Data Mining (W4240 Section 001)
Clustering (part 2)

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Outline

Outline

Mixture Models

The *Gaussian mixture model*: loosely, cluster with *soft* assignments

To generate data from a GMM:

- choose cluster with $c_i \sim Categorical(p_1, ..., p_p)$
- generate point x_i with $x_i | c_i = k \sim \mathcal{N}(\mu_k, \Sigma_k)$
- (μ_k is mean vector, Σ_k is covariance matrix)

As with K-Means, we generated data with:

- observation x_i in cluster c_i
- K clusters
- Our goal is use data to find μ_k (and Σ_k)

Mixture Models

Mixture models are fit using the following iterative steps:

1. E-step:

$$\mathbb{P}(c_i = k \,|\, x_i) = \frac{\pi_k N(x_i \,|\, \mu_k, \Sigma_k)}{\sum_{\ell=1}^{K} \pi_\ell N(x_i \,|\, \mu_\ell, \Sigma_\ell)}$$

π: Prior prob(y==k)

2. M-step:

$$\mu_k^{new} = \frac{1}{N_k} \sum_{i=1}^{n} \mathbb{P}(c_i = k \,|\, x_i) x_i$$

EM 算法

$$\pi_k^{new} = \frac{1}{N} \sum_{i=1}^{n} \mathbb{P}(c_i = k \,|\, x_i)$$

$$\Sigma_k^{new} = \frac{1}{N_k} \sum_{i=1}^{n} \mathbb{P}(c_i = k \,|\, x_i)(x_i - \mu_k^{new})(x_i - \mu_k^{new})^\top$$

- (the Expectation-Maximization algorithm)
- Let's compare this conceptually to K-Means

Clustering with Gaussian Mixture Models

- have real valued data, $X \in \mathbb{R}^{n \times p}$
- fit with a mixture of K clusters
- each observation x_i has cluster variable c_i
- given cluster k, fit data with a Gaussian distribution

