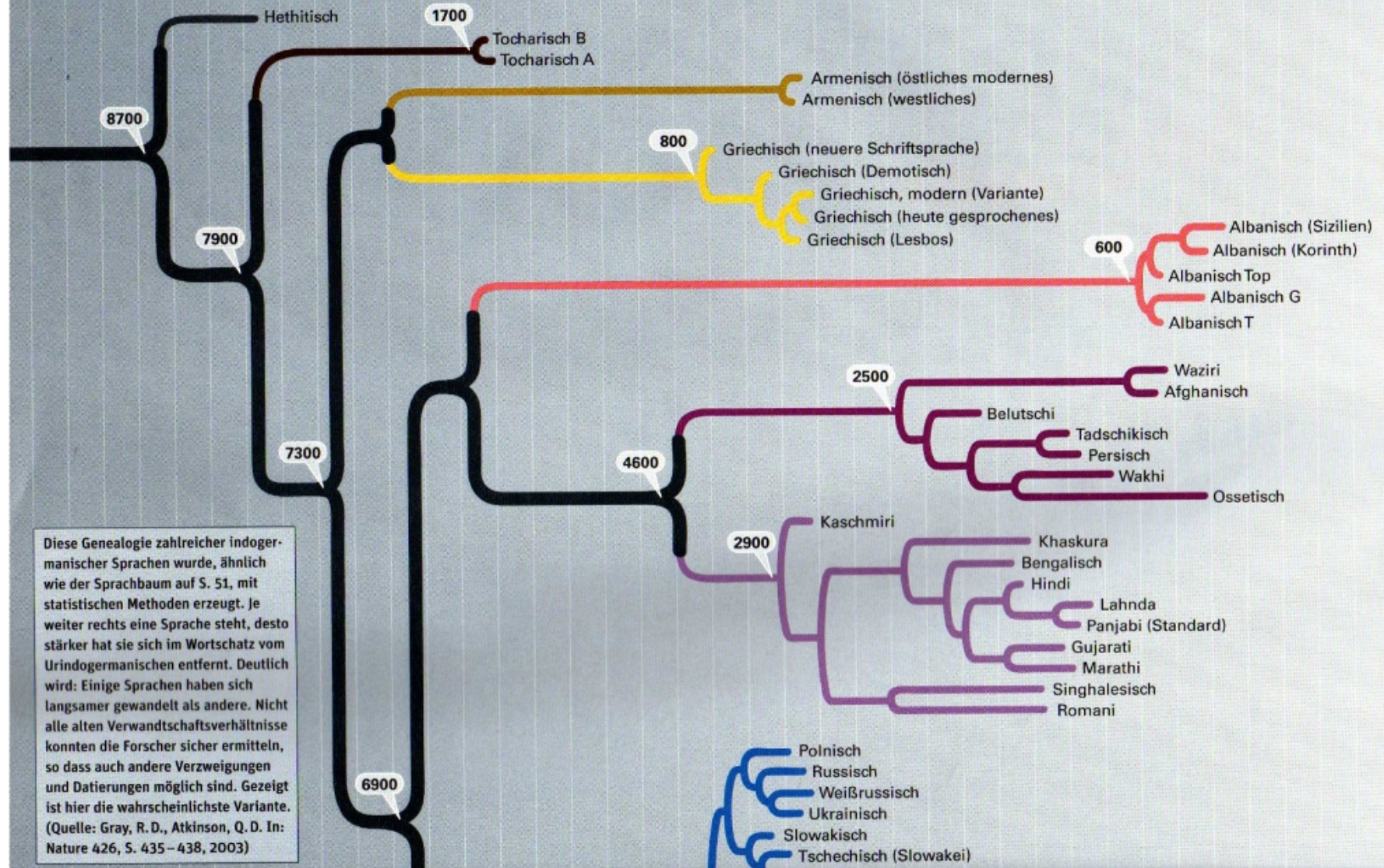


Hierarchical clustering - Dendrogram

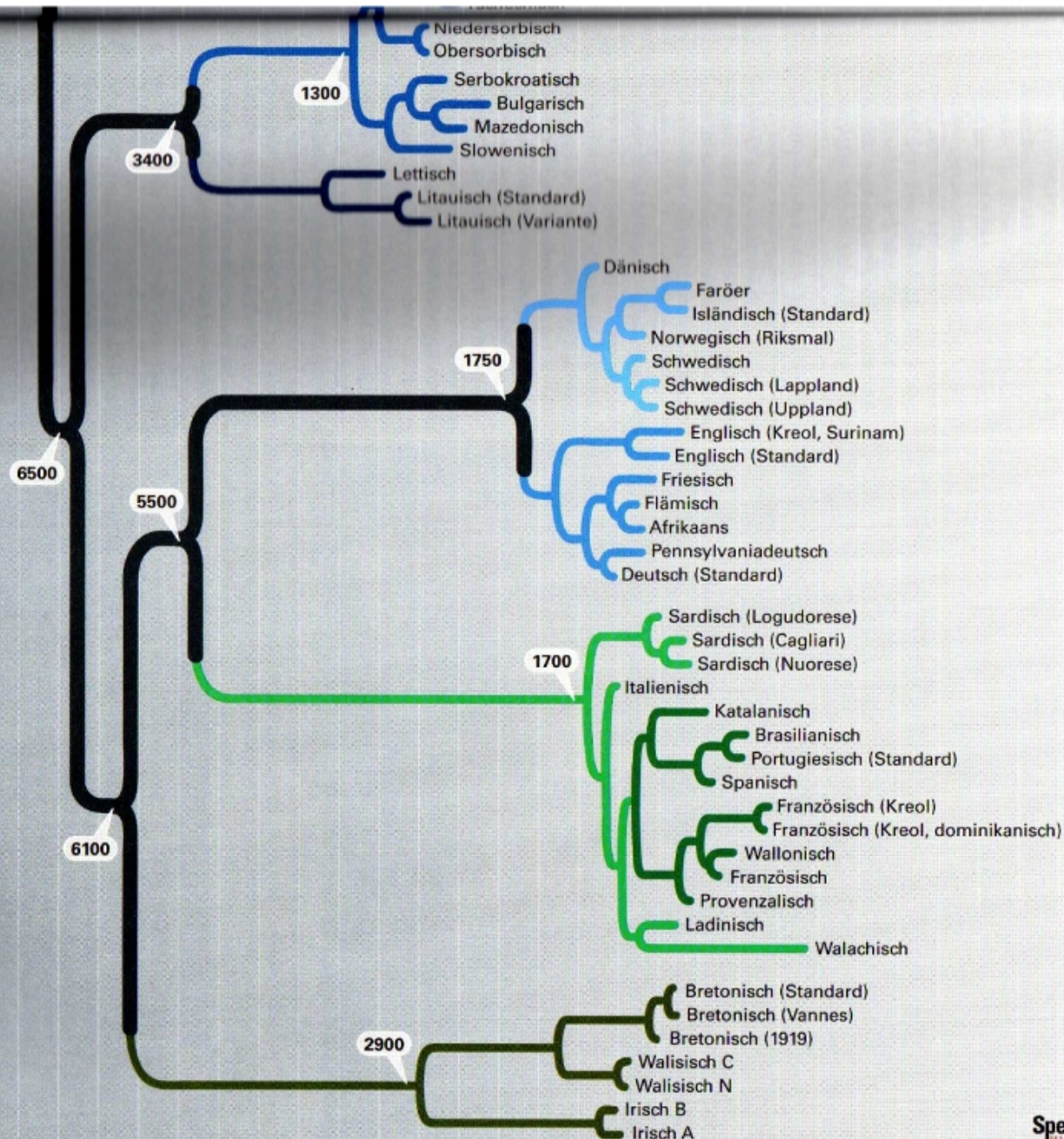
INTRODUCTION TO INTELLIGENT SYSTEMS 17/18

STAMMBAUM DER INDOGERMANISCHEN SPRACHEN



- Anatolisch
 - Tocharisch
 - Armenisch
 - Griechisch
 - Albanisch
 - Iranisch
 - Indisch
 - Slawisch
 - Baltisch
 - Norddeutsch
 - Westdeutsch
 - Französisch/Iberisch
 - Italisch
 - Keltisch
- Indoiranisch**
- Baltoslawisch**
- Germanisch**
- Italisch**

5500 errechnete mittlere Daten der jeweiligen Abspaltung in Jahren vor heute



How can we build such diagrams (called dendrograms) in which the objects cluster in groups of different size at different levels?

