Introduction to Statistical Modelling

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Table of contents

Preface

Most of the figures in this book are generated with R. If you are reading this book online, you can view the source code for each figure by clicking the little triangle next to the word "Code" above the figure. In the PDF version of this book the code is listed inline with the figure.

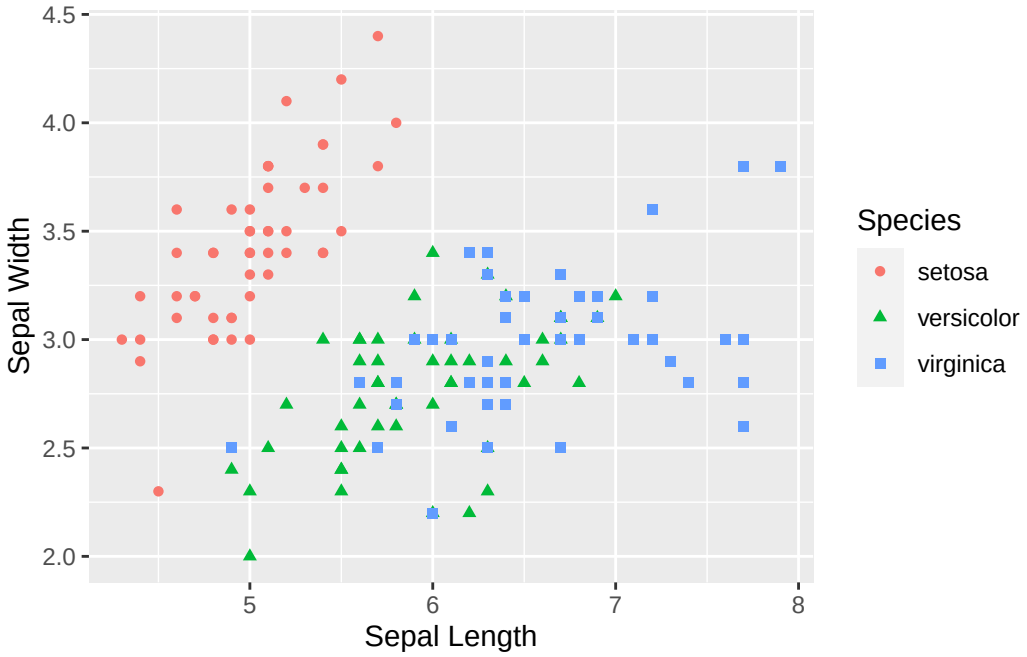


Figure 0.1: Length and width of the sepal petal of 150 Iris plants.

1 Principal component analysis

In the previous chapter we built a linear model to predict the amount of body fat, given measurements of the thickness of the triceps skin fold, the thigh circumference, and the midarm circumference. We saw that the dataset used for this model suffers from multicollinearity, meaning that some of the predictors (or linear combinations of predictors) are correlated with one another. Intuitively speaking, multicollinearity means that some variables don't contribute much to the expressivity of the data: we could omit them and end up with a dataset that is almost as informative as the original one.

To find out which combinations of variables contribute most to the variability of our data, we will turn to *principal component analysis*, one of the mainstays of statistical data analysis. Principal component analysis will allow us to identify the main sources of variability in our dataset, and will tell us which combinations of variables can be omitted with only little impact on the data itself. This allows us to reduce the number of features in the dataset, and makes principal component analysis into what is called a technique for *dimensionality reduction*. This is useful for a number of reasons:

- As a *pre-processing technique*: Many statistical techniques, such as multiple linear regression, do not perform well in the presence of highly correlated features. They either fail to converge outright, or they give unreliable results (for example, model coefficients and predictions that change drastically when the data is slightly perturbed). This is even more of an issue when there are more predictors than data points, a situation that often occurs when analysing gene expression data or spectroscopy data.
- To save on *computational processing time*: analyzing superfluous variables comes with a cost, which can often increase drastically with the number of features. We will see an example of this phenomenon in Section 1.4.3, where the data points are vectors with 4096 components. After principal component reduction, the dimensionality of the dataset can be reduced to 50-100 components, a reduction by more than 98%.
- To *visualize* the data: for datasets with a limited number of features, we can use a scatter matrix to view the distribution of the features and their relations with one another. Scatter matrices become uninformative, however, as soon as there are more than 4 or 5 features. Moreover, scatter matrices may hide correlations that occur between different linear combinations of variables, as we have seen in the chapter on linear modeling.

1.1 Intuition

Principal component analysis (PCA) finds a low-dimensional approximation to the dataset which retains as much as possible the variability of the original dataset. To understand what is meant by this, let's revisit the body fat dataset of chapter 1. In this dataset, the features are the measurements of the thickness of the triceps skin fold, the thigh circumference, and the midarm circumference. The total body fat is the outcome, but we will not consider it for the time being.

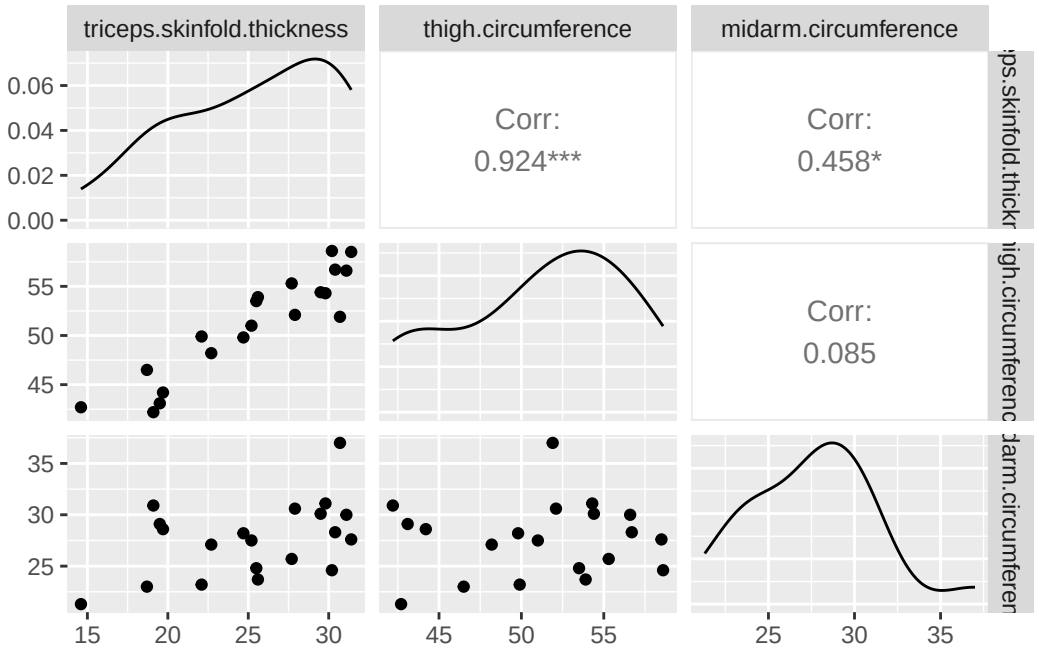
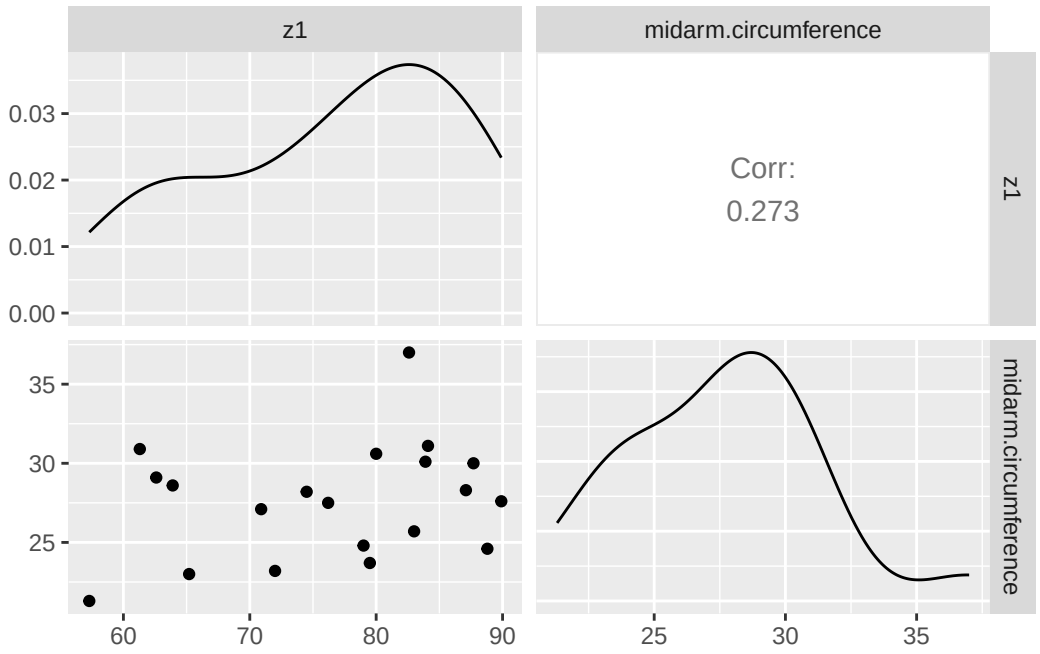


Figure 1.1: Correlations between the different variables in the body fat dataset. The variable `triceps.skinfold.thickness` is strongly correlated with the other two variables in the dataset and hence carries less information.

