Statistics - Week 2

Jimmy Tsz Ming Yue*

University of Sydney
jyue6728@uni.sydney.edu.au

Semester 2 Statistics 2018

Contents

1 What is clustering?

Definition. Clustering are methods of grouping samples (x) that are similar in nature, according to some pre-defined criteria. It is a form of unsupervised learning, in that there is no label information (y) to tell the algorithm which observations should be grouped together. As such it is often used for exploratory data analysis: for which we can look at patters or structures in the data set which may be of particular interest to us.

2 Basic Principles of Clustering

In clustering, we aim to group observations that are similar. There are certain issues that arise from this , which include consideration of the data types, the prescence of missing data, scaling and the similarity metric that we chose in doing our clustering. Examples of such metrics are: Euclidean, Manhattan, Pearson correlation, Spearman correlation. To do clustering we can employ many different algorithms, such as: Hierarchical clustering, K-means clustering, Fuzzy c-means clustering, semi-supervised clustering and bi-clustering.

*440159151

3 Commonly used similarity measures

Definition. Metric: A metric is a measure of the similarity or dissimilarity between two data objects and it is used to form data points into cluster. (Formally speaking a metric is a measure of the distance within a metric space). We have:

1. Correlation Coefficients, which compares the shape of expression curves; (Pearson's Correlation Coefficient):

$$\rho(x,y) = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}} \tag{1}$$

$$d_p = \frac{1 - \rho(x,y)}{2} \tag{2}$$

2. Distance Metrics, where we have;

   (a) Manhattan distance;

$$d(X,Y) = \sum_i |x_i - y_i|$$

   (b) Euclidean distance;

$$d(x,y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

We also have Spearman's and Kendall's correlation which we can use to define our metrics. We can use absolute correlation to capture both positive and negative correlation.

4 Distances between clusters

We can choose different measures for measuring between clusters, with:

1. Single: Which measures the closest distance between two clusters
2. Complete: Which measures the maximum distance between two clusters
3. Distance between centroids, which measures between the centroid of two clusters
4. Average Linkage: Which takes the average distance between clusters.

5 Clustering Algorithms

We have two different flavours of clusterings;

1. Partitioning
2. Hierarchical

5.1 Hierarchical methods

Hierarchical clustering methods produce a tree or dendrogram. They avoid specifying how many clusters are approrpriate by providing a partition for each k obtained from cutting the tree at some level. An example of hierarchical clustering is the bottom-up tree buidling. This is done as follows:

Bottom-Up Tree building procedure

1. Let us start with n samples for which we generate n clusters.
2. At each step, we merge the two closest clusters using a measure of between-cluster dissimilarity which reflects the shape of the clusters. (We may use different measures of distance as outlined above)

Let us give some examples first with some R code of the crime data given last week then with Gene expression data;

5.2 Partitioning methods

Partitioning clustering methods seeks to partition the data into pre-specified number k of mutually exclusive and exhuastive groups. This is done through iteratively reallocating the observations to clusters until some critierion is met, for example the minimisation of cluster sums of squares.

Typical Clustering Algorithm

1. Choose k objects as the initial cluster centers
2. Until no change,
3. Reassign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster.
4. Update the cluster means,

5.2.1 Problems with k-means

There are some issues with paritioning, namely the prescence of outliers. For example, objects with extremely large values may substantially distort the distribution of data.

6 Tutorial 2

The "ClueR" R package contains a time-course phosphoproteomics dataset "hES". Each column of in hES data is a time point and each row is a phosphorylation sites. We will perform clustering analysis on this dataset.

