Week 9 Clustering

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Cluster Analysis

- Cluster Analysis or Clustering is a form of ***unsupervised learning***. There is no specific response variable.
- The aim is to find groups in data; i.e. group observations in a data set into clusters with similar values of their variables.

We will look at

- k-means clustering
- hierarchical clustering
- distance metrics
- practical issues

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Cluster Analysis

Like Principle Components Analysis, Clustering is about simplifying a data set. PCA aims to reduce the dimensions of data set so that we can better see patterns without losing too much information.

Cluster Analysis seeks to find groups in a data set directly, where members of groups are more similar to members of the same group than other groups.

We need to define what it means to be a group and what it means to be similar.

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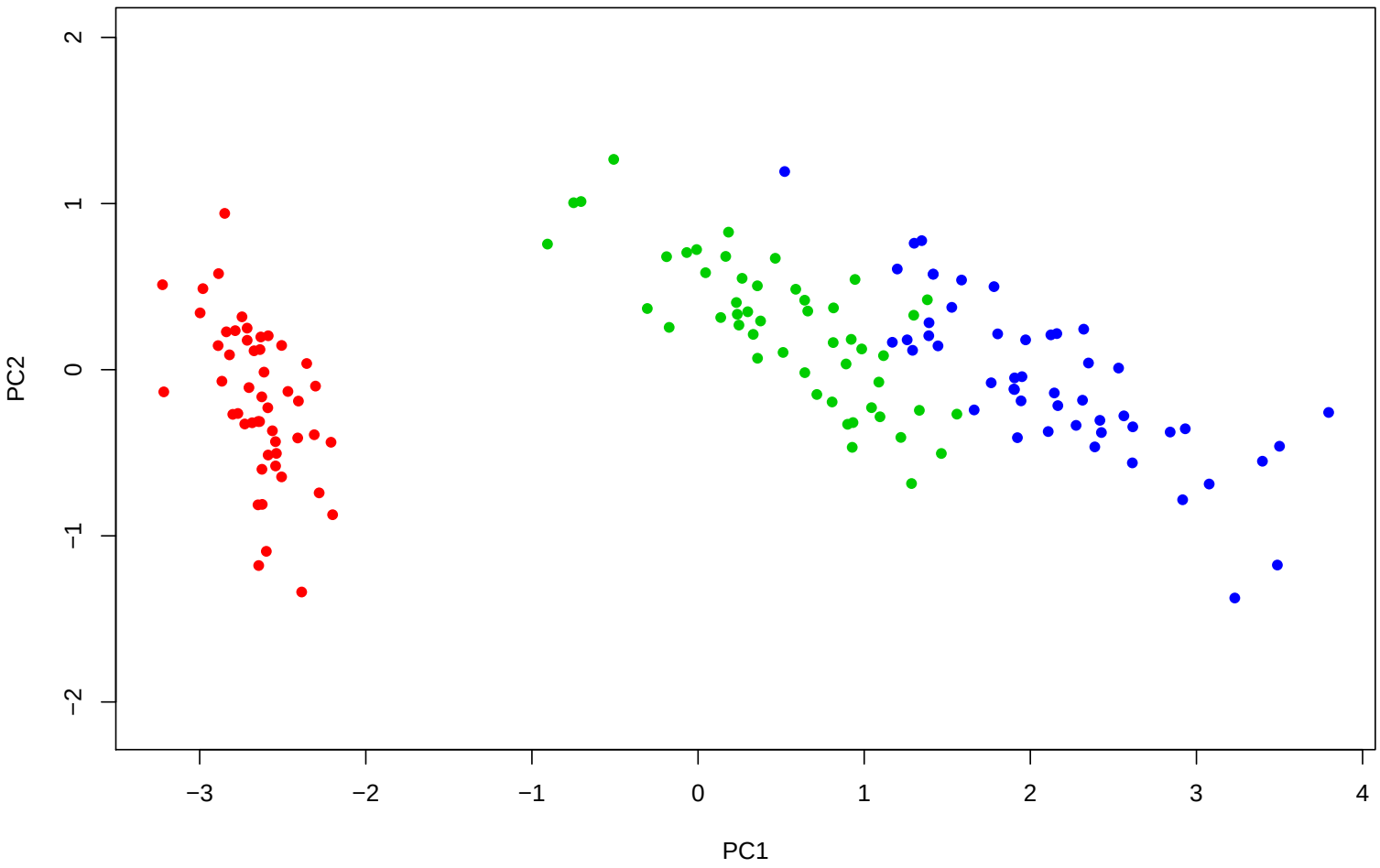
Clusters



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Similarity

In fact, we work with dissimilarity or distance. The simplest and most commonly used dissimilarity is ***Euclidean distance***. Euclidean distance is what we mean by distance when we measure it with a ruler or tape measure.

