Introduction to Clustering

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Contents

1 Introduction

1.1 Objective

Objective: grouping of observations into **clusters**, so that

- similar observations appear in the same cluster
- dissimilar observations appear in distinct clusters

$\longrightarrow$ need for a measure for **similarity** and **dissimilarity**?

1.2 Example 1

Single cell transcriptomics: $n \times p$ Matrix for which

- every column contains the expression levels of one of p genes for n cells
- every row contains the expression levels of p genes for one cell (**sample**)
- Research question: look for groups of cells that have similar gene expression patterns

- Or, look for groups of genes that have similar expression levels across the different cells. This can help us in understanding the regulation and functionality of the genes.

$\longrightarrow$ both **observations** (rows) and **variables** (columns) can be clustered

1.3 Example 2

Abundance studies: the abundances of n plant species are counted on p plots (habitats)

- look for groups that contain species that live in the same habitats, or, look for groups of habitats that have similar species communities

$\longrightarrow$ both **observations** (rows) and **variables** (columns) can be clustered

2 Partition Based Cluster Analysis

- Partition based cluster methods require the number of clusters (k) to be specified prior to the start of the algorithm.

2.1 K-means Methods

- To use the k-means clustering algorithm we have to pre-define k, the number of clusters we want to define.
- The k-means algorithm is iterative.
- The algorithm starts by defining k cluster centers (centroids).
- Then the algorithm proceeds as follows
  1. First each observation is assigned to the cluster with the closest center to that observation.
  2. Then the k centers are redefined using the observations in each cluster, i.e. the multivariate means (column means) of all observations in a cluster are used to define each new cluster center.
  3. We repeat these two steps until the centers converge.

2.2 Example

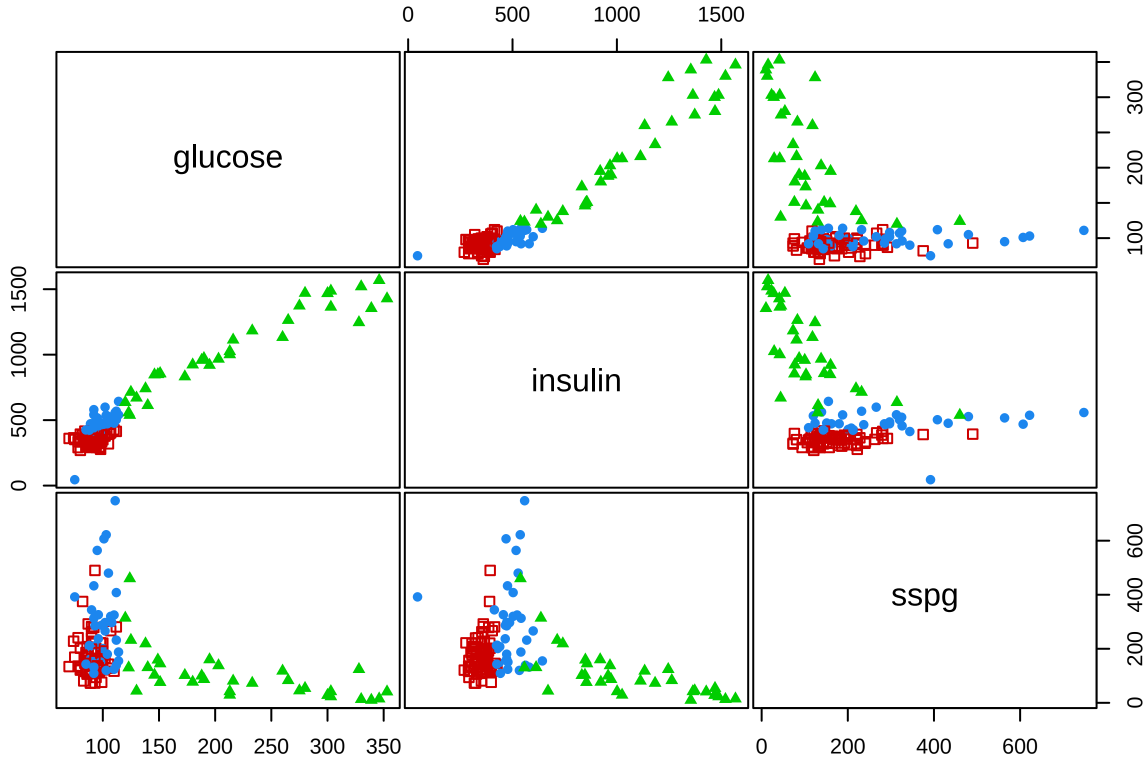
```r
library(tidyverse)
data(diabetes,package = "mclust")
class <- diabetes$class
table(class)
```

```
#> class
#> Chemical   Normal    Overt
#>       36       76       33
```

```r
head(diabetes)
```

```
#>    class glucose insulin sspg
#> 1 Normal      80     356  124
#> 2 Normal      97     289  117
#> 3 Normal     105     319  143
#> 4 Normal      90     356  199
#> 5 Normal      90     323  240
#> 6 Normal      86     381  157
```

```r
mclust::clPairs(diabetes[,-1], diabetes$class)
```

