Business 4720

Introduction to Unsupervised Machine Learning

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Learning Goals

After reading this chapter, you should be able to:

- Explain the aims principal components analysis, the importance of scaling data before the analysis, the concept of a principal component and how to choose an appropriate number of components.
- Carry out a principal component analysis and justify the number of components retained.
- Explain the process of k-means clustering, including the importance of the distance function and of scaling data before clustering.
- Carry out a k-means clustering and evaluate its quality.
- Explain hierarchical clustering, and the distance and linkage functions involved in clustering.
- Choose an appropriate clustering solution from a dendrogram.
- Carry out a hierarchical clustering and evaluate its quality.

Sources and Further Reading

The material in this chapter is based on the following sources. They are freely available. Consult them for additional information.

Gareth James, Daniel Witten, Trevor Hastie and Robert Tibshirani: *An Introduction to Statistical Learning with Applications in R*. 2nd edition, corrected printing, June 2023. (ISLR2)
`https://www.statlearning.com`
Chapter 12

The book by James et al. provides an easy introduction to machine learning at the introductory undergraduate level. It focuses on applications, not mathematics, and contains many exercises using R. Concepts are well explained and illustrated. There is a similar book available by the same authors with applications in Python. This book is a more accessible of the following book.

Trevor Hastie, Robert Tibshirani, and Jerome Friedman: *The Elements of Statistical Learning*. 2nd edition, 12th corrected printing, 2017. (ESL)
`https://hastie.su.domains/ElemStatLearn/`
Chapter 14

The book by Hastie et al. still sets the standard for statistical learning. It is widely used and cited. It's treatment is more technical than the previous book and there are no exercises in R or Python. However, it covers the concepts in more depth (and a few more formulas). However, it is still very accessible even to an undergraduate audience.

Kevin P. Murphy: *Probabilistic Machine Learning – An Introduction*. MIT Press 2022.
https://probml.github.io/pml-book/book1.html
Chapters 20, 21

Murphy's book is available under a creative-commons license. It is a somewhat more technical treatment of the material, but with many illustrations and examples. It is quite comprehensive in its coverage and targeted at the advanced undergraduate or graduate student.

1 Introduction

In unsupervised machine learning, there are no known correct outputs that can be used to train or fit statistical models. In that sense, there are no X and Y variables, but only the X variables. Unsupervised machine learning focuses on identifying patterns in the data, often in order to simplify the data. The two unsupervised methods considered here, principal components analysis (PCA) and cluster analysis or clustering, both do this. For example, PCA "summarizes" multiple variables or "dimensions" into fewer variables, the principal components, while cluster analysis finds similarities in the data and groups or clusters observations into fewer clusters than observations. The principal components and the clusters can be viewed as simpliciations or summaries of the data.

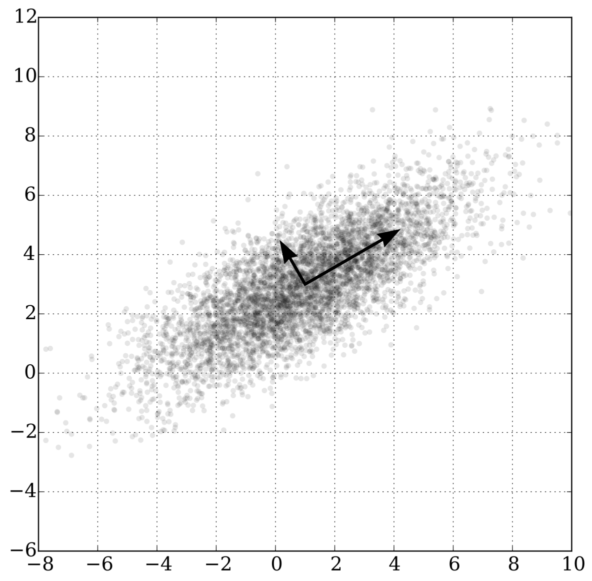
2 Principal Components Analysis

The aim of *principal component analysis* (PCA) is to create linear combinations of the input variables, the principal components (PC), that satisfy two conditions:

1. They are maximally variable, that is, their variance is maximal, and
2. They are orthogonal, that is, independent, of each other.

There are as many principal components as there are input variables. Generally, only a few of the principal components, the ones with the greatest variance, are retained for further analysis. It is not uncommon to reduce hundreds of variables to five or ten principal components for further analysis.

These principal components are considered summaries of the original data and can be used, for example, instead of the original input variables in a regression or classification model. This makes the model smaller and therefore easier to understand, interpret, and verify. Using fewer inputs for a regression or classification can also serve as a



https://commons.wikimedia.org/wiki/File:GaussianScatterPCA.svg

Figure 1: Scatterplot with Principal Components

regularization method, that is, a way to make the model less susceptible to overfitting. This is because models with fewer inputs generally have fewer parameters, all other things being equal. Additionally, the principal components are useful for data visualization. It is much easier to show a 2D or 3D summary of the data when the data has been summarized in two or three principal components, rather than visually depicting dozens or hundreds of variables.

Figure 1 shows an example visualization of a scatterplot of data on two variables and the two principal components. Technically, the two arrows shown are the *eigenvectors* of the covariance matrix of the data, scaled in length by the square root of the corresponding *eigenvalue* and then shifted to the mean of the data, details that will become clear below.

We first introduce an iterative method of computing principal components. Recall that principal components are linear combinations of the original input variables. Hence, the first principal component (PC) for $1 \leq i \leq n$ data values and p variables is defined as:

$$z_{i1} = w_{11}x_{i1} + w_{21}x_{i2} + \cdots + w_{p1}x_{ip}$$

Or, simpler, in matrix form:

$$Z_1 = Xw_1$$

The *weight vector* or *loading vector* $w_1 = (w_{11}, \ldots, w_{p1})$ is a $p \times 1$ column vector that is scaled to unit length, that is, $||w_1||_2 = 1$. X is a $n \times p$ data matrix and Z_1 is the first principal component of size $n \times 1$.

