Section 2
Unsupervised Learning:
Hierarchical Clustering

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11752 Aprendizaje Automático
11752 Machine Learning
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en Sistemas Inteligentes

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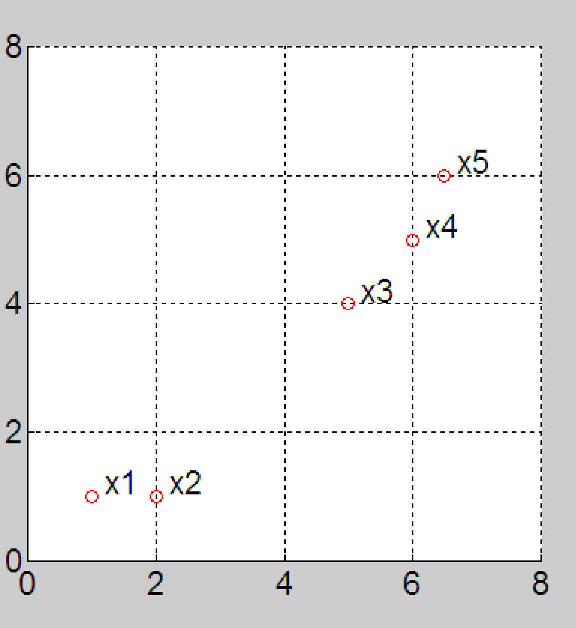
Contents

- Introduction
- Agglomerative clustering
- Divisive clustering
- Selection of a good clustering

Introduction

- Given a set of samples X, these algorithms produce a **set of clusterings**, not just one



R_0 : $\{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}, \{x_5\}$

R_1 : $\{x_1, x_2\}, \{x_3\}, \{x_4\}, \{x_5\}$

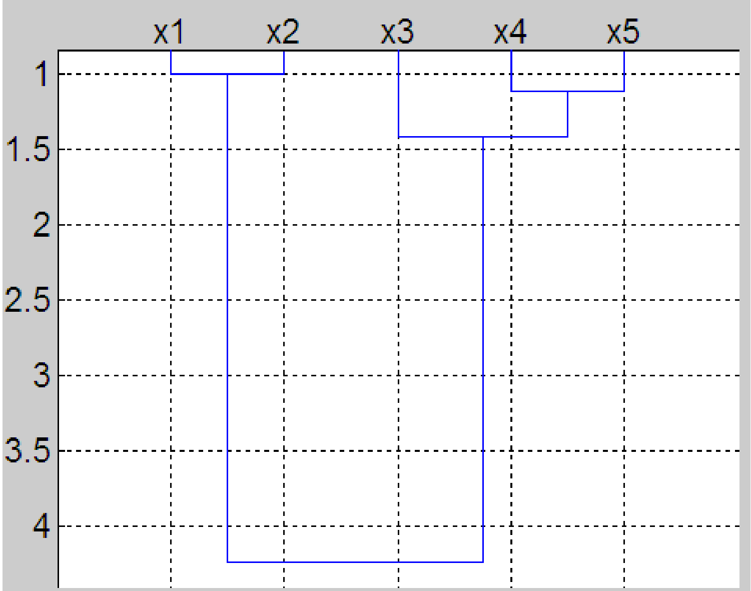
R_2 : $\{x_1, x_2\}, \{x_3\}, \{x_4, x_5\}$

R_3 : $\{x_1, x_2\}, \{x_3, x_4, x_5\}$

R_4 : $\{x_1, x_2, x_3, x_4, x_5\}$

Actually, it is a **hierarchy of clusterings,** as they can be considered **nested**:

$R_0 \subset R_1 \subset R_2 \subset R_3 \subset R_4 \subset R_5$



DENDROGRAM (binary tree)

- N samples ⇒ **N-level** hierarchy – **N** execution steps
- Essentially, two sorts of hierarchical clustering algorithms:
  - **Agglomerative** — $\{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}, \{x_5\} \to \{x_1, x_2, x_3, x_4, x_5\}$ (bottom-up process)
  - **Divisive** — $\{x_1, x_2, x_3, x_4, x_5\} \to \{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}, \{x_5\}$ (top-down process)
  - both are just heuristic, **not optimal**, i.e. they do not optimize any objective function
  - a hierarchy of clusterings is produced even if there is no structure in the data

Contents

- Introduction
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- Divisive clustering
- Selection of a good clustering

Agglomerative clustering

- Generic algorithm:

```
(1) $\mathcal{R}_0 = \{C_i = \{x_i\}, i = 1, \ldots, N\}$
(2) $t = 0$
(3) **repeat**
    (3.1) Choose the pair of **clusters** $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that

          $\wp(C_r, C_s) = \begin{cases} \min\limits_{i,j}\{\wp(C_i, C_j)\} & \wp \text{ is DM} \\ \max\limits_{i,j}\{\wp(C_i, C_j)\} & \wp \text{ is SM} \end{cases}$

    (3.2) $\mathcal{R}_{t+1} = (\mathcal{R}_t - \{C_r, C_s\}) \bigcup \{C_r \bigcup C_s\}$
    (3.3) $t = t + 1$
    **until** all samples are in a single **cluster**
```

OBSERVATIONS:

- when two samples get in the same cluster, they keep together until the end
- there is no way to recover from a bad merge

Agglomerative clustering

- At the level **t**, there are **N-t** clusters. therefore, one has to analyze:

$$\binom{N-t}{2} = \frac{(N-t)!}{2!(N-t-2)!} = \frac{(N-t)(N-t-1)}{2}$$

clusters to find the best merge for level **t+1**.

- The number of merges which have to be considered up to the end of the process can be easily calculated:

$$\sum_{t=0}^{N-1} \binom{N-t}{2} = \sum_{k=1}^{N} \binom{k}{2} = \sum_{k=1}^{N} \frac{k(k-1)}{2} = \frac{1}{2}\left(\sum_{k=1}^{N} k^2 - \sum_{k=1}^{N} k\right)$$

$$= \frac{1}{2}\left(\frac{N(N-1)(2N-1)}{12} - \frac{N(N-1)}{2}\right)$$

$$= \mathcal{O}(N^3)$$

$t = 0, \ldots, N-1$

$\Rightarrow k = N - t = 1, 2, \ldots, N$

This gives an idea of the complexity of the process.

Agglomerative clustering

- From an implementation point of view, there are two main approaches of agglomerative clustering:
  - ☞ based on **matrix** concepts
  - based on **graph** theory
  - We will consider the first approach. Some previous concepts first:
    - **data matrix**:

$$D(X) = \begin{array}{cc} \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1L} \\ x_{21} & x_{22} & \dots & x_{2L} \\ \vdots & \vdots & & \vdots \\ x_{N1} & x_{N2} & \dots & x_{NL} \end{bmatrix} & \begin{matrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{matrix} \end{array}$$

    - **proximity matrix**: (e.g. dissimilarity matrix)
      - point of departure for dendrogram construction

$$P(X) = \begin{bmatrix} \wp(x_1, x_1) & \wp(x_1, x_2) & \dots & \wp(x_1, x_N) \\ \wp(x_2, x_1) & \wp(x_2, x_2) & \dots & \wp(x_2, x_N) \\ \vdots & \vdots & & \vdots \\ \wp(x_N, x_1) & \wp(x_N, x_2) & \dots & \wp(x_N, x_N) \end{bmatrix}$$

Agglomerative clustering

- **Example**:
  - given X = {x_1,x_2,x_3,x_4,x_5} such that $D(X) = \begin{bmatrix} \boxed{1 \quad 1} \\ 2 \quad 1 \\ \boxed{5 \quad 4} \\ 6 \quad 5 \\ 6.5 \quad 6 \end{bmatrix}$

$$\sqrt{(5-1)^2 + (4-1)^2} = 5$$

  - [1] Using the **Euclidean distance**, the proximity matrix (**dissimilarity**) is
    - notice the diagonal elements are **0**

$$P(X) = \begin{bmatrix} 0.00 & 1.00 & 5.00 & 6.40 & 7.43 \\ 1.00 & 0.00 & 4.24 & 5.66 & 6.73 \\ 5.00 & 4.24 & 0.00 & 1.41 & 2.50 \\ 6.40 & 5.66 & 1.41 & 0.00 & 1.12 \\ 7.43 & 6.73 & 2.50 & 1.12 & 0.00 \end{bmatrix}$$

  - [2] Using the **Tanimoto measure**, the proximity matrix (**similarity**) is
    - notice the diagonal elements are **1**

$$P(X) = \begin{bmatrix} 1.00 & 0.75 & 0.26 & 0.21 & 0.18 \\ 0.75 & 1.00 & 0.44 & 0.35 & 0.30 \\ 0.26 & 0.44 & 1.00 & 0.96 & 0.90 \\ 0.21 & 0.35 & 0.96 & 1.00 & 0.98 \\ 0.18 & 0.30 & 0.90 & 0.98 & 1.00 \end{bmatrix}$$

Agglomerative clustering

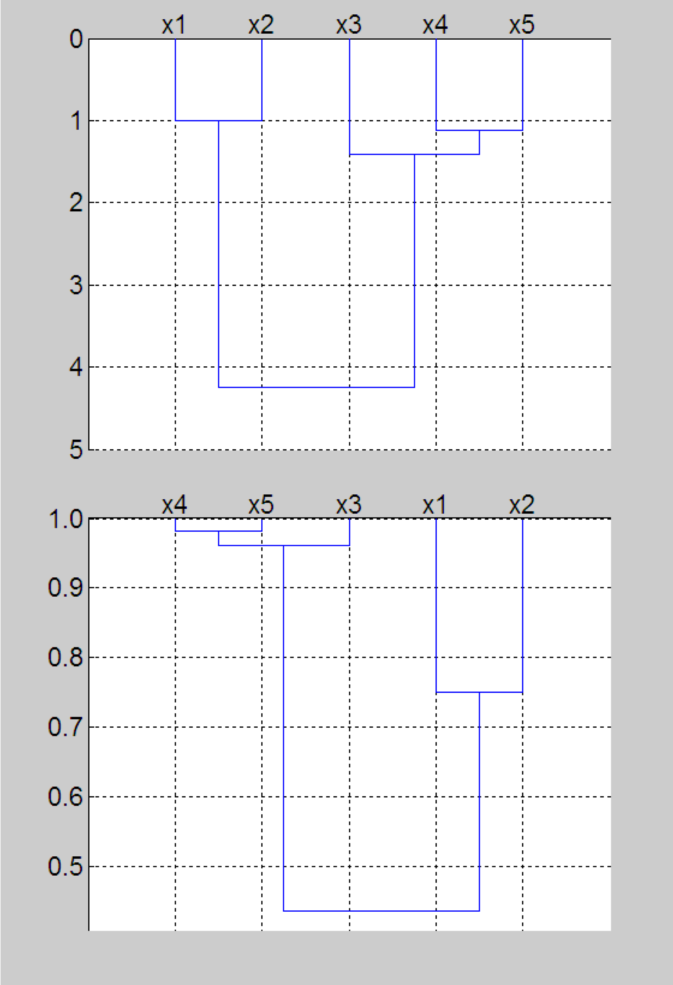
- **Example**: dendrograms for $\wp(C_1, C_2) = \min/\max_{a \in C_1, b \in C_2} \wp(a, b)$

[1] proximity function: **Euclidean distance** (d_2)

$$P(X) = \begin{bmatrix} 0.00 & 1.00 & 5.00 & 6.40 & 7.43 \\ 1.00 & 0.00 & 4.24 & 5.66 & 6.73 \\ 5.00 & 4.24 & 0.00 & 1.41 & 2.50 \\ 6.40 & 5.66 & 1.41 & 0.00 & 1.12 \\ 7.43 & 6.73 & 2.50 & 1.12 & 0.00 \end{bmatrix}$$

[2] proximity function: **Tanimoto similarity** (s_T)

$$P(X) = \begin{bmatrix} 1.00 & 0.75 & 0.26 & 0.21 & 0.18 \\ 0.75 & 1.00 & 0.44 & 0.35 & 0.30 \\ 0.26 & 0.44 & 1.00 & 0.96 & 0.90 \\ 0.21 & 0.35 & 0.96 & 1.00 & 0.98 \\ 0.18 & 0.30 & 0.90 & 0.98 & 1.00 \end{bmatrix}$$



dissimilarity dendrogram

↑

the sequence of mergings is different because $d_2 \neq 1 - s_T$!!