Euclidean distance between points **A** and **B** is:

- always zero or greater
- zero if and only if two points are the same (in the same place)
- less than the sum of the distances from **A** to **C** and **C** to **B** (*Triangle Inequality*)

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Euclidean Distance

If X is a data matrix, i.e. X_{ij} is the value of the j^{th} variable measured on the i^{th} individual, then Euclidean distance between the i^{th} and i'^{th} is;

$$d(X_i - X_{i'}) = \sqrt{\sum_{j=1}^{p}(X_{ij} - X_{i'j})^2}$$

with ***only 2 measurements*** (dimensions).

cf. Pythagoras Theorem

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k-means

The idea of k-means clustering is *to seek groupings or clusters so that the distance between points within clusters is as small as possible.* Although, in fact, the within cluster sum of squares is ***minimized***.

$$\sum_{(clusters)} \sum_{(i,i' in clusters)} d(X_i - X_{i'})^2$$

The set of clusters is chosen to minimize this sum.

Cluster Centroid

A cluster centroid is the centre of a cluster. It is found by averaging each variable for all the observations in the cluster.

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k-means

Start with a desired number of clusters k

1. Randomly assign a number between 1 and k to each point. These are initial cluster labels.
2. For each cluster, find the centroid.
3. Assign each observation a new cluster based on the centroid it is closest to.
4. Repeat 2 and 3 above until the centroids (or clusters) don't change.

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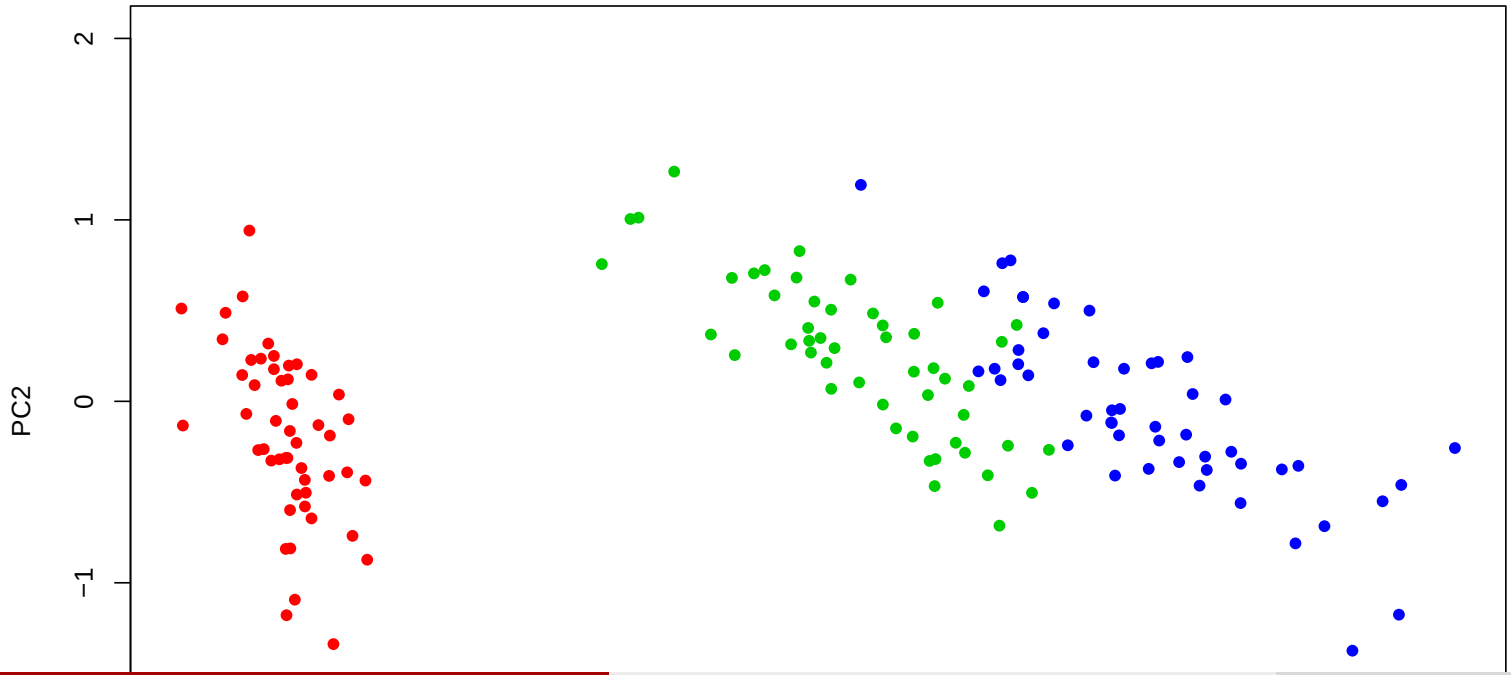
Iris Data - Plot PC1 against PC2

Colours represented by Species

```
 obj = prcomp(iris[,1:4])
plot(obj$x[,1:2], col=unclass(iris$Species)+1,
     pch=16, asp=1)
```



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k-means Clustering

k-means needs us to specify the number of clusters to seek. Example k=3

```
X = iris[,1:4]
km = kmeans(X, centers = 3)
```