From the scatter matrix, we see that `triceps.skinfold.thickness` and `thigh.circumference` are highly correlated: if you know one, you can predict the other one reasonably well. This makes it feel like a waste to analyze both: since they carry the same information, we can just as well throw one or the other away, or replace both by a linear combination. Let's do the latter, and introduce a new variable `z1` which is the sum of both. In terms of this variable and `midarm.circumference`, which we leave unchanged, the dataset has only two features that are mildly correlated, as shown on the scatter plot below.



We have succeeded in our aim to reduce the number of features in our dataset from 3 to 2, but a number of questions immediately pop up:

1. What is the meaning of the `z1` variable, and can we find it without looking at a scatter plot?
2. How much information do we lose by considering two variables instead of three? Will the conclusions from the reduced dataset still be valid for the full dataset?

It will turn out that the variable `z1`, which we constructed in an ad-hoc way, is remarkably close to the first principal component of the dataset, and we will discover a way to compute all principal components. We will also see that by discarding more or fewer principal components, as much variability of the original dataset can be retained as is needed.

1.2 Derivation of the PCA algorithm

PCA works by making linear combinations of the original variables so that the total amount of variation is maximal. There is another way of computing principal components, by minimizing the reconstruction error, and it can be shown that both approaches give the same principal components (Bishop (2006), section 12). In this course, we will develop the first method further.

We assume that we have N observations $\mathbf{x}_i$, where each $\mathbf{x}_i$ is a column vector in $\mathbb{R}^D$. We assemble these observations into an $N \times D$ *data matrix* $\mathbf{X}$, where each row of $\mathbf{X}$ is an observation

$\mathbf{x}_i$:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \cdots \\ \mathbf{x}_N^T \end{bmatrix}.$$

Keep in mind that the columns of $\mathbf{X}$ are the features (also referred to as independent variables or predictors) of the dataset. In the case of the body fat dataset, $\mathbf{X}$ is a 20×3 matrix, since there are 20 observations, with 3 features for each observation. We will refer to the jth column of $\mathbf{X}$ by the notation $\mathbf{X}_j$, where $j = 1, \ldots, D$. Note that $\mathbf{X}_j$ is a column vector, with N entries, and there are D such columns. For the body fat dataset, the columns correspond to the following features:

- $\mathbf{X}_1$: `triceps.skinfold.thickness`
- $\mathbf{X}_2$: `thigh.circumference`
- $\mathbf{X}_3$: `midarm.circumference`

1.2.1 The first principal component

The first principal component, $\mathbf{Z}_1$ is a linear combination of the features, so that the amount of variation in $\mathbf{Z}_1$ is maximized. Let's unpack these ideas one at a time. The fact that $\mathbf{Z}_1$ is a linear combination means that it can be written as

$$\mathbf{Z}_1 = v_1\mathbf{X}_1 + \cdots + v_D\mathbf{X}_D = \sum_{j=1}^{D} v_j\mathbf{X}_j.$$

where the v_j are coefficients that we have to determine. These coefficients are sometimes referred to as the principal component **loadings**, since v_j expresses how much of $\mathbf{X}_j$ is added ("loaded") to the principal component.

We can write this expression for $\mathbf{Z}_1$ in a compact way by assembling all the coefficients v_j into a vector $\mathbf{v}$, called the **loadings vector**:

$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \cdots \\ v_D \end{bmatrix}.$$

With this expression, $\mathbf{Z}_1$ can be written as a matrix-vector product:

$$\mathbf{Z}_1 = \mathbf{X}\mathbf{v}. \tag{1.1}$$

We will often use this way of expressing $\mathbf{Z}_1$ as a matrix-vector product, since it makes subsequent calculations easier.

Before we go on to determine the loadings v_j, let's focus on the geometry behind Equation 1.1. Each component of $\mathbf{Z}_1$ can written as

$$(\mathbf{Z}_1)_i = \mathbf{x}_i^T \mathbf{v}.$$

This is the dot product of the ith observation $\mathbf{x}_i$ with the loadings vector $\mathbf{v}$. This dot product tells us how much of the vector $\mathbf{x}_i$ is parallel to $\mathbf{v}$, as shown in Figure 1.2. For example, a data point that is at right angles to $\mathbf{v}$ will have dot product 0 (no component at all along $\mathbf{v}$), while one that is parallel to $\mathbf{v}$ will have a dot product that is maximal in magnitude.

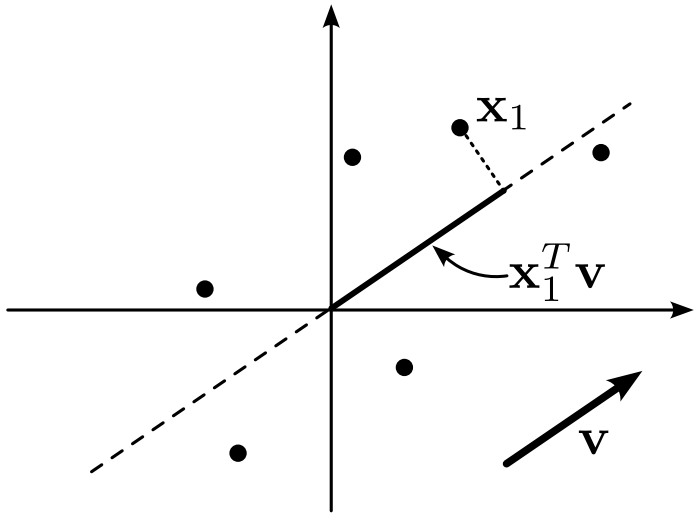


Figure 1.2: The ith component of the first principal component $\mathbf{Z}_1$ is the length of the orthogonal projection of $\mathbf{x}_i$ onto the line in the direction of $\mathbf{v}$.

In other words, we obtain $\mathbf{Z}_1$ by taking a fixed vector $\mathbf{v}$ and projecting all of our data points on the line through the origin in the direction of $\mathbf{v}$. If we choose another vector, $\mathbf{w}$, we obtain a different projection, as indicated on Figure 1.3.

Our goal is now to find the loadings vector $\mathbf{v}$ so that the variance of the projected dataset is maximal. To make this problem well-posed, we will assume that $\mathbf{v}$ has unit norm:

$$\mathbf{v}^T\mathbf{v} = 1. \tag{1.2}$$

If we did not impose this constraint, we could increase the amount of variance simply by making $\mathbf{v}$ longer.