↓

similarity dendrogram

Agglomerative clustering

- **Example**: dendrogram for $\wp(C_1, C_2) = \min_{a \in C_1, b \in C_2} \wp(a, b)$

$$P_0 = \begin{bmatrix} 0.00 & \boxed{1.00} & 5.00 & 6.40 & 7.43 \\ 1.00 & 0.00 & 4.24 & 5.66 & 6.73 \\ 5.00 & 4.24 & 0.00 & 1.41 & 2.50 \\ 6.40 & 5.66 & 1.41 & 0.00 & 1.12 \\ 7.43 & 6.73 & 2.50 & 1.12 & 0.00 \end{bmatrix}$$

$C_6 = \{x_1, x_2\}$

$$P_1 = \begin{bmatrix} \cancel{0.00} & \cancel{1.00} & \cancel{5.00} & \cancel{6.40} & \cancel{7.43} & \cancel{-\!-} \\ \cancel{1.00} & \cancel{0.00} & \cancel{4.24} & \cancel{5.66} & \cancel{6.73} & \cancel{-\!-} \\ \cancel{5.00} & \cancel{4.24} & 0.00 & 1.41 & 2.50 & 4.24 \\ \cancel{6.40} & \cancel{5.66} & 1.41 & 0.00 & \boxed{1.12} & 5.66 \\ \cancel{7.43} & \cancel{6.73} & 2.50 & 1.12 & 0.00 & 6.73 \\ \cancel{-\!-} & \cancel{-\!-} & 4.24 & 5.66 & 6.73 & 0.00 \end{bmatrix}$$

(a) $d(C_3,C_6)$
(b) $d(C_4,C_6)$
(c) $d(C_5,C_6)$

$C_7 = \{x_4, x_5\}$

(a) = $\min\{d(x_3,x_1)5.00,\ d(x_3,x_2)4.24\}$
(b) = $\min\{d(x_4,x_1)6.40,\ d(x_4,x_2)5.66\}$
(c) = $\min\{d(x_5,x_1)7.43,\ d(x_5,x_2)6.73\}$

¡¡ this information is available from P_0 !!

Agglomerative clustering

- **Example**: dendrogram for $\wp(C_1, C_2) = \min_{a \in C_1, b \in C_2} \wp(a, b)$

$$P_2 = \begin{bmatrix} 0.00 & 1.00 & 5.00 & 6.40 & 7.43 & -- & -- \\ 1.00 & 0.00 & 4.24 & 5.66 & 6.73 & & \\ 5.00 & 4.24 & 0.00 & 1.41 & 2.50 & 4.24 & \boxed{1.41} \\ 6.40 & 5.66 & 1.41 & 0.00 & 1.12 & 5.66 & \\ 7.43 & 6.73 & 2.50 & 1.12 & 0.00 & 6.73 & -- \\ -- & -- & 4.24 & 5.66 & 6.73 & 0.00 & 5.66 \\ -- & -- & 1.41 & -- & -- & 5.66 & 0.00 \end{bmatrix}$$

(a) $d(C_3,C_7)$ → $C_8 = \{x_3, \{x_4, x_5\}\}$

(b) $d(C_6,C_7)$

(a) = min{$d(x_3,x_4)$1.41, $d(x_3,x_5)$2.50}

(b) = min{$d(x_1,x_4)$6.40, $d(x_1,x_5)$7.43, $d(x_2,x_4)$5.66, $d(x_2,x_5)$6.73}

Agglomerative clustering

- **Example**: dendrogram for $\wp(C_1, C_2) = \min_{a \in C_1, b \in C_2} \wp(a, b)$

$$P_3 = \begin{bmatrix} 0.00 & 1.00 & 5.00 & 6.40 & 7.43 & -- & -- & -- \\ 1.00 & 0.00 & 4.24 & 5.66 & 6.73 & & & \\ 5.00 & 4.24 & 0.00 & 1.41 & 2.50 & 4.24 & 1.41 & -- \\ 6.40 & 5.66 & 1.41 & 0.00 & 1.12 & 5.66 & -- & -- \\ 7.43 & 6.73 & 2.50 & 1.12 & 0.00 & 6.73 & & \\ -- & -- & 4.24 & 5.66 & 6.73 & 0.00 & 5.66 & \boxed{4.24} \\ & & 1.41 & & & 5.66 & 0.00 & \\ -- & -- & -- & -- & -- & 4.24 & -- & -- \end{bmatrix}$$

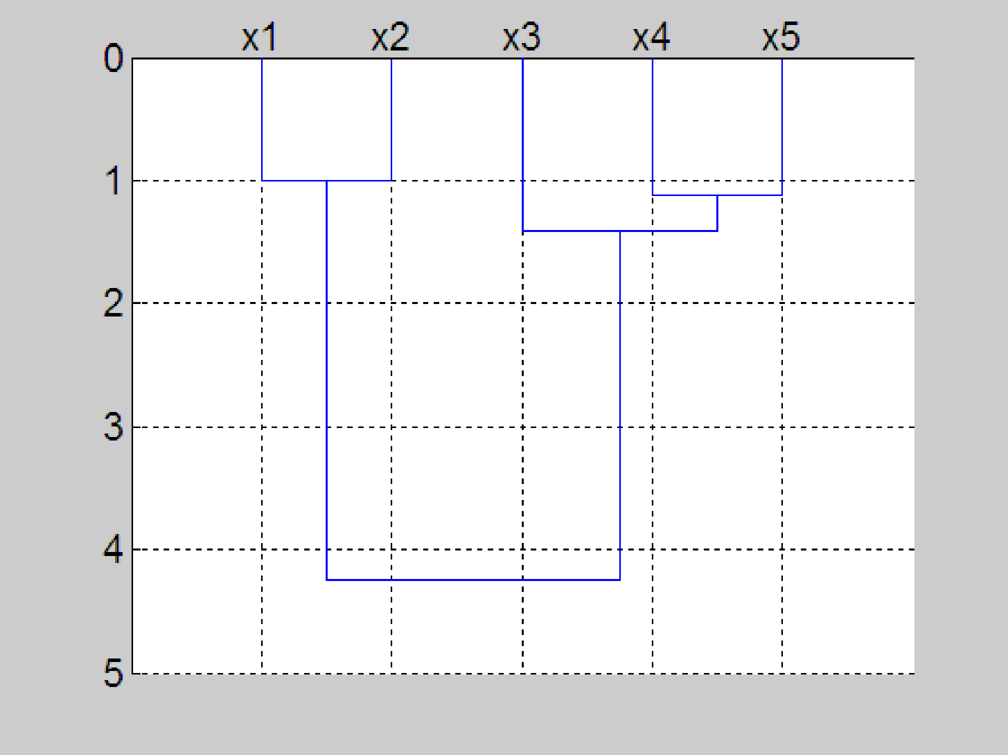
(a) d(C_6,C_8) $\rightarrow$ C_9 = {{x_1, x_2}, {x_3, {x_4, x_5}}}

(a) = min{d(x_1,x_3)5.00, d(x_1,x_4)6.40, d(x_1,x_5)7.43,
d(x_2,x_3)4.24, d(x_2,x_4)5.66, d(x_2,x_5)6.73}

Agglomerative clustering

- **Example**: dendrogram for $\wp(C_1, C_2) = \min_{a \in C_1, b \in C_2} \wp(a, b)$

$C_6 = \{x_1, x_2\}$ (1.00)
$C_7 = \{x_4, x_5\}$ (1.12)
$C_8 = \{x_3, \{x_4, x_5\}\}$ (1.41)
$C_9 = \{\{x_1, x_2\}, \{x_3, \{x_4, x_5\}\}\}$ (4.24)



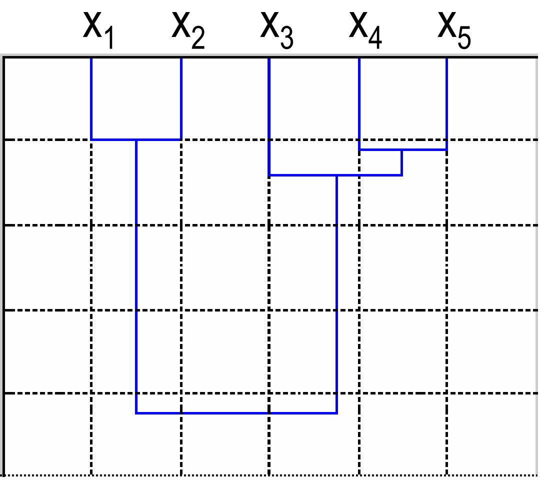
Agglomerative clustering

- In this way, the clustering algorithm turns out to be as follows:

```
(1) $\mathcal{R}_0 = \{C_i = \{x_i\}, i = 1, \ldots, N\}$
(2) $t = 0$
(3) repetir
    (3.1) Choose the pair of clusters $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that:
          $P_t(r,s) = \begin{cases} \min_{i,j} P_t(i,j) & P_t \text{ is DM} \\ \max_{i,j} P_t(i,j) & P_t \text{ is SM} \end{cases}$
    (3.2) $\mathcal{R}_{t+1} = (\mathcal{R}_t - \{C_r, C_s\}) \bigcup \{C_r \bigcup C_s\}$
    (3.3) Calculate $P_{t+1}$ from $P_t$:
          $P_{t+1} = P_t$
          remove row and column $r$ of $P_{t+1}$
          remove row and column $s$ of $P_{t+1}$
          open new row and column $P_{t+1}$ for $C_q = \{C_r \bigcup C_s\}$
          calculate $P_{t+1}(\cdot, q)$ and $P_{t+1}(q, \cdot)$
    (3.4) $t = t + 1$
until all examples are in a single cluster
```

