Clustering

Karen Mazidi

Modified from Kabacoff, “R in Action”, 2nd ed

K-means

Apply k-means to the wine data set, which contains 13 chemical measurements on 178 Italian wines.

The first column, Type, indicates 1 or 3 win varieties. We will drop this variable for the clustering.

```
data(wine, package="rattle")
names(wine)
```

```
##  [1] "Type"            "Alcohol"         "Malic"
##  [4] "Ash"             "Alcalinity"      "Magnesium"
##  [7] "Phenols"         "Flavanoids"      "Nonflavanoids"
## [10] "Proanthocyanins" "Color"           "Hue"
## [13] "Dilution"        "Proline"
```

```
head(wine)
```

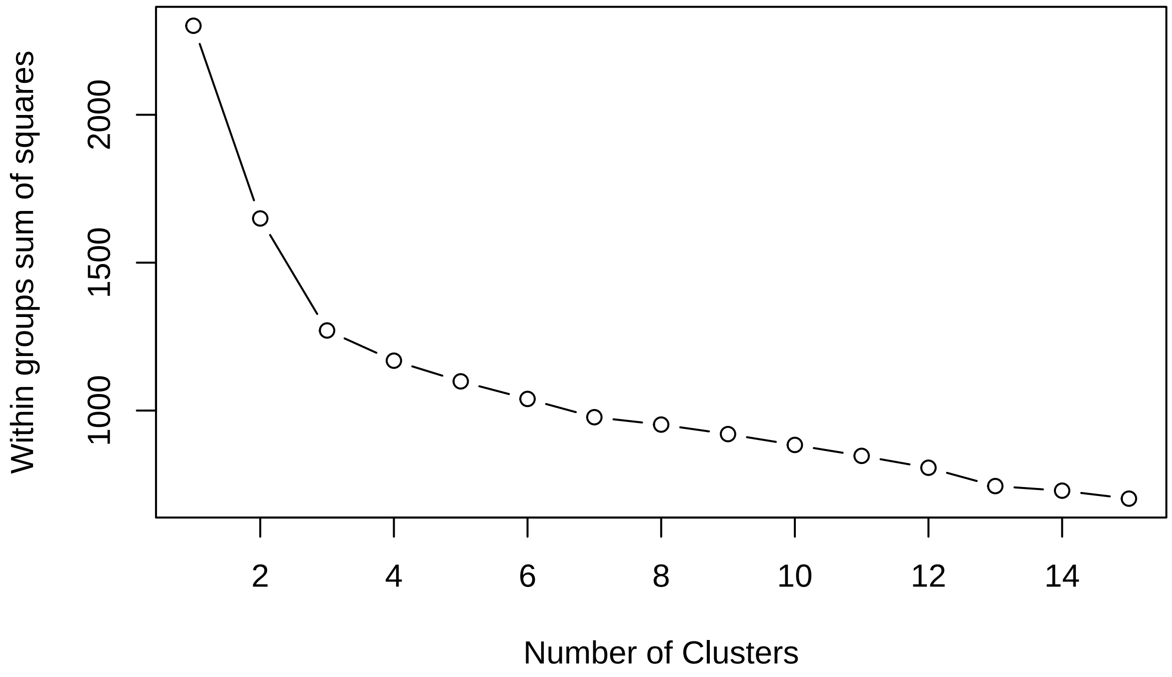
```
##   Type Alcohol Malic  Ash Alcalinity Magnesium Phenols Flavanoids
## 1    1   14.23  1.71 2.43       15.6       127    2.80       3.06
## 2    1   13.20  1.78 2.14       11.2       100    2.65       2.76
## 3    1   13.16  2.36 2.67       18.6       101    2.80       3.24
## 4    1   14.37  1.95 2.50       16.8       113    3.85       3.49
## 5    1   13.24  2.59 2.87       21.0       118    2.80       2.69
## 6    1   14.20  1.76 2.45       15.2       112    3.27       3.39
##   Nonflavanoids Proanthocyanins Color  Hue Dilution Proline
## 1          0.28            2.29  5.64 1.04     3.92    1065
## 2          0.26            1.28  4.38 1.05     3.40    1050
## 3          0.30            2.81  5.68 1.03     3.17    1185
## 4          0.24            2.18  7.80 0.86     3.45    1480
## 5          0.39            1.82  4.32 1.04     2.93     735
## 6          0.34            1.97  6.75 1.05     2.85    1450
```

```
df <- scale(wine[-1])
head(df)
```

```
##        Alcohol       Malic        Ash Alcalinity  Magnesium   Phenols
## [1,] 1.5143408 -0.56066822  0.2313998 -1.1663032 1.90852151 0.8067217
## [2,] 0.2455968 -0.49800856 -0.8256672 -2.4838405 0.01809398 0.5670481
## [3,] 0.1963252  0.02117152  1.1062139 -0.2679823 0.08810981 0.8067217
## [4,] 1.6867914 -0.34583508  0.4865539 -0.8069748 0.92829983 2.4844372
## [5,] 0.2948684  0.22705328  1.8352256  0.4506745 1.27837900 0.8067217
## [6,] 1.4773871 -0.51591132  0.3043010 -1.2860793 0.85828399 1.5576991
##      Flavanoids Nonflavanoids Proanthocyanins      Color        Hue
## [1,]  1.0319081    -0.6577078       1.2214385  0.2510088  0.3611585
## [2,]  0.7315653    -0.8184106      -0.5431887 -0.2924962  0.4049085
## [3,]  1.2121137    -0.4970050       2.1299594  0.2682629  0.3174085
## [4,]  1.4623994    -0.9791134       1.0292513  1.1827317 -0.4263410
## [5,]  0.6614853     0.2261576       0.4002753 -0.3183774  0.3611585
## [6,]  1.3622851    -0.1755994       0.6623487  0.7298108  0.4049085
##       Dilution     Proline
## [1,] 1.8427215  1.01015939
## [2,] 1.1103172  0.96252635
## [3,] 0.7863692  1.39122370
## [4,] 1.1807407  2.32800680
## [5,] 0.4483365 -0.03776747
## [6,] 0.3356589  2.23274072
```