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Random Start Function (*nstart*)

There are additional arguements for maximum number of iterations (*iter.max*) and the random start number (*nstart*).

```
km2 = kmeans(iris[,1:4], 3, nstart = 20, iter.max=100)
km2$cluster
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3 3 2 3 3 3 3 3 3 3 3
##  [71] 3 3 3 3 3 3 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
## [106] 2 3 2 2 2 2 2 2 3 3 2 2 2 2 3 2 3 2 3 2 2 3 3 2 2 2
## [141] 2 2 3 2 2 2 3 2 2 3
```

The Cluster Allocations

The cluster allocations can be obtained using the function (*fitted*).

```
fitted(km, "classes")
```

```
##   [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
##  [36] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 3 1 1 1 1 1 1 1 1
##  [71] 1 1 1 1 1 1 1 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [106] 3 1 3 3 3 3 3 3 1 1 3 3 3 3 1 3 1 3 1 3 3 1 1 3 3 3
## [141] 3 3 1 3 3 3 1 3 3 1
```

Plotting k-means Clusters

The colours indicate the observations according to the k-means cluster label depicting k-means clusters. Not according to the original variable Species

```
pp = prcomp(X)
plot(pp$x[,1:2], col=fitted(km, "classes")+1,
     xaxt="n", yaxt="n")
```

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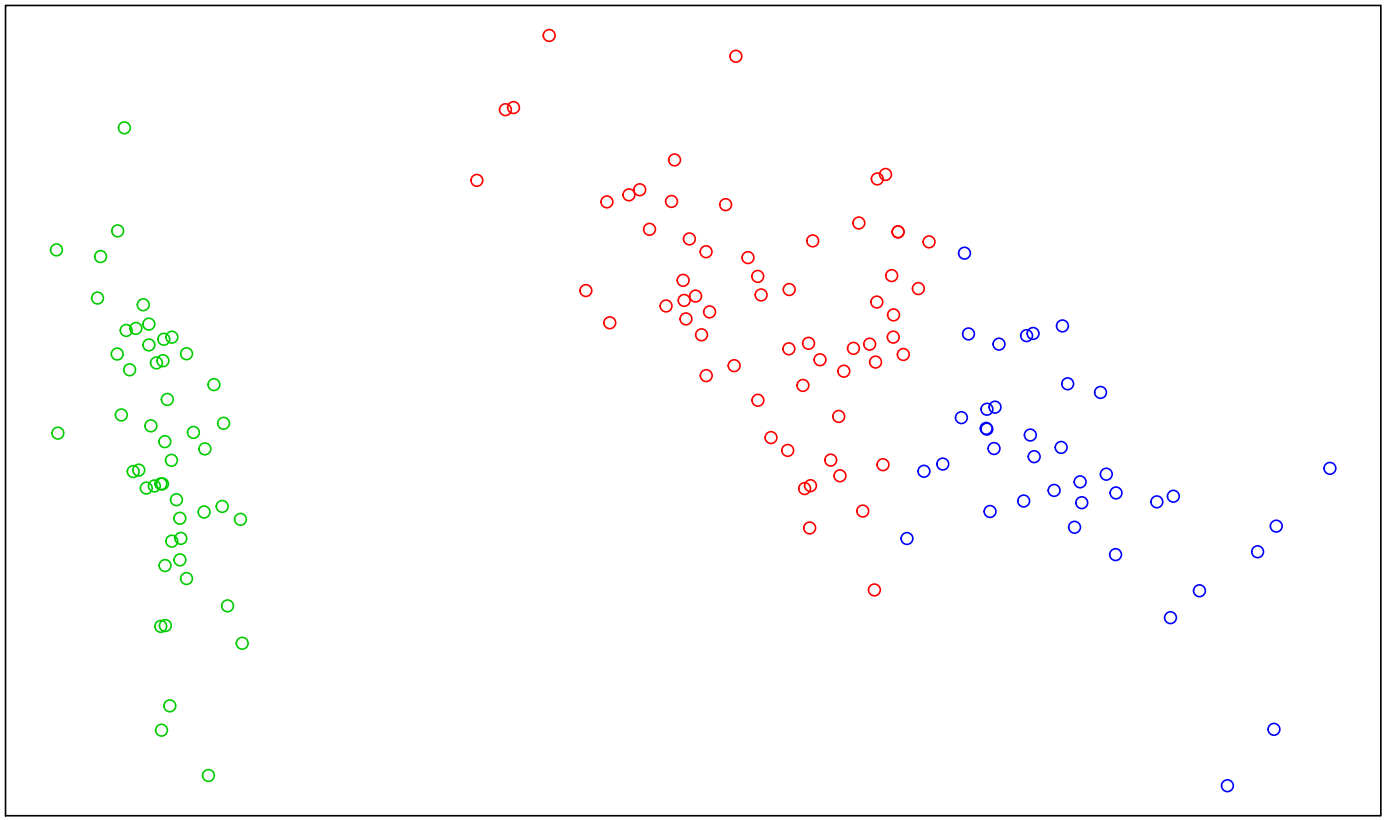
Plotting k-means (Continued...)



