A Handbook of Statistical Analyses Using ${\sf R}$

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CHAPTER 15

Cluster Analysis: Classifying the Exoplanets

- 15.1 Introduction
- 15.2 Cluster Analysis
- 15.3 Analysis Using R

Sadly Figure~15.2 gives no completely convincing verdict on the number of groups we should consider, but using a little imagination 'little elbows' can be spotted at the three and five group solutions. We can find the number of planets in each group using

```
R> planet_kmeans3 <- kmeans(planet.dat, centers = 3)
R> table(planet_kmeans3$cluster)
    1    2    3
28    10   63
```

The centers of the clusters for the untransformed data can be computed using a small convenience function

```
R> ccent <- function(cl) {
+         f <- function(i) colMeans(planets[cl == i,])
+         x <- sapply(sort(unique(cl)), f)
+         colnames(x) <- sort(unique(cl))
+         return(x)
+ }</pre>
```

which, applied to the three cluster solution obtained by k-means gets

R> ccent(planet_kmeans3\$cluster)

```
1 2 3
mass 7.0532143 3.4360 1.6540635
period 839.1644356 2420.5500 311.3897179
eccen 0.5184643 0.2718 0.1777984
```

for the three cluster solution and, for the five cluster solution using

```
R> planet_kmeans5 <- kmeans(planet.dat, centers = 5)</pre>
```

R> table(planet_kmeans5\$cluster)

```
1 2 3 4 5
28 5 7 49 12
```

R> ccent(planet_kmeans5\$cluster)

```
R> data("planets", package = "HSAUR")
R> library("scatterplot3d")
R> scatterplot3d(log(planets$mass), log(planets$period),
+ log(planets$eccen), type = "h", angle = 55,
+ pch = 16, y.ticklabs = seq(0, 10, by = 2),
+ y.margin.add = 0.1, scale.y = 0.7)
```

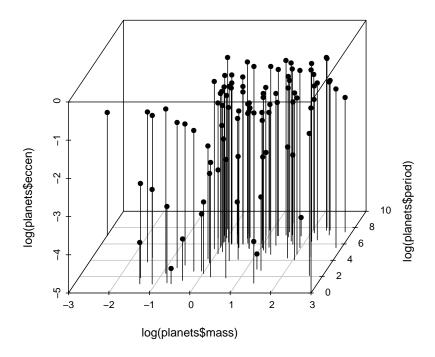
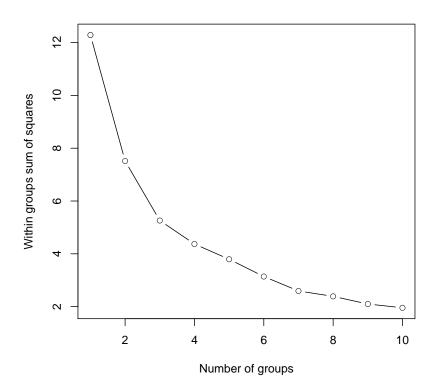


Figure 15.1 3D scatterplot of the logarithms of the three variables available for each of the exoplanets.

	1	2	3	4	5
mass	2.2617857	14.3480	2.185714	1.6846122	8.595
period	580.6828929	659.3976	2557.642857	282.2685965	1335.740
eccen	0.4910714	0.3268	0.199000	0.1221082	0.473



 ${\bf Figure~15.2} \quad {\bf Within\mbox{-}cluster~sum~of~squares~for~different~numbers~of~clusters~for~the~exoplanet~data}.$

```
R> plot(planet_mclust, planet.dat, what = "BIC", col = "black",
+ ylab = "-BIC", ylim = c(0, 350))
```

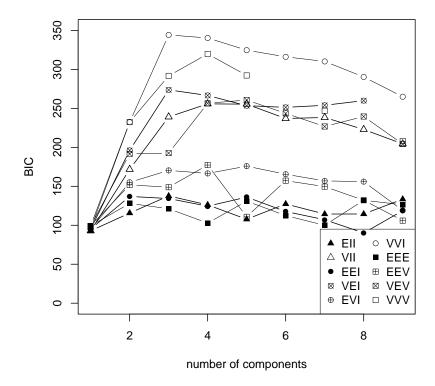


Figure 15.3 Plot of BIC values for a variety of models and a range of number of clusters.