Write a function to plot the within-groups sums of squares vs. the number of clusters.

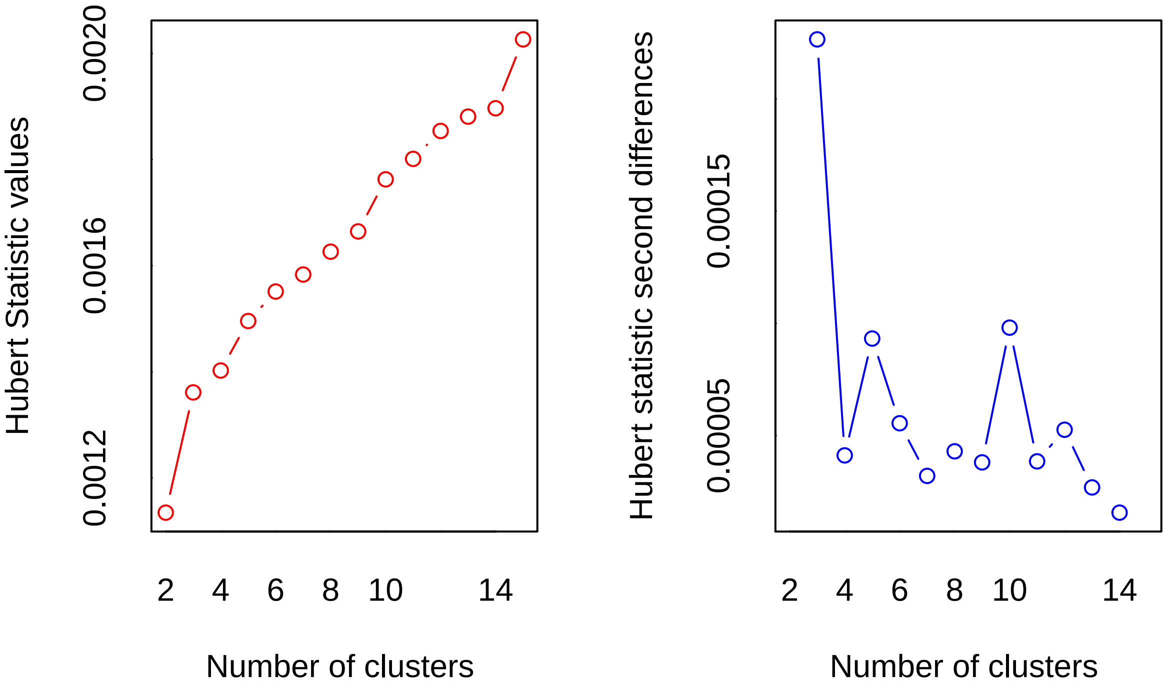
```
wsplot <- function(data, nc=15, seed=1234){
  wss <- (nrow(data)-1)*sum(apply(data,2,var))
  for (i in 2:nc){
    set.seed(seed)
    wss[i] <- sum(kmeans(data,centers=i)$withinss)
  }
  plot(1:nc, wss, type="b", xlab="Number of Clusters",
       ylab="Within groups sum of squares")
}
wsplot(df)
```