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Comparing Cluster Lables with Species

We can now compare the k-means cluster with the true species.

```
table(species=iris$Species, cluster=fitted(km, "classes"))
```

```
##                cluster
## species          1  2  3
##   setosa         0 50  0
##   versicolor    48  0  2
##   virginica     14  0 36
```

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km Output

```
km
```

```
## K-means clustering with 3 clusters of sizes 62, 50, 38
##
## Cluster means:
##   Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1     5.901613    2.748387     4.393548    1.433871
## 2     5.006000    3.428000     1.462000    0.246000
## 3     6.850000    3.073684     5.742105    2.071053
##
## Clustering vector:
##   [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
##  [36] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 3 1 1 1 1 1 1 1 1
##  [71] 1 1 1 1 1 1 1 3 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [106] 3 1 3 3 3 3 3 3 1 1 3 3 3 3 1 3 1 3 1 3 3 1 1 3 3 3
## [141] 3 3 1 3 3 3 1 3 3 1
```

km Output Continued

```
km$iter
```

```
## [1] 2
```

```
km$ifault
```

```
## [1] 0
```

```
km$size
```

```
## [1] 62 50 38
```

```
km$betweenss
```

```
## [1] 602.5192
```

```
km$tot.withinss
```

Hierarchical Clustering

- k-means implicitly uses Euclidean distance
- The data must be all *quantitative measurements*
- If some data is *qualitative*, more advanced algorithms exist
- hierarchical clustering uses an arbitrary distance

There are two types of hierarchical clustering

- ***agglomerative***
- ***divisive***

We discuss the first method here.

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Agglomerative Hierarchical Clustering

Suppose we have a possibly high dimensional data set X, and a distance defined between observations; e.g. Euclidean distance. The idea of agglomerative hierarchical clustering, is *to gradually merge clusters together to get a hierarchy of cluster solutions.*

1. Start with all observations in their own clusters - therefore, n clusters.
2. Merge the closest 2 clusters, to produce 1 fewer cluster.
3. Repeat 2, until all observations are in 1 cluster.

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Agglomerative Hierarchical Clustering (Continued...)

When the clusters contain more than one point, we have to consider what closest means.

How to measure the distance between two clusters **A** and **B**;

- The ***minimum*** of distances between points in **A** and points in **B**.
- The ***average*** of distances between points in **A** and points in **B**.
- The ***maximum*** of distances between points in **A** and points in **B**.
- Anything else.

Each of these definitions produces a different clustering methods.

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Distance Metrics

The most commonly used distance is ***Euclidean distance***. The distance between x and y is then;

$$\sqrt{\sum_j (y_j - x_j)^2}$$

Alternatives are,

- the ***City Block*** or ***Manhattan distance*** (The sum of the distances on each variable):

$$\sum_j (y_j - x_j)$$

- the ***Maximum distance***:

$$max_j (y_j - x_j)$$

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Distance Metrics (Continued...)

For binary data (e.g. presence/ absence), the binary metrics is often used. Suppose you have data where x and y are sets of indicators of the presence of somethings. E.g.

- Shopping baskets : each variable is "1" if an item is being bought
- Archaelogical sites : "0/1" indicates artefact found or not.
- Documents : "0/1" indicates word present or not.

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Distance Metrics (Continued...)

The binary metric compares two observations by looking at the number of things in common versus those not in common

$$d(x, y) = A/(A + B + C)$$

where

- A : items in both x and y
- B : items in x only
- C : items in y only
- D : items not in either x or y (not used)

