

Hierarchical clustering

Ting Huang

Adapted from the slides of
David M. Blei from Princeton University

[http://www.cs.princeton.edu/courses/archive/spr08/cos424/
slides/clustering-2.pdf](http://www.cs.princeton.edu/courses/archive/spr08/cos424/slides/clustering-2.pdf)

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- Visualizing this tree provides a useful summary of the data

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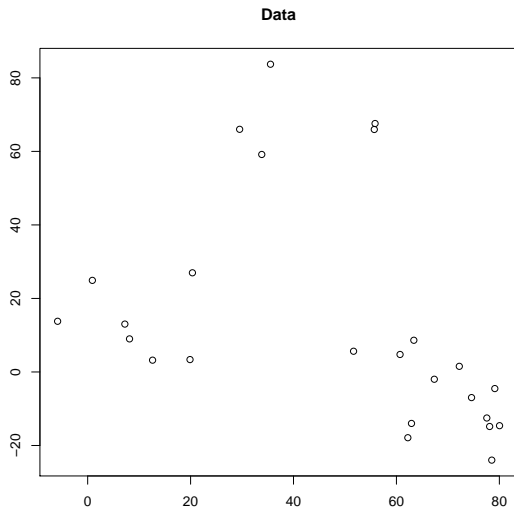
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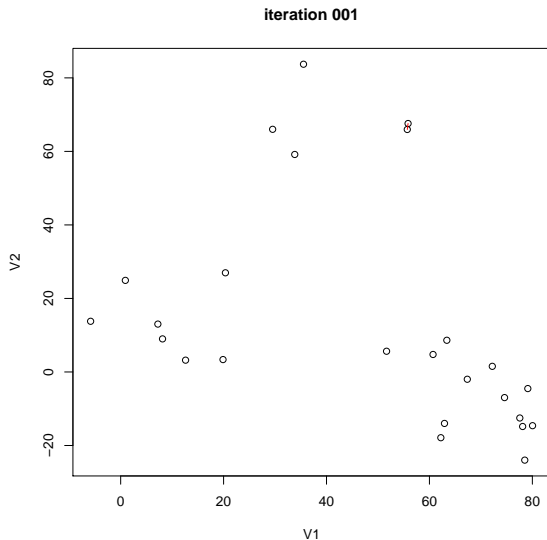
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- Algorithm:
 - ① Place each data point into its own singleton group
 - ② Repeat: iteratively merge the two closest groups
 - ③ Until: all the data are merged into a single cluster