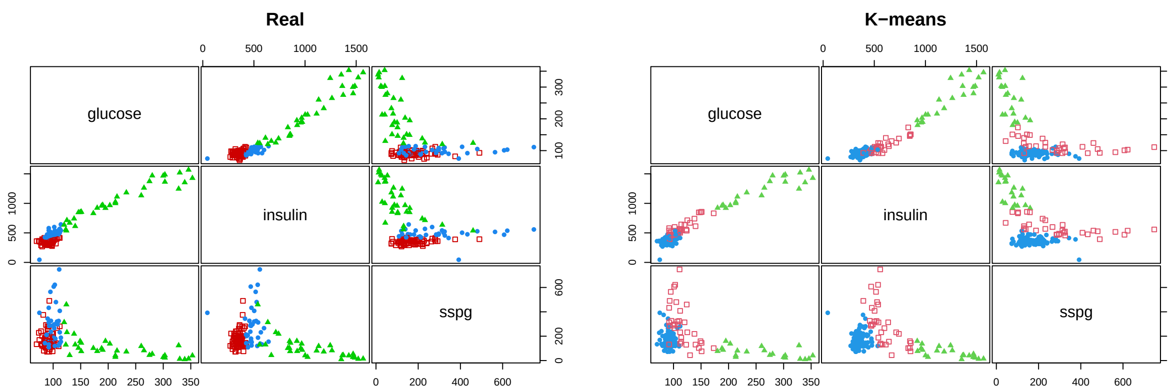



```r
diabetesKmeans <- kmeans(diabetes[,-1], centers = 3)
diabetesKmeans
```

```
#> K-means clustering with 3 clusters of sizes 34, 21, 90
#>
#> Cluster means:
#>     glucose   insulin      sspg
#> 1 115.73529  591.1176 294.97059
#> 2 262.52381 1225.5238  65.85714
#> 3  91.55556  362.0000 173.05556
#>
#> Clustering vector:
#>   1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
#>   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3
#>  21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36  37  38  39  40
#>   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3
#>  41  42  43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60
#>   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3
#>  61  62  63  64  65  66  67  68  69  70  71  72  73  74  75  76  77  78  79  80
#>   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3
#>  81  82  83  84  85  86  87  88  89  90  91  92  93  94  95  96  97  98  99 100
#>   3   1   3   3   3   1   1   1   1   1   1   1   1   1   1   3   1   1   1   1
#> 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
#>   1   1   3   3   3   1   1   1   1   3   1   3   2   2   1   2   2   2   1   2
#> 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140
#>   1   2   2   1   1   2   2   1   2   1   1   2   2   1   1   1   1   2   2   2
#> 141 142 143 144 145
```

```
#>   2   2   2   2   2
#> 
#> Within cluster sum of squares by cluster:
#> [1] 1571557.1 1098989.0  699088.9
#>  (between_SS / total_SS =  80.6 %)
#> 
#> Available components:
#> 
#> [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
#> [6] "betweenss"    "size"         "iter"         "ifault"
```

```
mclust::clPairs(diabetes[,-1], diabetes$class, main = "Real"); mclust::clPairs(diabetes[,-1], diabetesK
```



3 Hierarchical Cluster Analysis

- Distinction between agglomerative and divisive methods
- Agglomerative start from the situation where each individual observations forms its own cluster (so it starts with n clusters). In the next steps clusters are sequentially merged, until finally there is only one cluster with n observations.
- Divisive methods work just the other way around.
- The solution of an hierarchical clustering is thus a sequence of n nested cluster solutions.

3.1 General Algorithm of Agglomerative Hierarchical Clustering

- In step 0 each observations is considered as a cluster (i.e. n clusters).
- Every next step consists of:
    1. merge the two clusters with the smallest intercluster dissimilarity
    2. recalculate the intercluster dissimilarities

In step 0 the intercluster dissimilarity coincides with the dissimilarity between the corresponding observations

$\rightarrow$ intercluster dissimilarity?

3.2 Intercluster Dissimilarities

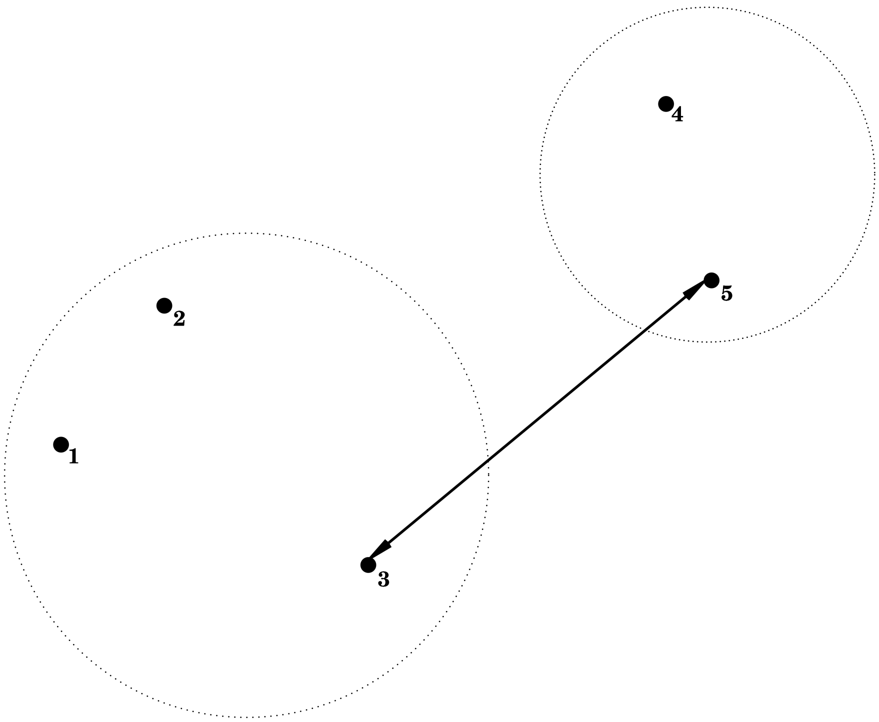
- Represent clusters (e.g. C_1 and C_2) as sets of points $\mathbf{x}_i$ which belong to that cluster
- $d(C_1, C_2)$: intercluster dissimilarity between

We consider three intercluster dissimilarities.

