Business 4720 - Class 13

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This Class

What You Will Learn:

- Unsupervised Machine Learning
  - Dimension Reduction using Principal Components Analysis
  - Clustering

Based On

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

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

Kevin P. Murphy: *Probabilistic Machine Learning – An Introduction*. MIT Press 2022.

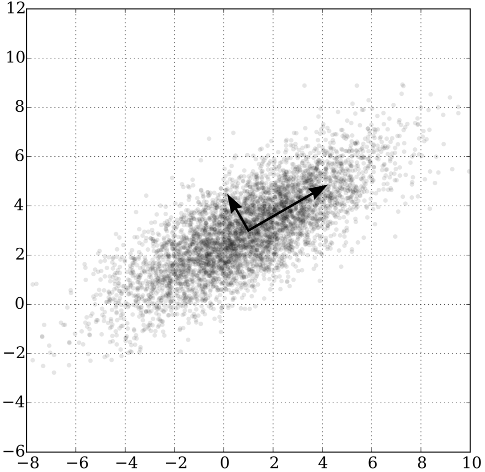
`https://probml.github.io/pml-book/book1.html`

Chapters 20, 21

Principal Components Analysis (PCA)

- Create linear combinations of predictors that are:
  - Maximally variable
  - Independent of each other
- Generally fewer components than predictors
- Can be used instead of original predictors in regression or classification models
- Useful when the problem dimensionality is too high (too many parameters)
  - Can be interpreted as a regularization method
- Useful for visualization to show 2D or 3D summaries of high-dimensional data

PCA [cont'd]



Scatterplot with **Principal Components**

(Eigenvectors of covariance matrix, scaled by the square root of the corresponding eigenvalue and shifted to mean)

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

PCA [cont'd]

- First principal component (PC) for $1 \leq i \leq n$ data values and p variables:

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

- **Loading vector** $\phi = (\phi_{11}, \ldots, \phi_{p1})$ scaled so that $||\phi||_2 = 1$
- Assume zero-centered variables
- Maximize:

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

- Subject to:

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

PCA [cont'd]

- For further components k, subtract the first $k - 1$ components from the data X (residualization), then repeat the maximization
- At most as many components as data variables p
- Each successive component explains a decreasing proportion of the variance in the data
- Information loss when using fewer components to represent data

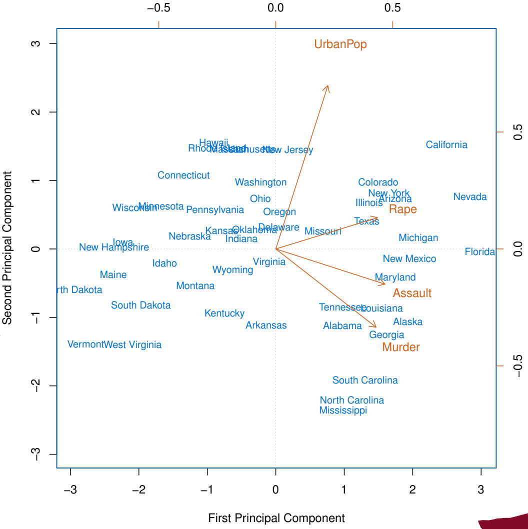
Tips

- Scale data prior to PCA
- Principle component signs can be ”flipped” (arbitrarily)

PCA – Example and Biplot

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

Source: ISLR2 Table 12.1



Source: ISLR2 Figure 12.1

PCA – Technicalities

- Each PC is an **eigenvector** of the data correlation matrix:

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

  where V are the eigenvectors, C is the 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:

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

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

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

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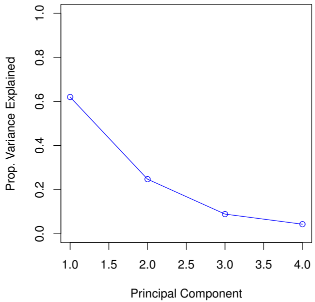
Choosing the Number of Principal Components

- Eigenvalue $\lambda > 1$
- Cumulative explained variance greater than threshold
- Cross-validation to find optimal K (lowest test error) in a linear regression or classification model
- ”Eyeballing” the screeplot