Agglomerative clustering

- **Additional remarks**:

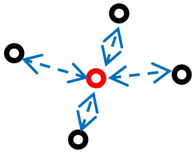


```
(1) $\mathcal{R}_0 = \{C_i = \{x_i\}, i = 1, \ldots, N\}$
(2) $t = 0$
(3) repeat
    (3.1) Choose the pair of clusters $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that
          $\wp(C_r, C_s) = \begin{cases} \min_{i,j}\{\wp(C_i, C_j)\} & \wp \text{ is DM} \\ \max_{i,j}\{\wp(C_i, C_j)\} & \wp \text{ is SM} \end{cases}$
    (3.2) $\mathcal{R}_{t+1} = (\mathcal{R}_t - \{C_r, C_s\}) \bigcup \{C_r \bigcup C_s\}$
    (3.3) $t = t + 1$
  until all samples are in a single cluster
```

- the dendrogram strongly depends on the chosen proximity measure between clusters $\wp(C_i,C_j)$
- the shape of the dendrogram itself indicates whether the clustering at a certain level is natural or not:
  - a great “jump” between levels suggests the existence of a **non-natural merging**
  - it is not necessary to build completely the dendrogram: one can stop at a certain level, before **reaching a non-natural clustering**, or when a **certain number of clusters has been found**
- regarding the adequateness of a merge, every step of the algorithm increases the **total variance of the clustering** E_t, defined by:

$$E_t = \sum_{r \in \mathcal{R}_t} e_r^2 \quad \text{[total variance of clustering } \mathcal{R}_t\text{]}$$

$$e_r^2 = \sum_{a \in C_r} \|a - \mu_r\|^2, \quad \mu_r = \frac{1}{n_r} \sum_{a \in C_r} a$$



Agglomerative clustering

- **Increase of total variance** from level t to level t+1:
  - Let us consider the merge between clusters C_i and C_j into cluster C_q at level t+1
  - Then, the increment of total variance can be stated as:

$$\Delta E^{ij}_{t+1} = E^{ij}_{t+1} - E_t = \left(\sum_{r\neq q} e_r^2\right) + e_q^2 - \left(\left(\sum_{r\neq i,j} e_r^2\right) + e_i^2 + e_j^2\right) = e_q^2 - e_i^2 - e_j^2$$

  - Taking into account that:

$$\begin{aligned} e_r^2 &= \sum_{a\in C_r} \|a-\mu_r\|^2 = \sum_{a\in C_r} (a-\mu_r)^T(a-\mu_r) \\ &= \sum_{a\in C_r} a^T a - 2\sum_{a\in C_r} \mu_r^T a + \sum_{a\in C_r} \mu_r^T \mu_r \\ &= \sum_{a\in C_r} a^T a - 2\mu_r^T(n_r\mu_r) + n_r(\mu_r^T\mu_r) \\ &= \sum_{a\in C_r} a^T a - n_r(\mu_r^T\mu_r) = \sum_{a\in C_r} \|a\|^2 - n_r\|\mu_r\|^2 \end{aligned}$$

$$\mu_r = \frac{1}{n_r}\sum_{a\in C_r} a \Rightarrow \sum_{a\in C_r} a = n_r\mu_r$$

Agglomerative clustering

- **Increase of total variance** from level t to level t+1:
  - Since C_q is the merge of C_i and C_j, the increment of total variance is given by:

$$\begin{aligned}\Delta E^{ij}_{t+1} &= \sum_{a\in C_q}\|a\|^2 - n_q\|\mu_q\|^2 - \left(\sum_{a\in C_i}\|a\|^2 - n_i\|\mu_i\|^2\right) - \left(\sum_{a\in C_j}\|a\|^2 - n_j\|\mu_j\|^2\right)\\ &= n_i\|\mu_i\|^2 + n_j\|\mu_j\|^2 - n_q\|\mu_q\|^2 = n_i(\mu_i^T\mu_i) + n_j(\mu_j^T\mu_j) - n_q(\mu_q^T\mu_q)\end{aligned}$$

  - Taking into account that:

$$n_q\mu_q = \sum_{a\in C_i} a + \sum_{b\in C_j} b = n_i\mu_i + n_j\mu_j \quad \textbf{and} \quad n_q = n_i + n_j$$

then we obtain:

$$\begin{aligned}\Delta E^{ij}_{t+1} &= n_i(\mu_i^T\mu_i) + n_j(\mu_j^T\mu_j) - n_q\left(\frac{n_i}{n_q}\mu_i + \frac{n_j}{n_q}\mu_j\right)^T\left(\frac{n_i}{n_q}\mu_i + \frac{n_j}{n_q}\mu_j\right)\\ &= \frac{n_i n_j}{n_i+n_j}\mu_i^T\mu_i + \frac{n_i n_j}{n_i+n_j}\mu_j^T\mu_j - 2\frac{n_i n_j}{n_i+n_j}\mu_i^T\mu_j\\ &= \frac{n_i n_j}{n_i+n_j}(\mu_i-\mu_j)^T(\mu_i-\mu_j) = \boxed{\frac{n_i n_j}{n_i+n_j}\|\mu_i-\mu_j\|^2 = \Delta E^{ij}_{t+1} > 0}\end{aligned}$$

Agglomerative clustering

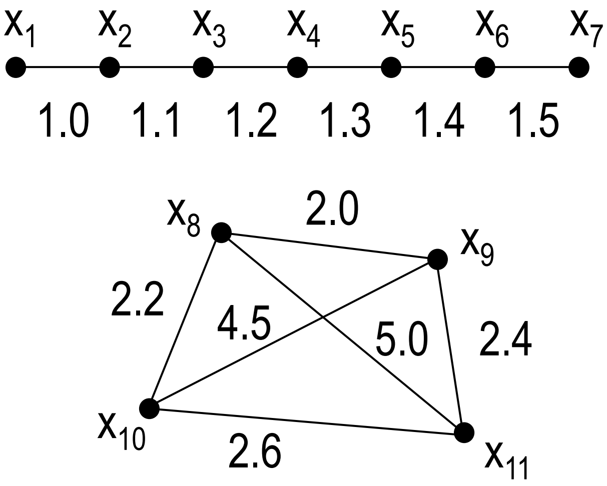
- Agglomerative algorithms **depending on the proximity function between clusters**
  - **Nearest neighbour** (or *single-link* / *single-linkage*)

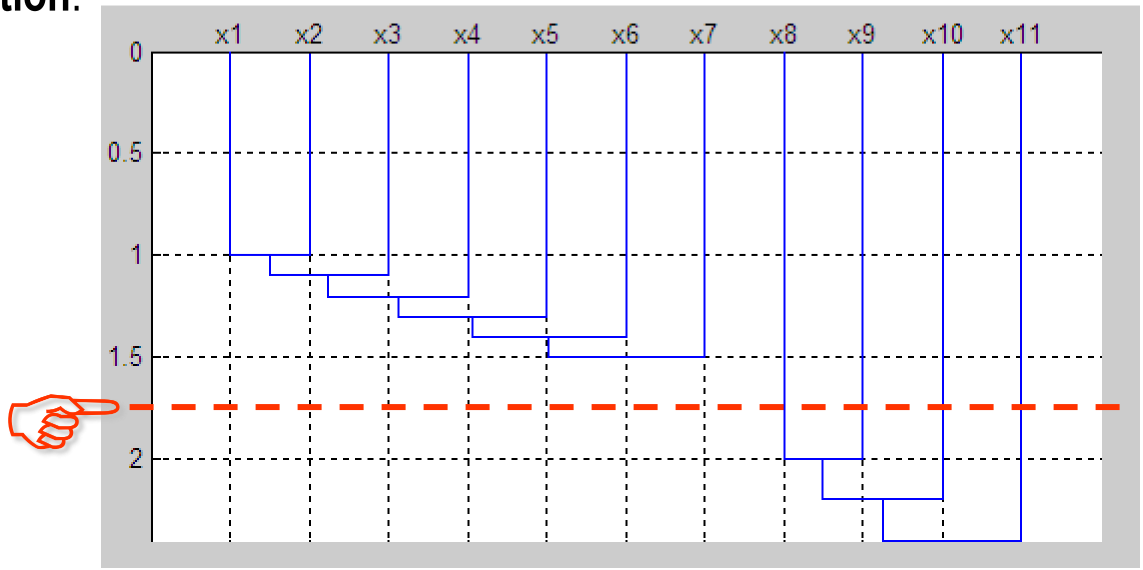
(3.1) Choose the pair of **clusters** $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that:

$$\wp(C_r, C_s) = \begin{cases} \min\limits_{i,j}\{\wp_{\min}(C_i, C_j) = \min\limits_{a \in C_i, b \in C_j} \wp(a,b)\} & (\wp \text{ is DM}) \\ \max\limits_{i,j}\{\wp_{\max}(C_i, C_j) = \max\limits_{a \in C_i, b \in C_j} \wp(a,b)\} & (\wp \text{ is SM}) \end{cases}$$

  - **favour elongated clusters** (chain effect)

- **Example of application**:





Agglomerative clustering

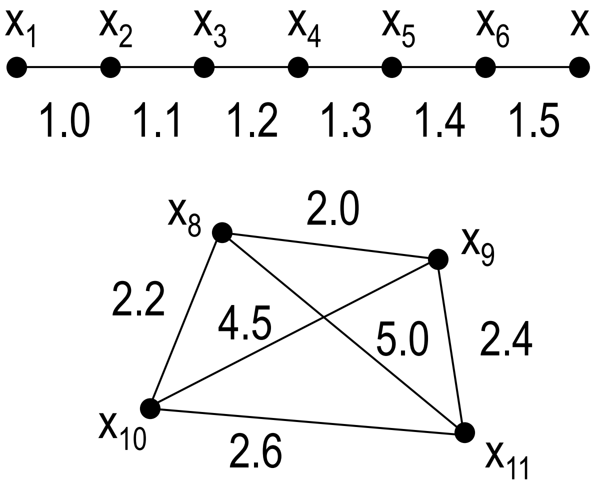
- Agglomerative algorithms **depending on the proximity function between clusters**
  - **Farthest neighbour** (or *complete-link / complete-linkage*)