3.2.1 Single Linkage = Nearest Neighbour

$$d(C_1, C_2) = \min_{\mathbf{x}_1 \in C_1; \mathbf{x}_2 \in C_2} d(\mathbf{x}_1, \mathbf{x}_2),$$

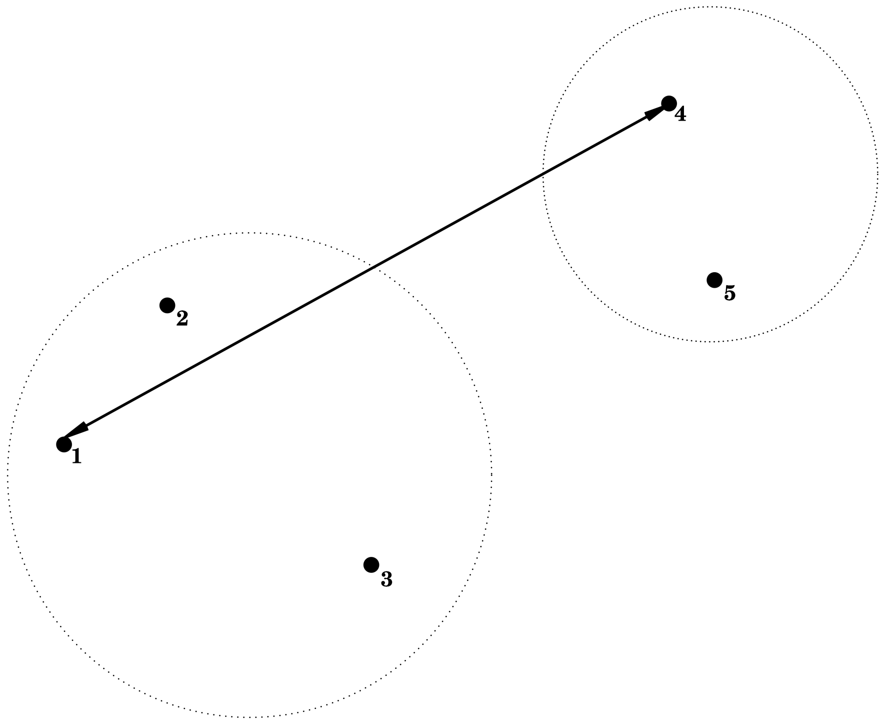
i.e. the dissimilarity between C_1 and C_2 is determined by the smallest dissimilarity between a point of C_1 and a point of C_2.



3.2.2 Complete Linkage = Furthest Neighbour

$$d(C_1, C_2) = \max_{\mathbf{x}_1 \in C_1; \mathbf{x}_2 \in C_2} d(\mathbf{x}_1, \mathbf{x}_2),$$

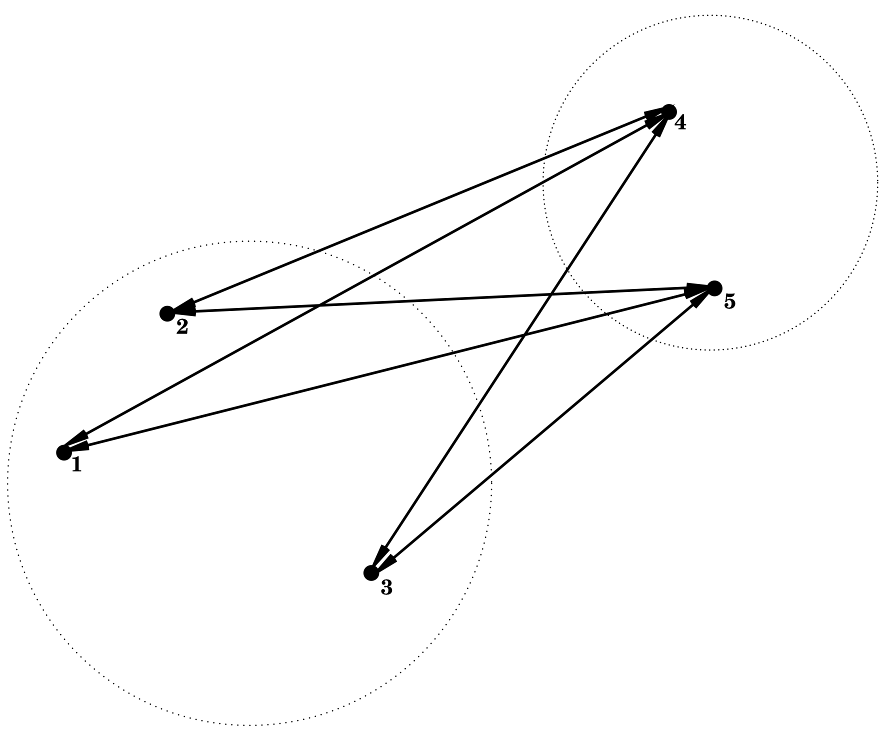
i.e. the dissimilarity between C_1 and C_2 is determined by the largest dissimilarity between a point of C_1 and a point of C_2.



3.2.3 Average Linkage = Group Average

$$d(C_1, C_2) = \frac{1}{|C_1||C_2|} \sum_{\mathbf{x}_1 \in C_1; \mathbf{x}_2 \in C_2} d(\mathbf{x}_1, \mathbf{x}_2),$$

i.e. the dissimilarity between C_1 and C_2 is determined by the average dissimilarity between all points of C_1 and all points of C_2.