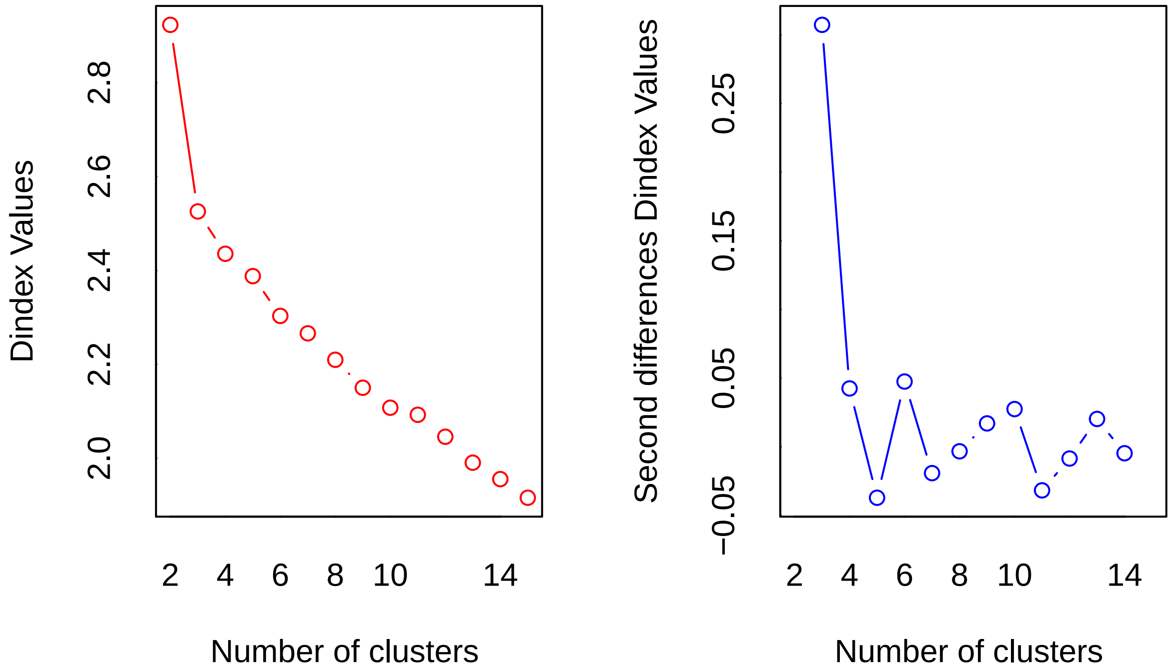
Use the NbClust() function to help determine the best number of clusters.

In the within-groups plot, we see an “elbow” around 3, suggesting that 3 clusters is a good choice.

```
library(NbClust)
set.seed(1234)
nc <- NbClust(df, min.nc=2, max.nc=15, method="kmeans")
```



```
## *** : The Hubert index is a graphical method of determining the number of clusters.
##                 In the plot of Hubert index, we seek a significant knee that corresponds to a
##                 significant increase of the value of the measure i.e the significant peak in Hubert
##                 index second differences plot.
##
```

