x = Rmat))
```

```
## [1] 3
```

This value is equal to the number of variables in the considered trivariate data set in $X$.

7 Eigenvalues and eigenvectors: orthonormal eigenbasis of sample correlation matrix

In the present case, the three eigenvalues of the sample correlation matrix $R$ are

```
evAnaCor <- eigen(x = Rmat, symmetric = "TRUE")
evAnaCor$values
```

```
## [1] 1.7382412 0.8838105 0.3779482
```

```
sum(evAnaCor$values)
```

```
## [1] 3
```
and they sum up to the very number of variables in the trivariate data set in $X$. The three mutually orthogonal, normalised eigenvectors of the sample correlation matrix $R$ are (columnwise, from left to right)$^4$

|   | [,1]   | [,2]   | [,3]   |
|---|--------|--------|--------|
| [1,] | -0.6504363 | 0.3033698 | 0.69634715 |
| [2,] | -0.6625952 | 0.2215906 | -0.71544756 |
| [3,] | 0.3713492 | 0.9267494 | -0.05688085 |

These are also referred to as the principal components of the trivariate data set in $X$. The eigenvectors span the orthonormal eigenbasis of the sample correlation matrix $R$ in Euclidian space $\mathbb{R}^3$; cf. Bronstein et al. (2005) [2].

With regard to Kaiser’s (1960) [12] eigenvalue criterion it is noted that in the present example only one of the three eigenvalues of the sample correlation matrix $R$ is greater than 1, implying that presently the trivariate data set in $X$ possesses only a single dominant principal component.

The proportions of total variance of the trivariate data set in $Z$ explained by each of the three principal components amount to

```r
round(x = (evAnaCor$values / sum(evAnaCor$values)), digits = 4)
## [1] 0.5794 0.2946 0.1260
```

i.e., 57.94 %, 29.46 % and 12.60 %, respectively, and in cumulative terms

```r
round(x = (cumsum(evAnaCor$values) / sum(evAnaCor$values)), digits = 4)
## [1] 0.5794 0.8740 1.0000
```

An interpretation for the eigenvalues of the sample correlation matrix $R$ will be given in the next section.

## 8 Rotation matrix $V$, diagonal eigenvalue matrix $\Lambda$ and inverse diagonal eigenvalue matrix $\Lambda^{-1}$

From the three eigenvectors of the sample correlation matrix $R$ one constructs an orthogonal rotation matrix $V$, by means of which one can perform (presently in Euclidian space $\mathbb{R}^3$) transformations to the right-handed oriented orthonormal eigenbasis of the sample correlation matrix $R$. The determinant of the rotation matrix $V$ has the value 1, i.e.,

```r
rotMatCor <- evAnaCor$vectors
rotMatCor[, 3] <- (-1) * rotMatCor[, 3] # re-scaling by a factor of (-1)
rotMatCor
```

$^4$Regrettably R does not return the components of the three identified eigenvectors according to the usual mathematical convention, i.e., so that the eigenvectors form a right-handed oriented orthonormal basis.
implying that transformations with the rotation matrix $V$ preserve volumes.

Per construction the rotation matrix $V$ satisfies the following two tests of orthogonality

$$1 = V^T V = V V^T,$$

viz.

By means of diagonalisation of the sample correlation matrix $R$ via transformation with the rotation matrix $V$, one obtains the diagonal eigenvalue matrix $\Lambda$ as

$$\Lambda = V^T R V,$$

viz.

The diagonal eigenvalue matrix $\Lambda$ is nothing but the representation of the sample correlation matrix $R$ with respect to its orthonormal eigenbasis in Euclidian space $\mathbb{R}^3$.

The diagonal eigenvalue matrix $\Lambda$ obtained above may be subjected to the consistency check

$$0 = \Lambda - \text{diag}(\lambda_1, \ldots, \lambda_m),$$

viz.
The inverse, \( \Lambda^{-1} \), of the diagonal eigenvalue matrix \( \Lambda \) is computed by

\[
\text{LambdaCorInv} \leftarrow \begin{pmatrix}
\frac{1}{\text{evAnaCor$values}}
\end{pmatrix}
\]

The three eigenvalues of the sample correlation matrix \( R \) amount to the variances of the data in \( Z \) along the three directions in Euclidean space \( \mathbb{R}^3 \) defined by the orthonormal eigenbasis of the sample correlation matrix \( R \). The following consideration makes this fact explicit.

**8.1 Visualisation of data in \( Z_{\text{rot}} \) via 3D scatter plot**

Transformation of the data in \( Z \) to the orthonormal eigenbasis of the sample correlation matrix \( R \) yields

\[
Z_{\text{rot}} = ZV
\]

viz.

\[
Z_{\text{rot}} \leftarrow Z \times \text{rotMatCor}
\]

Visualisation of the resultant data in \( Z_{\text{rot}} \) by means of a 3D scatter plot gives

\[
\text{fig3} \leftarrow \text{plotly::plot_ly}(
\text{data} = \text{tibble::as_tibble}(x = \text{Zrot}),
\text{type} = "scatter3d",
\text{x} = \text{Zrot}[1],
\text{y} = \text{Zrot}[2],
\text{z} = \text{Zrot}[3],
\text{mode} = "markers",
\text{size} = 1
)\]