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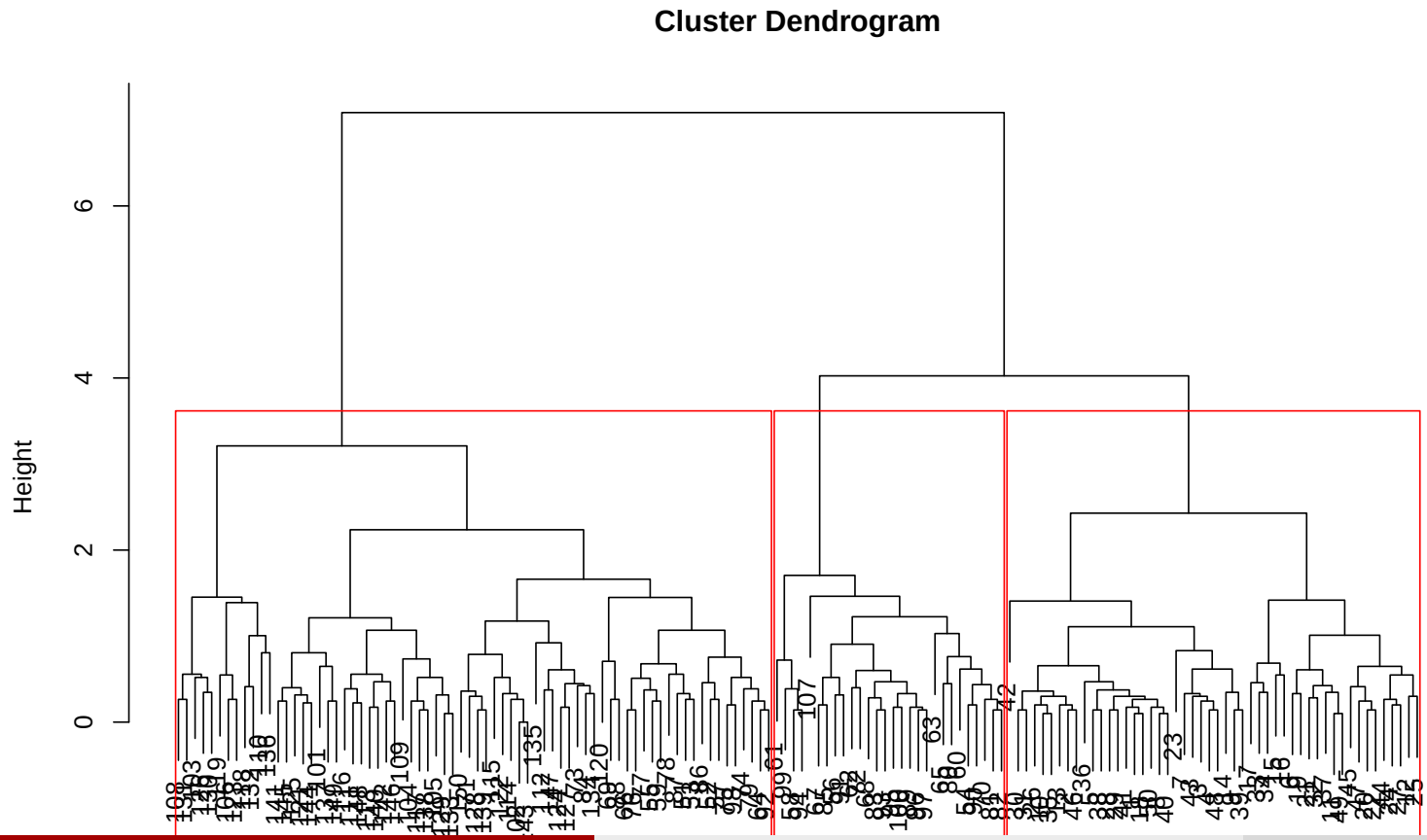
Examples Hierarchical Clustering

```
hh = hclust(dist(X))
plot(hh, main = "Cluster Dendrogram")
rect.hclust(hh, k=3)
```



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Examples Hierarchical Clustering (Continued...)

is a ***cluster dendrogram***; the height represents the ditance at which clusters were merged.

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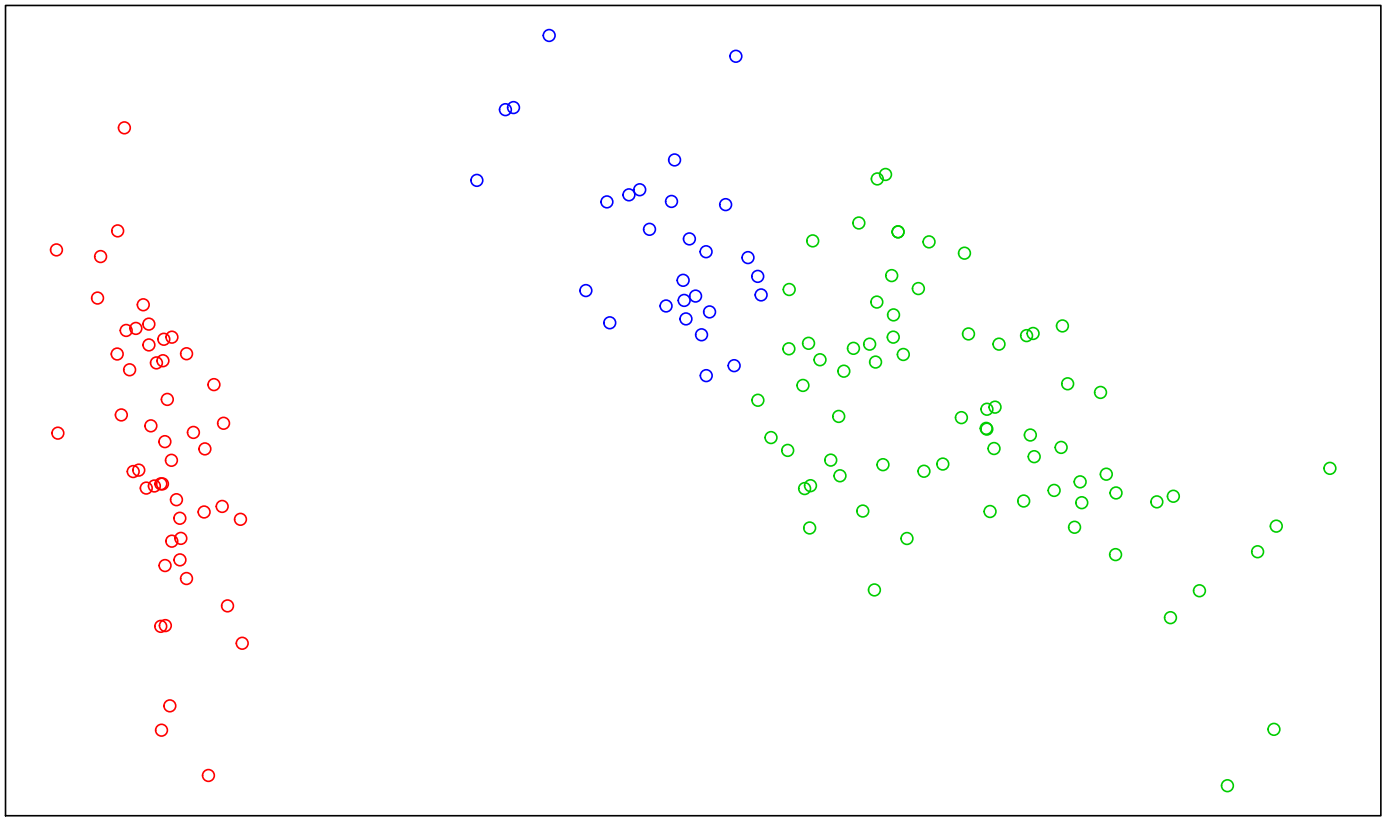
Examples Hierarchical Clustering - Iris Data