Assuming zero-centered variables, the variance of Z_1 and the optimization criterion can be expressed as follows:

$$\underset{w_{j1}}{\text{maximize}} \sum_{i=1}^{n} z_{i1}^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} w_{j1} x_{ij} \right)^2 \qquad \text{(Variance of } z_{i1}\text{)} \tag{1}$$

Subject to:

$$\sum_{j=1}^{p} w_{j1}^2 = 1 \qquad \text{(Scaling constraint)}$$

Or, simpler, in matrix form:

$$\underset{w_1}{\text{maximize}} \;\; Z_1^T Z_1 = w_1^T X_T X w_1 \quad \text{(Variance of } Z_1\text{)} \tag{2}$$

Subject to:

$$||w_1||_2 = 1 \qquad \text{(Scaling constraint)}$$

To derive the second PC, subtract the first PC from the data:

$$X_{\text{new}} \leftarrow X - Xw_1w_1^T$$

Then, repeat the maximization with the residual data X_{new}, that is the "left over" portion of the data.

This procedure can be repeated until as many principal components k are calculated as there are original data variables p. Because each iteration reduces the remaining data, the residual, by subtracting a component with maximum variance, the variance of the residual data shrinks. Hence, the variance of each successive principal component and therefore the proportion of the initial overall variance accounted for by each successive principal component shrinks. In other words, each successive component explains a decreasing proportion of the total original variance in the data.

There are two important considerations when working with PCA. First, the input data variables should be scaled to have equal or unit standard deviation, so that the measurement scale of different variables does not influence the outcome of the PCA. Second, the signs of the principal components can be ”flipped” arbitrarily. This can be seen in Figure 1, where one can easily imagine the two arrows pointing in opposite direction, and still providing the same good summary of the original data.

Variables in the data set should be scaled to identical standard deviations prior to PCA.

To give an applied example, consider four input variables extracted from a data set of police arrest data in the US for violent crimes in each of the 50 states of the US. While four principal components can be computed, the four input variables can be summarized pretty well by just the first two principal components that together explain more than 80% of the total variance. Figure 2 shows a plot of the data along the first two components which form the horizontal and vertical axis. This is known as a *biplot*. Overlayed are the four original variables. Table 1 shows the *component loadings*, that is the ϕ in the above formulas, for the first two principal components.

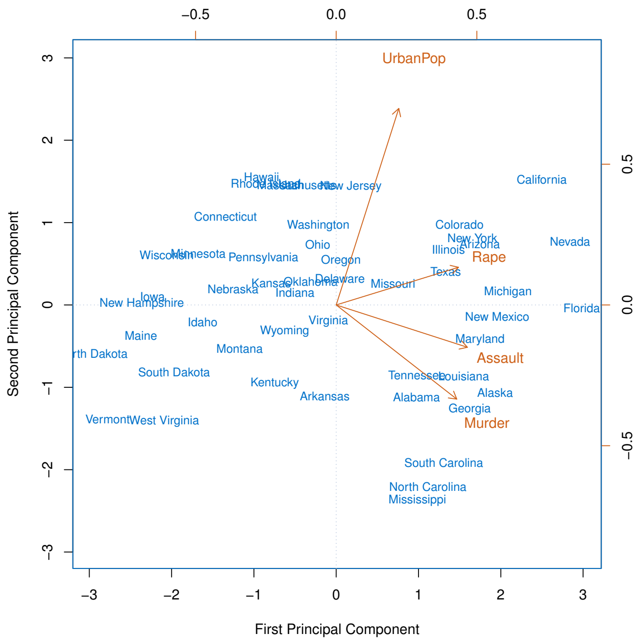
Interpretation of the principal components, which is important in explanation but less so in prediction, focuses on the loadings. For example, looking at the columns of the loadings in Table 1 shows that the first PC has high loadings on the variables ”Murder”, ”Assault”, and ”Rape”, and a much smaller loading on ”UrbanPop”. This suggests that PC1 expresses the overall prevalance of violent crime, as a summary of those three variables. In contrast, the second PC has a high loading on ”UrbanPop”, but a much lower (absolute) loading on the other three variables, indicating that it expresses primarily the one variable ”UrbanPop”. This interpretation is supported by Figure 2, which examines the rows of Table 1, plotting each variable as a two-component vector in the space spanned by PC1 and PC2 (recall that the principal components are by definition orthogonal). Here, the row vector for the variable ”UrbanPop” is visually distinct and separate from the row vectors for the other three variables.

While the iterative description of principal components above illustrates the properties of the components in terms of their variance, actual PCA is done by means of *eigendecomposition*. It turns out that the solution to the maximization problem in Equations 1

	PC1	PC2
Murder	.536	-0.418
Assault	.583	-0.188
UrbanPop	.278	0.873
Rape	.543	0.167

Source: ISLR2 Table 12.1

Table 1: US arrest data example – first two principal component loadings



Source: ISLR2 Figure 12.1

Figure 2: US arrests data example – Biplot with data plotted on first two principal components with original variables

and 2 are the principal components of the data correlation matrix. Each principal component is an *eigenvector* of the data correlation matrix such that:

$$V^{-1}X^TXV = V^{-1}CV = \Lambda$$

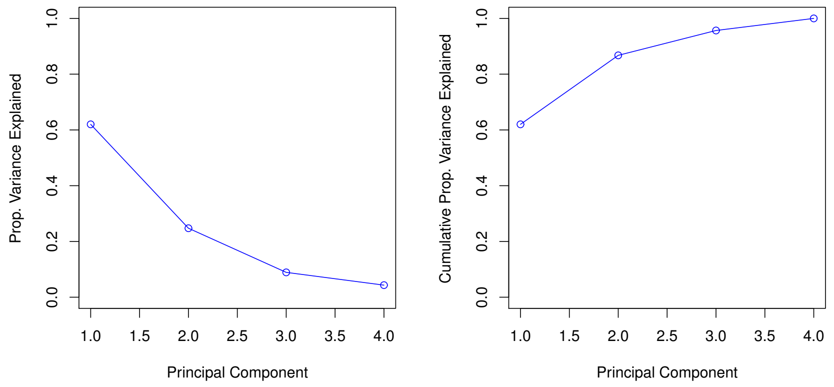
where V is the matrix whose columns are the *eigenvectors*, C is the data correlation matrix, and Λ is a diagonal matrix of *eigenvalues*.