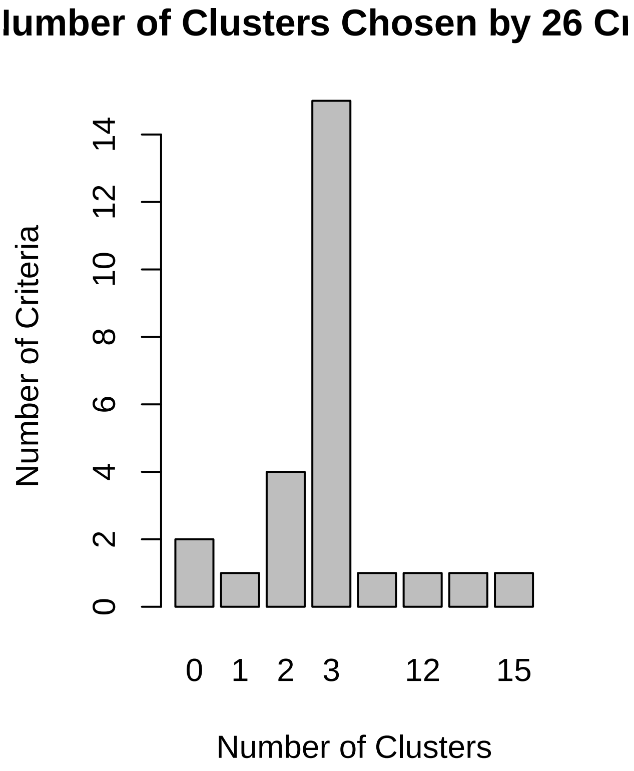


```
## *** : The D index is a graphical method of determining the number of clusters.
##                 In the plot of D index, we seek a significant knee (the significant peak in Dindex
##                 second differences plot) that corresponds to a significant increase of the value of
##                 the measure.
##
## *******************************************************************
## * Among all indices:
## * 4 proposed 2 as the best number of clusters
## * 15 proposed 3 as the best number of clusters
## * 1 proposed 10 as the best number of clusters
## * 1 proposed 12 as the best number of clusters
## * 1 proposed 14 as the best number of clusters
## * 1 proposed 15 as the best number of clusters
##
##                    ***** Conclusion *****
##
## * According to the majority rule, the best number of clusters is  3
##
##
## *******************************************************************
```

```
table(nc$Best.n[1,])
```

```
##
##  0  1  2  3 10 12 14 15
##  2  1  4 15  1  1  1  1
```

```
barplot(table(nc$Best.n[1,]),
        xlab="Number of Clusters", ylab="Number of Criteria",
        main="Number of Clusters Chosen by 26 Criteria")
```



KMeans

Fit the model using the kmeans() function. We set a seed first so we get reproducible results.

The centroids are found in fit.km$centers and we display those.

```
set.seed(1234)
fit.km <- kmeans(df, 3, nstart=25)
fit.km$size
```

```
## [1] 62 65 51
```

```
fit.km$centers
```

```
##      Alcohol      Malic        Ash Alcalinity   Magnesium     Phenols
## 1  0.8328826 -0.3029551  0.3636801 -0.6084749  0.57596208  0.88274724
## 2 -0.9234669 -0.3929331 -0.4931257  0.1701220 -0.49032869 -0.07576891
## 3  0.1644436  0.8690954  0.1863726  0.5228924 -0.07526047 -0.97657548
##    Flavanoids Nonflavanoids Proanthocyanins      Color        Hue
## 1  0.97506900   -0.56050853      0.57865427  0.1705823  0.4726504
## 2  0.02075402   -0.03343924      0.05810161 -0.8993770  0.4605046
## 3 -1.21182921    0.72402116     -0.77751312  0.9388902 -1.1615122
##     Dilution    Proline
## 1  0.7770551  1.1220202
## 2  0.2700025 -0.7517257
## 3 -1.2887761 -0.4059428
```

The centroids were calculated based on the scaled data. Next we use the aggregate() function along with the cluster membership to get variable means for each cluster in units of the original, unscaled, data.

```
aggregate(wine[-1], by=list(cluster=fit.km$cluster), mean)
```

```
##   cluster  Alcohol    Malic      Ash Alcalinity Magnesium  Phenols
## 1       1 13.67677 1.997903 2.466290   17.46290 107.96774 2.847581
## 2       2 12.25092 1.897385 2.231231   20.06308  92.73846 2.247692
## 3       3 13.13412 3.307255 2.417647   21.24118  98.66667 1.683922
##   Flavanoids Nonflavanoids Proanthocyanins    Color       Hue Dilution
## 1  3.0032258     0.2920968        1.922097 5.453548 1.0654839 3.163387
## 2  2.0500000     0.3576923        1.624154 2.973077 1.0627077 2.803385
## 3  0.8188235     0.4519608        1.145882 7.234706 0.6919608 1.696667
##     Proline
## 1 1100.2258
## 2  510.1692
## 3  619.0588
```

Model Analysis

If we cross-tabulate the Type in column 1 of the wine data with cluster membership, we see that the clusters are strongly correlated with the wine type.

```
ct.km <- table(wine$Type, fit.km$cluster)
ct.km
```

```
##
##      1  2  3
##   1 59  0  0
##   2  3 65  3
##   3  0  0 48
```

We can quantify the agreement between the type and the cluster using an adjusted Rand index. The adjusted Rand index provides a measure of the agreement between two partitions, adjusted for chance. The range of the index is from -1 (no agreement) to +1 (perfect agreement).

The results below show very good agreement!

```
library(flexclust)
```

```
## Loading required package: grid

## Loading required package: lattice

## Loading required package: modeltools

## Loading required package: stats4
```

```
randIndex(ct.km)
```

```
##      ARI
## 0.897495
```