1. Install "ClueR" R package and its dependent packages. Find out how to use it by typing "?runClue".

   Solution. Let us load the library:

```
> library("ClueR")
> ?runClue
```

□

2. Once you have installed the package load the hES dataset as follows:

```
> data(hES)
```

Solution. Find out the dimension of the hES dataset.

```
> dim(hES)

[1] 3416    5
```

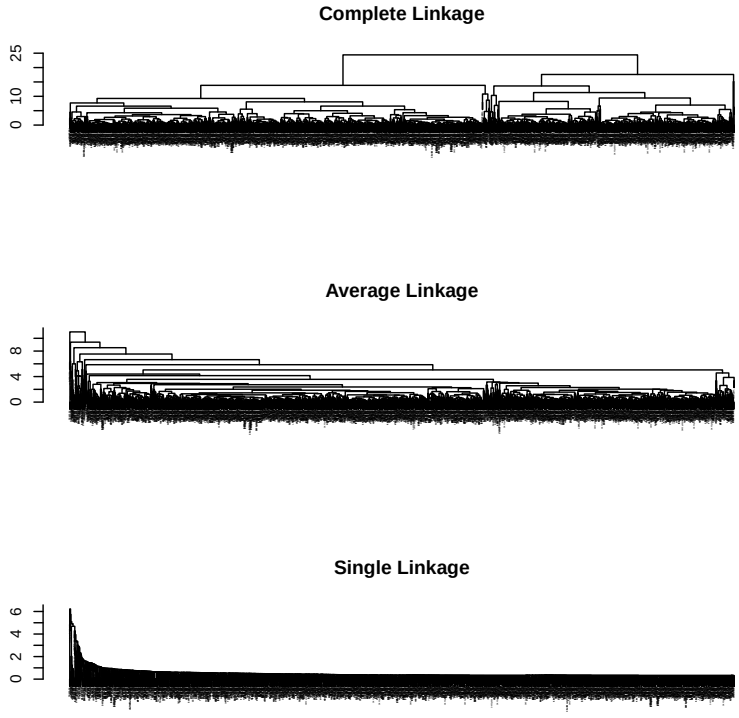
□

3. Create hierarchical clustering with respect to times (i.e. cluster the columns). How does time points cluster with each other? Does it make sense?

Solution. Let us have a look at the dataset to generate some perspective:

```
            0        30m        1hr       6hrs      24hrs
SFRS4;118;  0  0.5753123  0.6229304  0.5058909 -1.1844246
SFRS4;119;  0  0.5753123  0.7224660  0.5058909 -1.1844246
PPP2R5D;88; 0 -0.6665763 -1.3219281 -0.3219281  0.4329594
PPP2R5D;89; 0 -0.6214884 -1.4344028 -0.2688168  0.2986583
PPP2R5D;90; 0 -0.6214884 -1.4344028 -0.4150375  0.2986583
PPP2R5D;95; 0 -0.6214884 -1.4344028 -0.3219281  0.2986583

hc.clusters
   1    2    3    4    5
2121 1247   40    5    3
```



NB the t() function returns the transpose of a matrix

□

4. Install package "e1071" and apply c-means clustering to partition the data in to 9 groups ($c = 9$) with respect to phosphorylation sites (i.e. partition rows into c groups). Firstly, standardise the data to be unit free.