15.3.1 Model-based Clustering in R

We now proceed to apply model-based clustering to the planets data. R functions for model-based clustering are available in package <code>mclust</code> (Fraley et~al., 2006, Fraley and Raftery, 2002). Here we use the Mclust function since this selects both the most appropriate model for the data <code>and</code> the optimal number of groups based on the values of the BIC computed over several models and a range of values for number of groups. The necessary code is:

```
R> library("mclust")
R> planet_mclust <- Mclust(planet.dat)</pre>
```

and we first examine a plot of BIC values using The resulting diagram is

shown in Figure 15.3. In this diagram the numbers refer to different model assumptions about the shape of clusters:

- 1. Spherical, equal volume,
- 2. Spherical, unequal volume,
- 3. Diagonal equal volume, equal shape,
- 4. Diagonal varying volume, varying shape,
- 5. Ellipsoidal, equal volume, shape and orientation,
- 6. Ellipsoidal, varying volume, shape and orientation.

The BIC selects model 4 (diagonal varying volume and varying shape) with three clusters as the best solution as can be seen from the print output:

R> print(planet_mclust)

```
best model: diagonal, varying volume and shape with 3 components
```

This solution can be shown graphically as a scatterplot matrix The plot is shown in Figure 15.4. Figure 15.5 depicts the clustering solution in the three-dimensional space.

The number of planets in each cluster and the mean vectors of the three clusters for the untransformed data can now be inspected by using

R> table(planet_mclust\$classification)

```
1 2 3
19 41 41
```

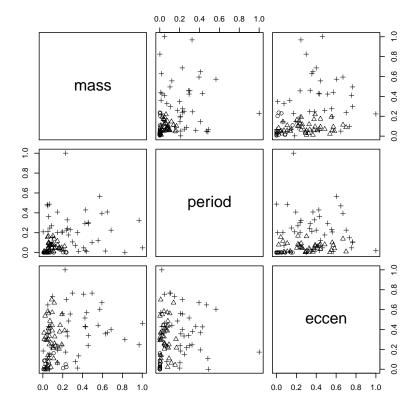
R> ccent(planet_mclust\$classification)

```
1 2 3
mass 1.16652632 1.5797561 6.0761463
period 6.47180158 313.4127073 1325.5310048
eccen 0.03652632 0.3061463 0.3704951
```

Cluster 1 consists of planets about the same size as Jupiter with very short periods and eccentricities (similar to the first cluster of the k-means solution). Cluster 2 consists of slightly larger planets with moderate periods and large eccentricities, and cluster 3 contains the very large planets with very large periods. These two clusters do not match those found by the k-means approach.

R> clPairs(planet.dat,

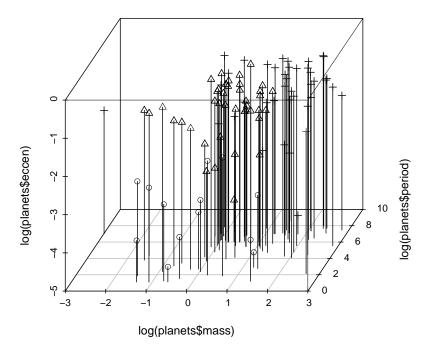
- + classification = planet_mclust\$classification,
- + symbols = 1:3, col = "black")



 $\begin{tabular}{ll} \textbf{Figure 15.4} & Scatterplot matrix of planets data showing a three cluster solution from Mclust. \end{tabular}$

```
{\tt R> \ scatterplot3d(log(planets\$mass), \ log(planets\$period),}\\
```

- + log(planets\$eccen), type = "h", angle = 55,
- + scale.y = 0.7, pch = planet_mclust\$classification,
- + y.ticklabs = seq(0, 10, by = 2), y.margin.add = 0.1)



 $\begin{tabular}{ll} \textbf{Figure 15.5} & 3D \ scatterplot \ of \ planets \ data \ showing \ a \ three \ cluster \ solution \ from \\ & \texttt{Mclust}. \end{tabular}$



Bibliography

Fraley, C. and Raftery, A.~E. (2002), "Model-based clustering, discriminant analysis, and density estimation," Journal of the American Statistical Association, 97, 611–631.

Fraley, C., Raftery, A.~E., and Wehrens, R. (2006), mclust: Model-based Cluster Analysis, URL http://www.stat.washington.edu/mclust, R package version 3.1-1.