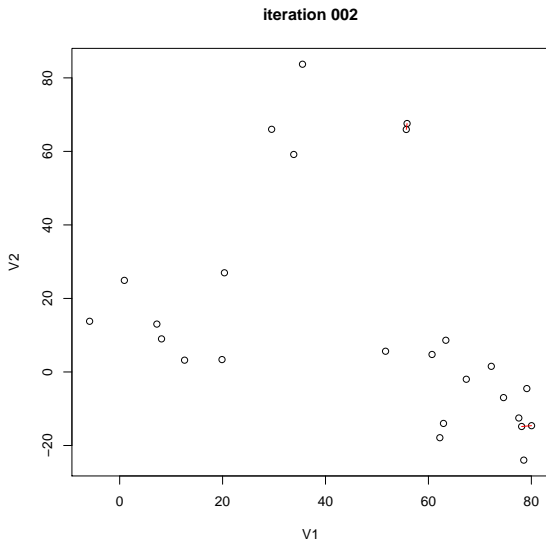
Example



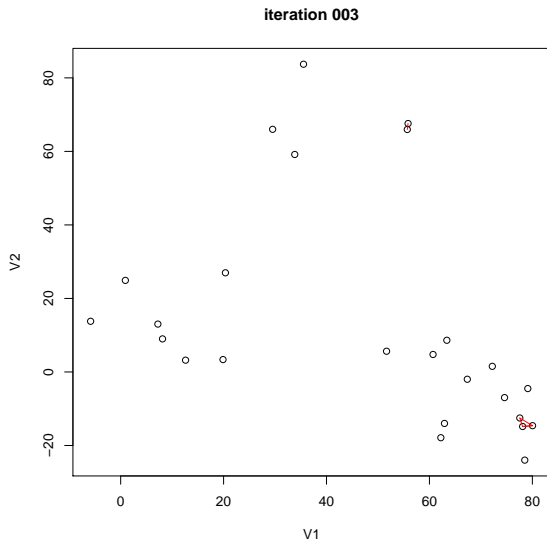
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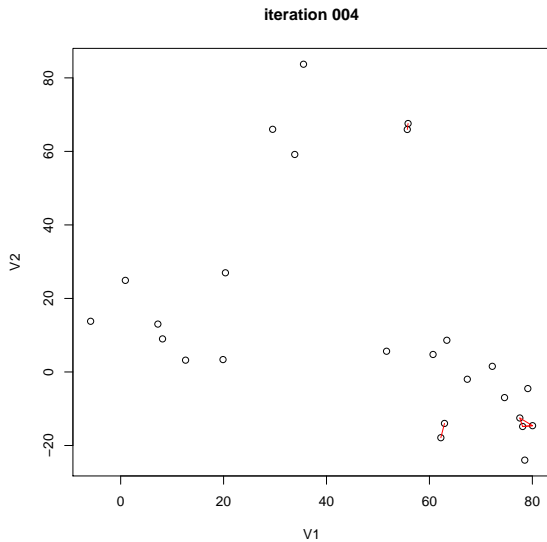
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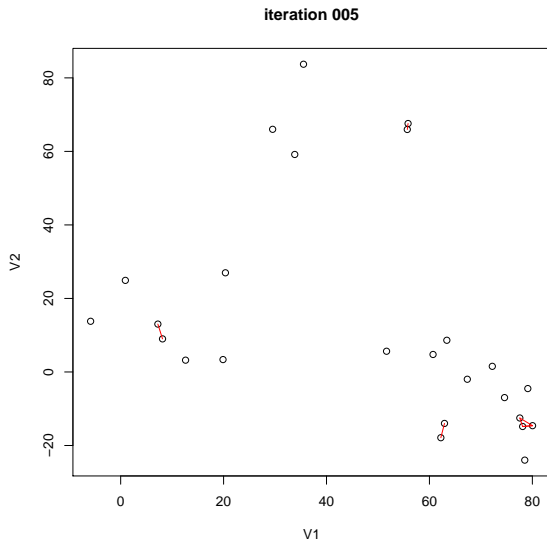
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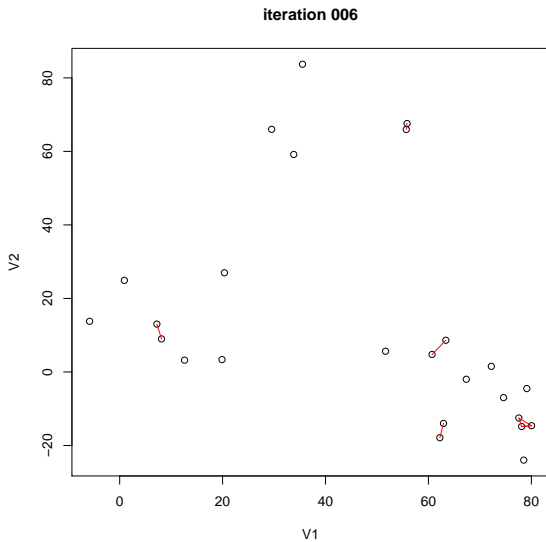
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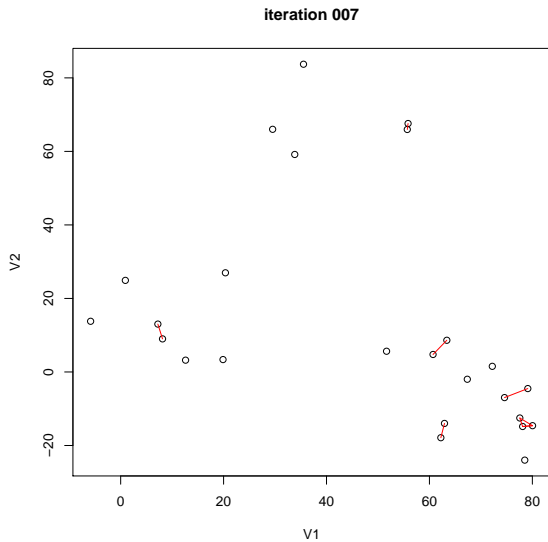