The mean of the projected data is given by

$$\bar{\mathbf{Z}}_1 = \frac{1}{N}\sum_{j=1}^{N}(\mathbf{Z}_1)_j = \frac{1}{N}\sum_{j=1}^{N}\mathbf{x}_j^T\mathbf{v} = \bar{\mathbf{x}}^T\mathbf{v},$$

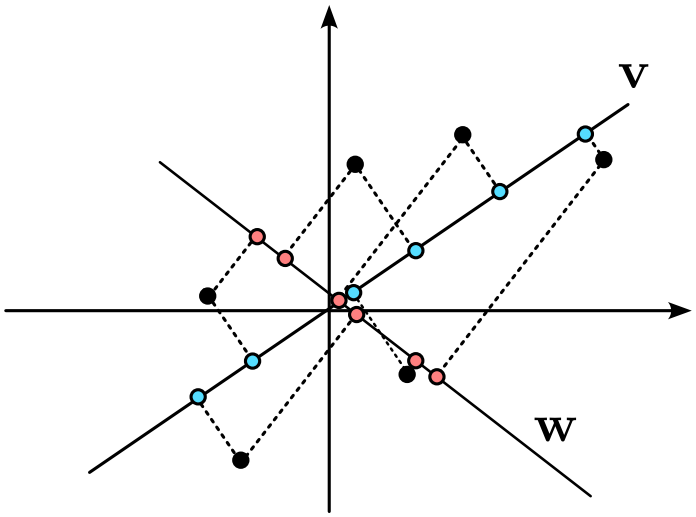


Figure 1.3: Two different projections, onto the loadings vector $\mathbf{v}$ (blue) and $\mathbf{w}$ (red).

where $\bar{\mathbf{x}}$ is the (sample) mean of the original data points. In other words, the mean $\bar{\mathbf{Z}}_1$ is just the mean $\bar{\mathbf{x}}$ of the data points, projected onto $\mathbf{v}$.

The variance of the projected data is given by

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}\left((\mathbf{Z}_1)_i - \bar{\mathbf{Z}}_1\right)^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{x}_i^T\mathbf{v} - \bar{\mathbf{x}}^T\mathbf{v}\right)^2.$$

This expression can be rewritten as a matrix product:

$$\sigma^2 = \mathbf{v}^T\mathbf{S}\mathbf{v}, \tag{1.3}$$

where $\mathbf{S}$ is the covariance matrix, given by

$$\mathbf{S} = \frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{x}_i\mathbf{x}_i^T - \bar{\mathbf{x}}\bar{\mathbf{x}}^T\right). \tag{1.4}$$

We are now ready to translate our problem into a mathematical form, so that we can solve it. To find the first principal component $\mathbf{Z}_1$, we want to find a loadings vector $\mathbf{v}$ so that the projected variance σ^2, given in Equation 1.3, is maximized. In addition, we want $\mathbf{v}$ to have unit length, as in Equation 1.2. In mathematical terms:

$$\mathbf{v} = \operatorname{argmax}\mathbf{v}^T\mathbf{S}\mathbf{v}, \quad \text{such that } \mathbf{v}^T\mathbf{v} = 1.$$

We can solve this optimization problem using the theory of Lagrange multipliers. If we introduce a Lagrange multiplier λ for the unit-length constraint, then the desired vector $\mathbf{v}$ is given by

$$\mathbf{v} = \operatorname{argmax} L(\mathbf{v})$$

where L is given by

$$L(\mathbf{v}) = \mathbf{v}^T\mathbf{S}\mathbf{v} - \lambda(\mathbf{v}^T\mathbf{v} - 1).$$

A necessary condition for $\mathbf{v}$ to be a maximum of L is that the gradient vanishes at $\mathbf{v}$. Taking the gradient of L with respect to $\mathbf{v}$ and setting the resulting expression equal to zero gives

$$\mathbf{S}\mathbf{v} = \lambda\mathbf{v}. \tag{1.5}$$

This is a very important result: it tells us that the $\mathbf{v}$ we are looking for is an **eigenvector** of the matrix $\mathbf{S}$, with corresponding **eigenvalue** λ. This will hold true generally, not just for the first principal component: finding the principal components of a data set will involve solving an eigenvalue problem, and selecting the largest eigenvalues.

Last, we have to find the Lagrange multiplier λ. This can be done by multiplying Equation 1.5 from the left by $\mathbf{v}^T$ to get

$$\mathbf{v}^T\mathbf{S}\mathbf{v} = \lambda\mathbf{v}^T\mathbf{v} = \lambda,$$

where we have used the unit-length constraint Equation 1.2.

We see that the Lagrange multiplier λ is precisely the variance σ^2 of the first principal component $\mathbf{Z}_1$. For this reason, we will refer to the eigenvalue λ as the amount of *retained variance*, since it expresses how much variance is captured by projecting the entire dataset onto the direction $\mathbf{v}$.

To sum up, the first principal component $\mathbf{Z}_1$ is a linear combination of the original features (columns) of our dataset, chosen so that the variance of $\mathbf{Z}_1$ is maximal. We can find $\mathbf{Z}_1$ by looking for the largest eigenvalue λ of the covariance matrix, with unit length eigenvector $\mathbf{v}$, and projecting the data matrix $\mathbf{X}$ onto $\mathbf{v}$.

1.2.2 The remaining principal components

Now that we've computed the first principal component, how do we compute the others? It probably won't come as a surprise that the next principal components, $\mathbf{Z}_2$, $\mathbf{Z}_3$, and so on, involve the amount of variation that is left in the data after $\mathbf{Z}_1$ has been removed, and that they involve the second, third, … largest eigenvalues.

Assuming that we have computed $\mathbf{Z}_1$ as in the previous section, and denote the loadings vector by $\mathbf{v}_1$. Recall that $\mathbf{v}_1$ points in the direction of the largest variance.

To find the next principal component, we consider the variability in the dataset that is not already accounted for by $\mathbf{Z}_1$. More precisely, we look for a loadings vector $\mathbf{v}_2$ which is orthogonal to $\mathbf{v}_1$, has unit length, and maximizes the amount of variability $\mathbf{v}_2^T\mathbf{S}\mathbf{v}_2$. By a similar reasoning as in the previous section, one can show that this $\mathbf{v}_2$ is an eigenvector associated

with the second largest eigenvalue of $\mathbf{S}$. The projection of the dataset onto this loadings vector then gives us the second principal component:

$$\mathbf{Z}_2 = \mathbf{X}\mathbf{v}_2.$$

This procedure can be applied to find all D principal components and results in the following algorithm to compute the principal components:

1. Compute the sample covariance matrix $\mathbf{S}$ using Equation 1.4.
2. Compute the eigenvalues of $\mathbf{S}$ and order them from largest to smallest: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$.
3. Find the corresponding eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_D$ and normalize them to unit length, if necessary. These vectors are the loading vectors and they point in the directions of highest variance.
4. Project the dataset onto the loading vectors to obtain the principal components $\mathbf{Z}_1, \mathbf{Z}_2, \ldots, \mathbf{Z}_D$.

Typically, we do not have to compute the principal components by hand: most data analysis packages will do this for us, either via a builtin command, such as in R (prcomp) or minitab, or via an extra package, such as scikit-learn (Python) or xlstat (Excel). It is instructive, however, to know the principles behind PCA, so that you can interpret and understand the results.

> **Note**
>
> Software packages that compute the principal components of a dataset typically do not compute the eigenvalues and eigenvectors of the covariance matrix, despite our derivation above. Instead, they rely on the so-called *singular value decomposition* (SVD) of the data matrix (after centering). The SVD is typically more accurate and easier to compute, and the principal components obtained in this way agree with the ones computed using the eigendecomposition (to within numerical roundoff).

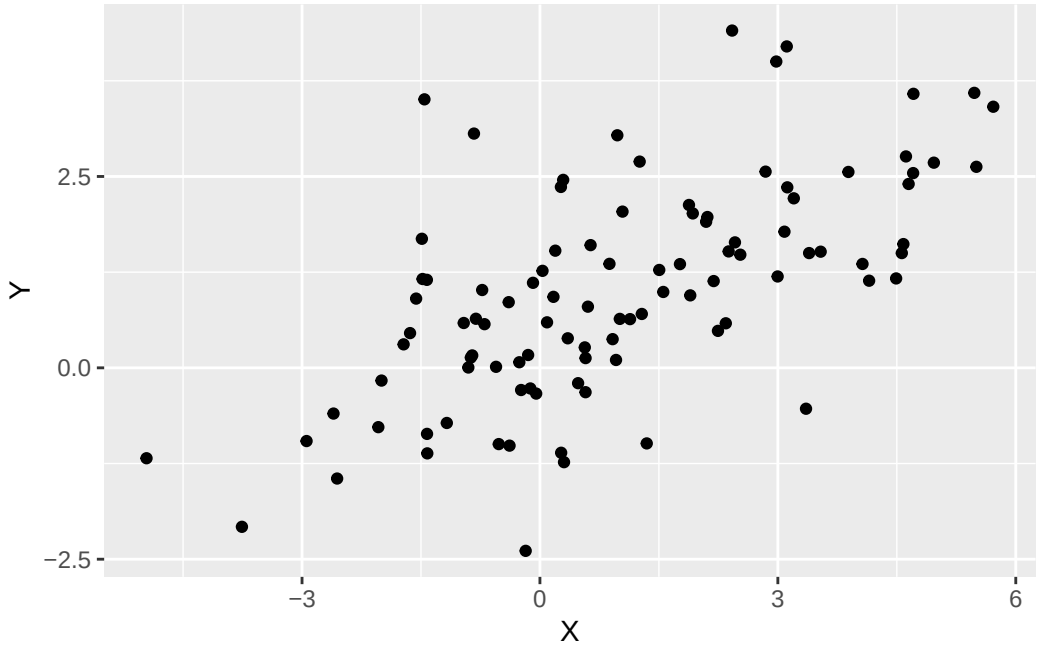
1.2.3 Worked-out example

For this example, we will calculate the principal components in two different ways. We will first compute the principal components by hand, by solving an eigenvalue problem. This is possible because the data are two-dimensional, and solving the characteristic equation for a two- or three-dimensional matrix can be done by hand. This is not practical for real-world datasets, which often contains dozens, thousands, or millions of features, and we will therefore also cover computing the principal components using R.