Source: ISLR2 Figure 12.3

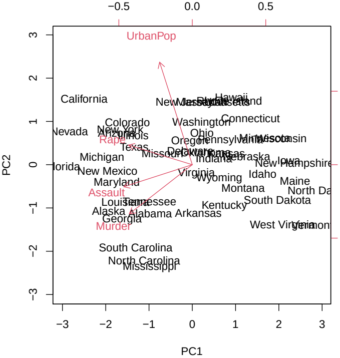
PCA in R

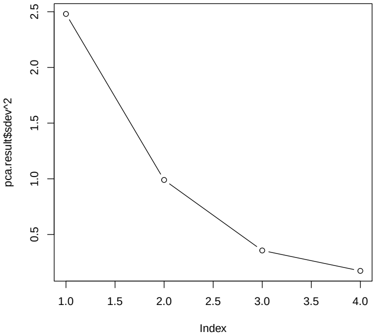
Use the `USArrests` dataset that contains data on the arrests (per 100,000 residents) for various violent crimes as well as the percentage of urban population in the 50 states of the US.

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

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

# Print the component loadings
pca.result$rotation

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

# Explained variance for each component
pca.result$sdev^2
# Scree plot (both points and lines)
plot(pca.result$sdev^2, type='b')
```

PCA in R [cont'd]

Biplot and Screeplot:





PCA in R [cont'd]

continued . . .

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

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

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

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

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Hands-On Exercises – PCA

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?

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Hands-On Exercises – PCA

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 Exercises – PCA

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.
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.

Clustering

Goals

- Form homogenous subgroups of data
- Based on *similarity* of (or *distance* between) observations
- Discover ”structure” in the data
- Clustering observations based on features, or clustering features based on observations (transpose of data matrix)

K-Means Clustering

- Number of clusters K is given

Hierarchical Clustering

- Unknown or variable number of clusters

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K-Means Clustering

- Minimize within-cluster variation $W(C_i)$:

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

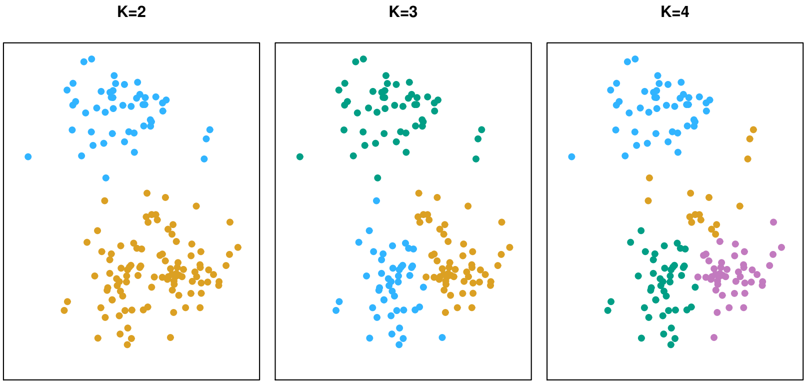
- Squared Euclidean Distance
  - Between every pair of observations in the cluster (equation 1)
  - Between every observation and the cluster **centroid** ("mean") (equation 2)

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

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

- Only for quantitative variables

K-Means Clustering



Source: ISLR2 Figure 12.7

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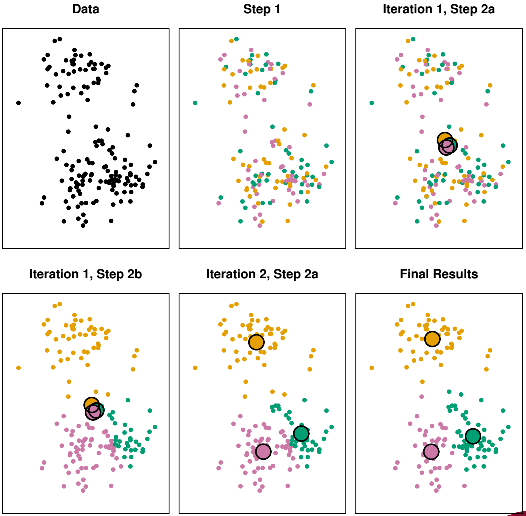
K-Means Clustering – Iterative Cluster Assignment

1. Randomly assign each observation to a cluster
2. Iterate until cluster assignments are stable
   - 2.1 Compute cluster means / centroid
   - 2.2 Assign each observation to cluster with closest centroid



Source: ISLR2 Figure 12.8

K-Means Clustering – Randomized Starting

- Different random initial starting clusters lead to different (suboptimal) solutions
- Run algorithm multiple times and select solution with lowest objective value

Source: ISLR2 Figure 12.9

K-Means Clustering in R

Simulated example:

```
# 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

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

K-Means Clustering in R [cont'd]

continued . . .

```
# Results show cluster means, cluster
# assignments, and sums of squares (distances)
# within and between
km.result
# Those values are also available in
# the result object
names(km.result)

# 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)
```