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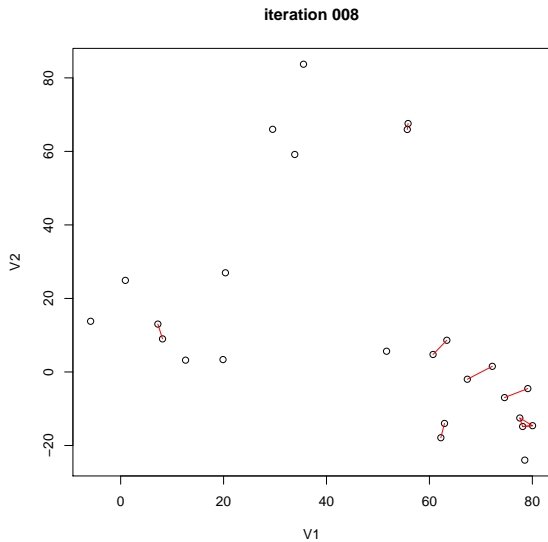
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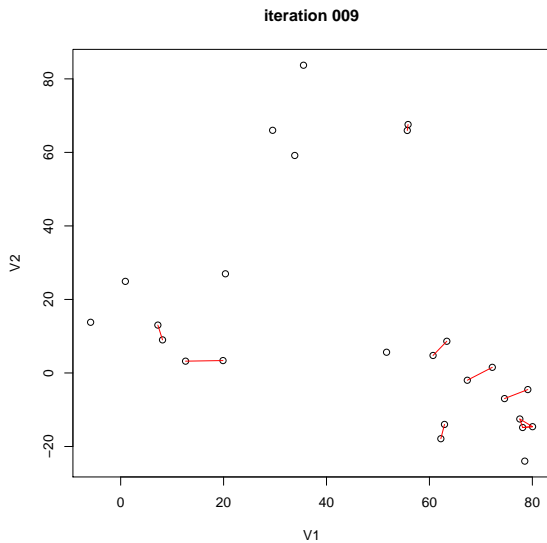
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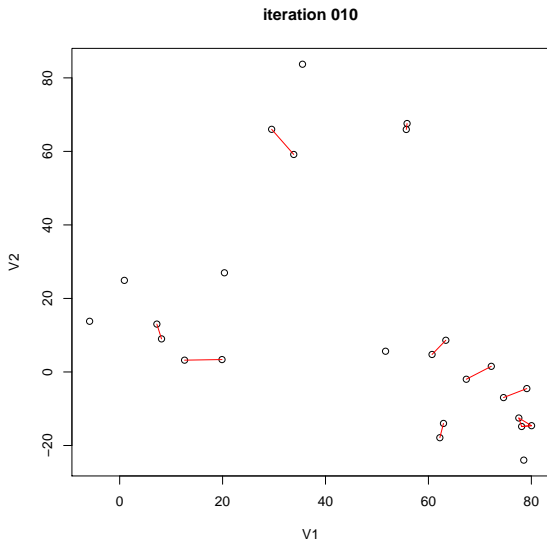
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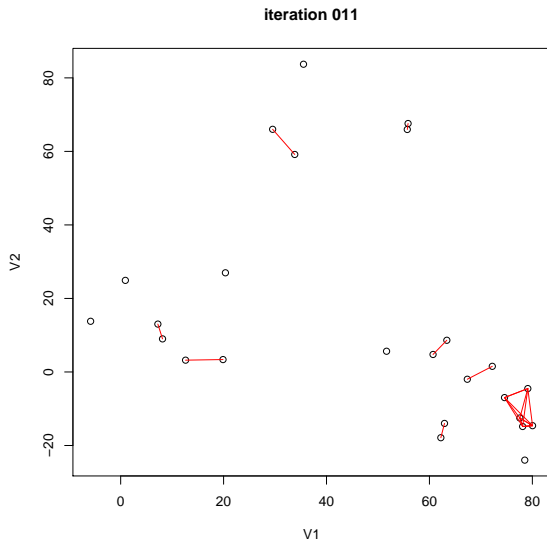