Dissimilarity between words

Let

$S_1 = \{a, e, i, o, u, y\}$ (vowels)

$S_2 = \{b, c, d, f, g, h, j, k, l, m, n, p, q, r, s, t, v, w, x, z\}$ (consonants)

We define the dissimilarity $d(x, x')$ between two characters x and x' as follows:

$d(x, x') = 0$ if $x == x'$

= 1 if $x \neq x'$ and both in S_1 (vowels)

= 2 if $x \neq x'$ and both in S_2 (consonants)

= 5 if $x \neq x'$ and in different sets (one is vowel, the other consonant)

= 7 if $x \neq \text{empty}$ and $x' == \text{empty}$ OR

$x == \text{empty}$ and $x' \neq \text{empty}$

Dissimilarity between words

Next we define the dissimilarity of two words as the sum of the dissimilarities of counterpart characters

- Example 1:
 - $\text{dissimilarity}(\text{'boy'}, \text{'bay'}) = 0 + 1 + 0 = 1$
- Example 2:
 - $\text{dissimilarity}(\text{'boss'}, \text{'bayes'}) = 0 + 1 + 5 + 5 + 7 = 18$

General requirements on (any) dissimilarity

- non-negativity

$$d(x, x') \geq 0$$

- reflexivity

$$d(x, x') = 0 \quad \text{if and only if} \quad x = x'$$

- symmetry

$$d(x, x') = d(x', x)$$

- triangle inequality:

$$d(x, x') + d(x', x'') \geq d(x, x'')$$

Dissimilarity matrix

| | <i>Baby</i> | <i>Day</i> | <i>Disc</i> | <i>Human</i> | <i>Mucus</i> | <i>Music</i> | <i>Mainly</i> | <i>People</i> |
|---------------|-------------|------------|-------------|--------------|--------------|--------------|---------------|---------------|
| <i>Baby</i> | | 12 | 10 | 11 | 11 | 11 | 22 | 23 |
| <i>Day</i> | | | 11 | 18 | 18 | 18 | 18 | 19 |
| <i>Disc</i> | | | | 15 | 15 | 13 | 20 | 20 |
| <i>Human</i> | | | | | 7 | 7 | 20 | 20 |
| <i>Mucus</i> | | | | | | 5 | 18 | 20 |
| <i>Music</i> | | | | | | | 18 | 20 |
| <i>Mainly</i> | | | | | | | | 7 |
| <i>People</i> | | | | | | | | |

Agglomerative clustering

Starting from individual objects, produce a sequence of clusters of increasing size.

We define the dissimilarity between two clusters as the smallest pair-wise dissimilarity of objects from these clusters, one object from each cluster (single linkage)

$$d_{\min}(D_i, D_j) = \min_{x \in D_i, x' \in D_j} \|x - x'\|$$

Dissimilarity matrix

| | <i>Baby</i> | <i>Day</i> | <i>Disc</i> | <i>Human</i> | <i>(Mucus, Music)₅</i> | <i>Mainly</i> | <i>People</i> |
|---------------------------------------|-------------|------------|-------------|--------------|---------------------------------------|---------------|---------------|
| <i>Baby</i> | | 12 | 10 | 11 | 11 | 22 | 23 |
| <i>Day</i> | | | 11 | 18 | 18 | 18 | 19 |
| <i>Disc</i> | | | | 15 | 13 | 20 | 20 |
| <i>Human</i> | | | | | 7 | 20 | 20 |
| <i>(Mucus, Music)₅</i> | | | | | | 18 | 20 |
| <i>Mainly</i> | | | | | | | 7 |
| <i>People</i> | | | | | | | |