Our dataset consists of 100 observations, where each observation has two components. The dataset is shown below and has been carefully constructed so that the covariance matrix $\mathbf{S}$

and mean $\bar{\mathbf{x}}$ are exactly equal to

$$\mathbf{S} = \begin{bmatrix} 5 & 2 \\ 2 & 2 \end{bmatrix}, \quad \text{and} \quad \bar{\mathbf{x}} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{1.6}$$



To find the loading vectors, we must find the eigenvalues of $\mathbf{S}$, which we can do via the characteristic equation:

$$\det(\mathbf{S} - \lambda \mathbf{I}) = 0.$$

Substituting the expression given in Equation 1.6 for the covariance matrix and expanding the determinant gives

$$\det \begin{bmatrix} 5-\lambda & 2 \\ 2 & 2-\lambda \end{bmatrix} = (5-\lambda)(2-\lambda) - 4 = 0.$$

The roots of this equation are $\lambda_1 = 6$ and $\lambda_2 = 1$. The corresponding eigenvectors are

$$\mathbf{v}_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ 2 \end{bmatrix}.$$

These are our loading vectors, and they indicate the direction in which the data varies the most (for $\mathbf{v}_1$) and the "second-most" (for $\mathbf{v}_2$). Figure Figure 1.4 shows the dataset again, now with the two loading vectors superimposed. Each loading vector has been rescaled by multiplying it with the square root of the corresponding eigenvalue. Why the square root? The eigenvalue itself represents the *variance* in that direction, the square root the standard deviation.

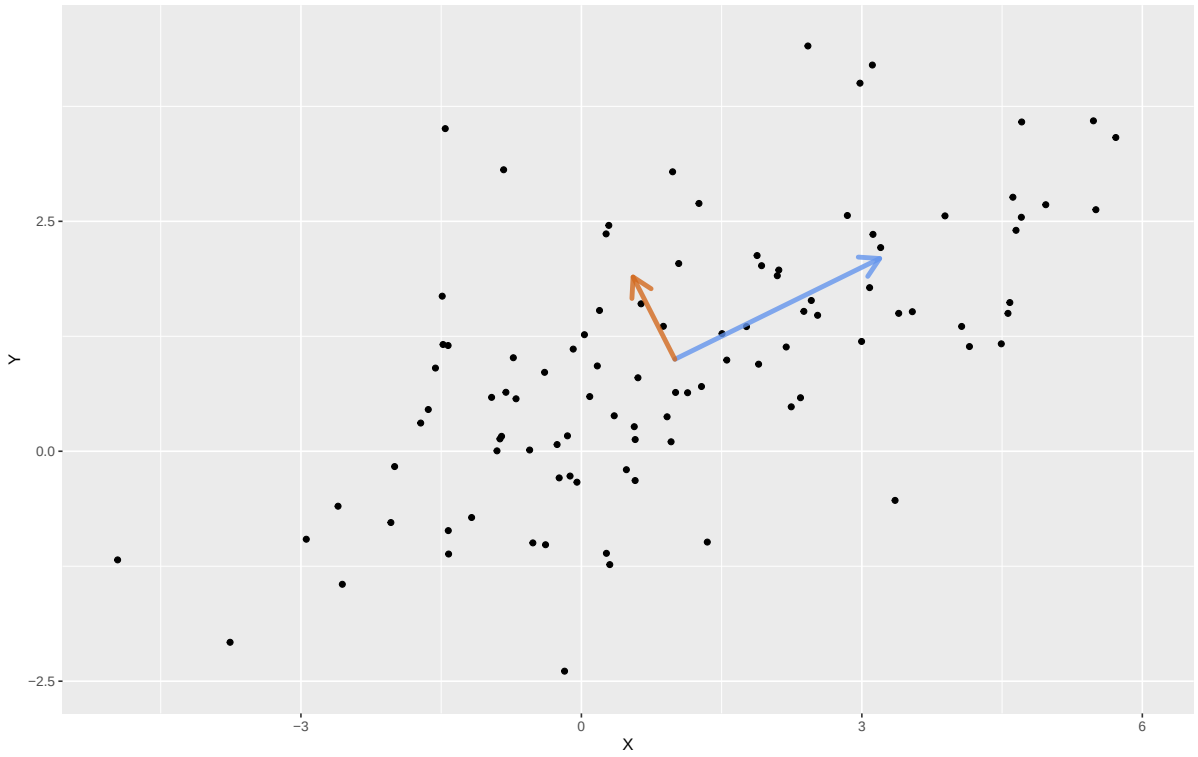


Figure 1.4: The dataset with the first loading vector (blue) and the second loading vector (orange) superimposed. Each loading vector has been rescaled by the square root of the corresponding eigenvalue, to give an indication of the variability in that direction.

To compute the principal components directly via R, we can use the `prcomp` command, as shown below. This is generally the preferred option over computing the eigenvalue decomposition by hand: `prcomp` is more flexible (allowing one, for example, to scale the data before computing the principal components) and is also numerically more stable.[1] For our simple dataset, the end result is the same:

```
pca <- prcomp(df)
pca
```

```
Standard deviations (1, .., p=2):
[1] 2.44949 1.00000

Rotation (n x k) = (2 x 2):
        PC1        PC2
X 0.8944272 -0.4472136
Y 0.4472136  0.8944272
```

> **Warning**
>
> Note that `prcomp` returns (among other things) the standard deviations, which are the square roots of the variances (eigenvalues). To compare the output of `prcomp` with the results of the eigenvalue analysis, **make sure to take the square of the standard deviations**, and you will see the eigenvalues appear:
>
> ```
> pca$sdev^2
> ```
>
> ```
> [1] 6 1
> ```

1.2.4 Standardizing the predictors

Prior to doing principal component analysis, the data are often standardized by subtracting the mean for each feature and dividing by the standard deviation. If the original predictors in our dataset are given by $\mathbf{X}_i$, $i = 1, \ldots, D$, this means that we introduce standardized variables $\mathbf{Y}_i$, given by

$$\mathbf{Y}_i = \frac{\mathbf{X}_i - \bar{\mathbf{X}}_i}{\sqrt{S_i^2}},$$

[1] R has two commands to compute the principal components: `prcomp` and `princomp`. The former computes principal components using the so-called singular value decomposition (SVD) and is preferred for numerical stability. The latter, `princomp`, uses the eigenvalue decomposition as is provided for backwards compatibility with SAS.

where S_i^2 is the variance of $\mathbf{X}_i$. If we put all of these variances S_i^2 into a diagonal matrix $\mathbf{V}$ given by

$$\mathbf{V} = \begin{bmatrix} \sqrt{S_1^2} & 0 & \dots & 0 \\ 0 & \sqrt{S_2^2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sqrt{S_D^2} \end{bmatrix}$$

then it can be shown that the covariance matrix $\mathbf{R}$ of the $\mathbf{Y}$ variables is related to the covariance matrix $\mathbf{S}$ of the original $\mathbf{X}$ variables by

...

This standardization often has a profound effect on the principal component analysis.