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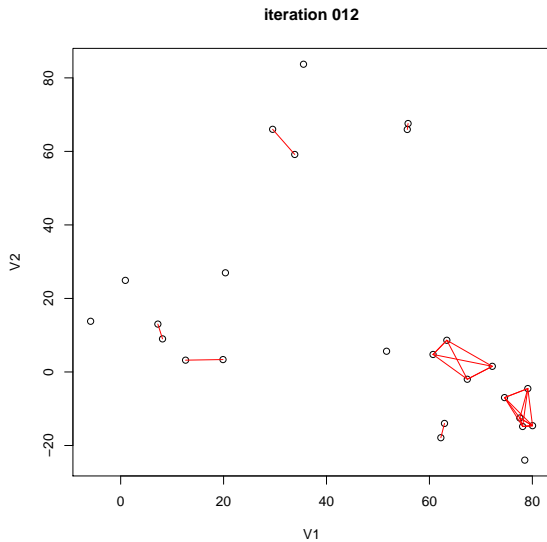
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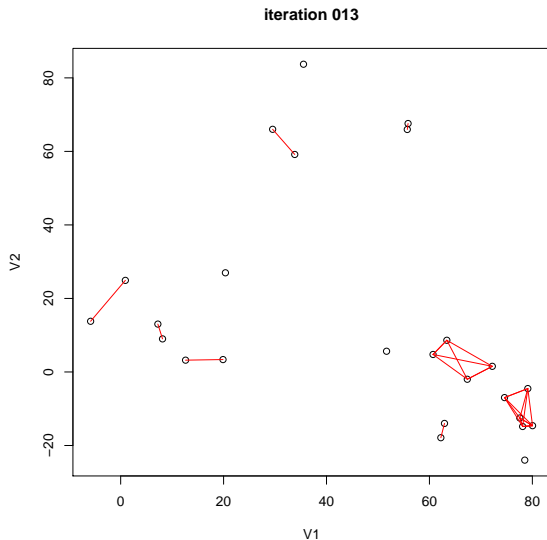
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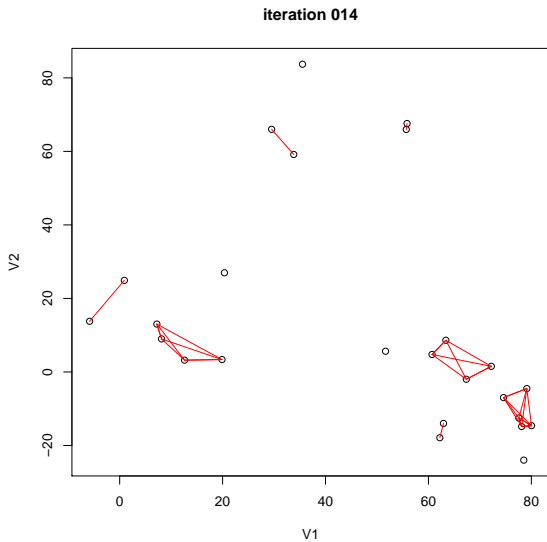
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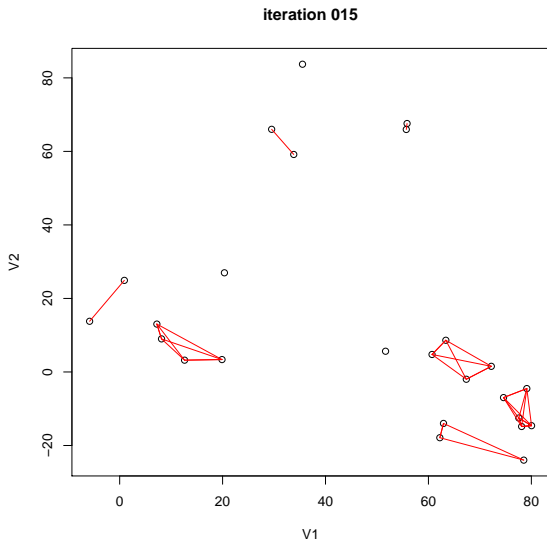
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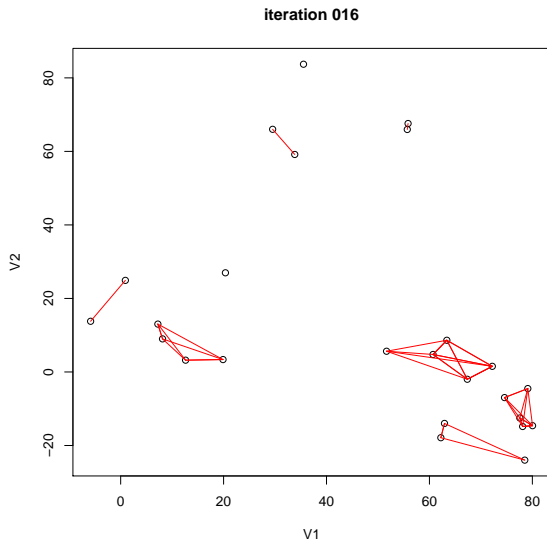