3.3 Cluster Tree

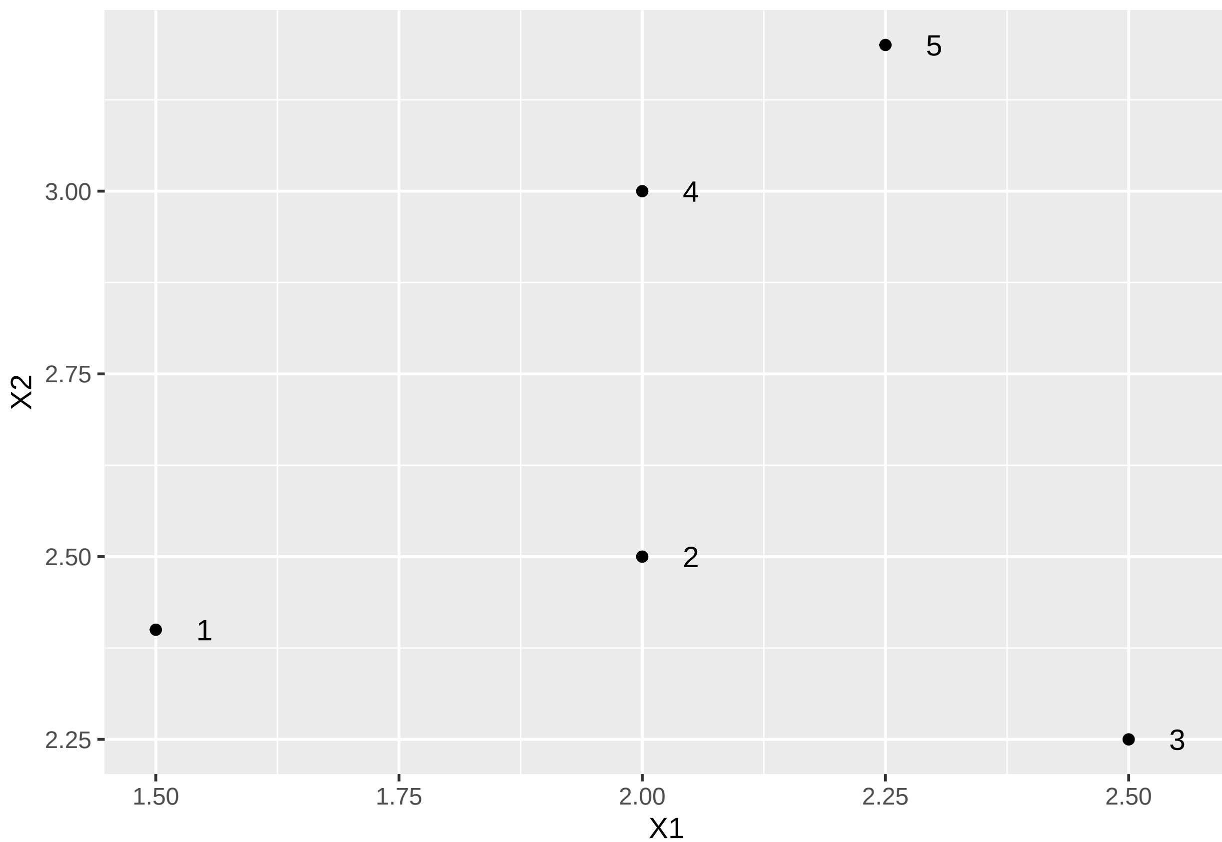
Hierarchical nature of the algorithm:

- Nested sequence of clusters $\longrightarrow$ visualisation via a tree
- Height of branches indicate the intercluster dissimilarity at which clusters are merged.
- Can used as instrument for deciding the number of clusters in the data

4 Toy example

X1	X2	label
1.50	2.40	1
2.00	2.50	2
2.50	2.25	3
2.00	3.00	4
2.25	3.20	5

```r
toy %>%
  ggplot(aes(X1, X2, label = label)) +
  geom_point() +
  geom_text(nudge_x = .05)
```



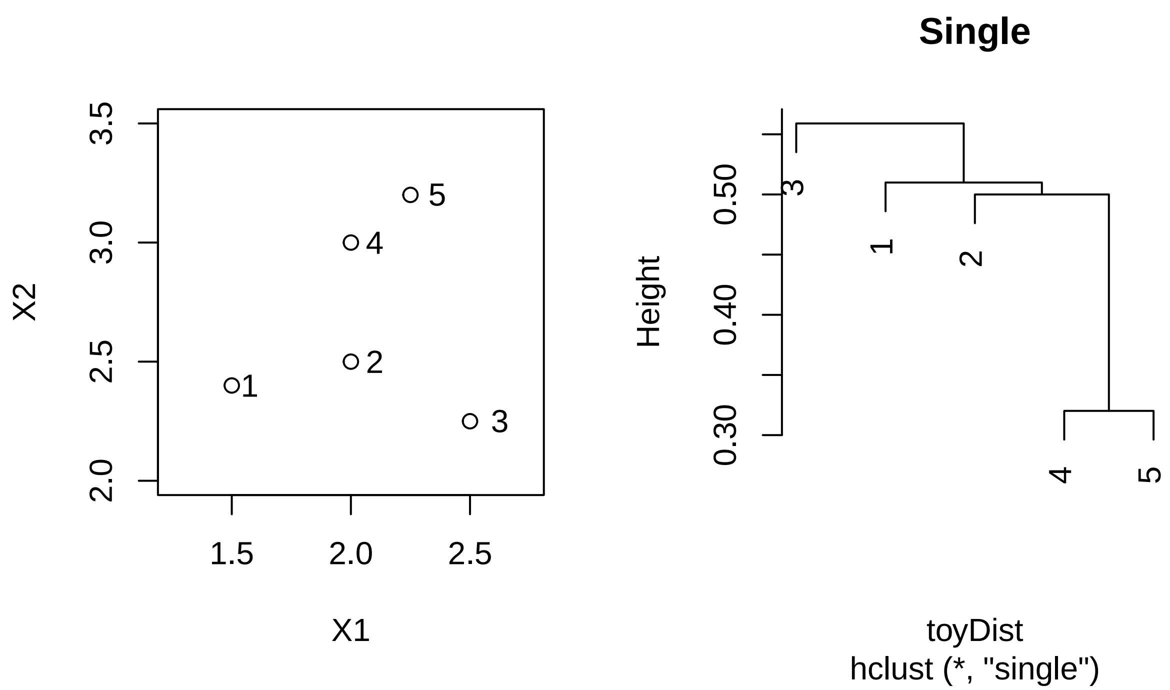

```r
toy[,1:2] %>% dist
```

```
#>           1         2         3         4
#> 2 0.5099020
```

```
#> 3 1.0111874 0.5590170
#> 4 0.7810250 0.5000000 0.9013878
#> 5 1.0965856 0.7433034 0.9823441 0.3201562
```