The *proportion of variance explained* f_k by each PC k is proportional to the corresponding *eigenvalue* λ_k, that is, the k-th entry of Λ:

$$f_k = \frac{\lambda_k}{\sum_{j=1}^{p} \lambda_j}$$

The *cumulative proportion of variance* F_k explained by the first k PC is then:

$$F_k = \frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{p} \lambda_j}$$



Source: ISLR2 Figure 12.3

Figure 3: US arrests data example – Scree plot and cumulative variance explained

There are different criteria for selecting the number of principal components to retain for further analyses:

- There may be a theoretical reason, especially in an explanation context, to retain a specific number of principal components
- The analyst retains those principal components that have an intuitive and relevant interpretation, as in the above example.
- The analyst retains those principal components whose eigenvalue $\lambda > 1$
- The analyst retains principal components until the cumulative proportion of variance explained by the components surpasses a given threshold, e.g. 80%. For example, the right panel in Figure 3 shows a plot of the cumulative variance explained. The first two principal components are necessary to explain 80% or more of the total variance in the original data.
- When used in subsequent regression or classification models, cross-validation may be used to identify the optimal K that shows the lowest test error.
- The analyst examines the "*scree plot*", that is, the plot of the eigenvalues or proportion of variance explained by each component. Oftentimes, there will be a clear point of inflection in this plot, indicating a useful cutoff. The left panel in Figure 3 shows such a scree plot. The proportion of variance explained diminishes for each additional principal component.

In practice, the number of principal components to retain is often subjective, and analysts use a combination of considerations and criteria to make their decision.

3 Principal Components Analysis in R

The `USArrests` in the `ISLR2` library contains data on the arrests (per 100,000 residents) for various violent crimes as well as the percentage of urban population in the 50 states of the US[1]. First, examine the data and the correlation between variables. In the correlation matrix, one can already see that ”UrbanPop” is not highly correlated with the other three variables, an indication that it will not load on the same principal component as those.

```
library(ISLR2)
?USArrests
summary(USArrests)
cor(USArrests)
```

The `prcomp()` function in R performs a PCA and can optionally scale and center the data before doing so:

```
# PCA using prcomp()
# Scaling is generally a good idea
pca.result <- prcomp(USArrests, scale=TRUE)

# Print the component loadings
pca.result$rotation
```

The results can be plotted in a biplot, similar to the one in Figure 2, using the `biplot()` function for the `prcomp` result object. By default, that function uses the first two principal components, but others can be specified using the `choices` argument. Note that the signs of the principal components may be arbitrarily flipped.

```
# Biplot for components 1 and 2
biplot(pca.result, choices=1:2, scale=0)
```

The explained variance can be computed from the result and plotted in a scree plot similar to the one in the left panel of Figure 3.

```
# Explained variance for each component
pca.result$sdev^2

# Scree plot (both points and lines)
plot(pca.result$sdev^2, type='b', col='blue')
```

Recall that the proportion of variance explained is the proportion of the variance of a principal component out of the total variance explained by all principal components.

[1]The R code for this example is based on material in Section 12.5 of ISLR2

The R function `cumsum()` can be used to conveniently calculate the cumulative value of this. The following code block computes a cumulative plot similar to the right panel in Figure 3.

```
# Proportion of variance explained
pve <- pca.result$sdev^2 / sum(pca.result$sdev^2)

# Cumulative sum of variance explained
plot(cumsum(pve), type='b', col='blue')
```

Using the `eigen(.)` function for eigenvalue decomposition shows that the principal component loadings correspond to the eigenvectors and the explained variance corresponds to the eigenvalues,

```
# Eigen-decomposition of correlation matrix
e <- eigen(cor(USArrests))
# Compare values and vectors to prcomp results
e$values
e$vectors
```

The component scores themselves are also available in the `prcomp` result for use in further analysis such as regression or classification:

```
# Print the component scores themselves
# For further use in regression, etc.
head(pca.result$x)
```

Hands-On Exercise

The `Boston` dataset in the `ISLR2` library describes house prices in the different suburbs of Boston. Use PCA to reduce the number of dimensions for this dataset:

1. Use the `prcomp` function to perform a PCA on the centered and standardized data. Limit yourself to quantitative inputs.
2. Produce a biplot of the first two components
3. Provide the proportion of variance explained by each component
4. How many components would you retain? Why? How much of the total variance would this explain?
5. Based on the loadings, can you ascribe meaning to the components? What do they represent?

Hands-On Exercise

The `Harmann74.cor` dataset in the `datasets` library contains the results of 24 psychological tests given to 145 school children. Use PCA to reduce the number of dimensions for this dataset:

1. Use the `prcomp` function to perform a PCA on the centered and standardized data. Limit yourself to quantitative inputs.
2. Produce a biplot of the first two components
3. Provide the proportion of variance explained by each component
4. How many components would you retain? Why? How much of the total variance would this explain?
5. Based on the loadings, can you ascribe meaning to the components? What do they represent?

Hands-On Exercise

The `Hitters` dataset in the `ISLR2` library contains the salary of 322 baseball players and season statistics. Use `salary` as the target variable and all other numerical variables as predictors.

1. Use PCA to reduce the number of dimensions for the predictors. Limit yourself to quantitative inputs.
2. Retain the first principal component.
3. Estimate and cross-validate a regression model using the first PC as predictor. What is the training and validation error?
4. Repeat steps (1) to (3), retaining 2, 3, . . . , all components
5. Plot the training and validation error agains the number of components. Describe and discuss your results.

4 Clustering

Whereas PCA tried to simplify a data set ”by column” through the identification of variables that can be summarized by principal components, cluster analysis tries to simply a data set ”by row” through the identification of observations that are similar and can be represented as a group, that is, a *cluster*. The aim is to form homogenous subgroups of observations and to discover ”structure” in the data.

There are a many different types of clustering. This chapter focuses on two simple and easy-to-understand methods. The *k-means clustering algorithm* is an example of centroid-based clustering, a method that assigns observations to clusters based on their distance from the cluster center (”centroid”), while *agglomerative clustering* is a form of hierarchical clustering which iteratively merges observations together to form larger and larger clusters.