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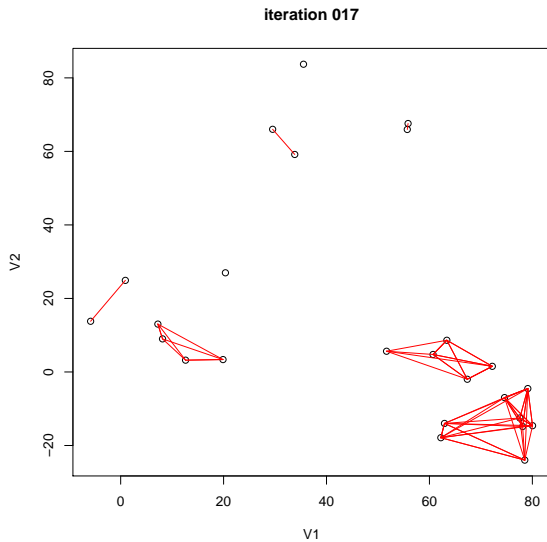
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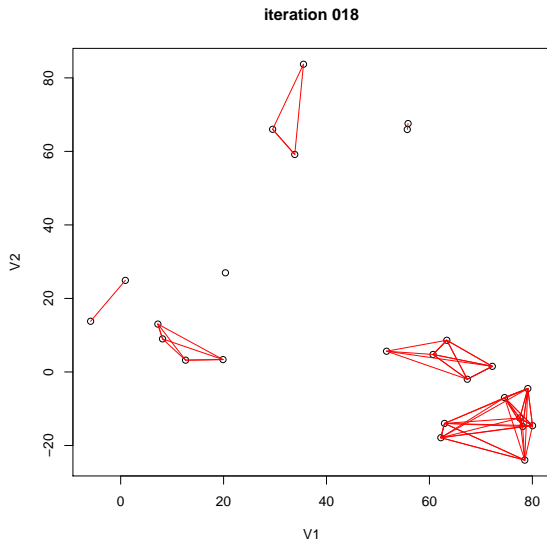
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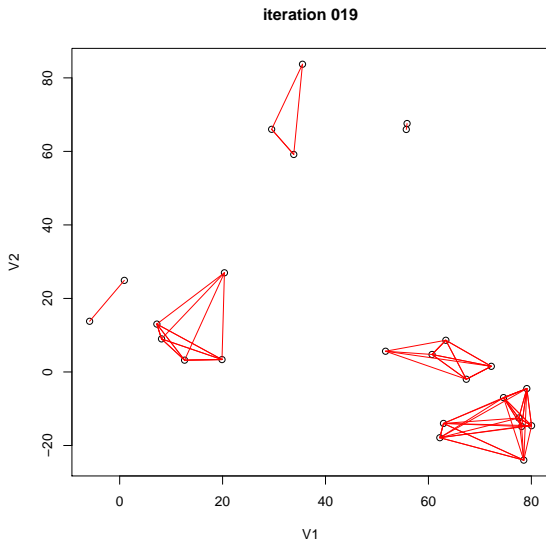
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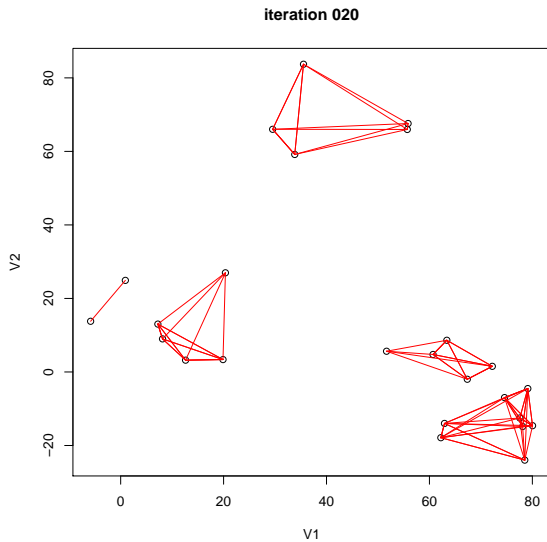