$$x_i \,|\, c_i = k \sim N(\mu_k, \Sigma_k)$$

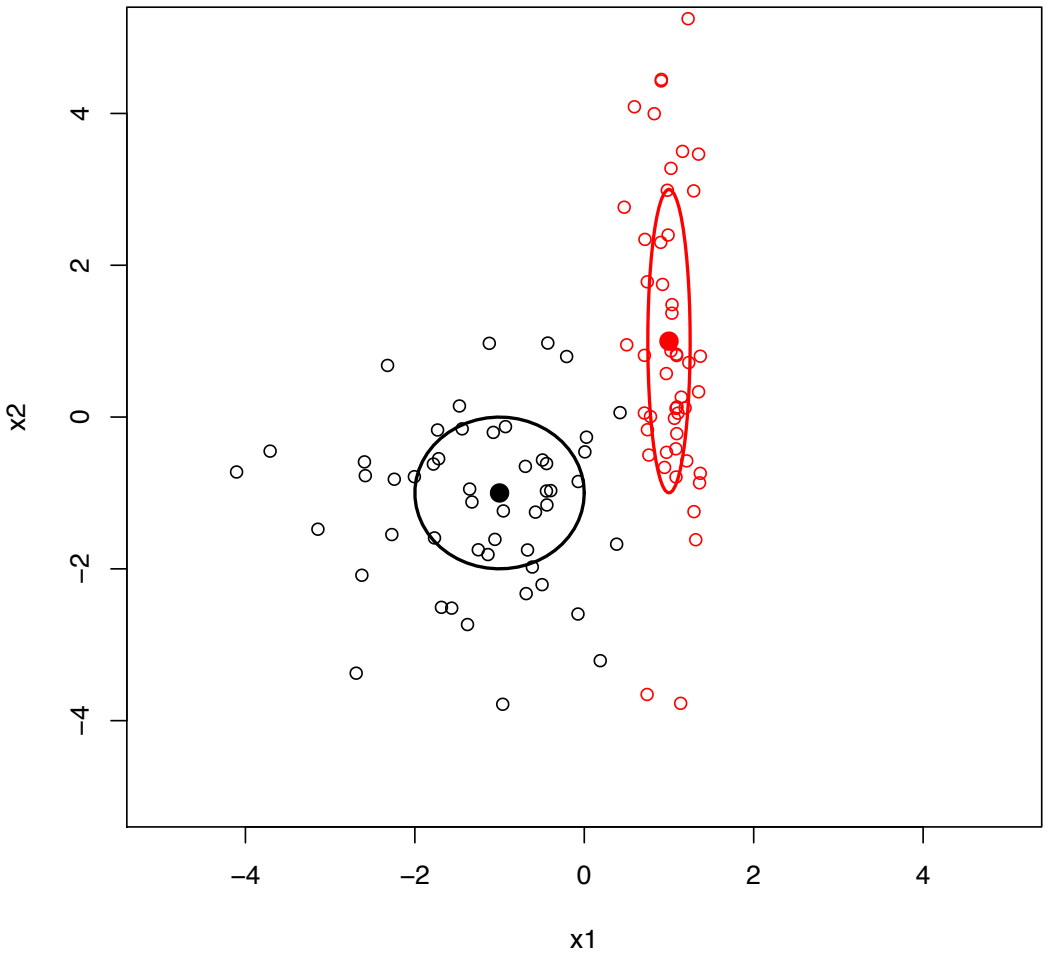
- density of data is

$$\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

Use iterative procedure to cluster distribution, update parameters, update cluster distribution, update parameters...

Mixture Models

Gaussian mixture model ($K = 2$):



Mixture Models

Extensions:

- if we have categorical data, we might model this with a multinomial distribution

$$x_i \,|\, c_i = k \sim Multi(p_{k,1}, \ldots, p_{k,M})$$

- actually, we can use any parametric distribution that we like
- creates a flexible model for mixed data types