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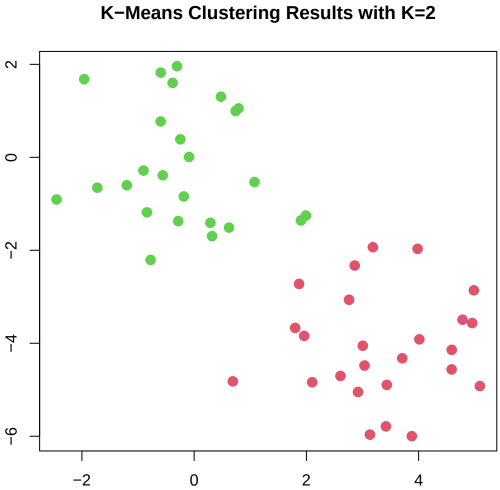
K-Means Clustering in R [cont'd]



Hands-On Exercises – K-Means Clustering

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.
2. Use different numbers of clusters *k* and identify which value of *k* gives you the best results. 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 Exercises – K-Means Clustering

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.
2. Use different numbers of clusters k and identify which value of k gives you the best results. 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.

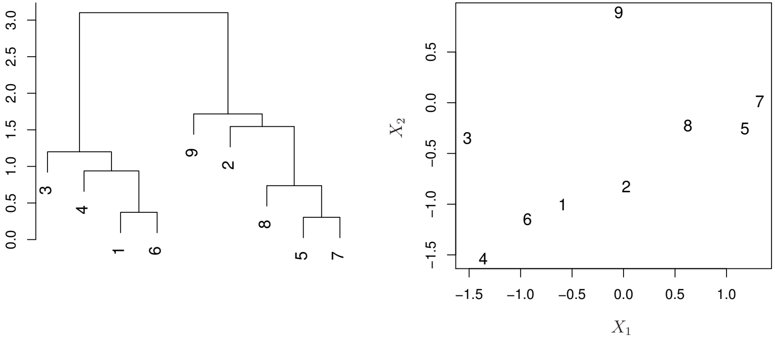
Hierarchical Clustering

Bottom-Up / Agglomerative Clustering

1. Begin with n observations and a dissimilarity or distance metric
2. Treat each observation as its own cluster
3. Repeat $n - 2$ times:
   3.1 Calculate dissimilarities or distances between all pairs of clusters
   3.2 Identify the pair of clusters that are least dissimilar (most similar)
   3.3 "Fuse" or merge these two clusters

Dendrogram

- Shows what clusters were fused at what dissimilarity



Source: ISLR2 Figure 12.12

Key Decisions

- How to measure dissimilarity/distance between observations?
- How to measure dissimilarity between clusters ("**linkage**")?
- How many clusters should we have?

Hierarchical Clustering – Common Distance Metrics

Common Distance Metrics or "Norms"

Taxicab / 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	$\|\|q-p\|\|_\infty$	$\lim_{p\to\infty} \left(\sum_i \|q_i - p_i\|^p\right)^{\frac{1}{p}} = \max_i(\|q_i - p_i\|)$
	$\|\|q-p\|\|_{-\infty}$	$\lim_{p\to-\infty} \left(\sum_i \|q_i - p_i\|^p\right)^{\frac{1}{p}} = \min_i(\|q_i - p_i\|)$

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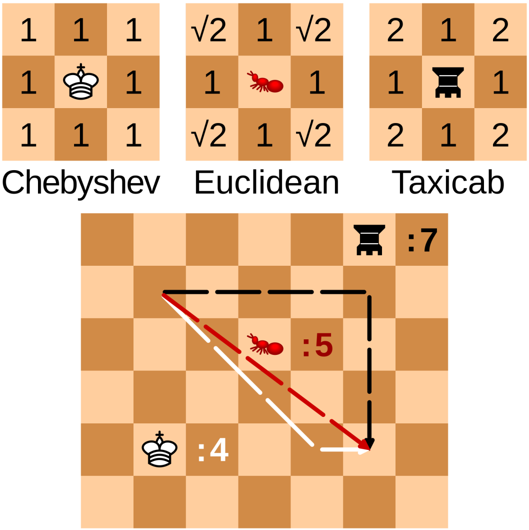
Hierarchical Clustering – Common Distance Metrics