```r
round(x = (\text{LambdaCor} - \text{diag}(x = \text{evAnaCor$values))), \text{digits} = 4)
## [,1] [,2] [,3]
## [1,] 0 0 0
## [2,] 0 0 0
## [3,] 0 0 0
```

```r
\text{LambdaCorInv} \leftarrow \begin{pmatrix}
\frac{1}{\text{evAnaCor$values}}
\end{pmatrix}
\]

## [,1] [,2] [,3]
## [1,] 0.5752941 0.000000 0.000000
## [2,] 0.000000 1.131464 0.000000
## [3,] 0.000000 0.000000 2.645865
```

\[
\text{Zrot} \leftarrow Z \times \text{rotMatCor}
\]

```r
\text{magrittr::set_colnames}(x = ., \text{value} = \text{c("PC1", "PC2", "PC3")})
```

Visualisation of the resultant data in \( Z_{\text{rot}} \) by means of a 3D scatter plot gives

```r
\text{plotly::plot_ly}(
\text{data} = \text{tibble::as_tibble}(x = \text{Zrot}),
\text{type} = "scatter3d",
\text{x} = \text{Zrot}[1],
\text{y} = \text{Zrot}[2],
\text{z} = \text{Zrot}[3],
\text{mode} = "markers",
\text{size} = 1
)\]

\text{plotly::layout}(
\text{title} = \text{paste0("Standardised data wrt. ",}
\text{"orthonormal eigenbasis of R")},
\text{scene} = \text{list}(
\text{xaxis} = \text{list(title = "Zrot1 [1]")},
\text{yaxis} = \text{list(title = "Zrot2 [1]")},
\text{zaxis} = \text{list(title = "Zrot3 [1]")})
```
Subsequent computation of the variances of the data in $Z_{\text{rot}}$ obtains

```r
apply(X = Zrot, MARGIN = 2, FUN = var)
```

```r
#> PC1 PC2 PC3
#> 1.7382412 0.8838105 0.3779482
```

i.e., the claimed result. Note that the data in the columns of $Z_{\text{rot}}$ is pairwise uncorrelated

```r
round(x = cor(x = Zrot), digits = 4)
```

```r
#> PC1 PC2 PC3
#> PC1 1 0 0
#> PC2 0 1 0
#> PC3 0 0 1
```

### 8.2 Visualisation of data in $Z_{\text{rot}}$ via scatter plot matrix

```r
GGally::ggpairs(data = tibble::as_tibble(x = Zrot)) + theme_bw()
```
8.3 Visualisation of data in $Z_{\text{rot}}$ via parallel box plots

```r
Zrot %>%
tibble::as_tibble(x = .) %>%
tidyr::pivot_longer(
  data = .,
  cols = c("PC1", "PC2", "PC3"),
  names_to = "dimension",
  values_to = "zscorerot"
) %>%
dplyr::mutate(
  dimension = forcats::fct_relevel(
    .f = dimension,
    c("PC1", "PC2", "PC3")
  )
) %>%
ggplot(data = .,
```
Note that in the orthonormal eigenbasis of the sample correlation matrix $R$ the heterogeneity of variances between the univariate data for each of the three variables in the rotated data matrix $Z_{rot}$ is more pronounced than the corresponding one in the original orthonormal basis between the univariate data for each of the three variables in the data matrix $Z$. This is a clear manifestation of the existing correlations between the latter three variables.

8.4 Descriptive statistics for data in $Z_{rot}$

Descriptive statistical measures are computed that characterise the observed univariate distributions for the data in $Z_{rot}$ (“rotated z-scores”):

1. Mean and standard deviation:
2. Standardised skewness and standardised excess kurtosis; cf. Joanes and Gill (1998) [10] and van Elst (2019) [4]:

```
standSkewness(Zrot)
## PC1  PC2  PC3
## -0.6580145 1.5543143 1.9033877

standKurtosis(Zrot)
## PC1  PC2  PC3
## -0.5119328 -0.3687139 -0.0712973
```

9 Principal component loadings matrix \( A \)

The principal component loadings matrix \( A \), defined in terms of the orthogonal rotation matrix \( V \) and the diagonal eigenvalue matrix \( \Lambda \) by

\[
A := V \Lambda^{1/2},
\]

provides the answer to the question: how strongly are the (presently) three original variables height, mass and age correlated with the identified three principal components of the trivariate data set considered?\(^5\)

```r
AmatCor <-
rotMatCor %>% abs(LambdaCor) ^ (1 / 2) %>%
magrittr::set_rownames(
  x = ., 
  value = c("height", "mass", "age")) %>%
magrittr::set_colnames(
  x = ., 
  value = c("PC1", "PC2", "PC3"))
AmatCor
## PC1  PC2  PC3
```

\(^5\)Generally: how strongly are the \( m \) original variables of a given metrically scaled multivariate data set correlated with the identified \( m \) principal components of this data set?
The fact that the principal component loadings matrix \( A \) may indeed be interpreted as a (formal) correlation matrix will become apparent later on.

The principal component loadings matrix \( A \) satisfies two consistency checks:

1. The sample correlation matrix \( R \) can be factorised by means of the principal component loadings matrix \( A \) as
   \[
   0 = R - AA^\top,
   \]
   viz.

   ```r
   round(x = (Rmat - AmatCor %*% t(AmatCor)), digits = 4)
   ## height_std [1] mass_std [1] age_std [1]
   ## height_std [1] 0 0 0
   ## mass_std [1] 0 0 0
   ## age_std [1] 0 0 0
   ```

2. The diagonal eigenvalue matrix \( \Lambda \) can be factorised by means of the principal component loadings matrix \( A \) as
   \[
   0 = \Lambda - A^\top A,
   \]
   viz.

   ```r
   round(x = (LambdaCor - t(AmatCor) %*% AmatCor), digits = 4)
   ## PC1 PC2 PC3
   ## PC1 0 0 0
   ## PC2 0 0 0
   ## PC3 0 0 0
   ```

10 Standardised data set in orthonormal eigenbasis of sample correlation matrix (matrix \( F \))

Finally, a transformation needs to be performed of the standardised trivariate data set in \( Z \) to the orthonormal eigenbasis of the sample correlation matrix \( R \), while respecting the conventional requirement that the resultant data shall likewise be standardised. This is realised in terms of a volume preserving rotation of the original reference frame with the rotation matrix \( V \), followed by a volume changing but directions preserving rescaling of the axes of the rotated reference frame with the (square root of the) inverse \( \Lambda^{-1} \) of the diagonal eigenvalue matrix \( \Lambda \). These two transformations performed in combination define the matrix \( F \),

\[
F := ZV\Lambda^{-1/2},
\]

viz.

---

6The effect of a pure transformation of the data in \( Z \) with the rotation matrix \( V \) was described and visualised before in Sec. 8.

7Equivalently, the matrix \( F \) can also be computed from the trivariate data set in \( Z \) by employing the principal component loadings matrix \( A \) and the inverse \( \Lambda^{-1} \) as \( F = ZAA^{-1} \).
FmatCor <-
    Z %*% rotMatCor %*% LambdaCorInv ^ (1 / 2) %>%
    magrittr::set_colnames(
        x = .,
        value = c("PC1_std [1]", "PC2_std [1]", "PC3_std [1]"))

dim(x = FmatCor)
## [1] 187 3

head(x = FmatCor)
## PC1_std [1] PC2_std [1] PC3_std [1]
## [1,] 1.8362245 0.4986426 1.1623874
## [2,] 2.6100451 0.2165376 0.8829885
## [3,] 0.6264361 0.3416280 0.8556499
## [4,] 0.2097674 -0.7040217 -0.7566757
## [5,] 0.4219218 -1.7223008 -1.2765885
## [6,] -1.1094795 1.0397559 0.7139017

which contains standardised and, by construction, mutually uncorrelated so-called “f-scores” in its columns.

10.1 Consistency checks for matrix $F$

The following consistency checks need to be satisfied by the matrix $F$:

1. The “f-scores” are standardised and mutually uncorrelated:

   $$0 = 1 - \frac{1}{n-1} F^\top F,$$

   viz.

   proxy <-
     (1 / (nrow(FmatCor) - 1)) * t(FmatCor) %*% FmatCor
   round(x = (diag(rep(x = 1, times = nrow(proxy))) - proxy),
       digits = 4)

   ## PC1_std [1] PC2_std [1] PC3_std [1]
   ## PC1_std [1] 0 0 0
   ## PC2_std [1] 0 0 0
   ## PC3_std [1] 0 0 0

2. The elements of the principal component loadings matrix $A$ represent, as algebraic projections of standardised and uncorrelated “z-scores” onto standardised and uncorrelated “f-scores”, bivariate correlations between the (presently three) original variables and the (presently three) principal components of the multivariate data set considered; cf. the remarks at the beginning of Sec. 9:

   $$0 = A - \frac{1}{n-1} Z^\top F,$$

   viz.
round(
  x = (AmatCor - (1 / (nrow(Z) - 1)) * t(Z) %*% FmatCor),
  digits = 4
)

## PC1 PC2 PC3
## height 0 0 0
## mass 0 0 0
## age 0 0 0

3. The “z-scores” may be perceived as linear combinations of the “f-scores”:

\[ 0 = Z - FA^T, \]

viz.

head(x = round(x = (Z - FmatCor %*% t(AmatCor)), digits = 4))

## height_std [1] mass_std [1] age_std [1]
## [1,] 0 0 0
## [2,] 0 0 0
## [3,] 0 0 0
## [4,] 0 0 0
## [5,] 0 0 0
## [6,] 0 0 0

tail(x = round(x = (Z - FmatCor %*% t(AmatCor)), digits = 4))

## height_std [1] mass_std [1] age_std [1]
## [182,] 0 0 0
## [183,] 0 0 0
## [184,] 0 0 0
## [185,] 0 0 0
## [186,] 0 0 0
## [187,] 0 0 0

10.2 Visualisation of data in \( F \) via 3D scatter plot

fig4 <-
plotly::plot_ly(
  data = tibble::as_tibble(x = FmatCor),
  type = "scatter3d",
  x = FmatCor[, 1],
  y = FmatCor[, 2],
  z = FmatCor[, 3],
  mode = "markers",
  size = 1
) %>%
plotly::layout(title = paste0("Standardised data in F ",

Standardised data in \( F \) (unit scale of measurement)

\[
\text{scene} = \text{list}(
  xaxis = \text{list}(\text{title} = "\text{PC1 std [1]}"),
  yaxis = \text{list}(\text{title} = "\text{PC2 std [1]}"),
  zaxis = \text{list}(\text{title} = "\text{PC3 std [1]}")
)
\]

10.3 Visualisation of data in \( F \) via scatter plot matrix

\[
\text{GGally::ggpairs(data} = \text{tibble::as_tibble(x) = FmatCor}) + \text{theme_bw()}\]
The scatter plot matrix shows nicely that the “f-scores” associated with each of the principal components are mutually uncorrelated.

10.4 Visualisation of data in $F$ via parallel box plots