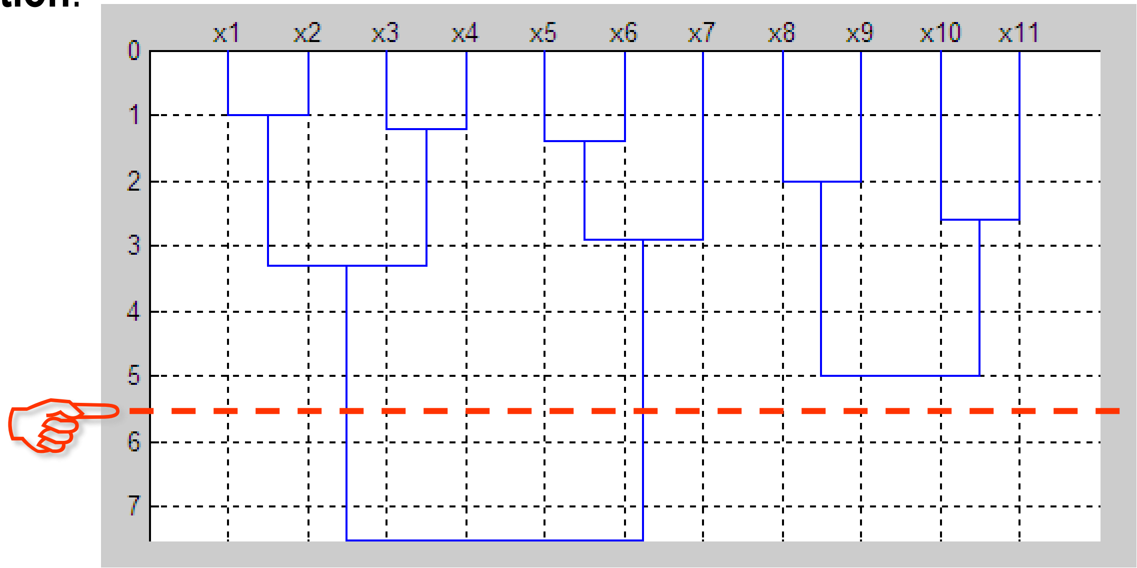
(3.1) Choose the pair of **clusters** $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that:

$$\wp(C_r, C_s) = \begin{cases} \min\limits_{i,j}\{\wp_{\max}(C_i, C_j) = \max\limits_{a\in C_i, b\in C_j} \wp(a,b)\} & (\wp \text{ is DM}) \\ \max\limits_{i,j}\{\wp_{\min}(C_i, C_j) = \min\limits_{a\in C_i, b\in C_j} \wp(a,b)\} & (\wp \text{ is SM}) \end{cases}$$

  - **favour compact clusters** (reduced diameter clusters)

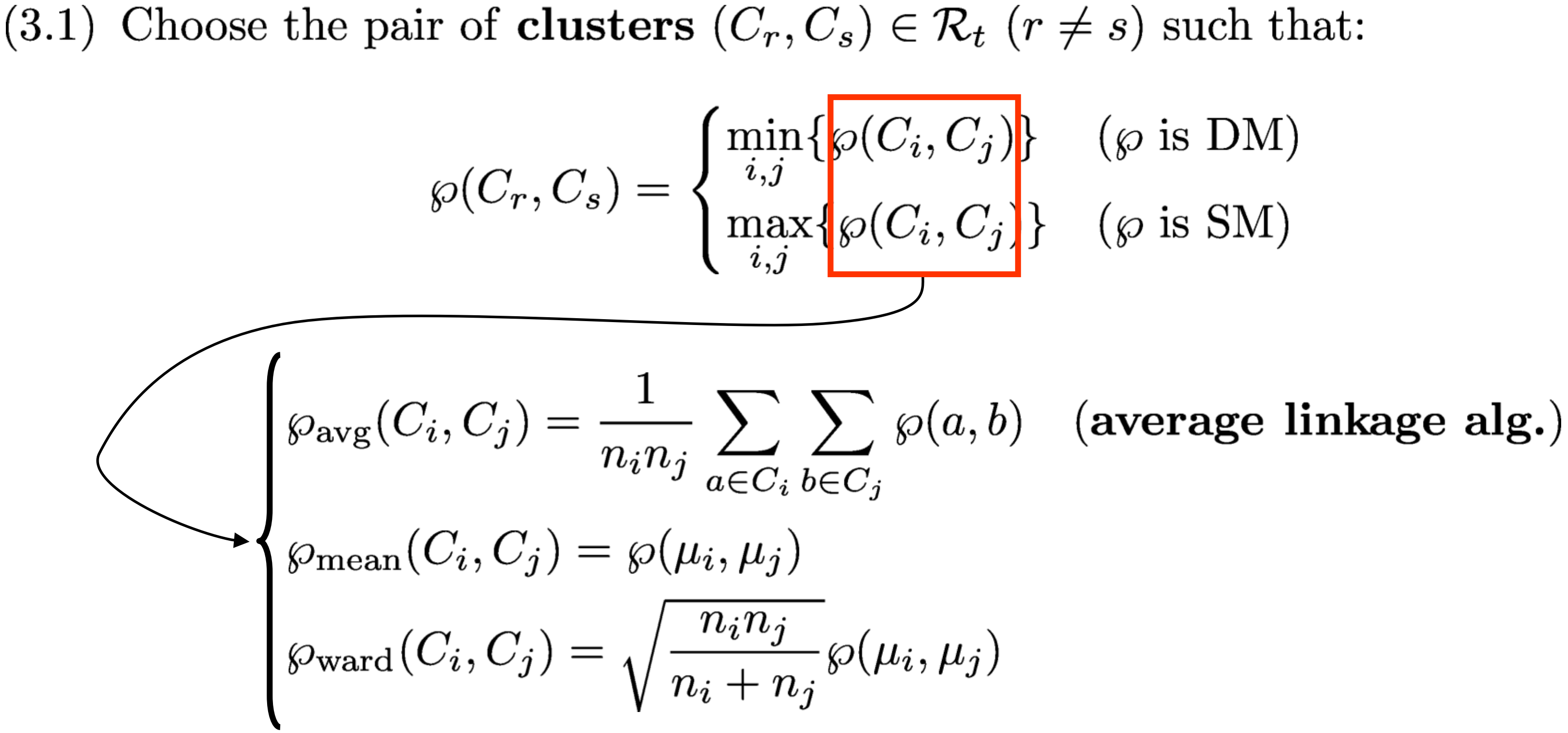
- **Example of application**:





Agglomerative clustering

- Agglomerative algorithms **depending on the proximity function between clusters**
  - NN and FN algorithms are at the **opposite ends of the spectrum** of measures cluster-to-cluster $\wp(C_i, C_j)$
  - Other algorithms, with intermediate behaviours, result for other distances:



(3.1) Choose the pair of **clusters** $(C_r, C_s) \in \mathcal{R}_t$ $(r \neq s)$ such that:

$$\wp(C_r, C_s) = \begin{cases} \min\limits_{i,j}\{\boxed{\wp(C_i, C_j)}\} & (\wp \text{ is DM}) \\ \max\limits_{i,j}\{\boxed{\wp(C_i, C_j)}\} & (\wp \text{ is SM}) \end{cases}$$

$$\begin{cases} \wp_{\text{avg}}(C_i, C_j) = \dfrac{1}{n_i n_j} \displaystyle\sum_{a \in C_i} \sum_{b \in C_j} \wp(a, b) & \textbf{(average linkage alg.)} \\ \wp_{\text{mean}}(C_i, C_j) = \wp(\mu_i, \mu_j) \\ \wp_{\text{ward}}(C_i, C_j) = \sqrt{\dfrac{n_i n_j}{n_i + n_j}}\, \wp(\mu_i, \mu_j) \end{cases}$$

Agglomerative clustering

- Agglomerative algorithms **depending on the proximity function between clusters**
  - In particular:

$$\wp_{\text{ward}}(C_i, C_j) = \sqrt{\frac{n_i n_j}{n_i + n_j}}\wp(\mu_i, \mu_j)$$

leads to the minimum total variance increase between steps if $\wp(\mu_i,\mu_j) = ||\mu_i - \mu_j||$:

- The algorithm chooses the pair of clusters that minimize $\sqrt{\frac{n_i n_j}{n_i + n_j}}||\mu_i - \mu_j||$

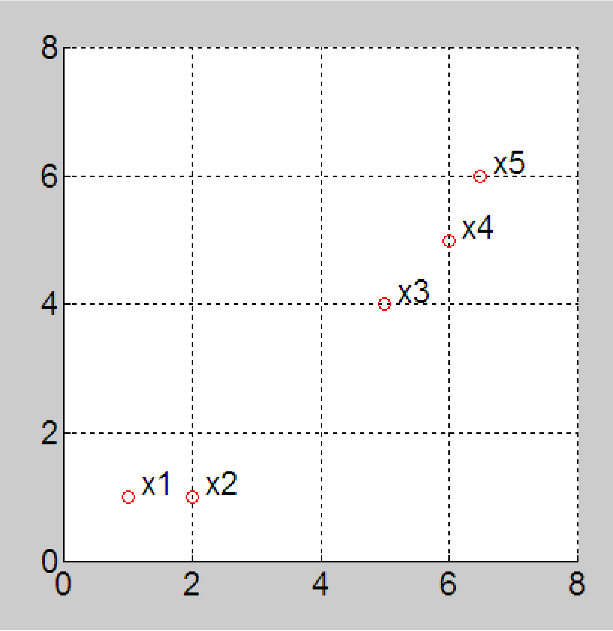
  and we have already seen that $\Delta E_{t+1}^{ij} = \frac{n_i n_j}{n_i + n_j}||\mu_i - \mu_j||^2$.

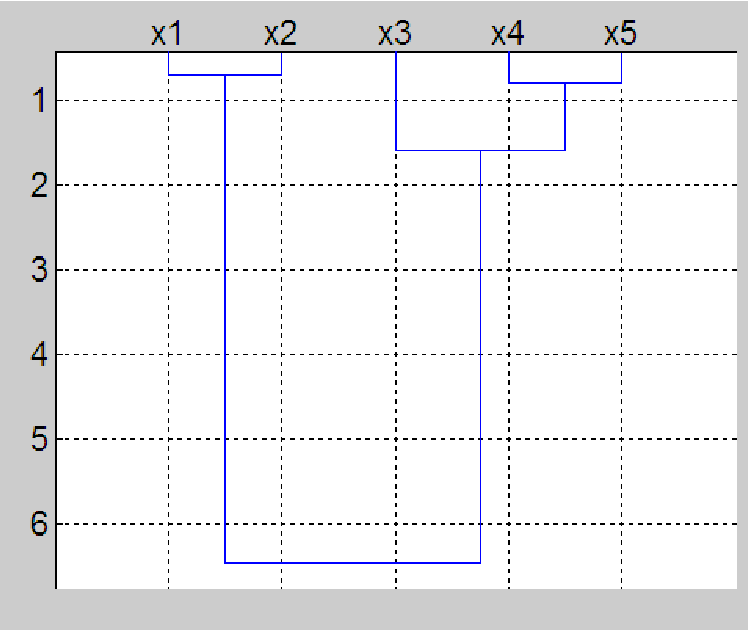
- Because of this, this algorithm is termed **algorithm** (of agglomerative hierarchical clustering) **of minimum variance**.