4.1 K-Means Clustering

In k-means clustering, the number of clusters K is assumed given, determined by the analysts knowledge of the data or the requirements of the analysis. The aim of k-means clustering is to minimize the *within-cluster variation* $W(C_i)$ in each cluster C_i:

$$\min_{C_i} \left\{ \sum_{k=1}^{K} W(C_k) \right\}$$

This within-cluster variation is defined as the squared Euclidean distance between every pair of observations in the cluster (Equation 3) or between every observation and the cluster *centroid* of the cluster it is assigned to, that is, its corresponding cluster mean $\bar{\mu}$ (Equation 4).

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \tag{3}$$

$$= 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{\mu}_{kj})^2 \tag{4}$$

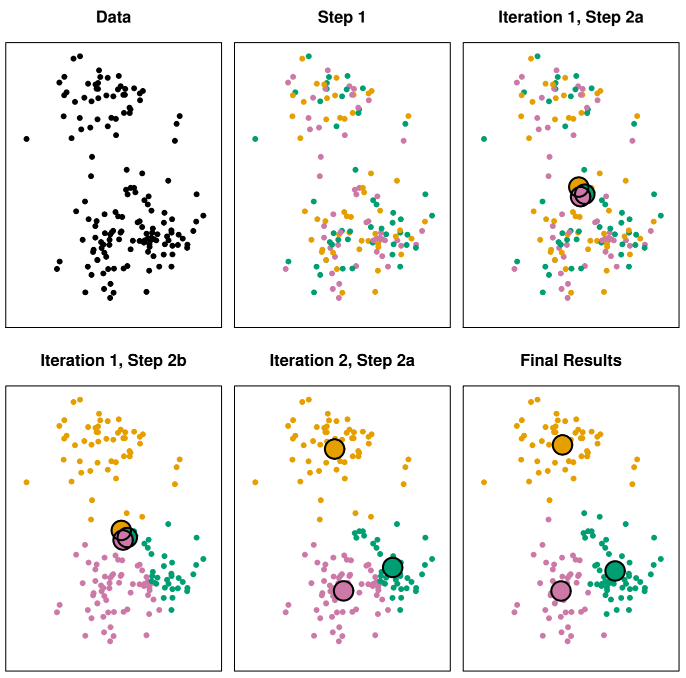
Here, i, i' range over observations within cluster C_k, j ranges over the p different variables that make up an observation, and $\bar{\mu}_k j$ is the mean of variable j for cluster k.

This definition of distance means that k-means cluster analysis is only applicable to quantitative variables.

When variables are measured on different scales, e.g. one variables in the range of $[0, 1]$ while another is measured between $[0, 1000000]$ it is important to *standardize or scale the variables to have similar standard deviations* (typically, unit standard deviation, i.e. 1). Otherwise, the Euclidean distance between observations is dominated by the variable with the largest range.

Variables in the data set should be scaled to identical standard deviations prior to k-means clustering.

K-means clustering uses an iterative algorithm, beginning with the random assignment of each observation i to one of the k clusters. From these cluster assignments, the cluster means (centroids) can be computed ($\bar{\mu}_{kj}$ in Equation 4). Next, each observation is assigned to that cluster whose centroid is closest. The last two steps are repeated until the cluster assignments no longer change.

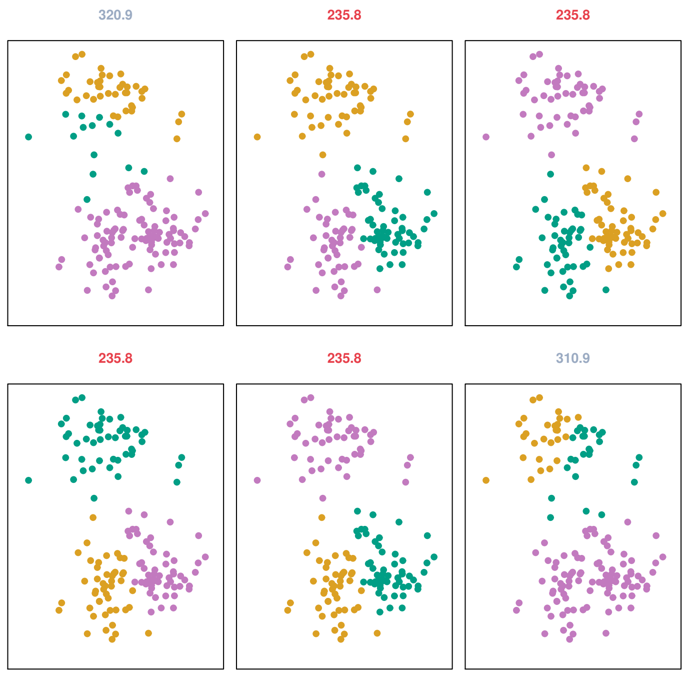


Source: ISLR2 Figure 12.8

Figure 4: K-means iterative cluster assignment example

This process is illustrated in Figure 4. The top left panel shows observations on two variables. The panel labeled ”Step 1” shows the initial random assignment of each observation to one of three clusters, indicated by the color. The top right panel, labelled ”Iteration 1, Step 2a” shows the cluster means or centroids computed based on this assignment as large coloured circles. As one might imagine, random assignment leads to cluster means that are very similar. The bottom left panel, ”Iteration 1, Step 2b” shows the cluster assignment of the observations based on the new cluster means. Each observation is assigned to that cluster whose mean is closest. The bottom middle panel, ”Iteration 2, Step 2a” shows the new cluster means based on the new cluster assignment of observations. The bottom right panel shows the final, stable cluster assignment. Repeated calculation of cluster means and assigning observations to clusters does not change cluster membership for any observation. Note that the cluster membership in this final panel is slightly different than the one in the bottom middle panel, indicating at least one more iteration between the two panels.

It should be clear from this description that the random initial cluster assignment has a significant impact on the final result. As the number of observations grow, the random effects generally diminish, but different random initial cluster assignments may yield different final clustering solutions.



Source: ISLR2 Figure 12.9

Figure 5: K-means clustering solutions from different initial cluster assignments

The k-means algorithm should be run multiple times and the optimal solution, that is, the one with the lowest within-cluster variability, should be chosen for further analysis.

This effect is shown in Figure 5. The data from the previous example was clustered six different times with different random initial cluster assignments. Each final solution is different, and may also have a different *within-cluster variability* as shown at the top of each panel. Note that some solutions are identical but permute the cluster assignments/colours. For example, the top middle and top right panels in Figure 5 are identical and also identical with the bottom left and bottom middle solution, except for the permutation of cluster assignments, indicated by the colours.