4.1 Single linkage

```
toyDist <- toy[,1:2] %>% dist
toySingle <- hclust(toyDist, method = "single")
par(mfrow=c(1,2),pty="s")
plot(X2 ~ X1, toy, xlim = c(1.25,2.75),ylim = c(2,3.5))
text(toy$X1*1.05,toy$X2,label=toy$label)
plot(toySingle, main = "Single")
```



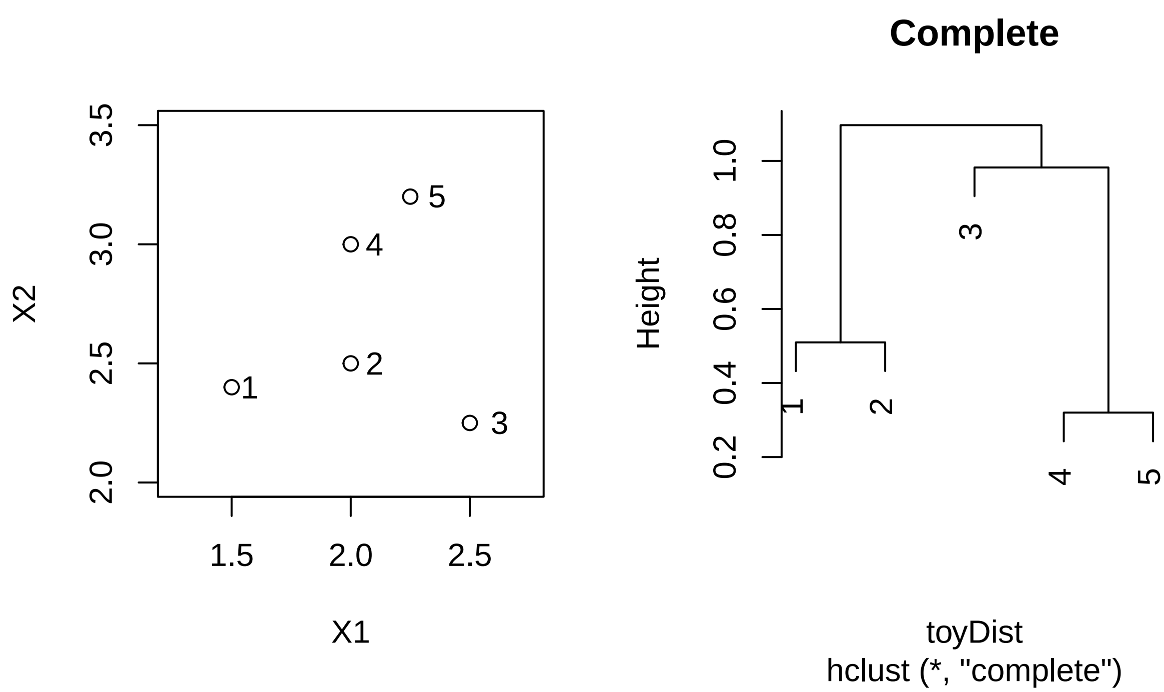

```
toyDist
```

```
#>           1         2         3         4
#> 2 0.5099020
#> 3 1.0111874 0.5590170
#> 4 0.7810250 0.5000000 0.9013878
#> 5 1.0965856 0.7433034 0.9823441 0.3201562
```

4.2 Complete linkage

```
toyComplete <- hclust(toyDist, method = "complete")
par(mfrow=c(1,2),pty="s")
plot(X2 ~ X1, toy, xlim = c(1.25,2.75),ylim = c(2,3.5))
```

```r
text(toy$X1*1.05,toy$X2,label=toy$label)
plot(toyComplete,  main = "Complete")
```

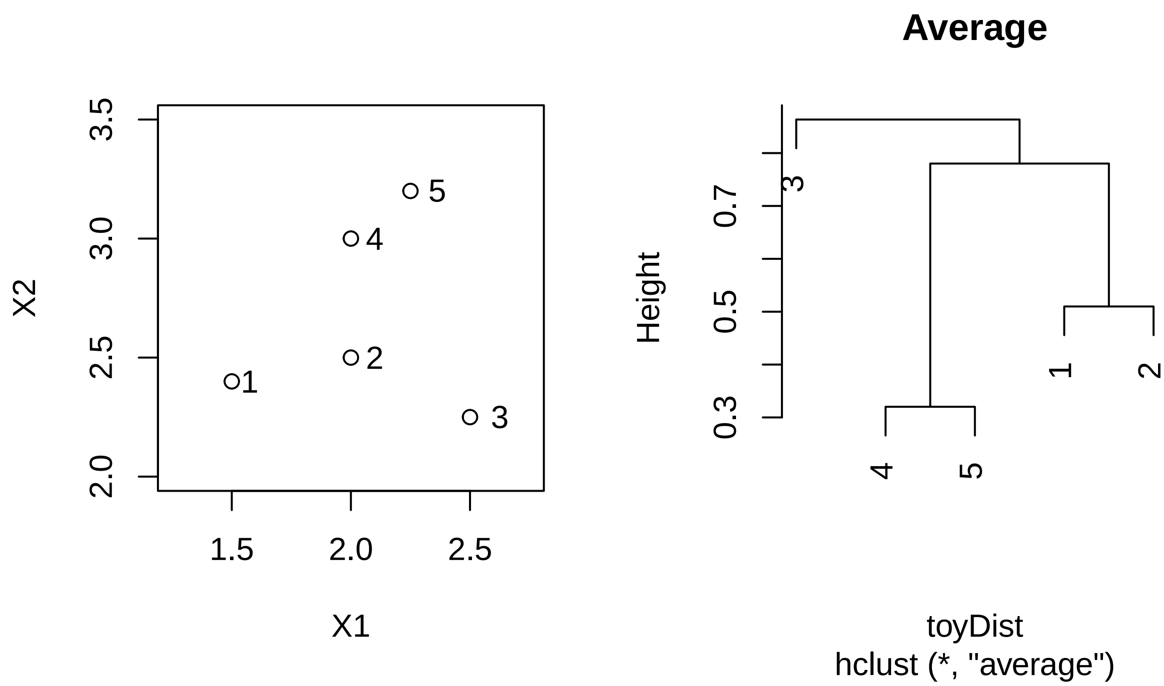



```r
toyDist
```

```
#>           1         2         3         4
#> 2 0.5099020
#> 3 1.0111874 0.5590170
#> 4 0.7810250 0.5000000 0.9013878
#> 5 1.0965856 0.7433034 0.9823441 0.3201562
```