Dissimilarity matrix

| | Baby | Day | Disc | ((Mucus,Music) ₅ Human) ₇ | (Mainly,People) ₇ |
|--|------|-----|------|--|------------------------------|
| Baby | | 12 | 10 | 11 | 22 |
| Day | | | 11 | 18 | 18 |
| Disc | | | | 13 | 20 |
| ((Mucus,Music) ₅ Human) ₇ | | | | | 18 |
| (Mainly, People) ₇ | | | | | |

Dissimilarity matrix

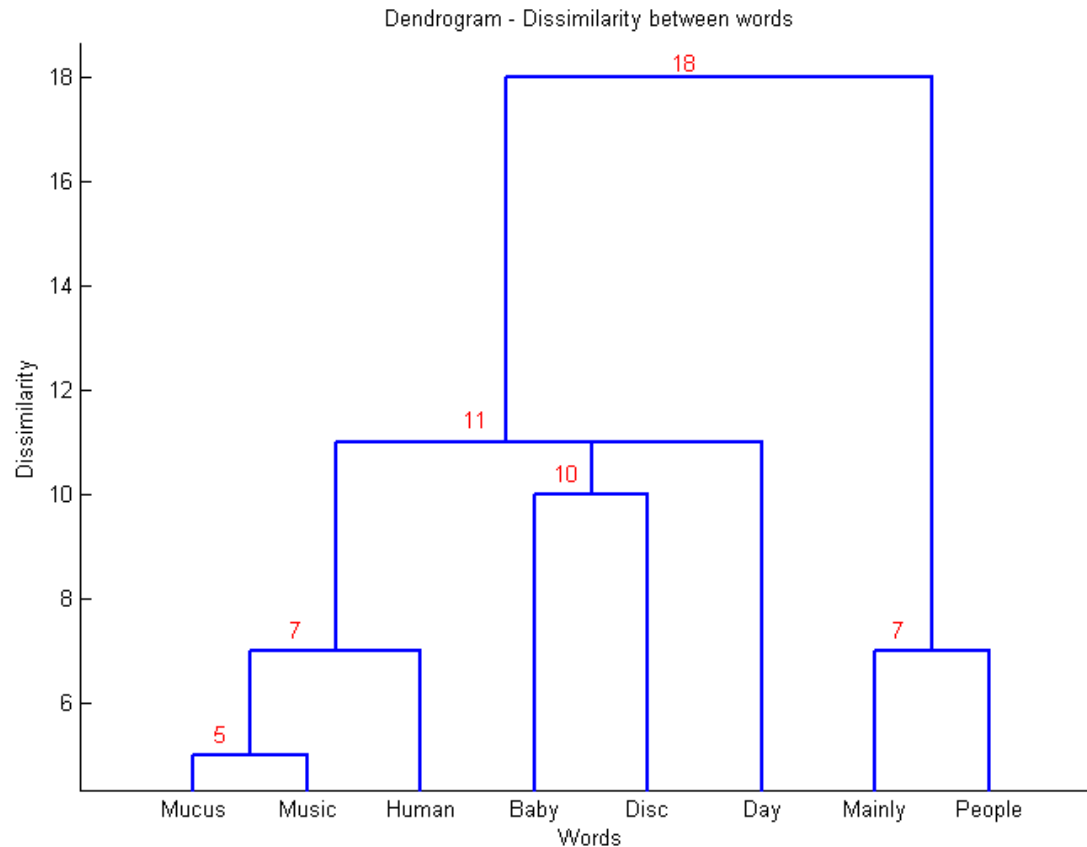
| | <i>(Baby,Disc)₁₀</i> | <i>Day</i> | <i>((Mucus,Music)₅ Human)₇</i> | <i>(Mainly, People)₇</i> |
|--|---------------------------------|------------|--|-------------------------------------|
| <i>(Baby,Disc)₁₀</i> | | 11 | 11 | 20 |
| <i>Day</i> | | | 18 | 18 |
| <i>((Mucus,Music)₅ Human)₇</i> | | | | 18 |
| <i>(Mainly,People)₇</i> | | | | |