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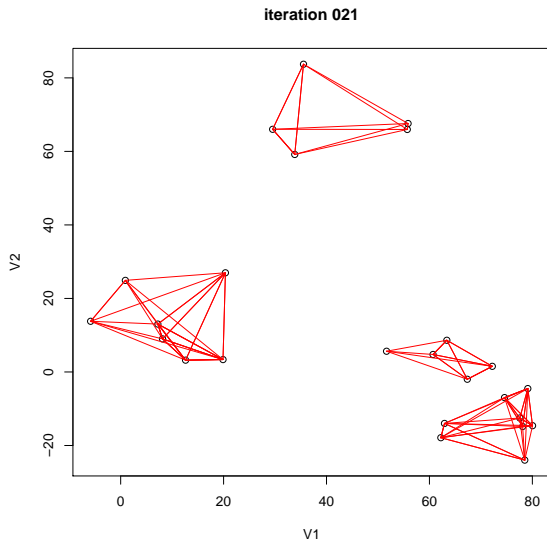
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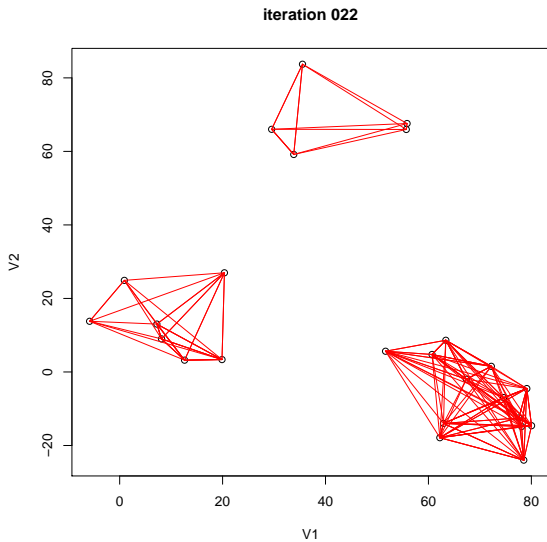
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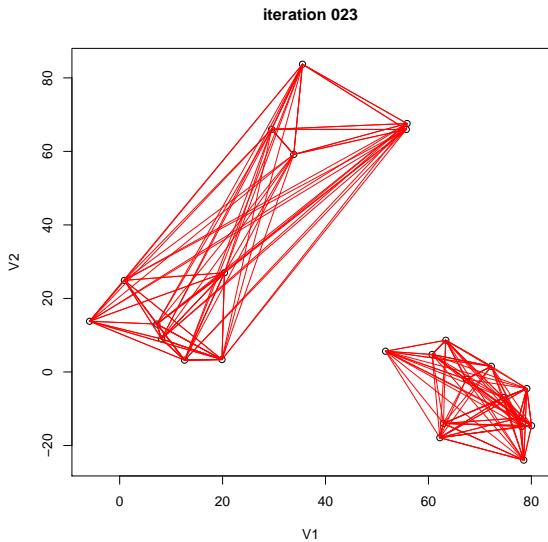
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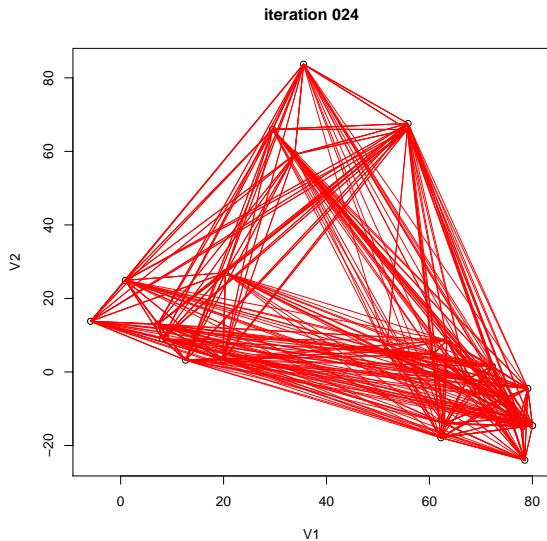
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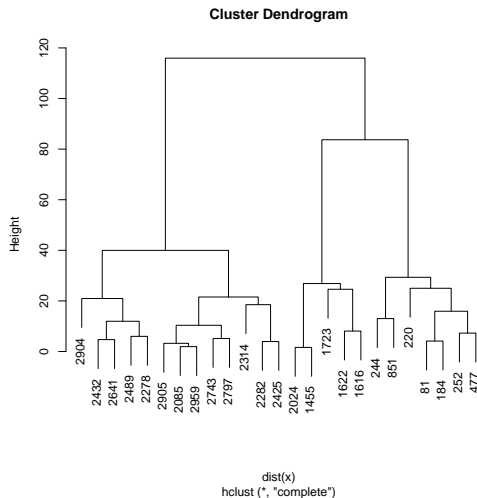
Example