```r
FmatCor %>%
  tibble::as_tibble(x = .) %>%
  tidyr::pivot_longer(
    data = .,
    cols = c('PC1_std [1]', 'PC2_std [1]', 'PC3_std [1]'),
    names_to = "dimension",
    values_to = "fscore"
  ) %>%
  dplyr::mutate(
    dimension = forcats::fct_relevel(
      .f = dimension,
      c("PC1_std [1]", "PC2_std [1]", "PC3_std [1]")))
```
Standardisation of the univariate data for each of the three variables in the orthonormal eigenbasis of the sample correlation matrix $R$ has neutralised the heterogeneity of variances observed in Subsec. 8.3.

11 Dimensional reduction: extraction of single dominant principal component

Secs. 4 to 10 featured in some detail the linear-algebraic methodology on which the principal component analysis of a metrically scaled multivariate data set is grounded. The discussion now turns to
describe the necessary steps involved in a dimensional reduction of such a data set, given that for the case considered the procedure proves conceptually and practically meaningful.

The dimensional reduction of the multivariate data set begins in the orthonormal eigenbasis of the sample correlation matrix $R$. In short, one only keeps those “$f$-scores” which are associated with the dominant principal components; the remaining ones are being discarded. The loss of information incurred in this way is generally perceived as being compensated by an overall reduction of complexity for the multivariate data set being analysed. The remaining “$f$-scores” will be transformed back to the original orthonormal basis and then expressed with respect to the original scales of measurement. The dimensionally reduced measured values so obtained may form the starting point of further statistical data analysis.\(^8\)

11.1 Qualitative criterion for extraction

The R package psych provides the function `VSS.scree()` for generating scree plots according to Cattell (1966) [3].