1.3 Interpreting the PCA results

In this section we will discuss a number of useful results that follow from PCA. We will use the bodyfat dataset as an illustration throughout.

```
pc <- prcomp(bodyfat_predictors)
pc
```

```
Standard deviations (1, .., p=3):
[1] 7.2046011 3.7432587 0.1330841

Rotation (n x k) = (3 x 3):
                                 PC1        PC2        PC3
triceps.skinfold.thickness 0.6926671  0.1511979  0.7052315
thigh.circumference        0.6985058 -0.3842734 -0.6036751
midarm.circumference       0.1797272  0.9107542 -0.3717862
```

We can also ask R to print a summary of the principal component analysis for us. This will give us a table with the proportion of variance explained by each principal component, as well as the cumulative proportion (the amount of variance retained by that principal component and all previous ones).

```
summary(pc)
```

```
Importance of components:
                          PC1    PC2     PC3
Standard deviation     7.2046 3.7433 0.13308
```

```
Proportion of Variance 0.7872 0.2125 0.00027
Cumulative Proportion  0.7872 0.9997 1.00000
```

1.3.1 The score plot

Perhaps the most useful visualization of the PCA is the so-called **score plot**, which is nothing but a scatter plot of the first two principal components. It often happens that the score plot is sufficient to discern patterns in the data, such as clusters.

Figure 1.5 shows a score plot for the bodyfat dataset. While no obvious patterns in this dataset stand out, the plot does show that the principal components are uncorrelated, and this is a good confirmation of what we already know on theoretical grounds. It is customary to put the percentages of variance explained on the axis labels of the score plot, so that the person interpreting it can have an idea of how well the first two principal components describe the data.

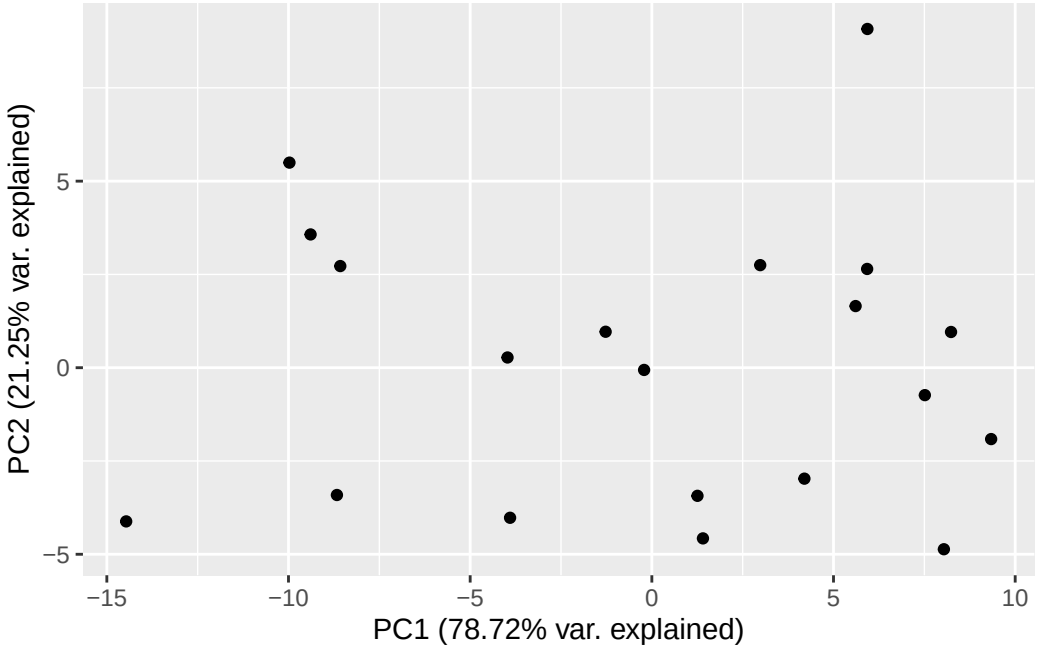


Figure 1.5: Score plot for the body fat dataset.

As an aside, above we noted that the principal components are uncorrelated with one another. We can also verify that this is the case numerically. The result is not exactly zero, but it is very small:

```
cov(pc$x[,1], pc$x[,2])
```

```
[1] -2.604824e-16
```

1.3.2 The loadings plot

A **loadings plot** shows the relations of the original variables and the principal components. This is often a useful visualization to see how each variable contributes to the principal components. Moreover, one can show that the loadings are proportional to the Pearson correlations between the principal components and the variables. Hence, if a loading is positive (negative), that variable will be positively (negatively) correlated with that principal component.[2]

At the beginning of this chapter we hypothesized that the variables `thigh.circumference` and `triceps.skinfold.thickness` would contribute about equally to the first principal component. From Figure 1.6 we see that this is indeed the case: both variables have loadings approximately equal to 0.7, when we consider the first principal component. We also see that the second principal component is mostly made up of the variable `midarm.circumference`.

Unfortunately there is no command in base R or ggplot to create a loadings plot – you have to make one yourself.

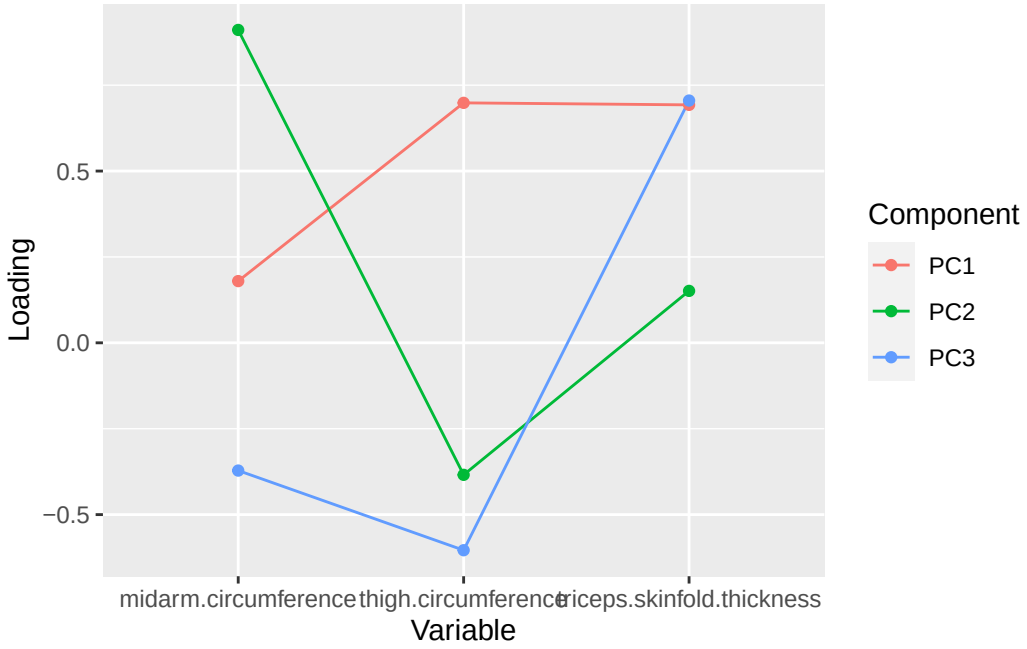


Figure 1.6: The loadings plot shows how the original variables are related to the principal components.

[2]There is a closely related plot type, the profile plot, which differs from the loadings plot in that it has the Pearson correlations on the y-axis. Otherwise the two plot types are identical.

1.3.3 The number of principal components

We now know how to calculate the D principal components for a given D-dimensional dataset, and we've seen that the principal components correspond to the directions in which the dataset varies the most. The real power of PCA, and the reason why it is so ubiquitous in data analysis, is that we can now selectively discard principal components that are not informative. By doing this, we obtain a dataset with fewer features, which is hence easier to analyze, and where the discarded features do not contribute too much to the expressivity of the data. This is what makes PCA into a *dimensionality reduction* method.