4.2 K-Means Clustering in R

To illustrate k-means clustering in R, consider the following simulated example, which uses the `kmeans()` function[2]. Data is simulated as 50 observations on two normally distributed variables. One half of the data is shifted by $+3$ on the first variables and

[2]The R code for this example is based on material in Section 12.5 of ISLR2

by -4 on the second variable. With a standard deviation of 1, this constitutes a large separation and should lead to clearly identifiable clusters.

```r
# Set RNG seed for replicability
set.seed(2)
# Create a 50 x 2 matrix of random variables
# Normally distributed, with 0 mean and SD=1
x <- matrix(rnorm(n=50*2, mean=0, sd=1), ncol=2)
# Clearly separate the first 25 points by shifting their coordinates
x[1:25, 1] <- x[1:25, 1] + 3
x[1:25, 2] <- x[1:25, 2] - 4
```

Next, the data is clustered using the `kmeans()` function into 2 clusters, 20 times with different random initial cluster assignments:

```r
# Cluster into 2 clusters, performing 20 random starting assignments
km.result <- kmeans(x, 2, nstart=20)
```

The result object `km.result` contains the cluster means, the cluster assignments for each observation and the sum-of-squares (distances) within each cluster and between clusters. Recall that the optimization objective is to minimize the within-cluster variation.

```r
# Results show cluster means, cluster assignments,
# and sums of squares (distances) within and between
print(km.result)
# Those values are also available as components in the result object
names(km.result)
print(km.result$centers)
print(km.result$withinss)
# etc.
```

Finally, it is easy to create colour-coded plot of the data (the following R code block adds 1 to every cluster number to avoid plotting black points). This generates a plot as shown in Figure 6, clearly indicating the well-separated clusters.

```r
# Plot the color-coded points
plot(x, col=(km.result$cluster+1),
     main = 'K-Means Clustering Results with K=2',
     xlab = '', ylab='', pch=20, cex=2)
```

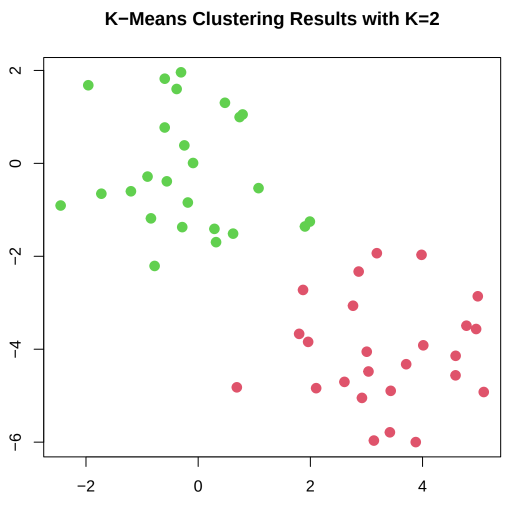


Figure 6: Result of k-means clustering on simulated data

Hands-On Exercise

The `Boston` dataset in the `ISLR2` library describes house prices in the different suburbs of Boston. Use K-Means Clustering to identify sets of similar suburbs using only the numerical variables in the data set.

1. Use the `kmeans` function to perform a cluster analysis, using multiple starting assignments. Limit yourself to quantitative inputs but do not scale the variables.
2. Use different numbers of clusters k and identify which value of k gives you the best results. Define what you mean by ”best” and justify your choice.
3. Scale the data so that each variable has the same variance or standard deviation, but do not change the variable means.
4. Repeat the cluster analysis with the best value of k and compare results.

Hands-On Exercise

The `Hitters` dataset in the `ISLR2` library contains the salary of 322 baseball players and season statistics. Use K-Means Clustering to identify sets of similar players, using only the numerical variables in the data set.

1. Use the `kmeans` function to perform a cluster analysis, using multiple starting assignments. Limit yourself to quantitative inputs but do not scale the variable.
2. Use different numbers of clusters k and identify which value of k gives you the best results. Define what you mean by ”best” and justify your choice.
3. Scale the data so that each variable has the same variance or standard deviation, but do not change the variable means.
4. Repeat the cluster analysis with the best value of k and compare results.

4.3 Hierarchical Clustering

Hierarchical clustering is either *agglomerative*, that is, it constructs clusters ”bottom-up” by joining observations or small clusters to larger clusters, or it may be *divisive*, that is, in ”top-down” fashion, starting from the whole set of observations, it iteratively divides the set into clusters. This section examines the use of agglomerative clustering, which is widely used because of its intuitive process and its flexibility.

Agglomerative clustering begins with n observations and a distance (or, alternatively, a similarity metric, which is just the inverse of distance – a large distance means a small similarity). The process is then as follows:

1. Treat each observation as its own cluster
2. Repeat the following steps $n - 2$ times:
   (a) Calculate distances between all pairs of clusters
   (b) Identify the pair of clusters that are least distant from each other
   (c) ”Fuse” or merge these two clusters

The process is usually visualized with a *dendrogram*, which literally means ”tree graph”, such as the one shown in the left panel of in Figure 7. A dendrogram is read bottom-up, showing which clusters are merged in which order. The vertical axis shows the distance between clusters as they are merged. Consider the observations on two variables shown in the right panel of Figure 7. In the example, clusters 5 and 7 are merged first, from a distance of ≈ 0.3. This distance is the smallest distance between all clusters, indicated as the lowest merging point in the dendrogram in the left panel of Figure 7. Cluster 5 is just observation 5, and cluster 7 is just observation 7. The two together form a new cluster. Next, clusters 1 and 6 are merged, from a distance of ≈ 0.4, the second lowest merging point in the dendrogram. Then, cluster 8 (which is observation 8) is added to the cluster consisting of observations 5 and 7, at a distance of ≈ 0.8. After this,

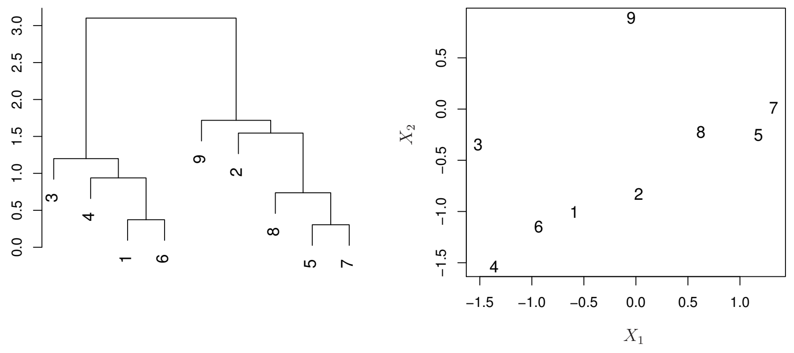

Source: ISLR2 Figure 12.12

Figure 7: Example dendrogram and data for agglomerative clustering

observation 4 is added to the cluster consisting of observations 1 and 6, etc. The final two clusters are at a distance of ≈ 3 when they are merged into a single cluster.