Example



Dendrogram of example data



Groups that merge at high values relative to the merger values of their subgroups are candidates for natural clusters. (Tibshirani et al., 2001)

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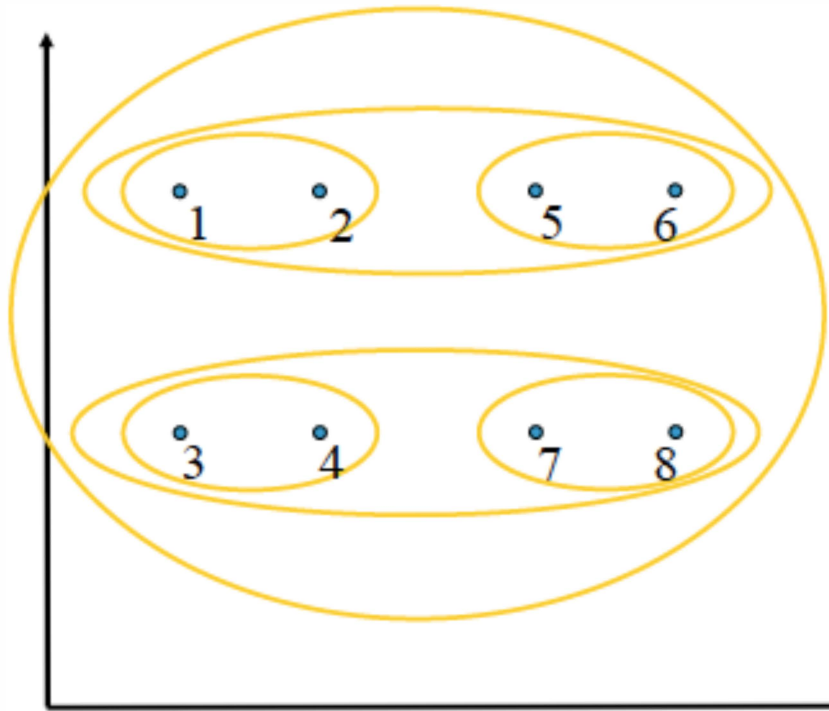
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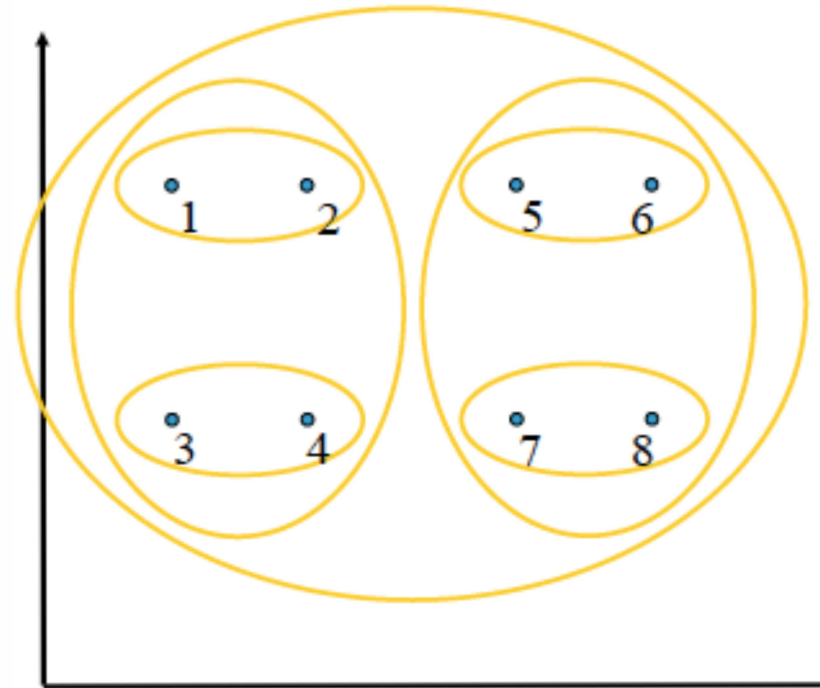
- *Group average*: the average similarity between groups

$$d_{GA} = \frac{1}{N_G N_H} \sum_{i \in G} \sum_{j \in H} d_{i,j}$$

Closest pair
(single-link clustering)



Farthest pair
(complete-link clustering)