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

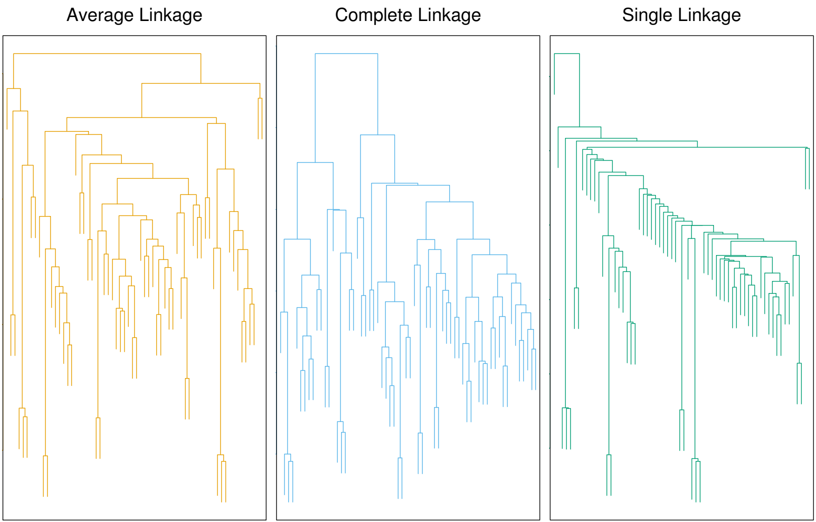
Hierarchical Clustering – Common Linkage Criteria

Common Linkages

Single	$d_{SL}(G,H) = \min_{i \in G, i' \in H} d_{i,i'}$
Complete	$d_{CL}(G,H) = \max_{i \in G, i' \in H} d_{i,i'}$
Average	$d_{AL}(G,H) = \operatorname{mean}_{i \in G, i' \in H} d_{i,i'}$

There are many other linkage functions: `https://en.wikipedia.org/wiki/Hierarchical_clustering`

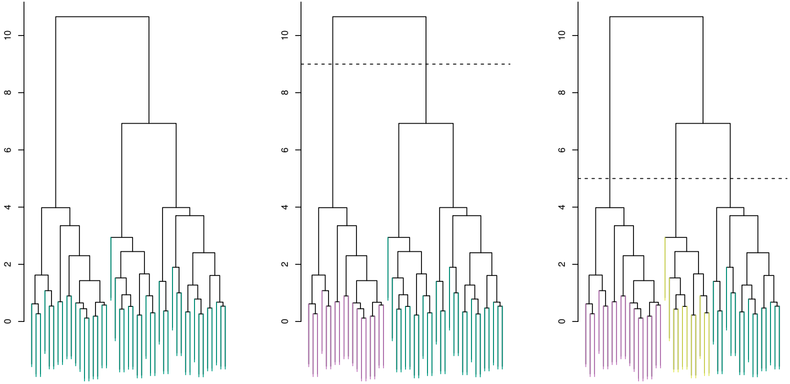
Hierarchical Clustering – Common Linkage Criteria



Source: ISLR2 Figure 12.14

Hierarchical Clustering – How Many Clusters?

- ”Cut” the dendrogram at a dissimilarity value



Source: ISLR2 Figure 12.11

Hierarchical Clustering in R

```r
# 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')

# 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')
```

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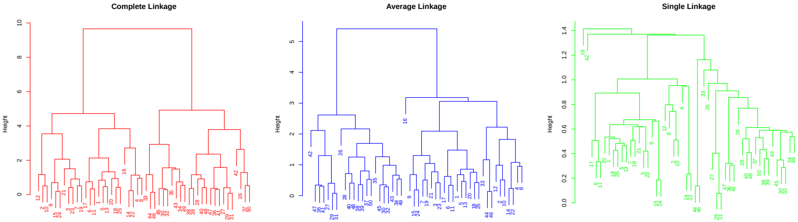
continued . . .

```
# 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)
```

Hierarchical Clustering in R [cont'd]



Hierarchical Clustering in R [cont'd]

Cutting the tree and identifying clusters:

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

Hands-On Exercises – Hierarchical Clustering

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.
2. Examine the dendrograms and identify which combination of distance metric and linkage function gives you the ”cleanest” separation of clusters.
3. How many factors k would you retain?
4. Using this value for k, perform a K-Means Clustering and compare the results.

Hands-On Exercises – Hierarchical Clustering

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.

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Hands-On Exercises – Hierarchical Clustering

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.
2. Examine the dendrograms and identify which combination of distance metric and linkage function gives you the ”cleanest” separation of clusters.
3. How many factors *k* would you retain?
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