The follwing key decisions need to be made by the analyst for agglomerative clustering:

- How to measure similarity or distance between observations?
- How to measure distance between clusters (”*linkage*”)?
- How many clusters should there be?

Table 2 shows a set of common distance metrics or vector norms that are frequently used in agglomerative clustering. Figure 8 is a visualization of the intuition behind some of these distance metrics. For example, the Chebyshev distance allows diagonal ”moves” to count as a single step with a distance of 1, wheres the taxicab metric counts a ”move” in each direction as a single step, so that diagonal ”moves” have a distance of 2. In principle, any of these distance metrics could also be used in k-means clustering, but this is rarely done.

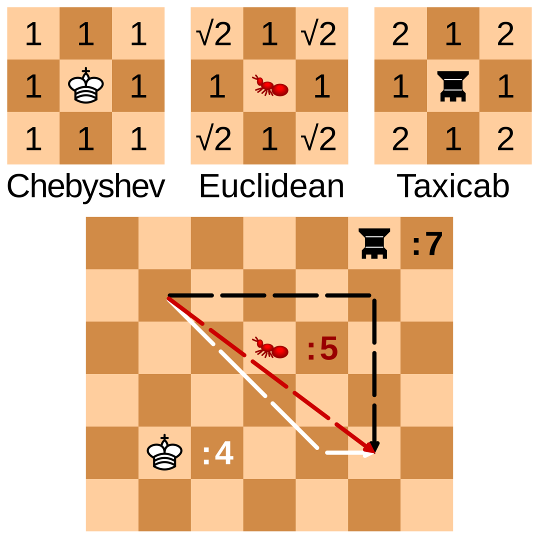
Because the distance function is heavily influenced by the measurement scale of the variables, when these are not equal, it is possible for one variable to dominate others, simply because it is measured on a different scale. As with PCA and k-means clustering, it is therefore important to scale the variables in the data set to identical standard deviation (typically, unit standard deviation, i.e. 1).

Variables in the data set should be scaled to identical standard deviations prior to hierarchical clustering.

Table 3 shows a set of the most commonly used *linkage functions*, that is, functions that express the distance between two clusters G and H. The *single linkage* is based on the minimum distance of any pair of observations where one observation is in cluster G and the other in cluster H. In other words, the distance of two clusters is the distance

Taxicab or Manhattan	$\|\|q-p\|\|_1$	$\sum_i \|q_i - p_i\|$
Euclidean	$\|\|q-p\|\|_2$	$\sqrt{\sum_i (q_i - p_i)^2}$
Minkowski	$\|\|q-p\|\|_p$	$\left(\sum_i \|q_i - p_i\|^p\right)^{\frac{1}{p}}$
Chebyshev	$\|\|q-p\|\|_\infty$	$\lim_{p\to\infty}\left(\sum_i \|q_i - p_i\|^p\right)^{\frac{1}{p}} = \max_i(\|q_i - p_i\|)$
	$\|\|q-p\|\|_{-\infty}$	$\lim_{p\to-\infty}\left(\sum_i \|q_i - p_i\|^p\right)^{\frac{1}{p}} = \min_i(\|q_i - p_i\|)$

Table 2: Common distance metrics or ”norms” in clustering



https://commons.wikimedia.org/wiki/File:Minkowski_distance_examples.svg

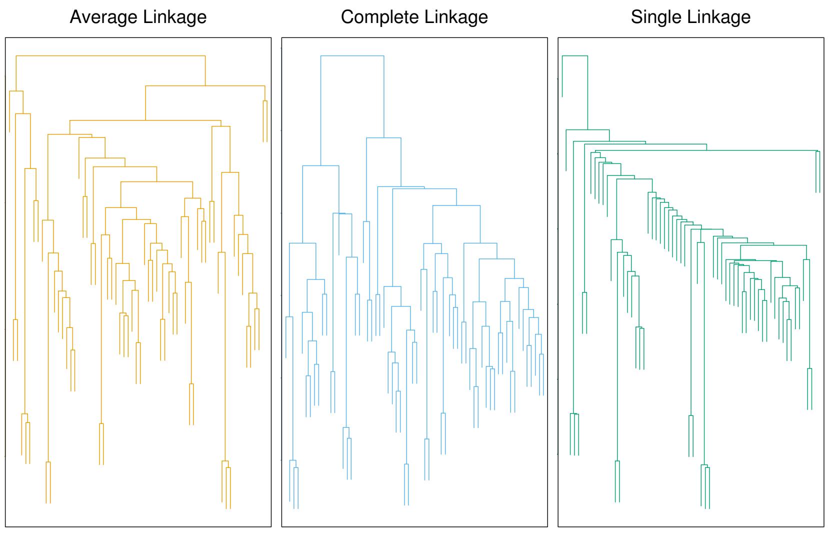
Figure 8: Different distance metrics and their intuition

between the two closest observations from each cluster. In contrast, *complete linkage* uses the maximum; the distance between clusters is the maximal distance between any of their member observations. Finally, *average linkage* uses the mean distance between all pairs of observations. There are many other, less commonly used linkage functions available[3].