4.3 Average linkage

```r
toyAvg <- hclust(toyDist, method = "average")
par(mfrow=c(1,2),pty="s")
plot(X2 ~ X1, toy, xlim = c(1.25,2.75),ylim = c(2,3.5))
text(toy$X1*1.05,toy$X2,label=toy$label)
plot(toyAvg, main = "Average")
```

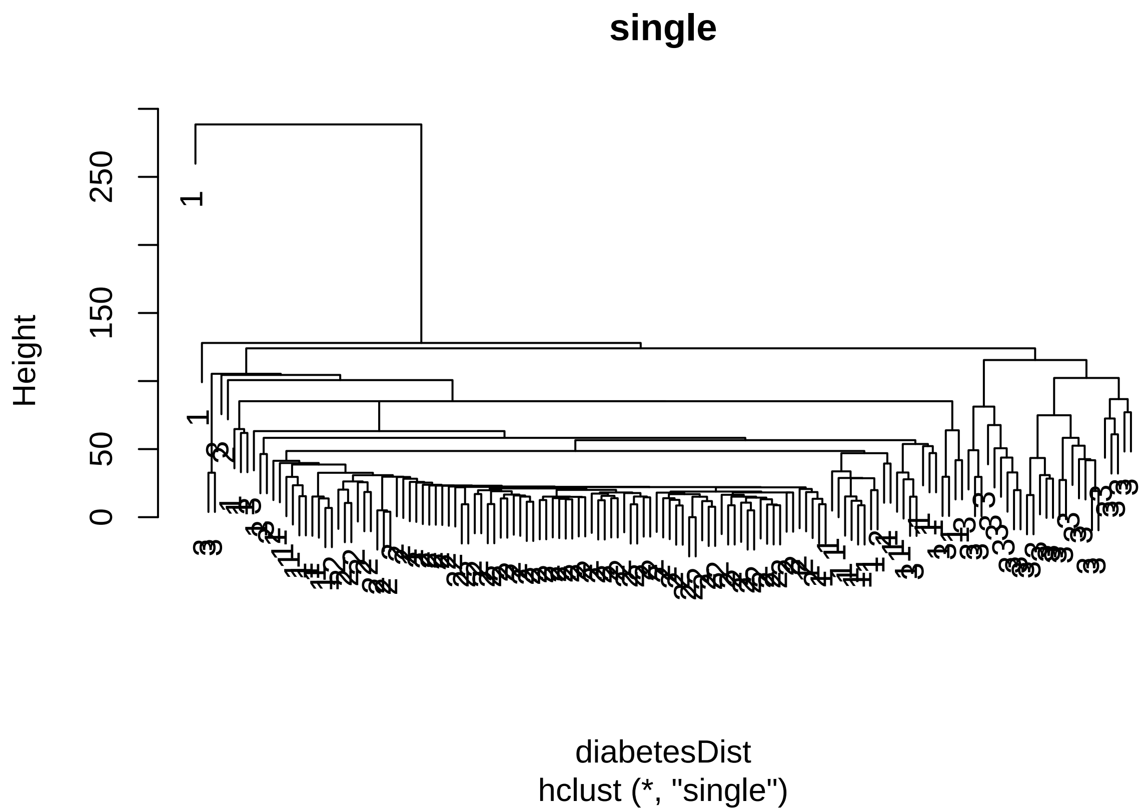



```
toyDist
```

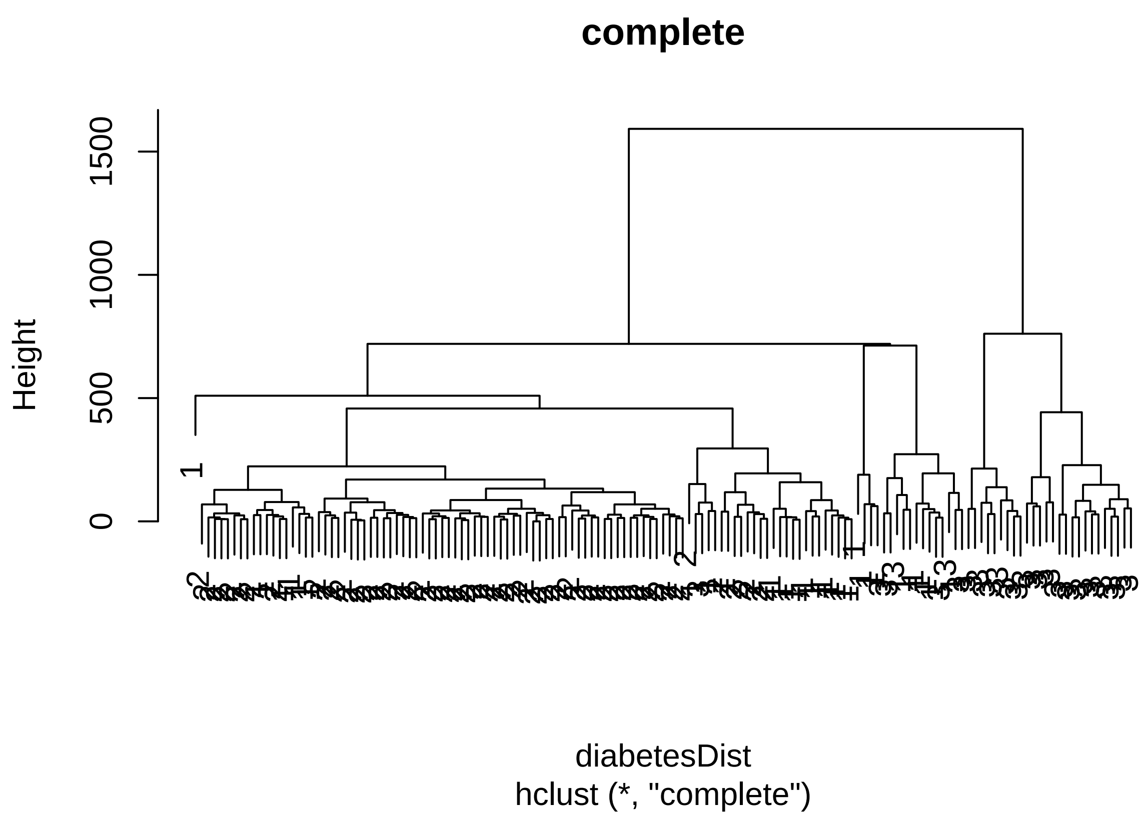
```
#>           1         2         3         4
#> 2 0.5099020
#> 3 1.0111874 0.5590170
#> 4 0.7810250 0.5000000 0.9013878
#> 5 1.0965856 0.7433034 0.9823441 0.3201562
```

4.4 Example

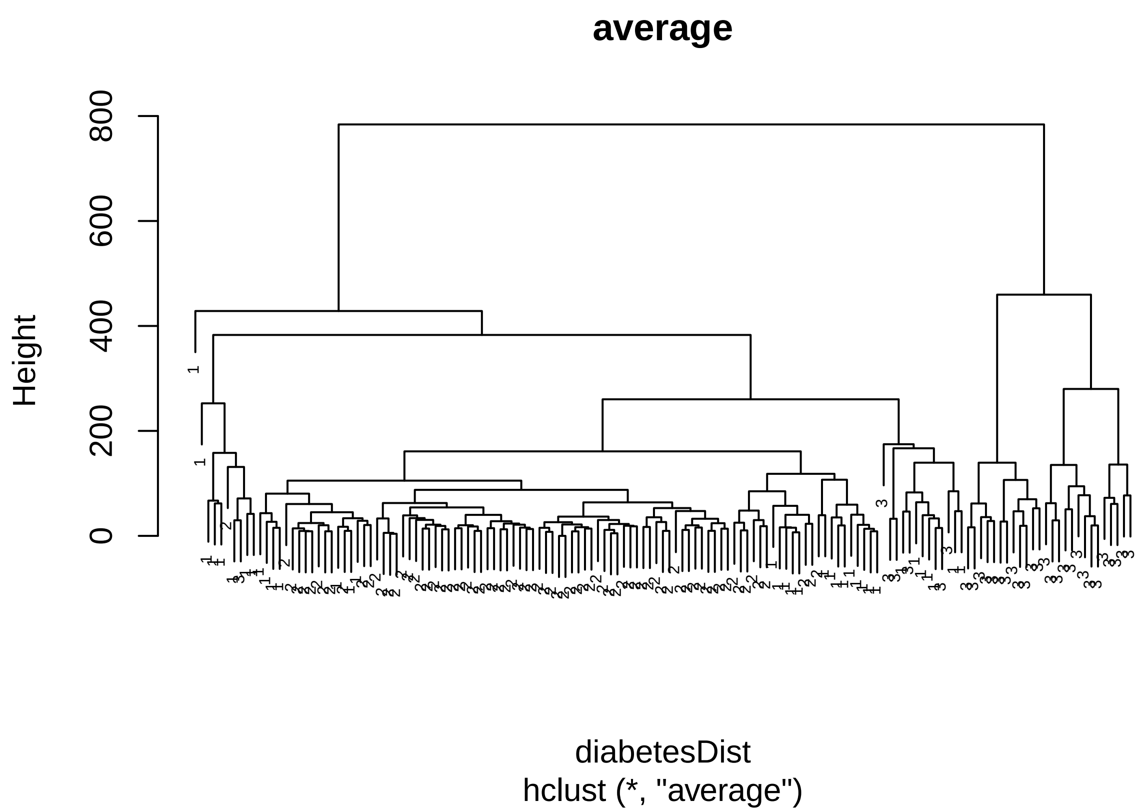
```
diabetesDist <- dist(diabetes[,-1])
diabetesSingle <- hclust(diabetesDist, method = "single")
plot(diabetesSingle, labels = as.double(diabetes$class), main="single")
```




```r
diabetesComplete <- hclust(diabetesDist, method = "complete")
plot(diabetesComplete, labels = as.double(diabetes$class), main="complete")
```




```r
diabetesAverage <- hclust(diabetesDist, method = "average")
plot(diabetesAverage, labels = as.double(diabetes$class), main = "average",cex=0.5)
```



5 Model-based clustering

- Paper: Fraley and Raftery (1998). How Many Clusters? Which Clustering Method? Answers Via Model-Based Cluster Analysis. The Computer Journal, (41)8:578-588.
- EM algorithm [PDF]
- Example: see tutorial session