Dissimilarity matrix

| | | |
|--|--|-------------------------------------|
| | <i>(Day, (Baby, Disc)₁₀, ((Mucus, Music)₅ Human)₇)₁₁</i> | <i>(Mainly, People)₇</i> |
| <i>(Day, (Baby, Disc)₁₀, ((Mucus, Music)₅ Human)₇)₁₁</i> | | 18 |
| <i>(Mainly, People)₇</i> | | |

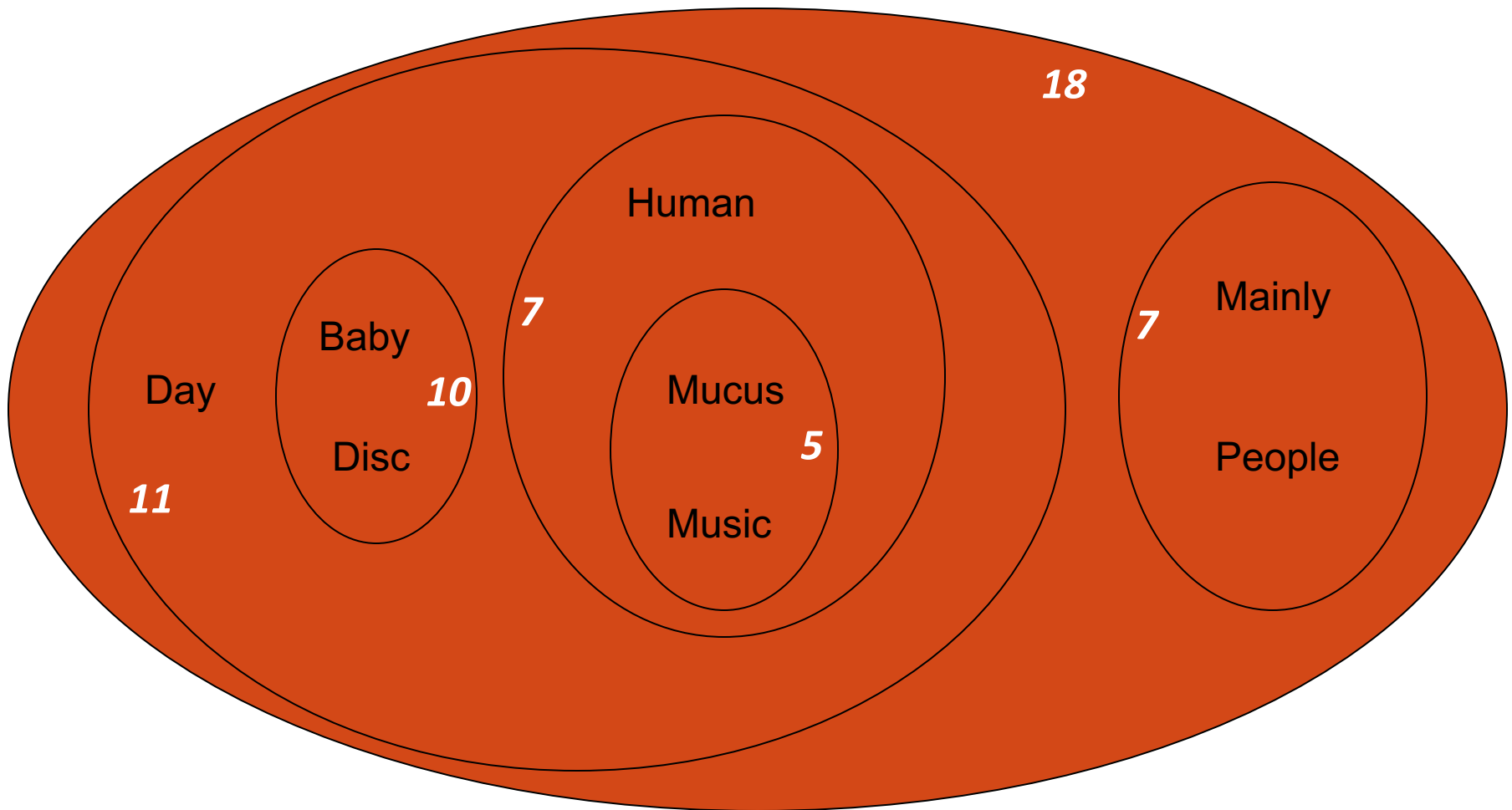
Dendrogram

Representation of the clustering hierarchy



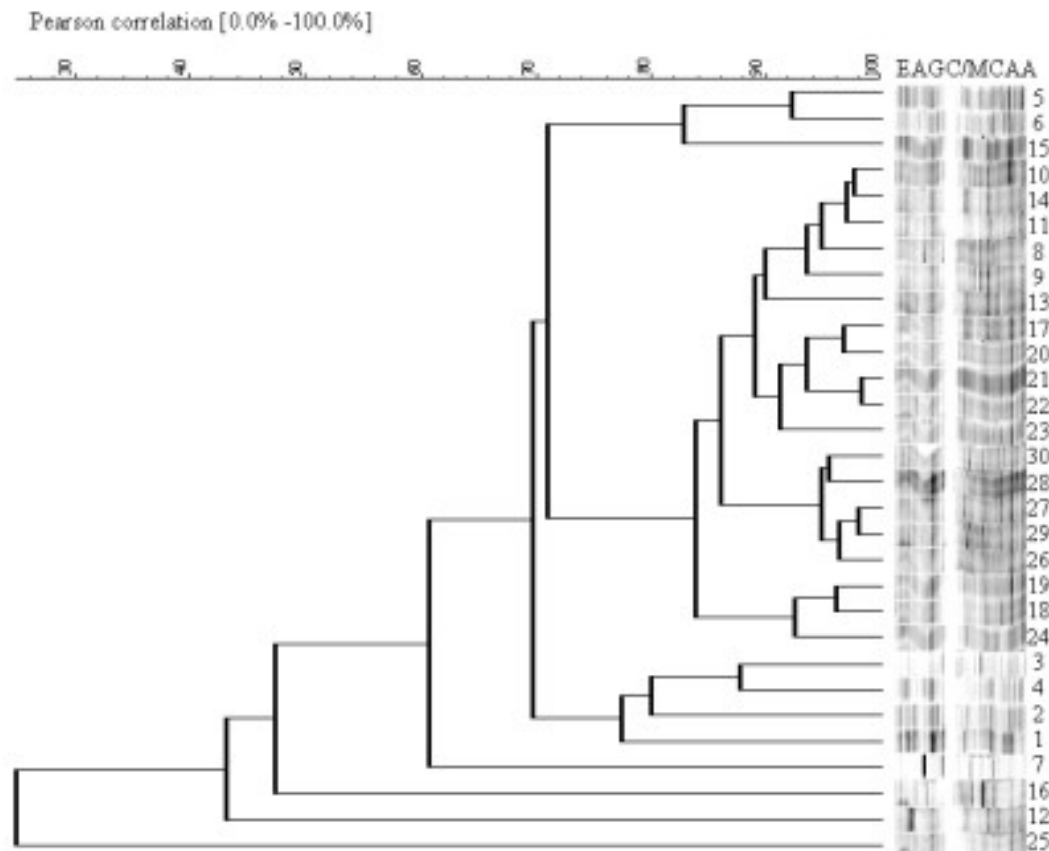
Venn diagram

$(((((\text{Baby}, \text{Disc})_{10}, ((\text{Mucus}, \text{Music})_5, \text{Human})_7)_{11}, \text{Day})_{11}, (\text{Mainly}, \text{People})_7)_{18}$



Black pepper cultivars using AFLP analysis along with digital fingerprint profile

(<http://www.pubmedcentral.nih.gov/articlerender.fcgi?artid=1948014>)



The clustering pattern obtained for the major cultivars of black pepper.