The question remains what principal components to discard. There are no universally accepted rules for this, but there are a couple of rules of thumb that can help us make an informed choice. Most of these rules take into account the total amount of variance retained by the first K principal components, defined as

$$S_K = \frac{\sum_{i=1}^{K} \lambda_i}{\sum_{j=1}^{D} \lambda_j},$$

Recall that the total amount of variance can be computed directly within R by using the `summary` command (and look for the "Cumulative Proportion" row):

```
summary(pc)
```

```
Importance of components:
                          PC1    PC2     PC3
Standard deviation     7.2046 3.7433 0.13308
Proportion of Variance 0.7872 0.2125 0.00027
Cumulative Proportion  0.7872 0.9997 1.00000
```

The number K of principal components can be chosen so that a fixed amount of variance (for example, 95%) is retained. To see this idea in action, let's apply it to the body fat dataset. The relative amount of variance explained by each principal component can then be calculated as follows:

```
var_explained <- pc$sdev^2 / sum(pc$sdev^2)
var_explained
```

```
[1] 0.787222422 0.212508963 0.000268615
```

and the total amount of variance explained cumulatively by

```
total_var <- cumsum(var_explained)
total_var
```

```
[1] 0.7872224 0.9997314 1.0000000
```

Note that these numbers agree with the output of the `summary` command. For what follows, it will be easier to have access to these quantities as straightforward R vectors.

We see that the first two principal components explain 78.7% and 21.3% of the total variance, respectively, and together they explain more than 99.97% of variance in the dataset. It therefore seems reasonable to discard the last principal component, which contributes less than 0.03% of variance.

For datasets with many features, a **scree plot** or **elbow plot** can be helpful to identify high-variance principal components. In a scree plot, the amounts of variance are plotted in descending order, so that one can identify at a glance the amount of variability contributed by each principal component. Some scree plots also include the total amount of variability, S_K, as a function of K.

R can make a pretty basic scree plot for you, via the screeplot command.

```
screeplot(pc, main = "Principal components", type = "lines")
```

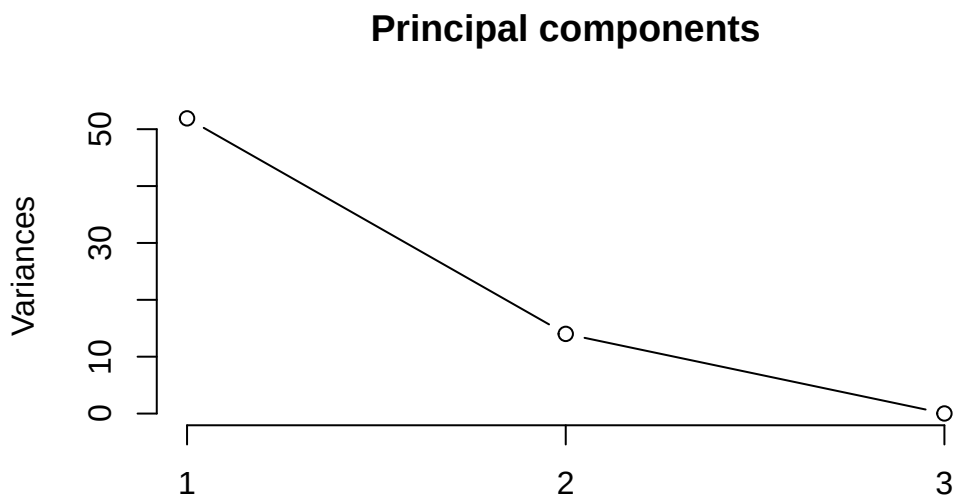


Figure 1.7: A scree plot made with the base R `screeplot` command.

With a bit more work, you can build your own scree plot, which is often preferable if you want to customize the plot, to include for example the cumulative variance, as in figure Figure 1.8.

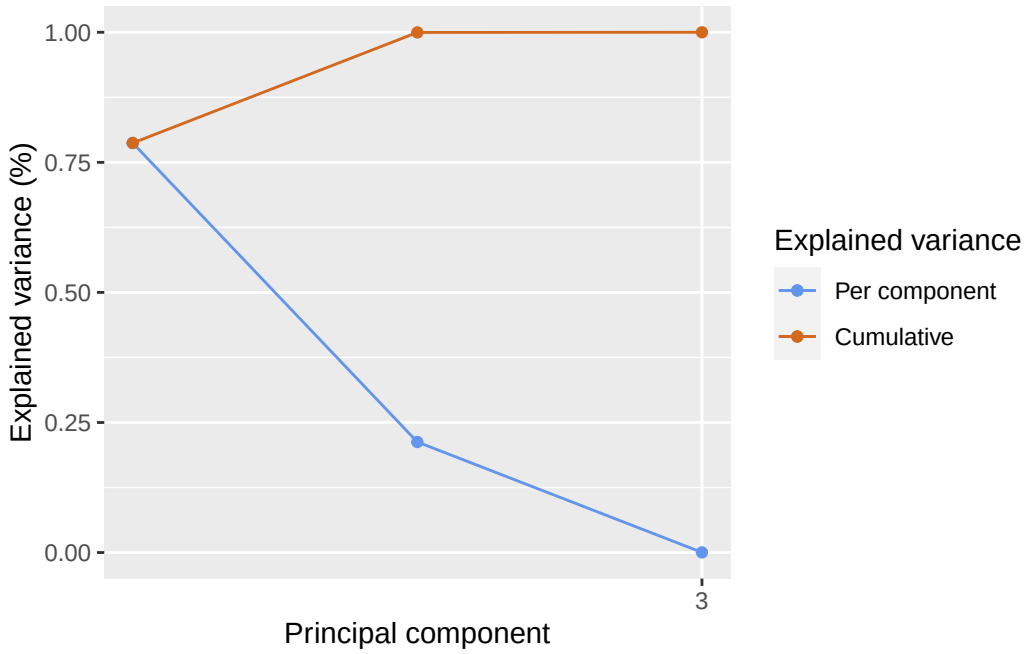


Figure 1.8: A scree plot for the body fat dataset confirms that the first two principal components explain almost all of the variance in the data.

Scree plots are often also referred to as "elbow plots", since the plot typically (but not always) shows an "elbow" where the explained variance levels off. However, spotting the exact location of the elbow is very subjective, and it is typically more appropriate to take the point where the remaining principal components only contribute some small percentage of variation, for example 5%.

1.3.4 Biplots

The **biplot** consists of a loadings plot overlaid on a score plot. By default, it shows the first two principal components as a scatter plot, together with a set of vectors, one for each original variable, showing the contribution of that variable to the first two principal components. Biplots are relatively complex, but it is worth understanding what they encode.

```
biplot(pc)
```

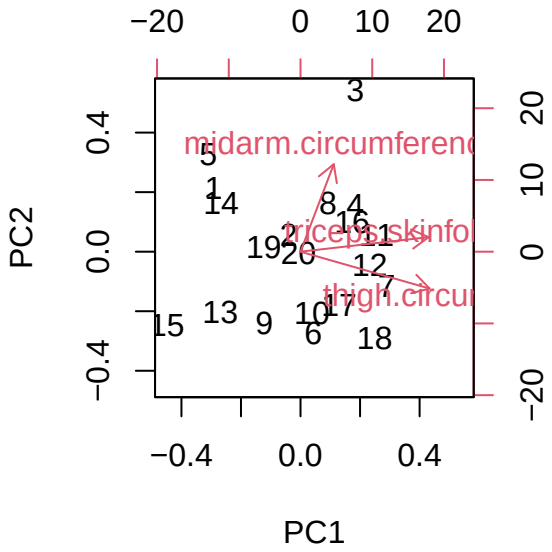


Figure 1.9: The biplot provides information about the transformed data and the loadings.

The numbers on the plot represent the data points from the original dataset, expressed relative to the first two principal components. This is the part of the biplot that is like a score plot. The red arrows, on the other hand, represent the original variables in the dataset (as shown by the labels attached to them) and are expressed on the top and right-most axis, which show how much each variable contributes to the first two principal components. The red arrows carry the same information as a loadings plot (in a different form), when you consider only the first two principal component.

At one glance, we see that `triceps.skinfold` and `thigh.circumference` are the most important contributors to the first principal component, and that the second principal component is almost entirely made up by `midarm.circumference`. This confirms our intuition from the beginning of this chapter, as well as the conclusions that we drew from the loadings plot.

1.4 Applications of principal component analysis

1.4.1 Principal component regression

1.4.2 Partial least squares regression

1.4.3 Eigenfaces

Our last example is not life sciences based, but serves as an illustration to show that PCA is a powerful technique in data analysis, which can be used to reduce the number of degrees of freedom in a large dataset.

We use the Olivetti dataset of human faces, which contains 400 frontal photographs of human faces. Each face is a grayscale image of 64 by 64 pixels, where the intensity of each pixel is a value between 0 (completely black) to 255 (completely white). Each image can be represented as a 64×64 matrix, but it will be more convenient to take the columns of this matrix and lay them out one after the other to obtain a vector with $64 \times 64 = 4096$ entries, as in Figure 1.10.