[3]https://en.wikipedia.org/wiki/Hierarchical_clustering

Single	$d_{SL}(G,H) = \min\limits_{i \in G, i' \in H} d_{i,i'}$
Complete	$d_{CL}(G,H) = \max\limits_{i \in G, i' \in H} d_{i,i'}$
Average	$d_{AL}(G,H) = \operatorname*{mean}\limits_{i \in G, i' \in H} d_{i,i'}$

Table 3: Commonly used linkage functions in hierarchical clustering

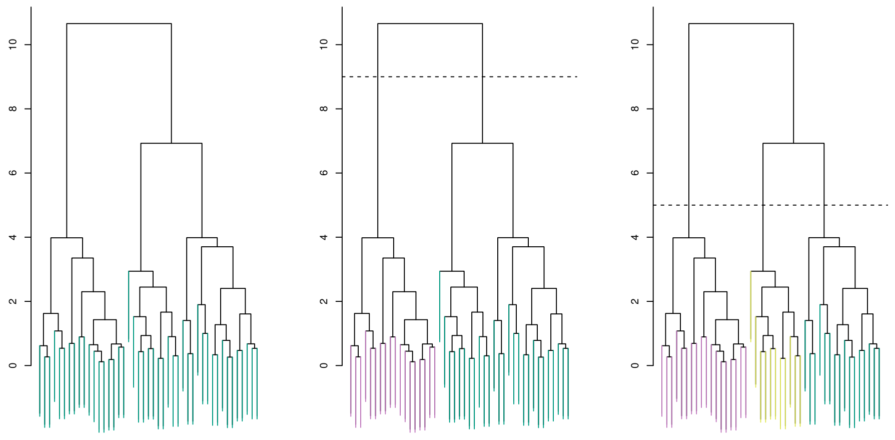


Source: ISLR2 Figure 12.14

Figure 9: The effect of different linkage functions in agglomerative clustering

The linkage function has a significant effect on the process of clustering a set of observations. Consider the three examples shown in the different panels of Figure 9. Merging two observations into a cluster is always done at the same distance, as this is determined purely by the distance metric, not the linkage function. However, the decision which clusters (of multiple observations) to combine is heavily influenced by the linkage function as can be seen in the very different dendrograms in Figure 9.

The final question concerns the choice of the number of clusters. The answer to this question may be driven by theory (typically in explanatory applications), by requirements of the subsequent data analysis or the subsequent use of the resulting clusters, or by examining the distances at which clusters are merged, that is, the height in the dendrogram. Choosing a number of clusters is called ”cutting the dendrogram” at a specific point. Consider the example in Figure 10. The left panel shows the solution of the agglomerative clustering. In the end, a single cluster containing all the observations remains, with the last two clusters merged at a distance of ≈ 10.5. The middle and right panel show two different ”cuts” of the dendrogram, one resulting in two clusters and the other resulting in three clusters. The cuts may be determined by a desired



Source: ISLR2 Figure 12.11

Figure 10: Cutting a dendrogram to determine the number of clusters

number of clusters, by considerations of distance, or both. It should be clear that lowering the ”cut” height further beyond what is shown in the right panel, that is reducing the distance between clusters, would result in many small clusters with a much smaller distance between them.

4.4 Hierarchical Clustering in R

This example uses the same simulated data as the example for k-means clustering[4]. First, generate 50 observations on two variables from a normal distribution. One half of the observations are shifted on both variables to provide a known cluster structure.

```
# Set RNG seed for replicability
set.seed(2)
# Create a 50 x 2 matrix of random variables
# Normally distributed, with 0 mean and SD=1
x <- matrix(rnorm(n=50*2, mean=0, sd=1), ncol=2)
# Clearly separate the first 25 points by shifting their coordinates
x[1:25, 1] <- x[1:25, 1] + 3
x[1:25, 2] <- x[1:25, 2] - 4
```

The `dist()` function is used to calculate differences between the observations. The names for the `method` argument to `dist()` are the same as in Table 2. Additionally, the `'maximum'` distance in R uses the greatest distance among all the variables of the two observations.

[4]The R code for this example is based on material in Section 12.5 of ISLR2

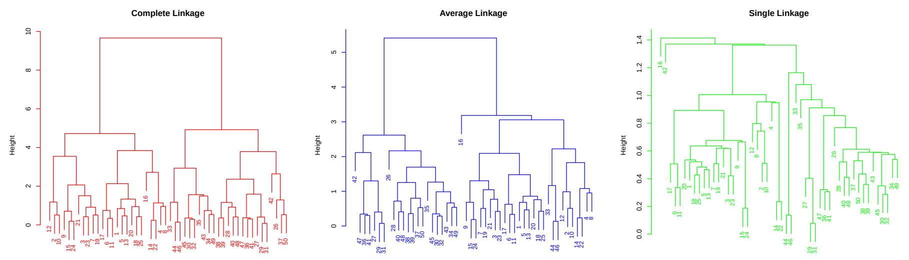


Figure 11: Dendrogram of three clustering solutions for simulated data

```
# The dist() function calculated distances
# according to a variety of metrics/norms
euclid.dist <- dist(x, method='euclidean')
pnorm.dist <- dist(x, method='minkowski', p=3)
manh.dist <- dist(x, method='manhattan')
max.dist <- dist(x, method='maximum')
```

The `hclust()` function performs the hierarchical agglomerative clustering. The `method` argument specifies the type of linkage, according to Table 3. The `hclust()` function can use a few additional linkages not listed in that table, see the documentation (`?hclust`) for details.

```
# Use the hclust() function with a distance metric
hc.complete <- hclust(euclid.dist, method='complete')
hc.single <- hclust(euclid.dist, method='single')
hc.average <- hclust(euclid.dist, method='average')
```

The dendrograms for the three different clustering solutions can be plotted to produce Figure 11.

```
# Plot the dendrograms in a single plot
par(mfrow = c(1, 3))
plot(hc.complete , col='red',
   main = "Complete Linkage", xlab = "", sub = "", cex = .9)
plot(hc.average , col='blue',
   main = "Average Linkage", xlab = "", sub = "", cex = .9)
plot(hc.single , col='green',
   main = "Single Linkage", xlab = "", sub = "", cex = .9)
```

The complete linkage and average linkage solutions are visually quite similar, but upon careful examination of which observations and clusters are merged in which order, they are actually very different from each other. The single linkage solution is visually very different from the others. Note the ”height” of the dendrogram on the vertical axis. Because the single linkage focuses on the minimal distance between a pair of observations from each cluster, the heights in this dendrogram are the smallest among the three dendrograms. Because the average linkage focuses on the mean of distances of pairs of observations of two clusters, its height values are generally larger, but still smaller than the range of heights for the complete linkage solution, which focuses on the maximum distance between pairs of observations from two clusters.