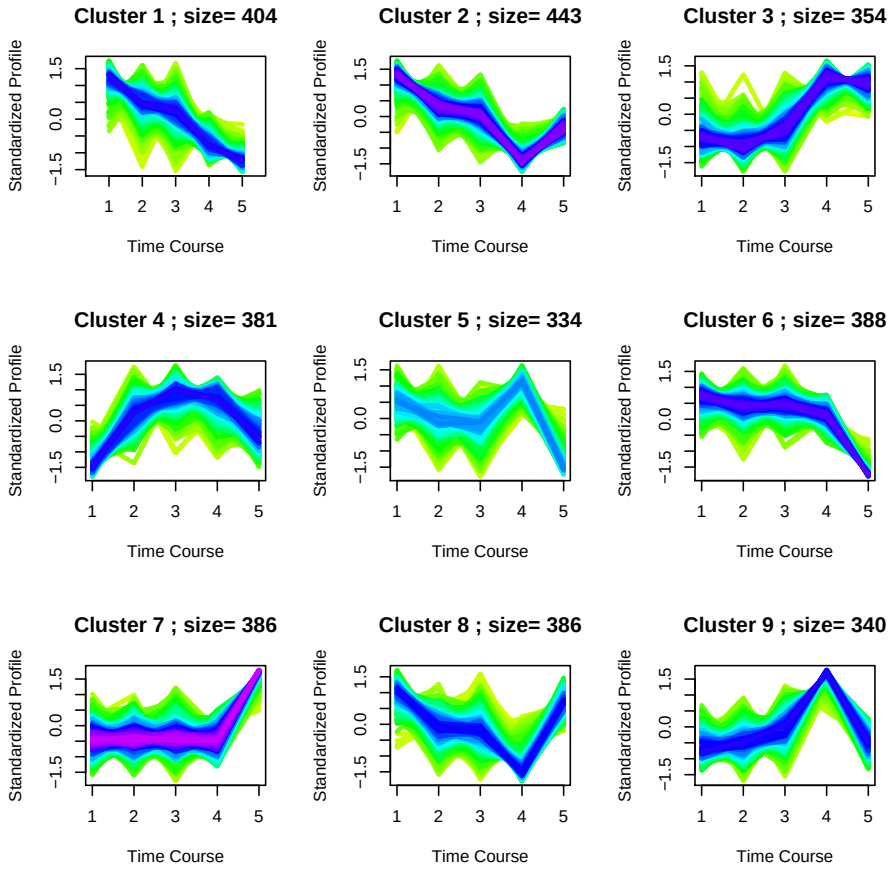
```
> standardize <- function(mat) {
+ means <- apply(mat, 1, mean)
+ stds <- apply(mat, 1, sd)
+ tmp <- sweep(mat, 1, means, FUN="-")
+ mat.stand <- sweep(tmp, 1, stds, FUN="/")
+ return(mat.stand)
+ }
> hES.scaled <- standardize(hES)
```

Once the data is standardised the data to be unit free, perform clustering.

```
> library(e1071)
> fc <- cmeans(hES.scaled, centers=9)
```

Visualise the clustering results using ClueR package function "fuzzPlot" as follows:

```
> fuzzPlot(hES.scaled, fc, mfrow = c(3, 3))
```



Solution. □

5. Is $k = 9$ the best choice of k? Apply Dunn index to validate k-means clustering using different k values. Which K gives best clustering results according to Dunn index? Does it differ if we use other validation index such as Connectivity or APN?

Solution. Let us quickly generate the dunn index for the dataset for differing k values:

```
> library(cluster)
> library(clValid)
> intern <- clValid(hES.scaled, nClust=2:9, validation=c("internal", "stability"), clMethods=
> summary(intern)

Clustering Methods:
 kmeans

Cluster sizes:
 2 3 4 5 6 7 8 9

Validation Measures:
```

```
                          2        3        4        5        6        7        8        9

kmeans APN             0.2125   0.2323   0.2781   0.3804   0.3788   0.3941   0.4789   0.4774
       AD              2.3322   2.0901   1.9332   1.9398   1.8315   1.7491   1.7392   1.7008
       ADM             0.6133   0.5991   0.6283   0.8393   0.7811   0.7722   0.9256   0.9159
       FOM             0.8531   0.8155   0.7979   0.7923   0.7354   0.7176   0.7167   0.6926
       Connectivity  210.3500 332.8917 395.2639 427.1460 495.8353 516.9726 576.8060 639.4250
       Dunn            0.0289   0.0158   0.0246   0.0037   0.0121   0.0130   0.0159   0.0253
       Silhouette      0.3086   0.2974   0.2833   0.2893   0.2932   0.3041   0.2768   0.2685

Optimal Scores:

               Score    Method Clusters
APN             0.2125 kmeans 2
AD              1.7008 kmeans 9
ADM             0.5991 kmeans 3
FOM             0.6926 kmeans 9
Connectivity  210.3500 kmeans 2
Dunn            0.0289 kmeans 2
Silhouette      0.3086 kmeans 2
```

As we can see, in Dunn Index, Silhouette and APN, the optimal score is 2 clusters. (We recall that Dunn index is between $[0, \infty)$) and should be maximised. In contrast connectivity should be miniised with APN between 0 and 1 and minimial values indicating consistent clustering. □