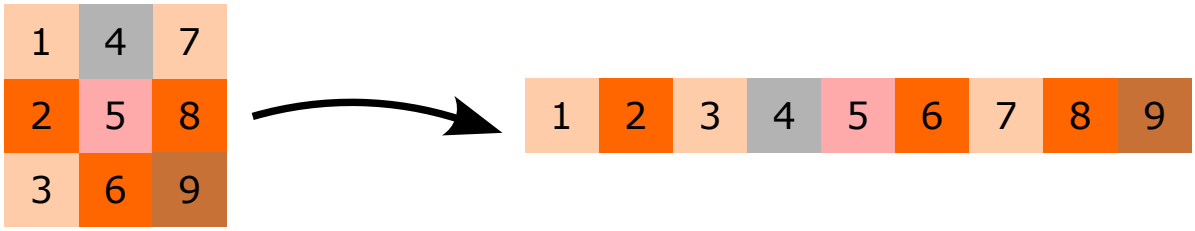


Figure 1.10: An image that is N pixels high and M pixels wide can be viewed as a matrix with N rows and M columns, or as a vector with $N \times M$ elements. Here, N and M are both equal to 3.

First, we load the dataset. Note that the dataset comes as a data matrix with 4096 rows and 400 columns.

```
library(loon.data)
data(faces)
dim(faces)
```

```
[1] 4096  400
```

Each column in the data matrix represents a face, laid out as a column vector with 4096 as in Figure 1.10. We can assemble these vectors back into images and visualize them. This requires some R commands that we haven't covered; you don't have to understand what this code does.

Doing a principal component analysis is a simple matter of running `prcomp`. Despite the size of the dataset, this component should not take more than a second to run.

```
pc_olivetti <- prcomp(faces)
```

Note that there are 400 principal components in this dataset. We can visualize their relative importance via a scree plot, which we limit to the first 50 components for clarity, since the remaining 350 components contribute almost no variance. This indicates that we can probably discard most of the principal components without losing much of the expressivity of our dataset. We will see further down that this is indeed the case!

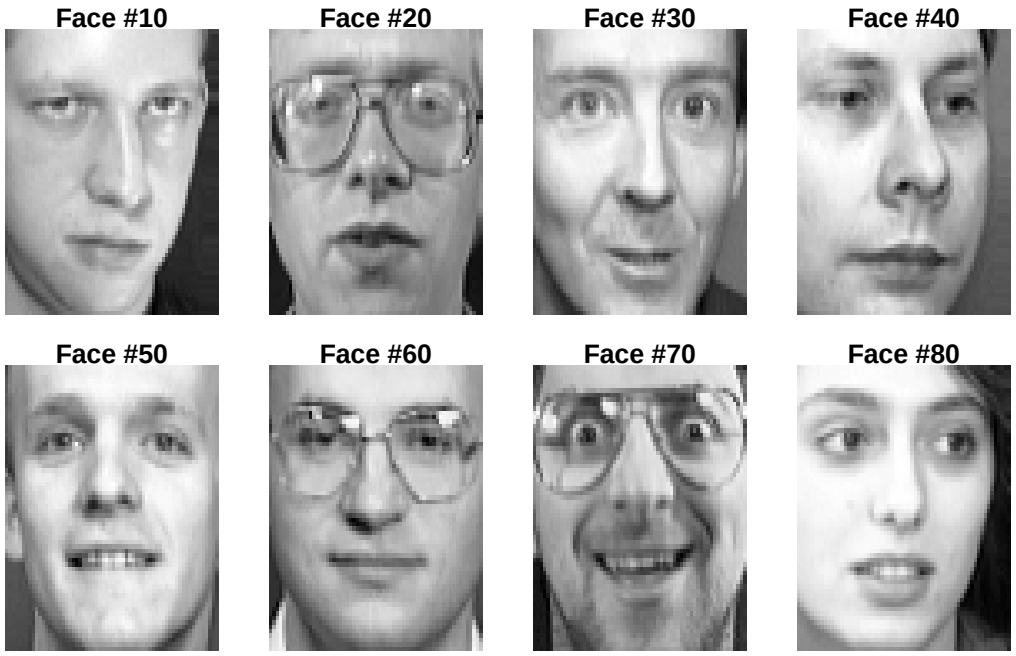
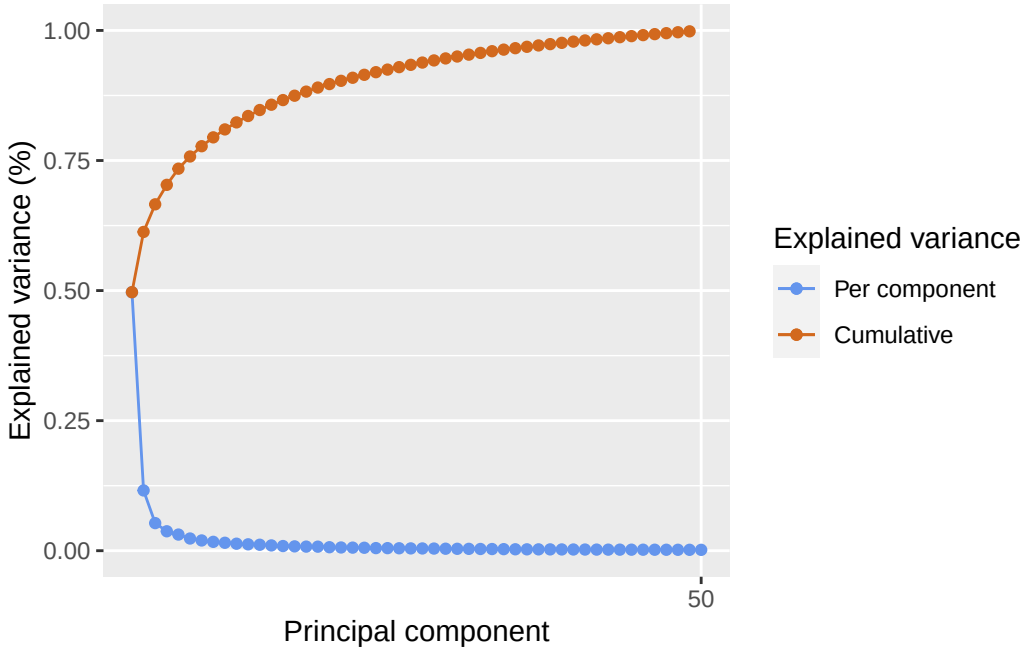


Figure 1.11: Six faces from the Olivetti dataset.



One of the advantages of the faces dataset is that the principal components can be represented graphically, and that we can reason about them. Figure 1.12 shows the first 8 principal components, represented as images. How should we interpret these images? Each principal

component represents a particular *pattern* in the dataset of all faces: the first principal component, for example, captures the overall structure of a human face, while the second represents the illumination from right to left. Probably there were some photos in the dataset that were illuminated from the left or the right. Principal component three does the same for the top-down illumination, and principal components four through eight capture particular patterns involving the eyes or the eyebrows. *By selectively "mixing" all 400 principal components, we can recreate any face in the dataset.*

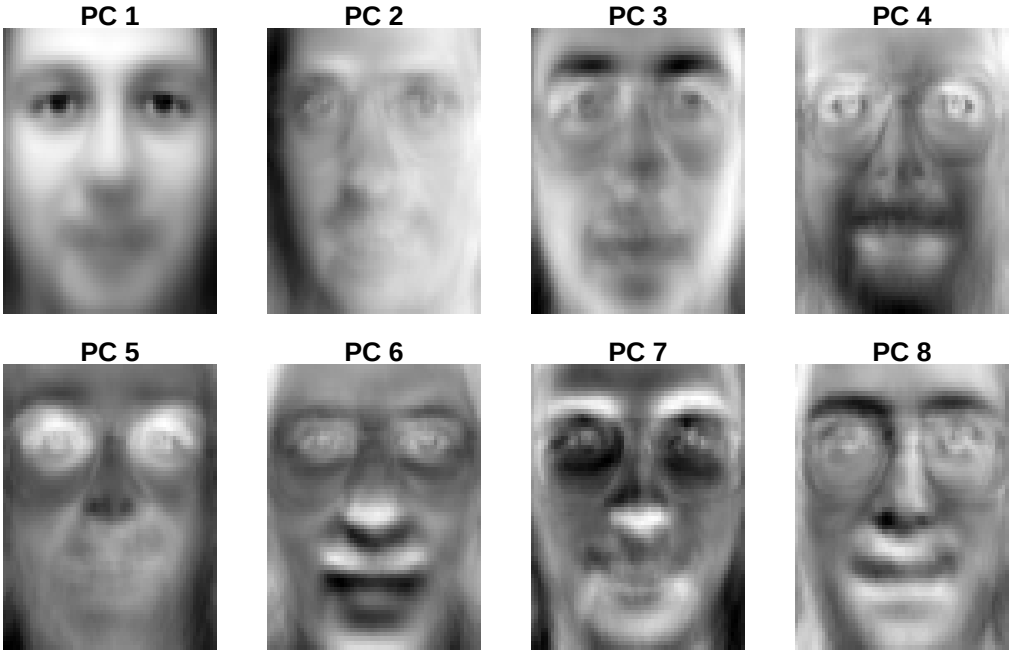


Figure 1.12: The first 8 principal components of the Olivetti dataset represent particularly expressive patterns in the dataset.