Finally, cutting the dendrogram is done with the `cutree()` function by specifying either the number of clusters k or the height h at which the dendrogram is to be cut. The function returns a vector with the cluster membership for each observation.

```
# Cut by number of groups/clusters
cutree(hc.complete, k=4)
# Cut by height (distance)
cutree(hc.complete, h=6)
```

Hands-On Exercise

The `Boston` dataset in the `ISLR2` library describes house prices in the different suburbs of Boston. Use Hierarchical Clustering to identify sets of similar suburbs using only the numerical variables in the data set.

1. Use the `hclust` function to perform a cluster analysis, exploring different distance metrics and linkage functions. Limit yourself to quantitative inputs.
2. Examine the dendrograms and identify which combination of distance metric and linkage function gives you the ”best” solution. Define ”best” and justify your decision.
3. How many clusters k would you choose?
4. Using this value for k, perform a k-means Clustering and compare the results. Remember that k-means clustering uses the Euclidean distance.

Hands-On Exercise

The `Hitters` dataset in the `ISLR2` library contains the salary of 322 baseball players and season statistics. Use Hierarchical Clustering to identify sets of similar players, using only the numerical variables in the data set.

1. Use the `hclust` function to perform a cluster analysis, exploring different distance metrics and linkage functions. Limit yourself to quantitative inputs and make sure you scale the data.
2. Examine the dendrograms and identify which combination of distance metric and linkage function gives you the ”best” solution. Define ”best” and justify your decision.
3. How many clusters k would you choose?
4. Using this value for k, perform a k-means clustering and compare the results. Remember that k-means clustering uses the Euclidean distance.

Hands-On Exercise

The `Auto` dataset in the `ISLR2` library contains information on 392 vehicles. Use Hierarchical Clustering to identify sets of similar vehicles, using only the numerical variables in the data set.

1. Use the `hclust` function to perform a cluster analysis, exploring different distance metrics and linkage functions. Limit yourself to quantitative inputs.
2. Examine the dendrograms and identify which combination of distance metric and linkage function gives you the ”best” solution. Define ”best” and justify your decision.
3. How many clusters k would you choose?
4. Using this value for k, perform a k-means Clustering and compare the results. Remember that k-means clustering uses the Euclidean distance.

5 Review Questions

Principal Components Analysis

1. Explain how unsupervised machine learning differs from supervised machine learning in terms of data requirements and outcomes.
2. What are the main goals of Principal Component Analysis (PCA) in data analysis?
3. Explain the concept of "variance" in the context of PCA. Why is maximizing variance an important objective?
4. How can PCA be used to simplify a complex dataset? Give an example based on a hypothetical dataset.
5. How can PCA contribute to improving the interpretability of complex models?

6. Describe the process of calculating the first principal component in PCA. What role do the loading vectors play? What optimization problem does PCA solve?
7. How does one interpret the loadings of a principal component and what do they signify about the variables involved?
8. Discuss the importance of scaling input variables before performing PCA. What could potentially happen if the variables are not scaled?
9. Describe the relationship between eigenvalues and the variance explained by the principal components. How does one interpret these eigenvalues in practical terms?
10. Provide several criteria that could be used to decide how many principal components to retain in an analysis.
11. Discuss the relevance of the ”scree plot” in determining the number of principal components to retain. What does an inflection point in the scree plot typically indicate?
12. Explain how the biplot can be used to visualize both the principal components and the original variables. What insights can one gain from such a visualization?
13. Explain how PCA can be used as a feature extraction technique in machine learning models.

K-Means Clustering

14. Define clustering in the context of unsupervised machine learning and explain its main purpose.
15. Compare and contrast the goals of principal component analysis (PCA) and clustering.
16. What are centroid-based clustering and hierarchical clustering? Provide examples of each.
17. Describe the k-means clustering algorithm. What objective does it aim to achieve?
18. Explain the concept of within-cluster variation in the context of k-means clustering.
19. What are the implications of variable scales on the performance of the k-means clustering algorithm? Why might scaling be necessary?
20. Illustrate the iterative process of the k-means clustering algorithm. What happens in each step?
21. Explain why the initial random assignment of observations to clusters can affect the final clustering solution in k-means.
22. Discuss the importance of running the k-means algorithm multiple times. How does this practice influence the reliability of the clustering results?
23. What are the computational complexities of k-means and hierarchical clustering? How do these affect their scalability to large datasets?
24. Discuss the limitations of k-means clustering and possible scenarios where it might not perform well.

Hierarchical Clustering

25. Describe a scenario in which hierarchical clustering would be more beneficial

than k-means clustering. Consider aspects such as data structure and analysis goals.

26. Describe hierarchical clustering and differentiate between agglomerative and divisive clustering.
27. Explain the initial steps in an agglomerative clustering process. How does it begin, and what happens in the initial stages?
28. Define a dendrogram and explain how it is used in hierarchical clustering.
29. Discuss the significance of distance measures in hierarchical clustering. How do they affect the clustering process?
30. How might the concept of distance be adapted when clustering categorical data using hierarchical methods?
31. What are the different types of linkage methods in hierarchical clustering? Describe at least three and explain how they influence the clustering results.
32. Provide an overview of common distance metrics used in agglomerative clustering. How might the choice of distance metric influence the outcome of clustering?
33. Explain the process of creating a dendrogram and interpreting its structure in the context of hierarchical clustering.
34. Explore the relationship between the number of observations and the interpretability of the dendrogram in hierarchical clustering. How does increasing the number of observations affect the clarity and usefulness of the dendrogram?
35. Explain the concept of ”cutting the tree” in hierarchical clustering. How does this process determine the number of clusters?
36. Discuss how the choice of linkage method might impact the sensitivity of hierarchical clustering to outliers and noise in the dataset.
37. How does the analyst decide on the number of clusters in hierarchical clustering? What factors might influence this decision?
38. Consider the distance metrics shown in Table 2. Which metric would be most appropriate for clustering data with extreme outliers and why?
39. Explain why it might be necessary to standardize variables before performing hierarchical clustering.
40. Evaluate the computational complexity of hierarchical clustering. How does this complexity influence the scalability of the method to large datasets?