```r
psych::VSS.scree(rx = Z)
```

\(^8\)The performance of a dimensional reduction of a given multivariate data set, when meaningful, does not really require computation of the matrix $F$, respectively the “$f$-scores”. For this purpose it fully suffices to transform the “$z$-scores” from the original orthonormal basis to the orthonormal eigenbasis of the sample correlation matrix $R$ and then keep only those values (columns) associated with the dominant principal components. Standardisation of values in the orthonormal eigenbasis merely corresponds to a convenient convention.
Based on numerous applications in practice, it is recommended to extract as many principal components from a given multivariate data set as correspond to the number of eigenvalues to be found left of the “ellbow” in a scree plot. In the present example this is just one, and thus proves consistent with Kaiser’s (1960) [12] eigenvalue criterion, which recommends extraction of all principal components that are associated with an eigenvalue greater than 1.

The procedure of a dimensional reduction of a given multivariate data set is now exemplified for the trivariate data set in \( X \). It is demonstrated on the basis of extraction of the single dominant principal component identified in Sec. 7.

### 11.2 Dimensionally reduced matrixes

The procedure of a dimensional reduction of a given multivariate data set is reflected in the first place in the matrixes of the aforementioned linear-algebraic methodology.

1. Dimensionally reduced rotation matrix \( V_{\text{red}} \) — only those eigenvectors of a sample correlation matrix \( R \) that are associated with eigenvalues greater than 1 will be employed in the construction of a rotation matrix:
2. Dimensionally reduced diagonal eigenvalue matrix $\Lambda_{\text{red}}$ — generated from the sample correlation matrix $R$ via transformation with the dimensionally reduced rotation matrix:

$$
\text{LambdaCorRed} \leftarrow \text{t(rotMatCorRed) $\%\% Rmat $\%\% rotMatCorRed}
$$

3. Inverse of dimensionally reduced diagonal eigenvalue matrix, $\Lambda_{\text{red}}^{-1}$

$$
\text{LambdaCorRedInv} \leftarrow \text{solve(LambdaCorRed)}
$$

4. Dimensionally reduced principal component loadings matrix $A_{\text{red}}$

$$
\text{AmatCorRed} \leftarrow \text{rotMatCorRed $\%\% \Lambda_{\text{red}}^{1/2}}
$$

5. Dimensionally reduced matrix $F$, $F_{\text{red}}$

$$
\text{FmatCorRed} \leftarrow \text{Z $\%\% \text{AmatCorRed $\%\% \Lambda_{\text{red}}^{-1}}}
$$
### Dimensional Reduction

#### 11.3 Comparison of trivariate example data set with its dimensionally reduced variant

The “f-scores” remaining in the dimensionally reduced matrix $F_{\text{red}}$ need to be transformed back to the original orthonormal basis, and then expressed with respect to the original scales of measurement. For illustrative purposes, a sample of the corresponding dimensionally reduced data will be contrasted with the original “z-scores,” and with the original measured values for the three variables height, mass and age.

**Standardised scale of measurement $Z_{\text{red}}$ vs $Z$**

```r
Zapprox <-
  FmatCorRed %*% t(AmatCorRed) %>%
  magrittr::set_colnames(x = .,
                         value = c("height_std [1]", "mass_std [1]", "age_std [1]"))
```

**head(x = Z)**

|       | height_std [1] | mass_std [1] | age_std [1] |
|-------|---------------|--------------|-------------|
| [1,]  | -1.9300562    | -0.9889505   | 1.3740963   |
| [2,]  | -2.5544936    | -1.8466045   | 1.4974016   |
| [3,]  | -0.8060688    | -0.0997265   | 0.6342642   |
| [4,]  | -0.0567439    | -0.6627263   | -0.5371365  |
| [5,]  | -0.3065189    | -1.2888663   | -1.3386213  |
| [6,]  | 0.9423560     | 1.4998244    | 0.3876535   |

**head(x = Zapprox)**

|       | height_std [1] | mass_std [1] | age_std [1] |
|-------|---------------|--------------|-------------|
| [1,]  | -1.5746556    | -1.6040913   | 0.8990074   |
| [2,]  | -2.2382460    | -2.2800865   | 1.2778665   |
| [3,]  | -0.5372007    | -0.5472428   | 0.3067003   |
| [4,]  | -0.1798862    | -0.1832489   | 0.1027012   |
Original scales of measurement

This requires a backward transformation (de-standardisation) of the data in \( Z_{\text{red}} \) respectively in \( Z \) to the original scales of measurement used for the three variables height, mass and age:

```r
b <- attr(x = Z, "scaled:scale")
a <- attr(x = Z, "scaled:center")
Xapp_int <- Zapprox * rep(x = b, each = nrow(Zapprox)) + rep(x = a, each = nrow(Zapprox))
XapproxCor <-
data.frame(Xapp_int)```

\[ X_{\text{red}} \] vs \( X \)

```r
head(x = X[, 1:3])
```

```r
## height [cm] mass [kg] age [yr]
## 1 139.700 36.48581 63
## 2 136.525 31.86484 65
## 3 145.415 41.27687 51
## 4 149.225 38.24348 32
## 5 147.955 34.86988 19
## 6 154.305 49.89512 47
```
11 DIMENSIONAL REDUCTION

head(x = XapproxCor)

## height [cm] mass [kg] age [yr]
## 1 141.5071 33.17148 55.29411
## 2 138.1330 29.52927 61.43916
## 3 146.7821 38.86569 45.68695
## 4 148.5989 40.82686 42.37810
## 5 147.6738 39.82830 44.06286
## 6 154.3512 47.03627 31.90171
tail(x = X[, 1:3])

## height [cm] mass [kg] age [yr]
## 1 156.210 44.02677 33.0
## 2 146.050 39.40581 37.4
## 3 152.400 40.82328 49.0
## 4 162.560 47.03182 27.0
## 5 142.875 34.24620 31.0
## 6 156.210 54.06250 21.0
tail(x = XapproxCor)

## height [cm] mass [kg] age [yr]
## 1 153.8304 46.47414 32.85012
## 2 147.3195 39.44581 44.70818
## 3 149.7042 42.01998 40.36509
## 4 158.1934 51.18383 24.90404
## 5 144.3624 36.25369 50.09386
## 6 158.8207 51.86096 23.76159

11.4 Visualisation of dimensionally reduced data via 3D scatter plot

Standardised scale of measurement

fig5 <-
plotly::plot_ly(
data = tibble::as_tibble(x = Zapprox),
type = "scatter3d",
x = Zapprox[, 1],
y = Zapprox[, 2],
z = Zapprox[, 3],
mode = "markers",
size = 1)
  ) %>%
plotly::layout(title = paste0("Dimensionally reduced ",
                             "standardised data in Zapprox"),
               scene = list(
xaxis = list(title = "height std [1]")
               ,
yaxis = list(title = "mass std [1]")
               ,
zaxis = list(title = "age std [1]")
               ))
fig5

Dimensionally reduced standardised data in Zapprox

Original scales of measurement

fig6 <-
plotly::plot_ly(
data = tibble::as_tibble(x = XapproxCor),
type = "scatter3d",
x = XapproxCor[, 1],
y = XapproxCor[, 2],
z = XapproxCor[, 3],
mode = "markers",
size = 1
) %>%
plotly::layout(title = paste0("Dimensionally reduced data ",
    "in XapproxCor"),
scene = list(
xaxis = list(title = "height [cm]")e
yaxis = list(title = "mass [kg]"),
zaxis = list(title = "age [yr]"
))
fig6
11 DIMENSIONAL REDUCTION

11.5 Visualisation of dimensionally reduced data via scatter plot matrix

Standardised scale of measurement

\[
\text{GGally::ggpairs(data = tibble::as_tibble(x = Zapprox)) + theme_bw()}
\]
Original scales of measurement

`GGally::ggpairs(data = tibble::as_tibble(x = XapproxCor)) + theme_bw()`
12 Conclusion

In the example considered, the dimensional reduction performed results in an extremal case: the trivariate data set in $X$ was effectively reduced to a univariate data set, which can explain $57.94\ %$ of the total variance of the original data set. The dimensionally reduced data set exhibits the maximal (minimal) possible values for the bivariate correlations between any pair of the three original variables height, mass and age.

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Constructive comments by Jana Orthey and Laurens van der Woude have helped to focus this tutorial on the specific needs of the targeted audience.
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