- At a practical level, this algorithm **favours the fusion of small clusters with large clusters** against fusing large or medium-size *clusters*, because of the involvement of cluster sizes in the proximity measure.

Agglomerative clustering

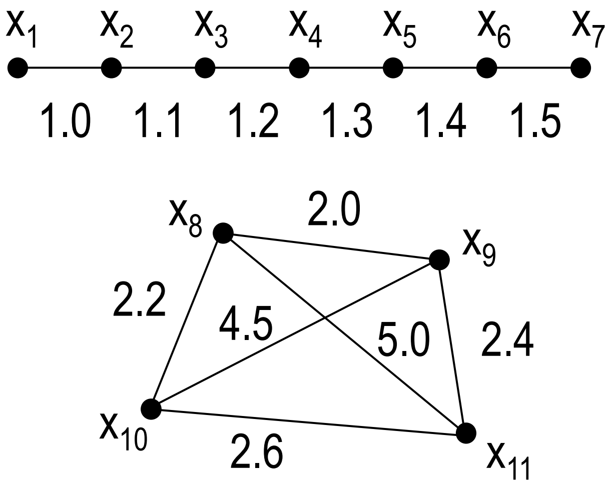
- Agglomerative algorithms **depending on the proximity function between clusters**
  - **Example** (of Ward distance use):

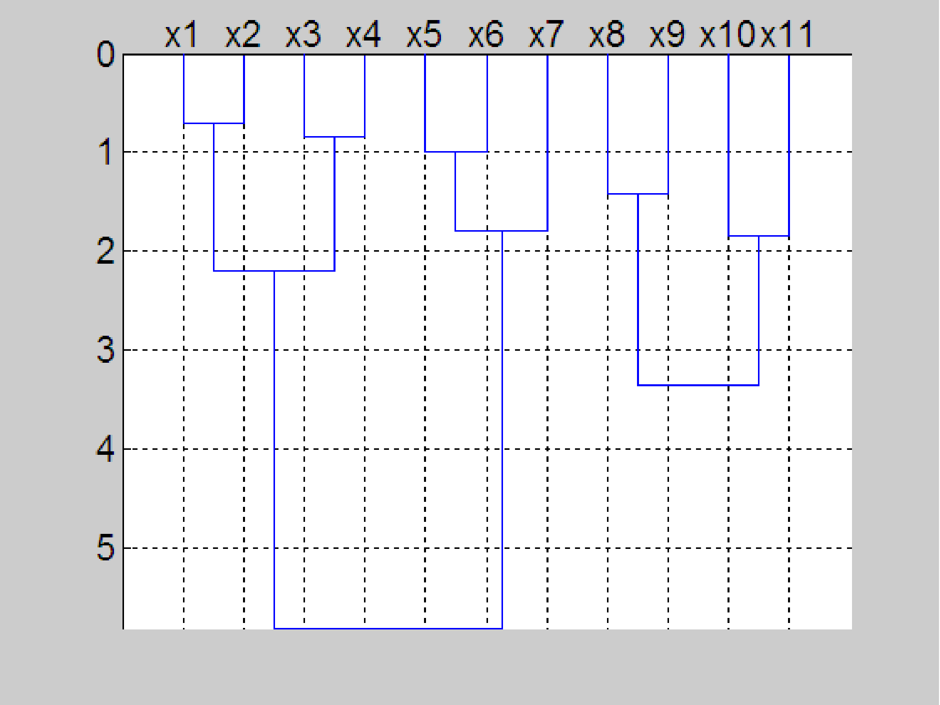




Agglomerative clustering

- Agglomerative algorithms **depending on the proximity function between clusters**
  - **Example** (of Ward distance use):

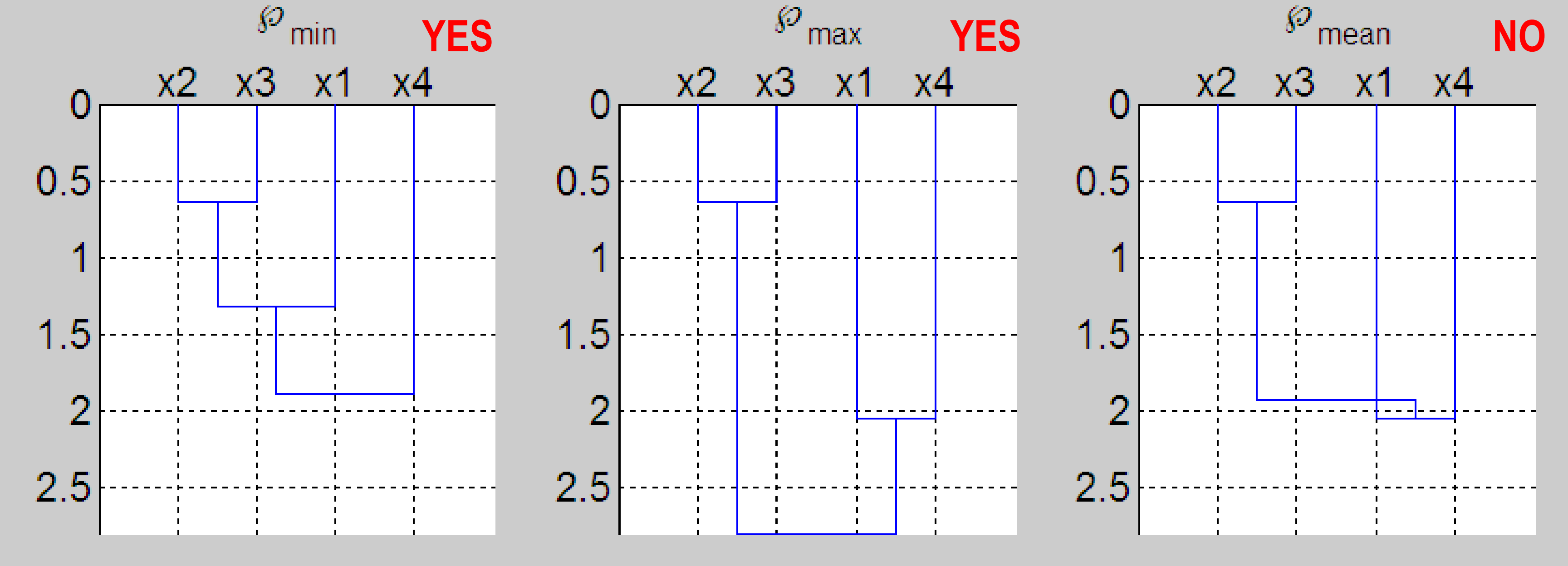




  - In clear cases (compact and well separated clusters), all alternatives lead to the same results. **Differences appear for *extreme cases***.

Agglomerative clustering

- **Monotonicity**
  - If the clustering algorithm selects clusters C_i y C_j to build a new cluster C_q so that $d(C_q,C_k) \geq d(C_i,C_j)$, $\forall k \neq i, j, q$, then the resulting dendrogram is said to be **monotonous**
  - If monotonicity holds, clusters are created at higher dissimilarity levels than its constituents



  - $\wp_{\text{min}}$, $\wp_{\text{max}}$, $\wp_{\text{avg}}$ and $\wp_{\text{ward}}$ can be proved to always give rise to monotonous dendrograms.
  - Monotonicity has been considered to be necessary for a clustering algorithm to be useful.

Agglomerative clustering

- **Ties in the proximity matrix P(X)**

$$P_0 = \begin{bmatrix} 0 & 4 & 9 & 6 & 5 \\ 4 & 0 & 3 & 8 & 7 \\ 9 & 3 & 0 & 3 & 2 \\ 6 & 8 & 3 & 0 & 1 \\ 5 & 7 & 2 & 1 & 0 \end{bmatrix}$$

$$P_1^{\wp\min} = \begin{bmatrix} 0 & 4 & 9 & \cancel{6} & \cancel{5} & 5 \\ 4 & 0 & 3 & \cancel{8} & \cancel{7} & 7 \\ 9 & 3 & 0 & \cancel{3} & \cancel{2} & 2 \\ \cancel{6} & \cancel{8} & \cancel{3} & \cancel{0} & \cancel{1} & \cancel{-} \\ \cancel{5} & \cancel{7} & \cancel{2} & \cancel{1} & \cancel{0} & \cancel{-} \\ 5 & 7 & 2 & \cancel{-} & \cancel{-} & 0 \end{bmatrix}$$

$$P_1^{\wp\max} = \begin{bmatrix} 0 & 4 & 9 & \cancel{6} & \cancel{5} & 6 \\ 4 & 0 & 3 & \cancel{8} & \cancel{7} & 8 \\ 9 & 3 & 0 & \cancel{3} & \cancel{2} & 3 \\ \cancel{6} & \cancel{8} & \cancel{3} & \cancel{0} & \cancel{1} & \cancel{-} \\ \cancel{5} & \cancel{7} & \cancel{2} & \cancel{1} & \cancel{0} & \cancel{-} \\ 6 & 8 & 3 & \cancel{-} & \cancel{-} & 0 \end{bmatrix}$$