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Examples Hierarchical Clustering - Iris Data (Continued...)

We apply *dist* first to get distances, then *hclust*. The result has the solution for all cluster numbers.

```
hh = hclust(dist(X), method="complete")
```

method can be "single", "average" and "complete" (plus others) the distance between two clusters **A** and **B** is

- ***single*** - The minimum of distances between points in **A** and points in **B**.
- ***average*** - The average of distances between points in **A** and points in **B**.
- ***complete*** - The maximum of distances between points in **A** and points in **B**.

Cluster Membership

To extract cluster membership, we have to decide how many clusters.

```
cutree(hh, k=3)
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [36] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 3 2 3 2 3 2 3 3 3
##  [71] 2 3 2 2 2 2 2 2 2 3 3 3 3 2 3 2 2 2 3 3 3 2 3 3 3 3 3
## [106] 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
## [141] 2 2 2 2 2 2 2 2 2 2
```

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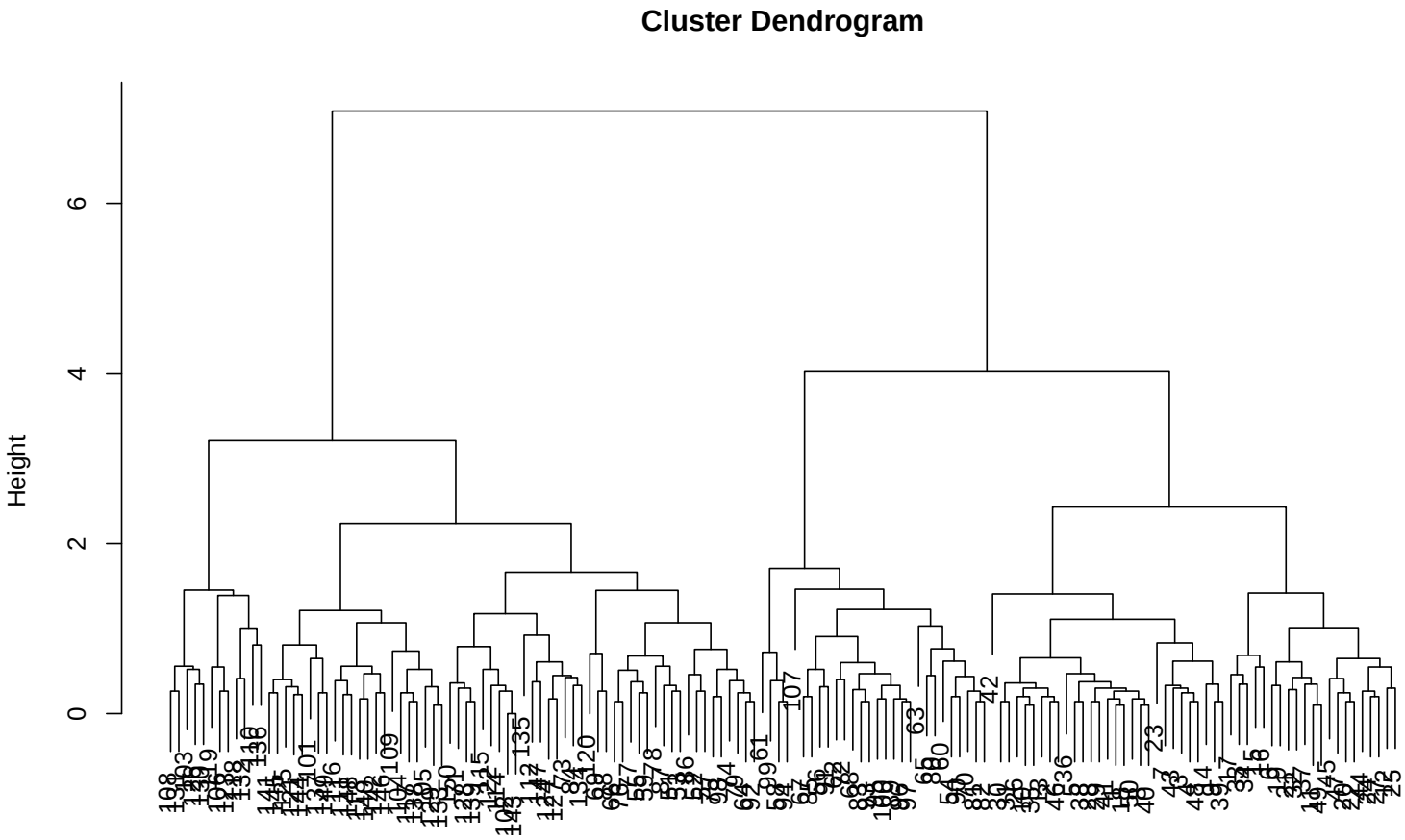
Plotting