(<http://www.pubmedcentral.nih.gov/articlerender.fcgi?artid=1948014>)

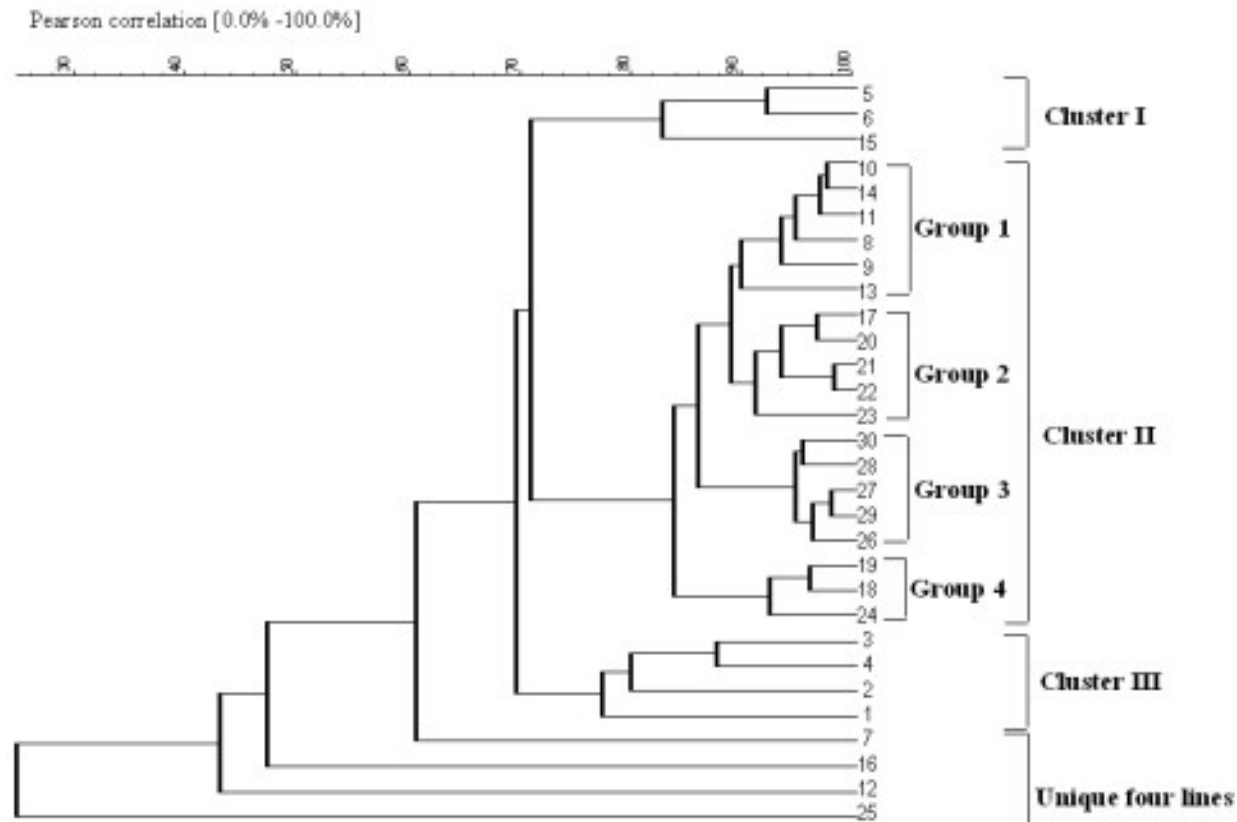


Figure 3b

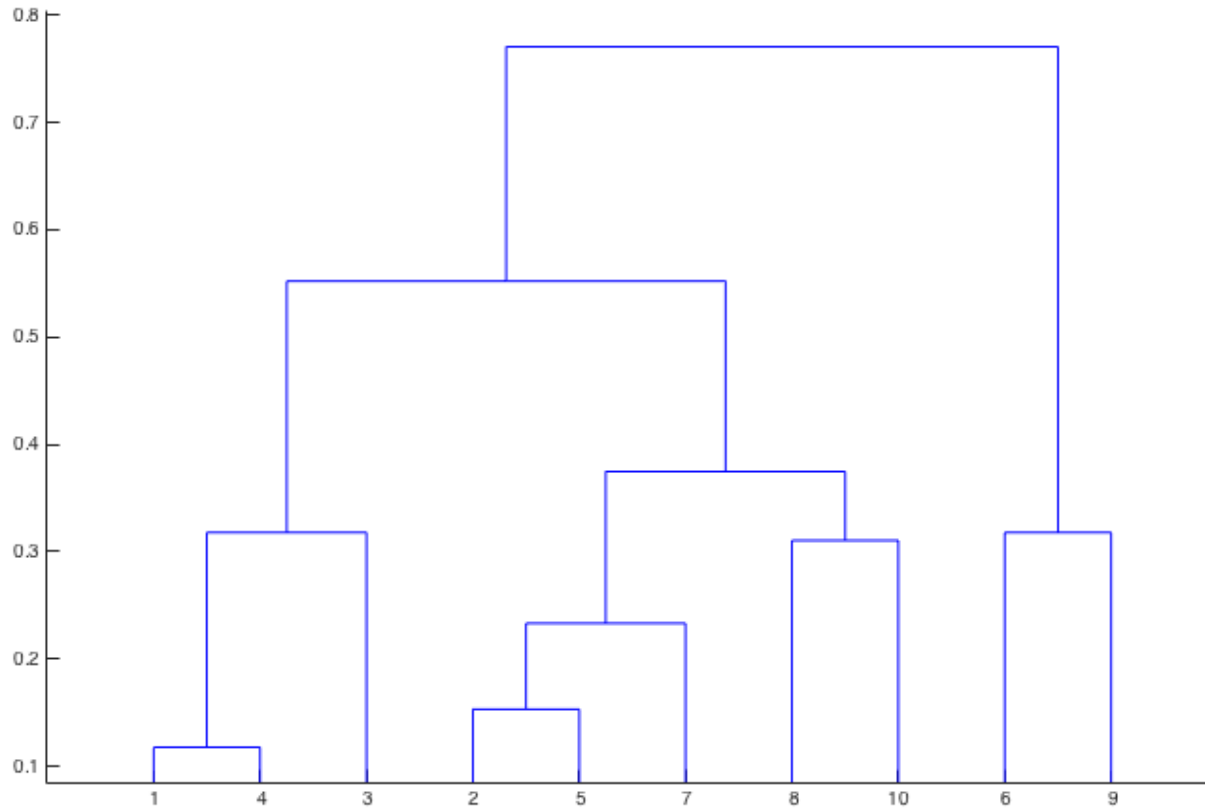
UPGMA dendrograms. A: black pepper cultivars using AFLP analysis along with digital fingerprint profile. B: the clustering pattern obtained for the major cultivars of black pepper.

Dendrogram in Matlab (example)

Let x_i , $i = 1 \dots 10$, be $n = 10$ feature vectors representing 10 objects. We will make a dendrogram for this set.

1. Put x_i , $i = 1 \dots 10$, to become the rows of a matrix X .
(E.g. $X = \text{rand}(10,2)$; (10 2-dim feature vectors))
2. Compute the pairwise distances of all observations in matrix X using a given distance metric: $Y = \text{pdist}(X, 'cityblock')$;
(Y is a row vector that includes the off-diagonal elements of a pair-wise distance matrix. It has $n(n-1)/2$ elements.)
3. Using the pair-wise distances, compute a $(n-1)*3$ matrix Z that represents a hierarchical binary cluster tree:
 $Z = \text{linkage}(Y, 'average')$; % 'average' – type of linkage used
4. Compute and plot a dendrogram using
 $[H, T] = \text{dendrogram}(Z)$; ($T = n*1$; H – vector of line handles)

Dendrogram in Matlab (example)



```
X = [0.3477  0.7363;  
      0.1500  0.3947;  
      0.5861  0.6834;  
      0.2621  0.7040;  
      0.0445  0.4423;  
      0.7549  0.0196;  
      0.2428  0.3309;  
      0.4424  0.4243;  
      0.6878  0.2703;  
      0.3592  0.1971]
```