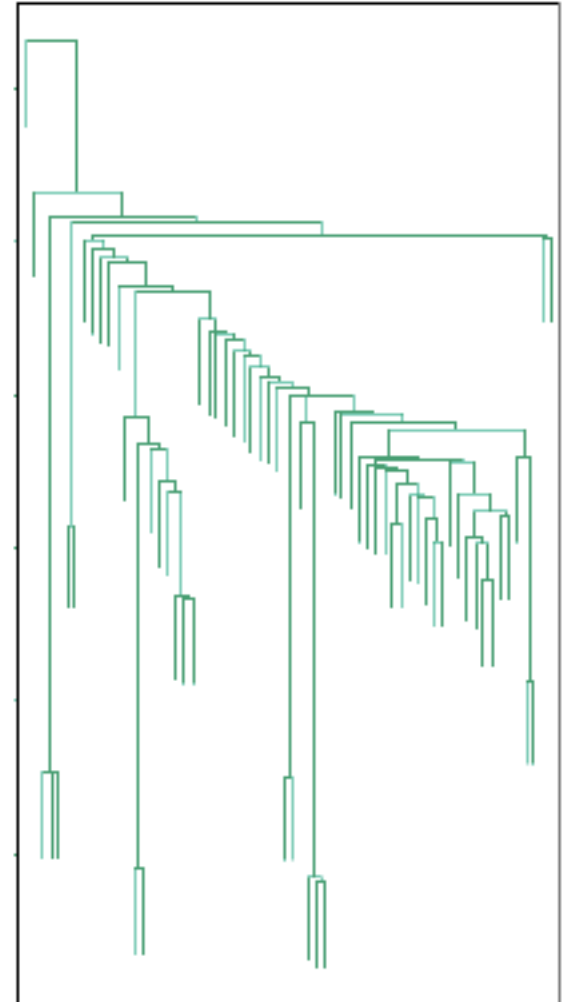
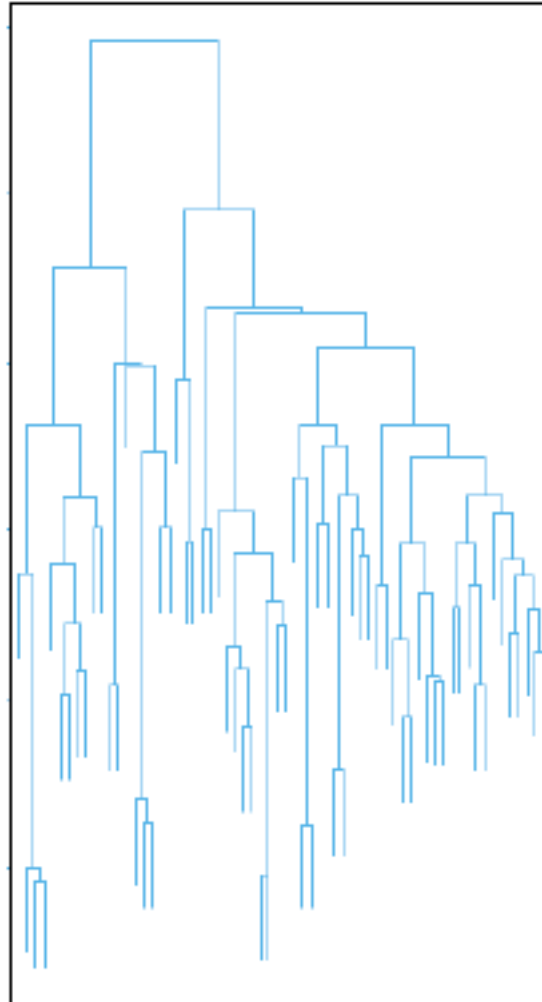
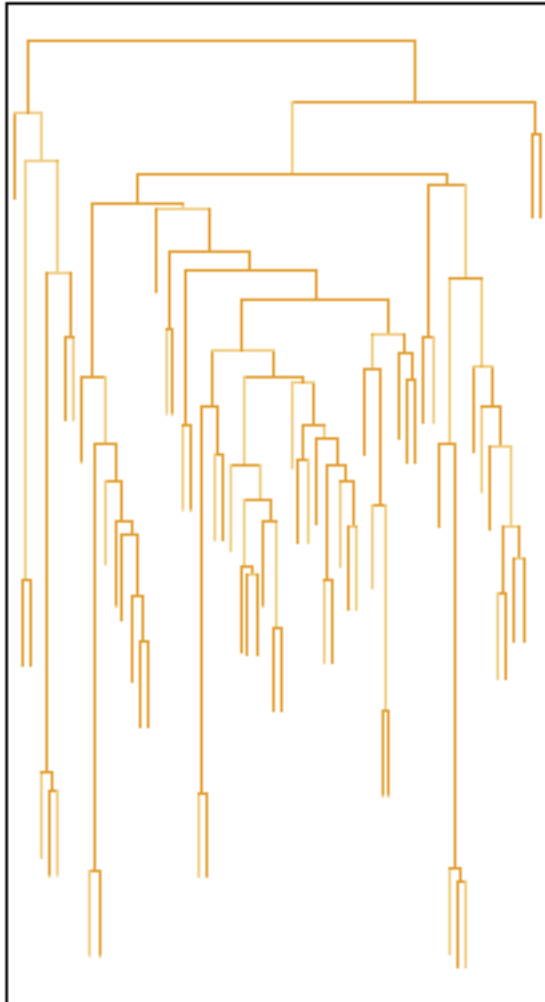
[Pictures from Thorsten Joachims]

Slide from Lu Wang's machine learning course

Average

Farthest

Nearest



Slide from Lu Wang's machine learning course
Mouse tumor data from [Hastie *et al.*]

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- Complete linkage has the opposite problem. It might not merge close groups because of outlier members that are far apart.
- Group average represents a natural compromise, but depends on the scale of the similarities. Applying a monotone transformation to the similarities can change the results.