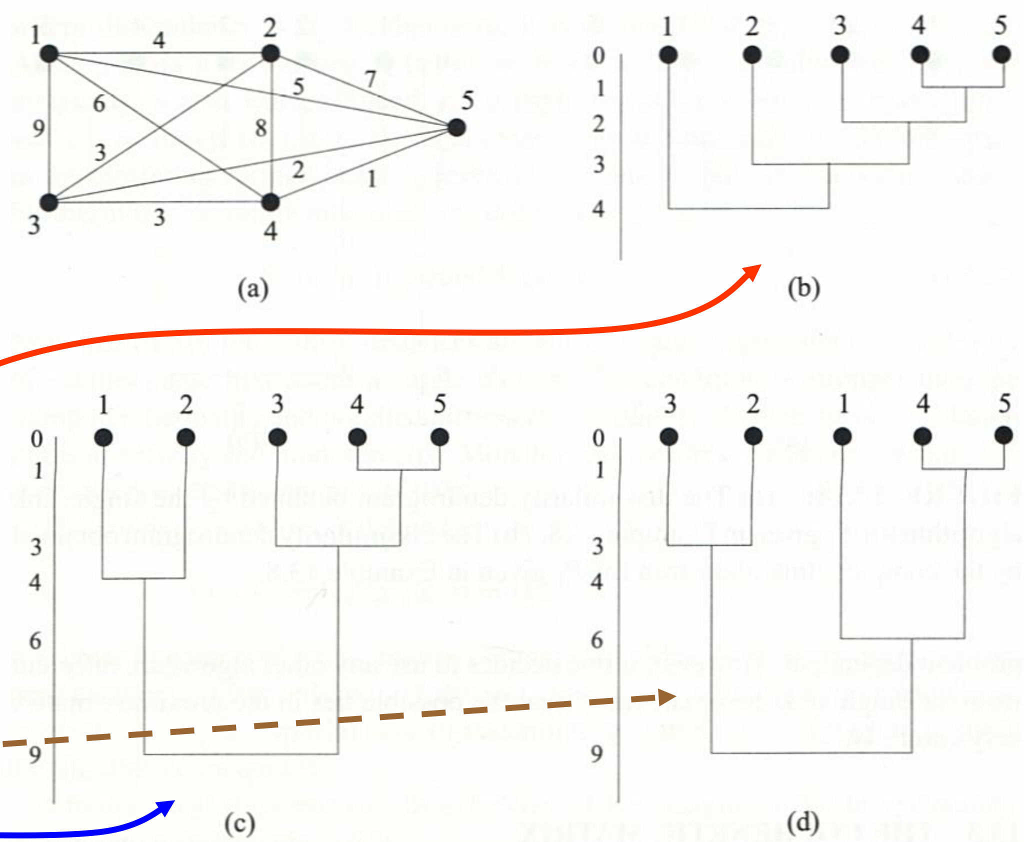


FIGURE 13.13: (a) The dissimilarity graph ($G(9)$) for the dissimilarity matrix given in Example 13.8. (b) The dissimilarity dendrogram obtained by the single link algorithm. (c) The dissimilarity dendrogram obtained by the complete link algorithm when edge (3, 4) is considered first. (d) The dissimilarity dendrogram obtained by the complete link algorithm when edge (2, 3) is considered first.

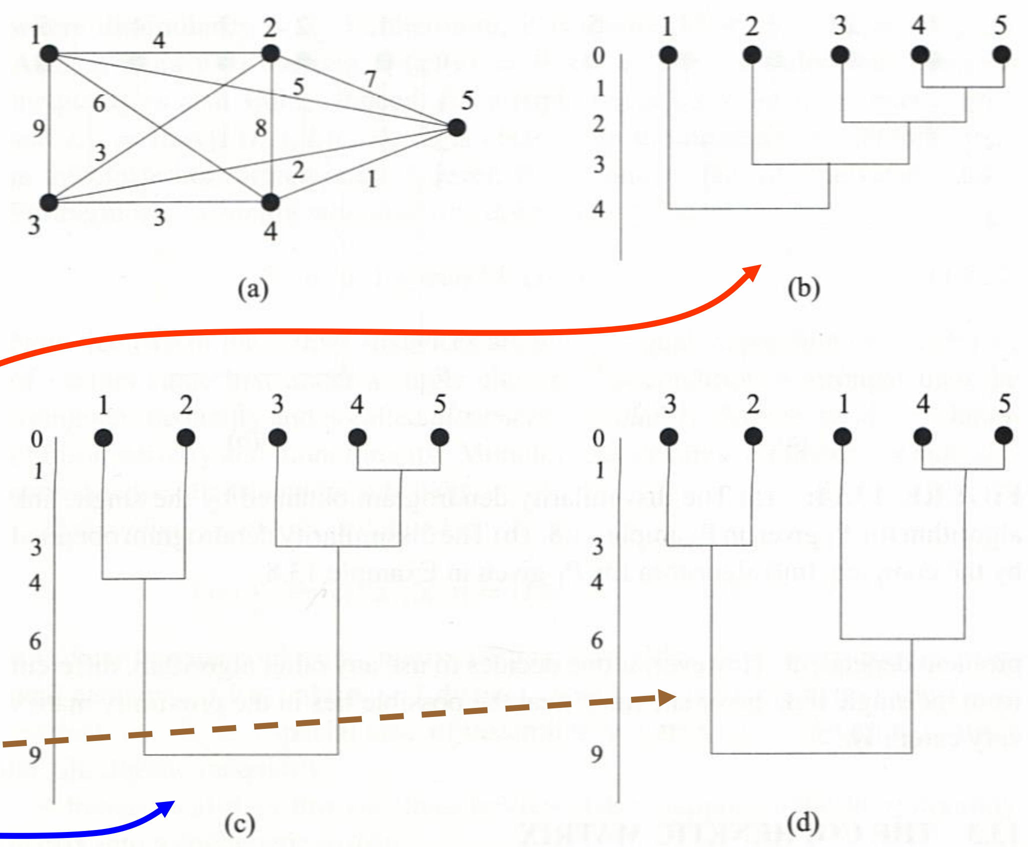
Agglomerative clustering

- **Ties in the proximity matrix P(X)**

$$P_0 = \begin{bmatrix} 0 & 4 & 9 & 6 & 5 \\ 4 & 0 & 3 & 8 & 7 \\ 9 & 3 & 0 & 3 & 2 \\ 6 & 8 & 3 & 0 & \boxed{1} \\ 5 & 7 & 2 & 1 & 0 \end{bmatrix}$$

$$P_1^{\wp_{\min}} = \begin{bmatrix} 0 & 4 & 9 & \cancel{6} & \cancel{5} & 5 \\ 4 & 0 & 3 & \cancel{8} & \cancel{7} & 7 \\ 9 & 3 & 0 & \cancel{3} & \cancel{2} & \boxed{2} \\ \cancel{6} & \cancel{8} & \cancel{3} & \cancel{0} & \cancel{1} & \cancel{-} \\ \cancel{5} & \cancel{7} & \cancel{2} & \cancel{1} & \cancel{0} & \\ 5 & 7 & 2 & \cancel{-} & \cancel{-} & 0 \end{bmatrix}$$

$$P_1^{\wp_{\max}} = \begin{bmatrix} 0 & 4 & 9 & \cancel{6} & \cancel{5} & 6 \\ 4 & 0 & \boxed{3} & \cancel{8} & \cancel{7} & 8 \\ 9 & 3 & 0 & \cancel{3} & \cancel{2} & \boxed{3} \\ \cancel{6} & \cancel{8} & \cancel{3} & \cancel{0} & \cancel{1} & \cancel{-} \\ \cancel{5} & \cancel{7} & \cancel{2} & \cancel{1} & \cancel{0} & \\ 6 & 8 & 3 & \cancel{-} & \cancel{-} & 0 \end{bmatrix}$$



- All agglomerative algorithms are more or less affected by this defect, although the **nearest neighbour algorithm** seems to be the least affected.

Contents

- Introduction
- Agglomerative clustering
- Divisive clustering
- Selection of a good clustering

Divisive Clustering

- Generic **algorithm**:

```
(1) $\mathcal{R}_0 = \{X\}$
(2) $t = 0$
(3) repeat
    (3.1) for all clusters $C_q$ of $\mathcal{R}_t$:
            Find $C_r^q$ and $C_s^q$ s.t. $C_q = C_r^q \bigcup C_s^q$, $C_r^q \bigcap C_s^q = \emptyset$ and
                $\wp(C_r^q, C_s^q) = \begin{cases} \max\limits_{i,j}\{\wp(C_i, C_j)\} & (\wp \text{ is DM}) \\ \min\limits_{i,j}\{\wp(C_i, C_j)\} & (\wp \text{ is SM}) \end{cases}$
          end
    (3.2) Find the cluster $C_{q*}$ whose splitting is the best
    (3.3) $\mathcal{R}_{t+1} = (\mathcal{R}_t - \{C_{q*}\}) \bigcup \{C_r^{q*}, C_s^{q*}\}$
    (3.4) $t = t + 1$
  until all samples are in a different cluster
```

  - Very high **cost** at the computational level
  - Different alternatives available, which try to reduce the cost of (3.1)

Contents

- Introduction
- Agglomerative clustering
- Divisive clustering
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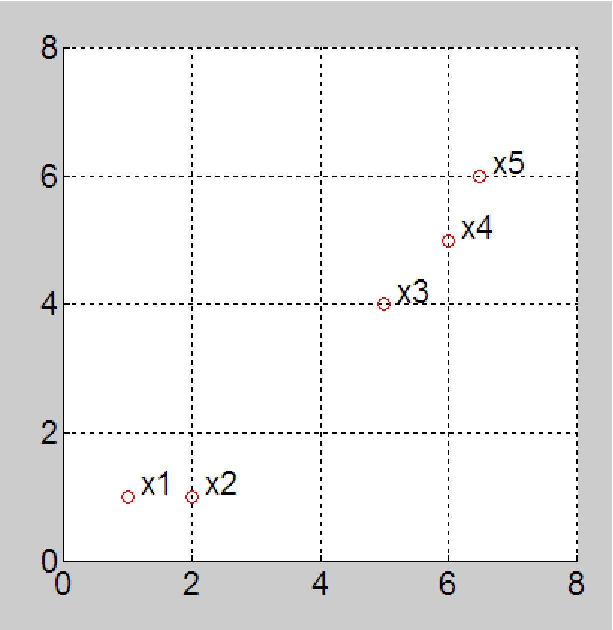
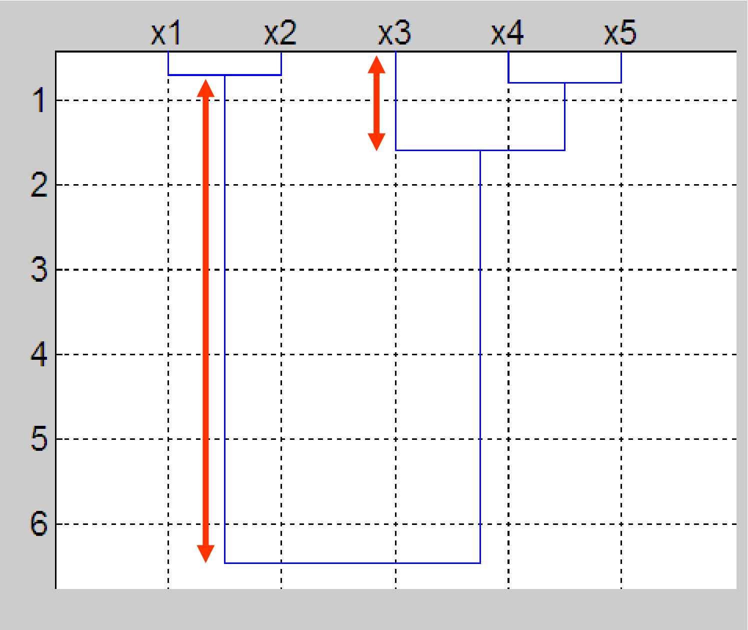
Selection of a good clustering (in the hierarchy)

- We turn our attention to the determination of a **good clustering within a given hierarchy**. This can help to identify the natural structure of the data.