We use plot to get the dendrogram.

```
plot(hh, xlab=" ", sub="Complete link cluster analysis")
```



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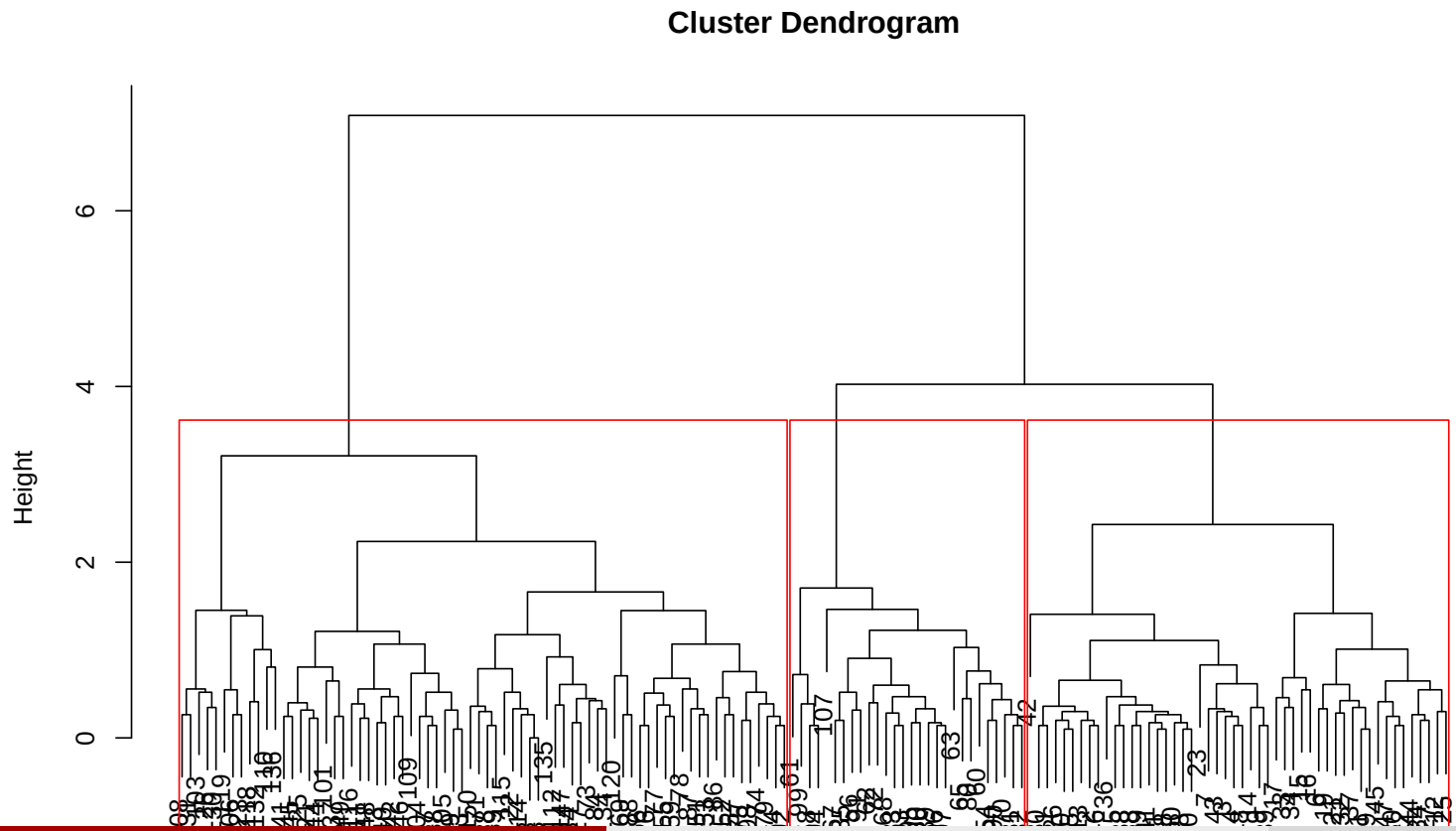
Plotting (Continued...)