To finish, let's also investigate how well PCA performs as a data reduction method. By retaining only a limited number of principal components, we can build "reduced" versions of the images that involve only a number of principal components. Figure 1.13 shows two original faces from the dataset (left), together with compressed versions involving the first 10, 40, and 80 most significant principal components. The version that uses only 10 components is quite generic and it is difficult even to distinguish the male and female face. The version with 80 components, on the other hand, is very close to the original.

It is worth realizing the amount of data compression realized by using PCA. The original images had 4096 degrees of freedom, whereas the rightmost versions in Figure 1.13 are described by 80 loadings, more than a 50-fold reduction in degrees of freedom! Clearly there are some visual artifacts that appear in the compressed versions, but the faces are clearly distinguishable, and it seems very reasonable at this point that a machine learning algorithm (for example, to classify the faces, or to do segmentation) could take these compressed images as input and

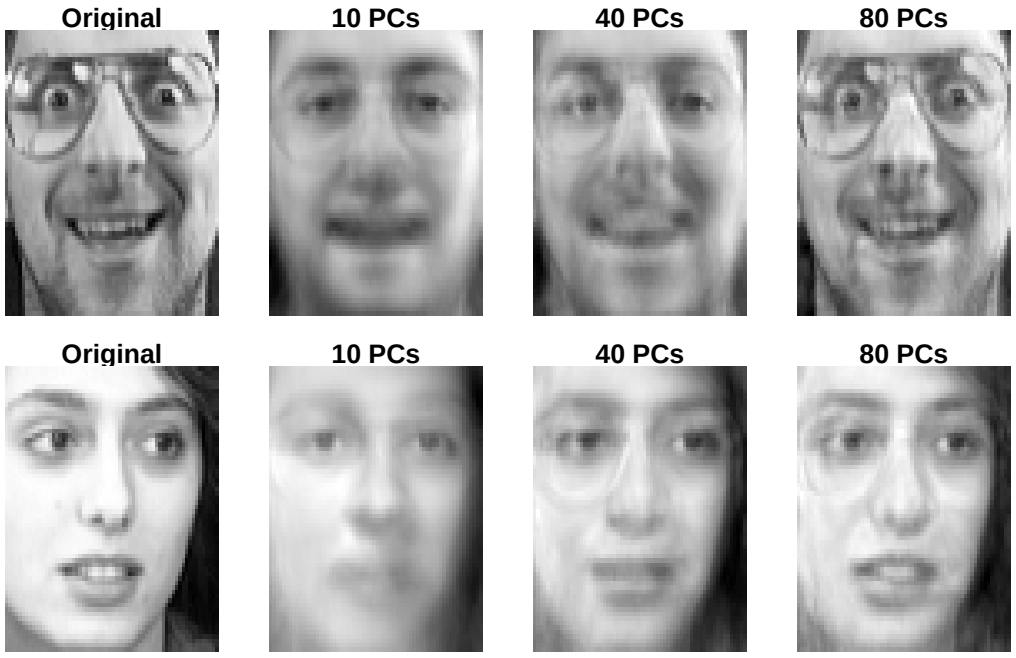


Figure 1.13: Original images (left), and 3 PCA-reduced images with increasing numbers of principal components.

still perform well.

1.5 Other methods for dimensionality reduction

1.5.1 Multidimensional scaling (MDS)

1.5.2 t-SNE and UMAP

References

Bishop, Christopher M. 2006. *Pattern Recognition and Machine Learning.* Vol. 2. Information Science and Statistics. Springer, New York.

A Datasets

A.1 Point clouds with specific mean and covariance

The `rmvnorm` command, part of the mvtnorm package, provides a way to sample points from a multivariate normal distribution with a specific population mean and standard deviation. For example, the code snippet below generates 100 sample points from a distribution with mean μ and covariance matrix Σ given by

$$\mu = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}. \tag{A.1}$$

The `mean` and `sigma` parameters are the *population* mean and covariance, and the *sample* mean and covariance will be slightly different:

```
bar_x <- colMeans(samples)
bar_x
```

```
[1] 0.9661279 0.7986743
```

```
sigma_x <- cov(samples)
sigma_x
```

```
         [,1]     [,2]
[1,] 2.162411 1.201452
[2,] 1.201452 3.173997
```

In some cases, we require a dataset whose sample mean and covariance are *exactly* equal to some given parameters. It turns out that we can achieve this by means of a judiciously chosen linear transformation. Assume that we have n datapoints $x_i \in \mathbb{R}^p$, and let A be an arbitrary $p \times p$ matrix and $b \in \mathbb{R}^p$ a vector. The transformed data points

$$y_i = Ax_i + b, \tag{A.2}$$

have sample mean $\overline{y}$ and covariance matrix Σ_y given

$$\overline{y} = A\overline{x} + b \quad \text{and} \quad \Sigma_y = A\Sigma_x A^T,$$

where $\overline{x}$ and Σ_x are the sample mean and covariance matrix of the x variables.

To make the sample mean equal to a given vector μ, and the sample covariance matrix equal to a given matrix Σ, we have to solve the following equations for A and b:

$$A\overline{x} + b = \mu \quad \text{and} \quad A\Sigma_x A^T = \Sigma.$$

Let's focus on the second equation first, since it only involves the matrix A. Since the covariance matrices Σ and Σ_x are positive definite, it turns out that there exist unique upper-triangular matrices R and R_x such that

$$\Sigma_x = R_x^T R_x \quad \text{and} \quad \Sigma = R^T R.$$

This is the so-called Cholesky decomposition; we don't have to worry about the details here, since R can compute R and R_x for us. Using this decomposition, the equation for A can be written as

$$AR_x^T R_x A^T = (R_x A^T)^T R_x A^T = R^T R,$$

so that it is sufficient to find a matrix A such that $R_x A^T = R$. This we know how to do: we just multiply both sides from the left by $(R_x)^{-1}$ and take the transpose to find

$$A = (R_x^{-1} R)^T.$$

With this expression for A, we can find b by setting

$$b = \mu - (R_x^{-1} R)^T \overline{x}.$$

We can code up these equations in R as in the snippet below. This approach works well for data points in low dimensions. For higher-dimensional data it is recommended (for reasons of numerical efficiency and stability) to avoid computing the inverse R_x^{-1} directly. Instead, we can solve a system of linear equations that yield the transformed points y_i directly. We will not pursue this alternative any further.

```
add_to_rows <- function(X, b) {
  t(apply(X, 1, function(row) row + b))
}

R <- chol(sigma)
R_x <- chol(cov(samples))
A <- t(solve(R_x) %*% R)
b <- mean - A %*% bar_x
```

```
samples_y <- samples %*% t(A)
samples_y <- add_to_rows(samples_y, b)
```

The resulting datapoints have mean and covariance exactly as given by Equation A.1:

```
colMeans(samples_y)
```

```
[1] 1 1
```

```
cov(samples_y)
```

```
     [,1] [,2]
[1,]    2    1
[2,]    1    3
```

Last, we can take a look at the relative location of the original and adjusted data points. We see that our procedure selectively moves points around to make the mean and covariance matrix equal to what we imposed on it.