1. Find in the dendrogram clusters with a **long lifetime**:
   - **lifetime of a cluster** ≡ absolute diference between the proximity level at which a cluster is generated and the level at which it is absorbed

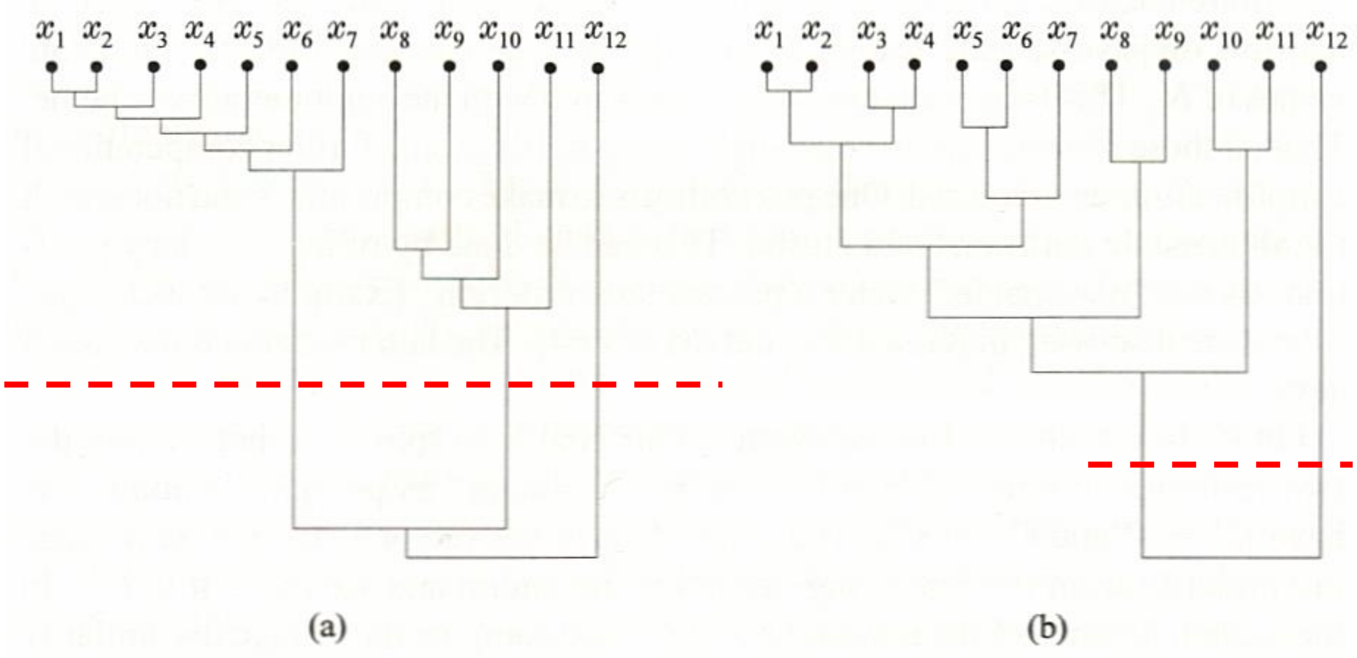




⇒ final clustering should be: {x_1,x_2}, {x_3,x_4,x_5}

Selection of best clustering

1. Find in the dendrogram clusters with a **long lifetime**:
   - **lifetime of a cluster** ≡ absolute difference between the proximity level at which a cluster is generated and the level at which it is absorbed
   - another example:



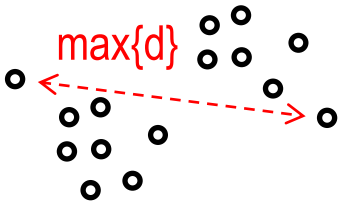
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10} x_{11} x_{12}
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10} x_{11} x_{12}

(a) (b)

Selection of best clustering

2. Stop before a **low-quality cluster** results:

   – Determine the disimilarity within a cluster by means of an appropriate measure **h**. Several possibilities:



$$h_1(C) = \max\{d(x,y),\ x,y \in C\} \qquad \text{— diameter of C}$$

$$h_2(C) = \text{median}\{d(x,y),\ x,y \in C\} \qquad \text{— robust to outliers}$$

$$h_3(C) = \frac{2}{n_C(n_C-1)} \sum_{x \neq y \in C} d(x,y)$$

   – In this way, every time a cluster is going to be created, one can check its internal dissimilarity and decide not to create it if it is above a threshold τ, and the process is stopped:

$$C_q = C_i \bigcup C_j \in \mathcal{R}_{t+1} : h(C_q) > \tau \Rightarrow \text{ STOP at level } t$$

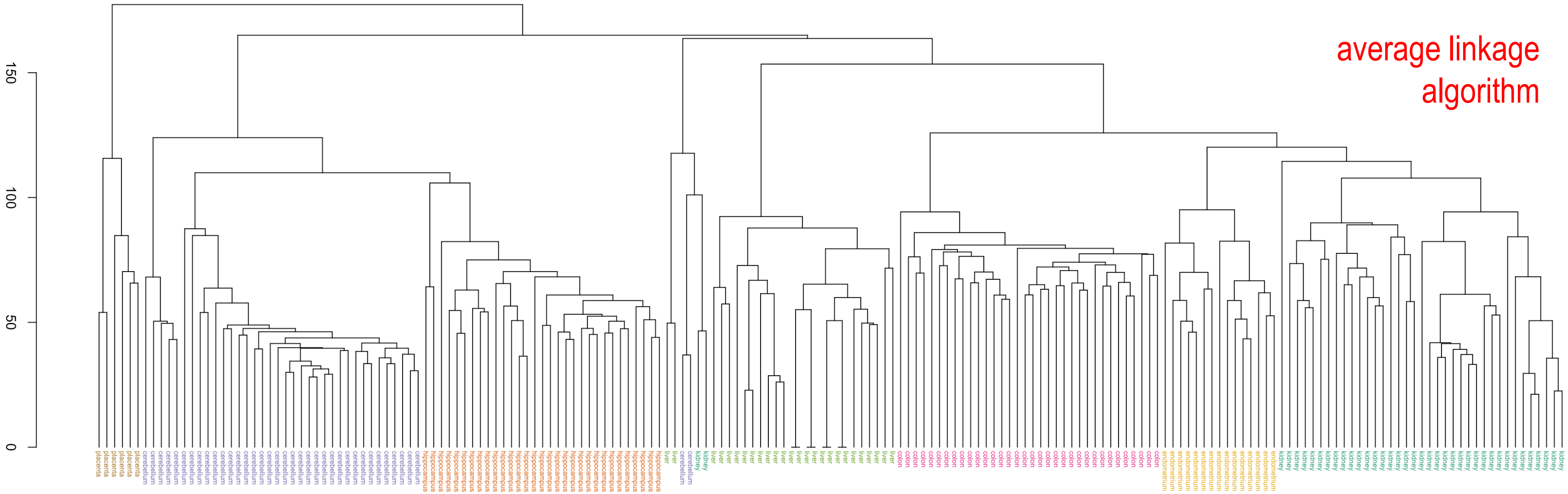
   – It is usually useful to define $\tau = \mu + \lambda\sigma$, where μ is the average distance among elements of X and σ is the standard deviation.

   – Typically, it is easier to set λ than τ.

Example

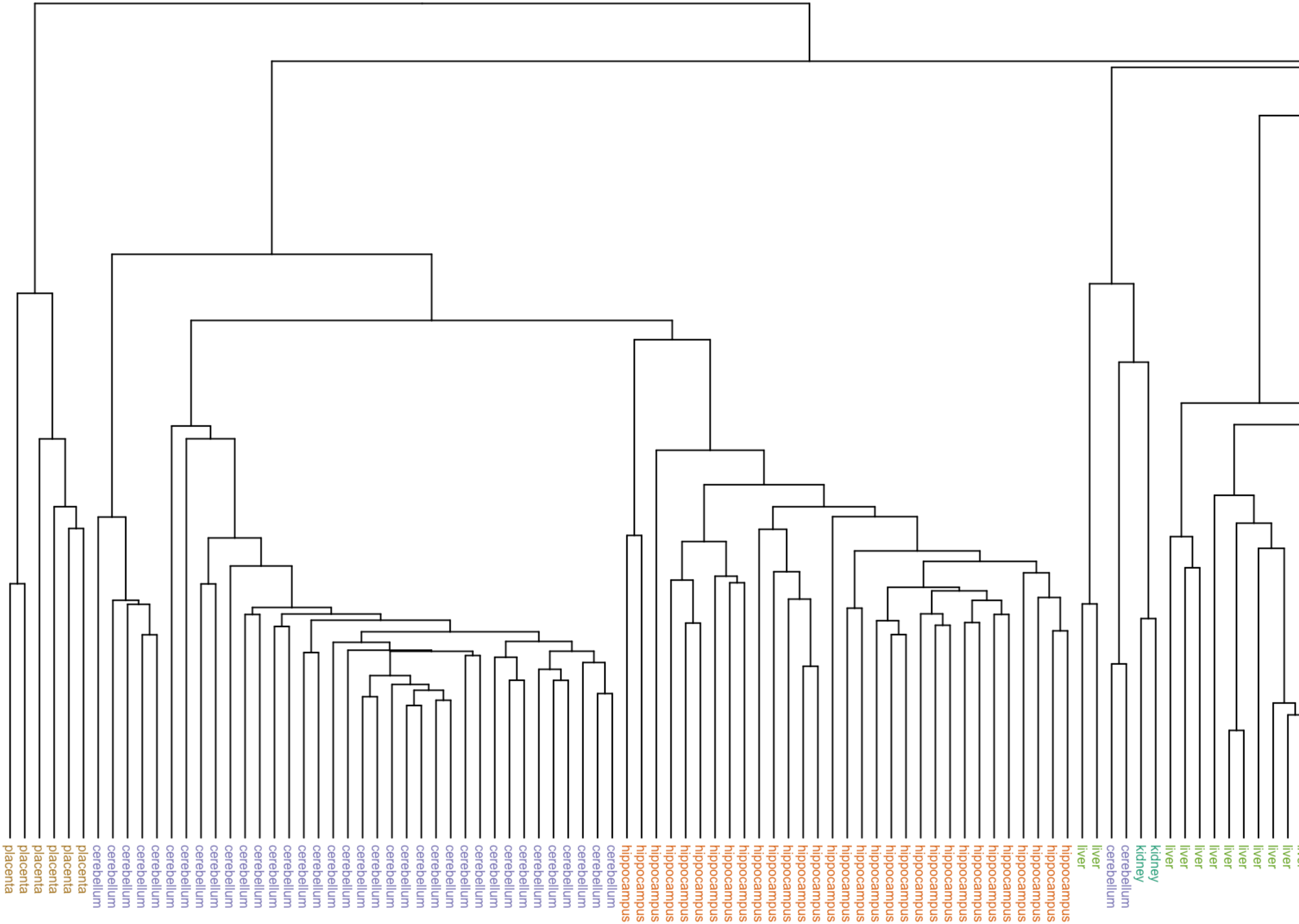
- <u>Example</u>: gene expression profiling of human tissues
  - Each row is a gene expression profile and each column is a different gene. The column names are the gene symbols. The outcome is a character vector representing the tissue.
  - Subset of the original dataset comprising 22.215 samples
  - 189 samples chosen at random, with L = 500
  - 7 tissues:

	cerebellum	colon	endometrium	hippocampus	kidney	liver	placenta
189 =	38	34	15	31	39	26	6



average linkage algorithm

  - source: https://github.com/genomicsclass/tissuesGeneExpression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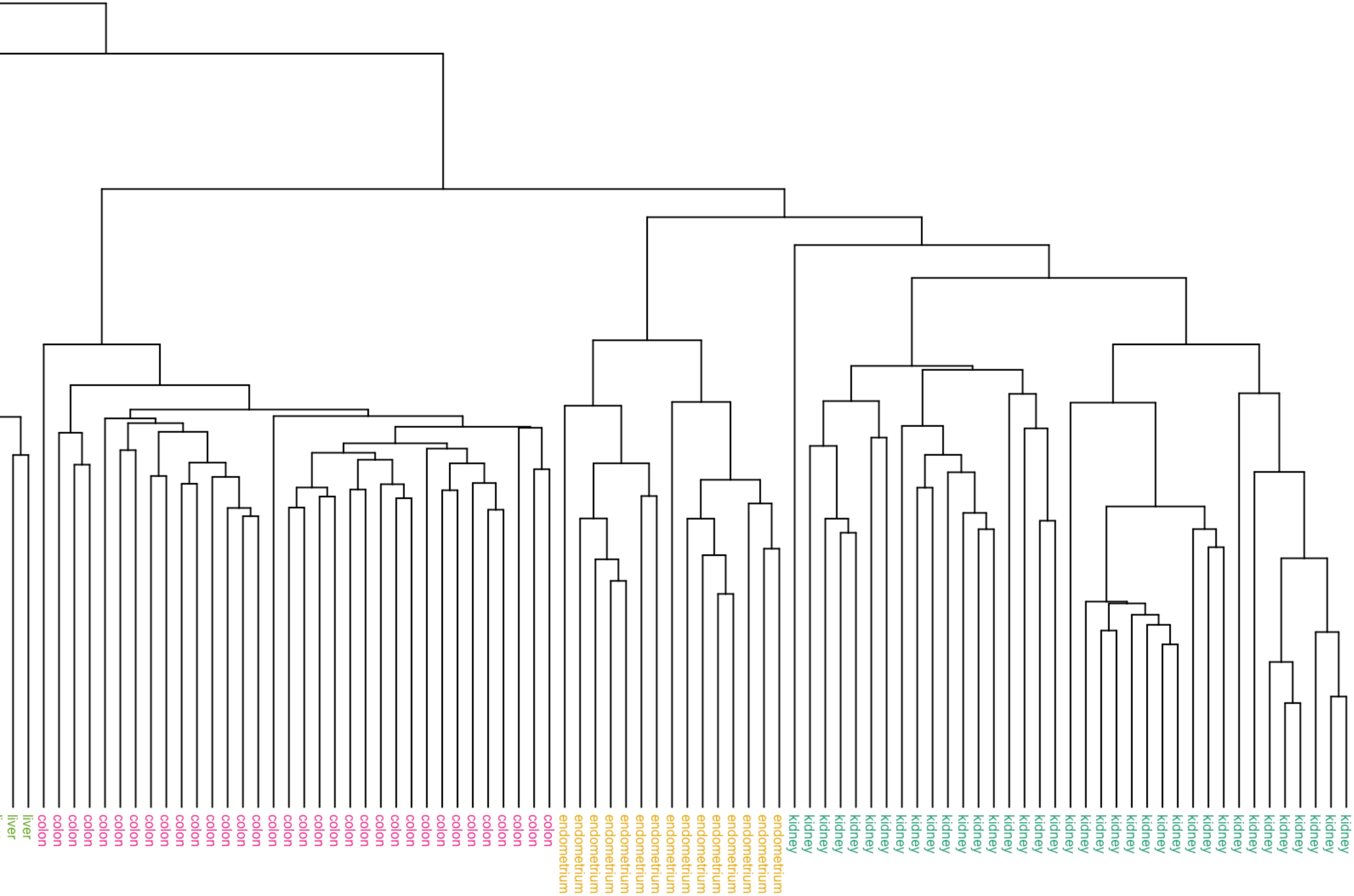
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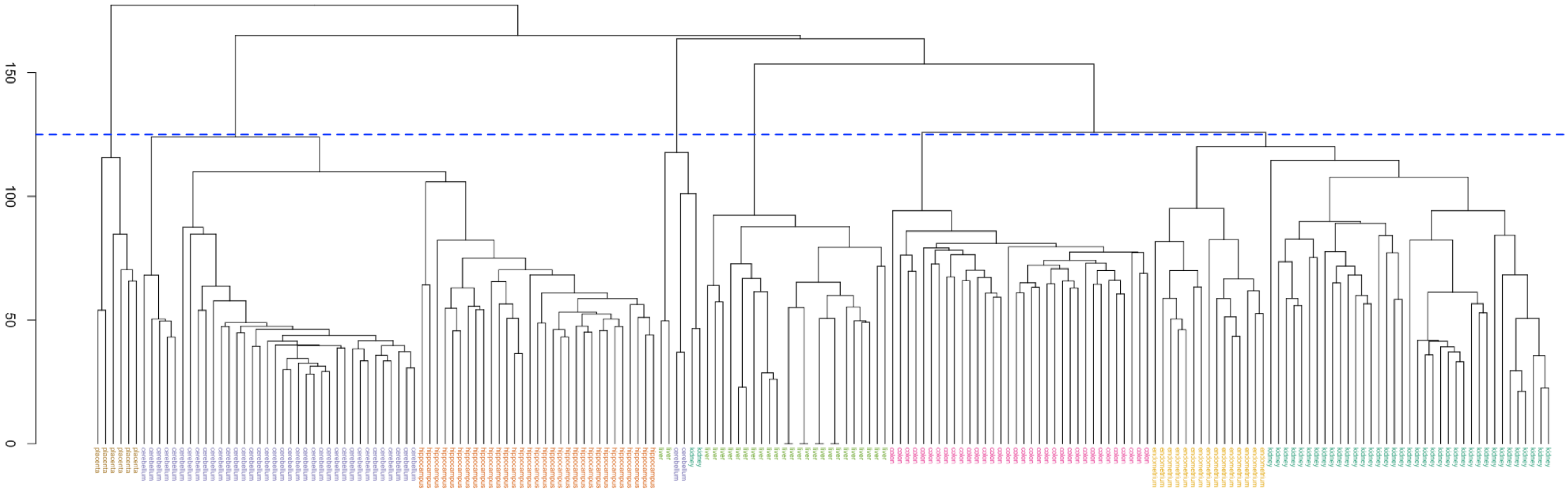
Example

- “Cutting” the dendrogram at height = 125:

contingency table →
(or contingency matrix)

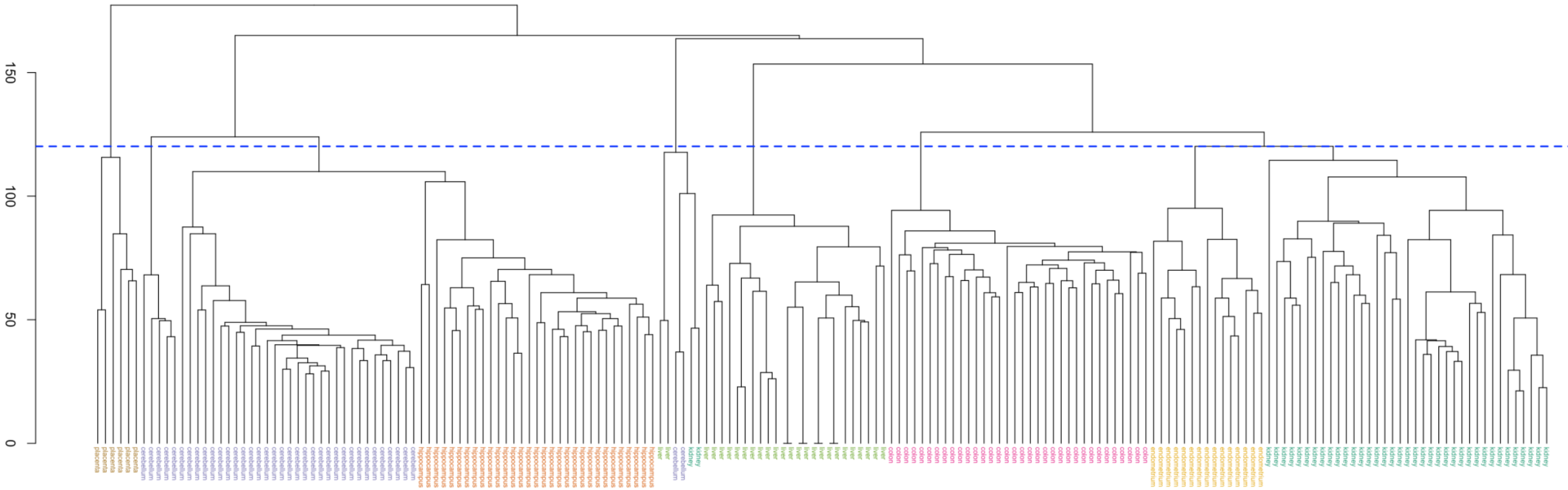
```
##                  cluster
## tissue            1  2  3  4  5  6
## 1.cerebellum      0 36  0  0  2  0
## 2.colon           0  0 34  0  0  0
## 3.endometrium    15  0  0  0  0  0
## 4.hippocampus     0 31  0  0  0  0
## 5.kidney         37  0  0  0  2  0
## 6.liver           0  0  0 24  2  0
## 7.placenta        0  0  0  0  0  6
```



Example

- “Cutting” the dendrogram so as to have 8 clusters:

```
##                       cluster
## tissue          1  2  3  4  5  6  7  8
## 1.cerebellum    0 31  0  0  2  0  5  0
## 2.colon         0  0 34  0  0  0  0  0
## 3.endometrium   0  0  0  0  0 15  0  0
## 4.hippocampus   0 31  0  0  0  0  0  0
## 5.kidney       37  0  0  0  2  0  0  0
## 6.liver         0  0  0 24  2  0  0  0
## 7.placenta      0  0  0  0  0  0  0  6
```



Section 2
Unsupervised Learning: Hierarchical Clustering

Universitat de les Illes Balears

Departament de Ciències Matemàtiques i Informàtica

11752 Aprendizaje Automático

11752 Machine Learning

Máster Universitario
en Sistemas Inteligentes

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