Session info

Session info

```
#> [1] "2024-10-07 12:41:05 CEST"
```

```
#> - Session info ---------------------------------------------------------------
#>  setting  value
#>  version  R version 4.4.0 RC (2024-04-16 r86468)
#>  os       macOS Big Sur 11.6
#>  system   aarch64, darwin20
#>  ui       X11
#>  language (EN)
#>  collate  en_US.UTF-8
#>  ctype    en_US.UTF-8
#>  tz       Europe/Brussels
#>  date     2024-10-07
#>  pandoc   3.1.1 @ /Applications/RStudio.app/Contents/Resources/app/quarto/bin/tools/ (via rmarkdown)
```

```
#>
#> - Packages -------------------------------------------------------------------
#>  package     * version date (UTC) lib source
#>  bookdown      0.40    2024-07-02 [1] CRAN (R 4.4.0)
#>  bslib         0.8.0   2024-07-29 [1] CRAN (R 4.4.0)
#>  cachem        1.1.0   2024-05-16 [1] CRAN (R 4.4.0)
#>  cli           3.6.3   2024-06-21 [1] CRAN (R 4.4.0)
#>  colorspace    2.1-1   2024-07-26 [1] CRAN (R 4.4.0)
#>  digest        0.6.37  2024-08-19 [1] CRAN (R 4.4.1)
#>  dplyr       * 1.1.4   2023-11-17 [1] CRAN (R 4.4.0)
#>  evaluate      1.0.0   2024-09-17 [1] CRAN (R 4.4.1)
#>  fansi         1.0.6   2023-12-08 [1] CRAN (R 4.4.0)
#>  farver        2.1.2   2024-05-13 [1] CRAN (R 4.4.0)
#>  fastmap       1.2.0   2024-05-15 [1] CRAN (R 4.4.0)
#>  fontawesome   0.5.2   2023-08-19 [1] CRAN (R 4.4.0)
#>  forcats     * 1.0.0   2023-01-29 [1] CRAN (R 4.4.0)
#>  generics      0.1.3   2022-07-05 [1] CRAN (R 4.4.0)
#>  ggplot2     * 3.5.1   2024-04-23 [1] CRAN (R 4.4.0)
#>  glue          1.8.0   2024-09-30 [1] CRAN (R 4.4.1)
#>  gtable        0.3.5   2024-04-22 [1] CRAN (R 4.4.0)
#>  highr         0.11    2024-05-26 [1] CRAN (R 4.4.0)
#>  hms           1.1.3   2023-03-21 [1] CRAN (R 4.4.0)
#>  htmltools     0.5.8.1 2024-04-04 [1] CRAN (R 4.4.0)
#>  jquerylib     0.1.4   2021-04-26 [1] CRAN (R 4.4.0)
#>  jsonlite      1.8.9   2024-09-20 [1] CRAN (R 4.4.1)
#>  knitr         1.48    2024-07-07 [1] CRAN (R 4.4.0)
#>  labeling      0.4.3   2023-08-29 [1] CRAN (R 4.4.0)
#>  lifecycle     1.0.4   2023-11-07 [1] CRAN (R 4.4.0)
#>  lubridate   * 1.9.3   2023-09-27 [1] CRAN (R 4.4.0)
#>  magrittr      2.0.3   2022-03-30 [1] CRAN (R 4.4.0)
#>  mclust        6.1.1   2024-04-29 [1] CRAN (R 4.4.0)
#>  munsell       0.5.1   2024-04-01 [1] CRAN (R 4.4.0)
#>  pillar        1.9.0   2023-03-22 [1] CRAN (R 4.4.0)
#>  pkgconfig     2.0.3   2019-09-22 [1] CRAN (R 4.4.0)
#>  purrr       * 1.0.2   2023-08-10 [1] CRAN (R 4.4.0)
#>  R6            2.5.1   2021-08-19 [1] CRAN (R 4.4.0)
#>  readr       * 2.1.5   2024-01-10 [1] CRAN (R 4.4.0)
#>  rlang         1.1.4   2024-06-04 [1] CRAN (R 4.4.0)
#>  rmarkdown     2.28    2024-08-17 [1] CRAN (R 4.4.0)
#>  rstudioapi    0.16.0  2024-03-24 [1] CRAN (R 4.4.0)
#>  sass          0.4.9   2024-03-15 [1] CRAN (R 4.4.0)
#>  scales        1.3.0   2023-11-28 [1] CRAN (R 4.4.0)
#>  sessioninfo   1.2.2   2021-12-06 [1] CRAN (R 4.4.0)
#>  stringi       1.8.4   2024-05-06 [1] CRAN (R 4.4.0)
#>  stringr     * 1.5.1   2023-11-14 [1] CRAN (R 4.4.0)
#>  tibble      * 3.2.1   2023-03-20 [1] CRAN (R 4.4.0)
#>  tidyr       * 1.3.1   2024-01-24 [1] CRAN (R 4.4.0)
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#>  tidyverse   * 2.0.0   2023-02-22 [1] CRAN (R 4.4.0)
#>  timechange    0.3.0   2024-01-18 [1] CRAN (R 4.4.0)
#>  tzdb          0.4.0   2023-05-12 [1] CRAN (R 4.4.0)
#>  utf8          1.2.4   2023-10-22 [1] CRAN (R 4.4.0)
#>  vctrs         0.6.5   2023-12-01 [1] CRAN (R 4.4.0)
#>  withr         3.0.1   2024-07-31 [1] CRAN (R 4.4.0)
```

```
#>  xfun          0.47    2024-08-17 [1] CRAN (R 4.4.0)
#>  yaml          2.3.10  2024-07-26 [1] CRAN (R 4.4.0)
#>
#>  [1] /Library/Frameworks/R.framework/Versions/4.4-arm64/Resources/library
#>
#> ------------------------------------------------------------------------------
```