rect.hclust can be used to box in the clusters.

```
plot(hh, xlab=" ", sub = "Complete link cluster analysis")
rect.hclust(hh, k=3)
```



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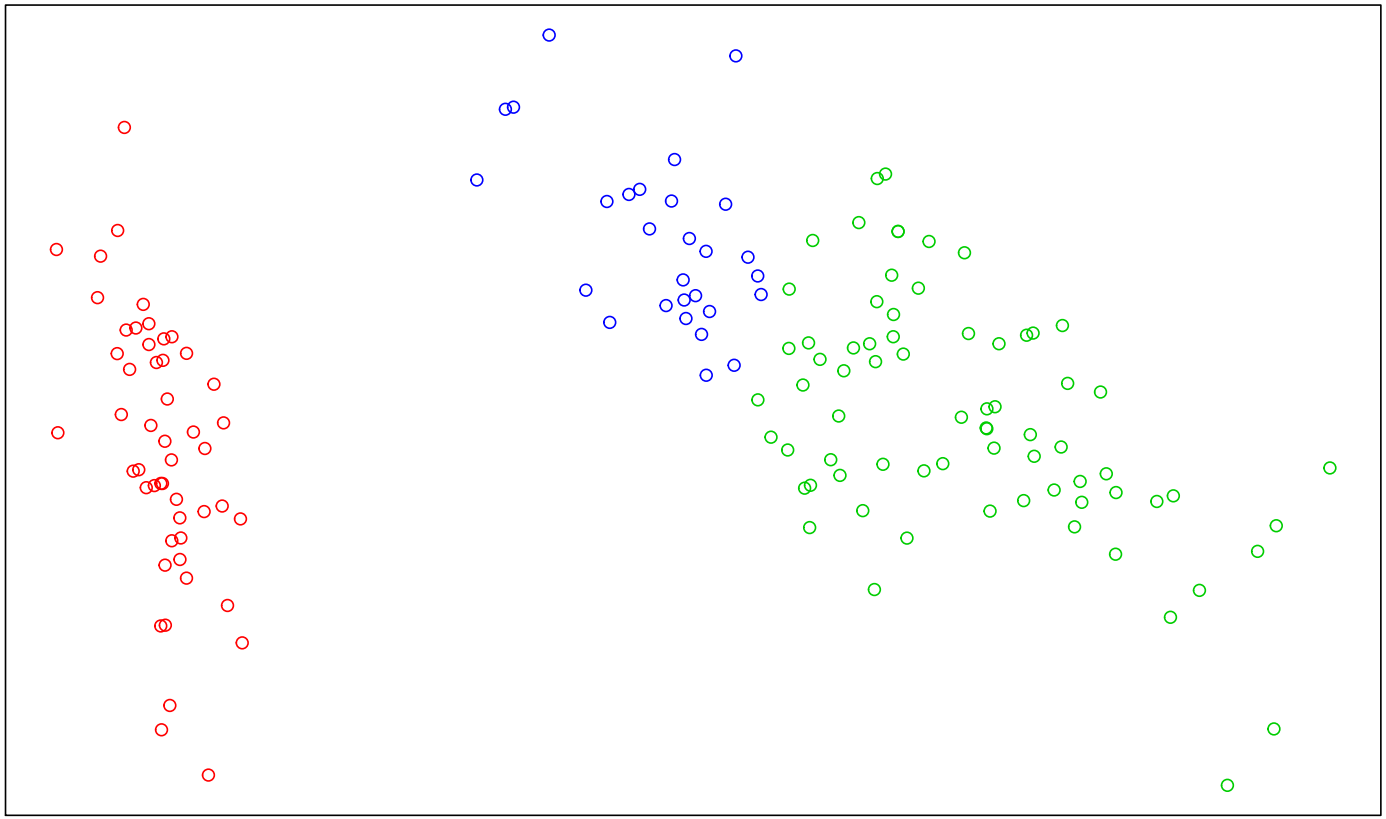
Principle Components Again

```
plot(pp$x[,1:2], col=cutree(hh,  k=3)+1,
     xaxt="n", yaxt="n")
```



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TEXT BOOK

Lecture notes are based on the textbook.

For further reference refer;

Prescribed Textbook - Chapter 10

- James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An Introduction to Statistical Learning: with Applications in R Springer.

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