Important Caveat: clusters need to be well-modeled by components of a mixture

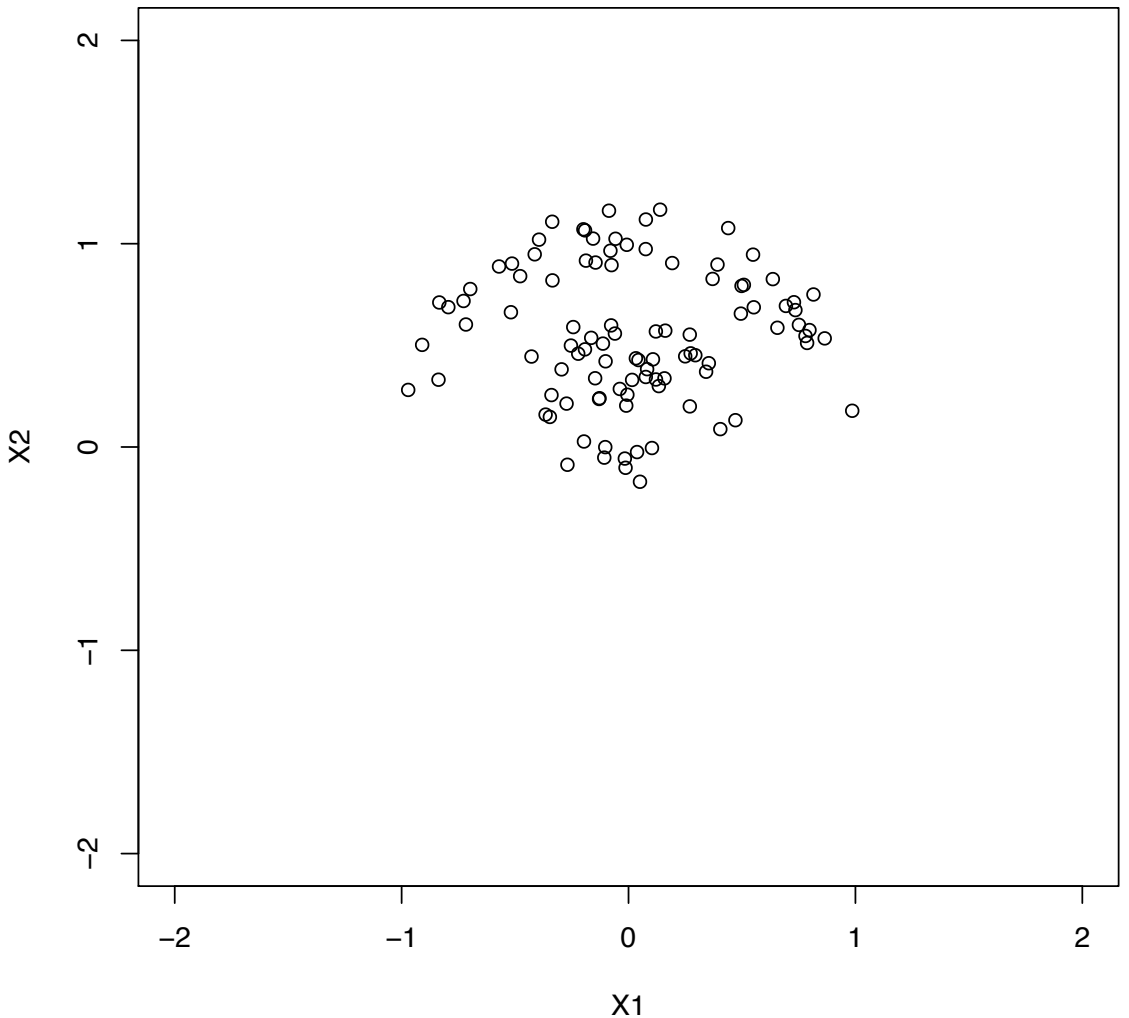
Mixture Models in R

We can use the mclust package in R to fit a mixture model

```
> library(datasets)
> library(mclust)
> faithful.mm <- Mclust(faithful)
> summary(faithful.mm)
> plot(faithful.mm)
> faithful.mm2 <- Mclust(faithful,G=2)
```

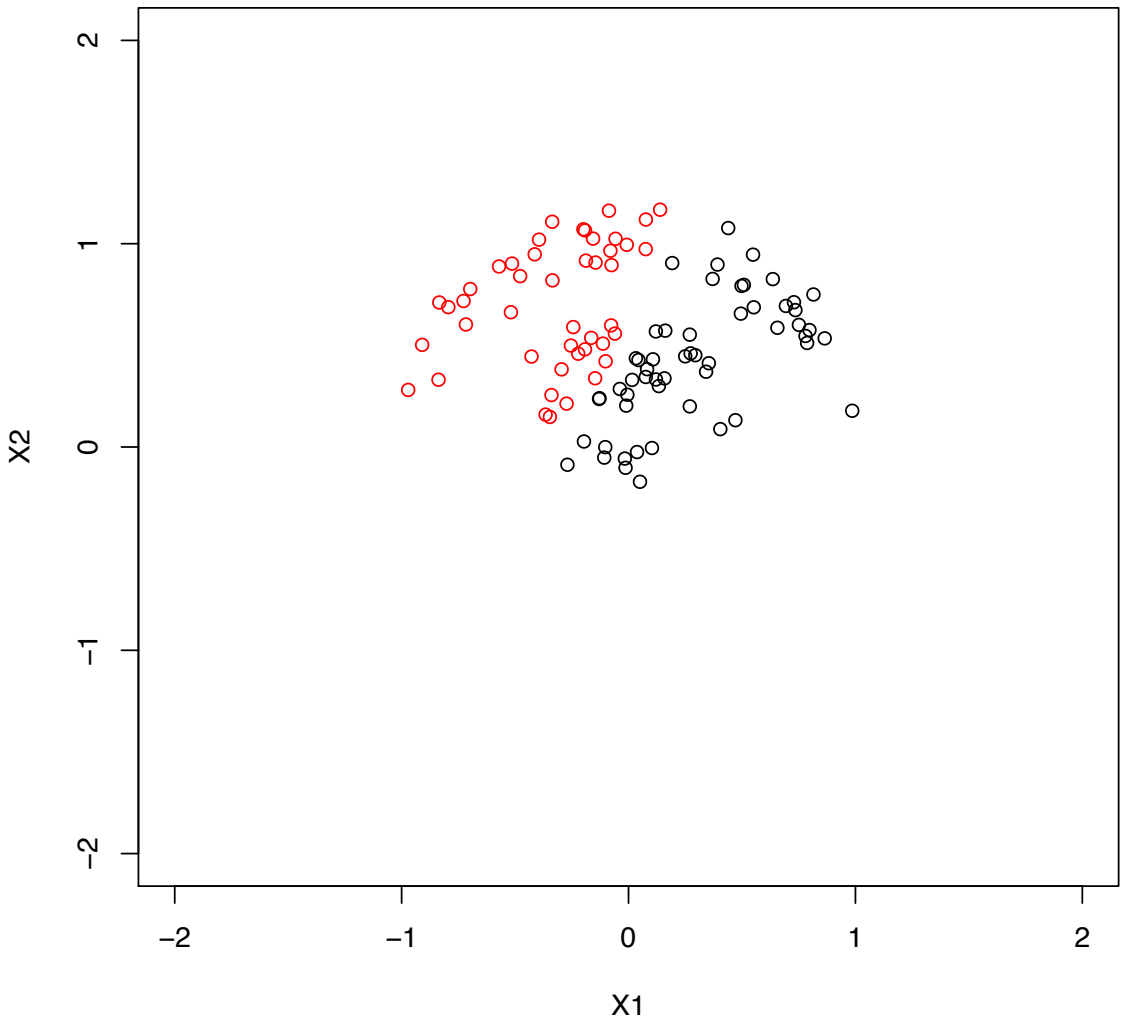
New Data

So what about this data?



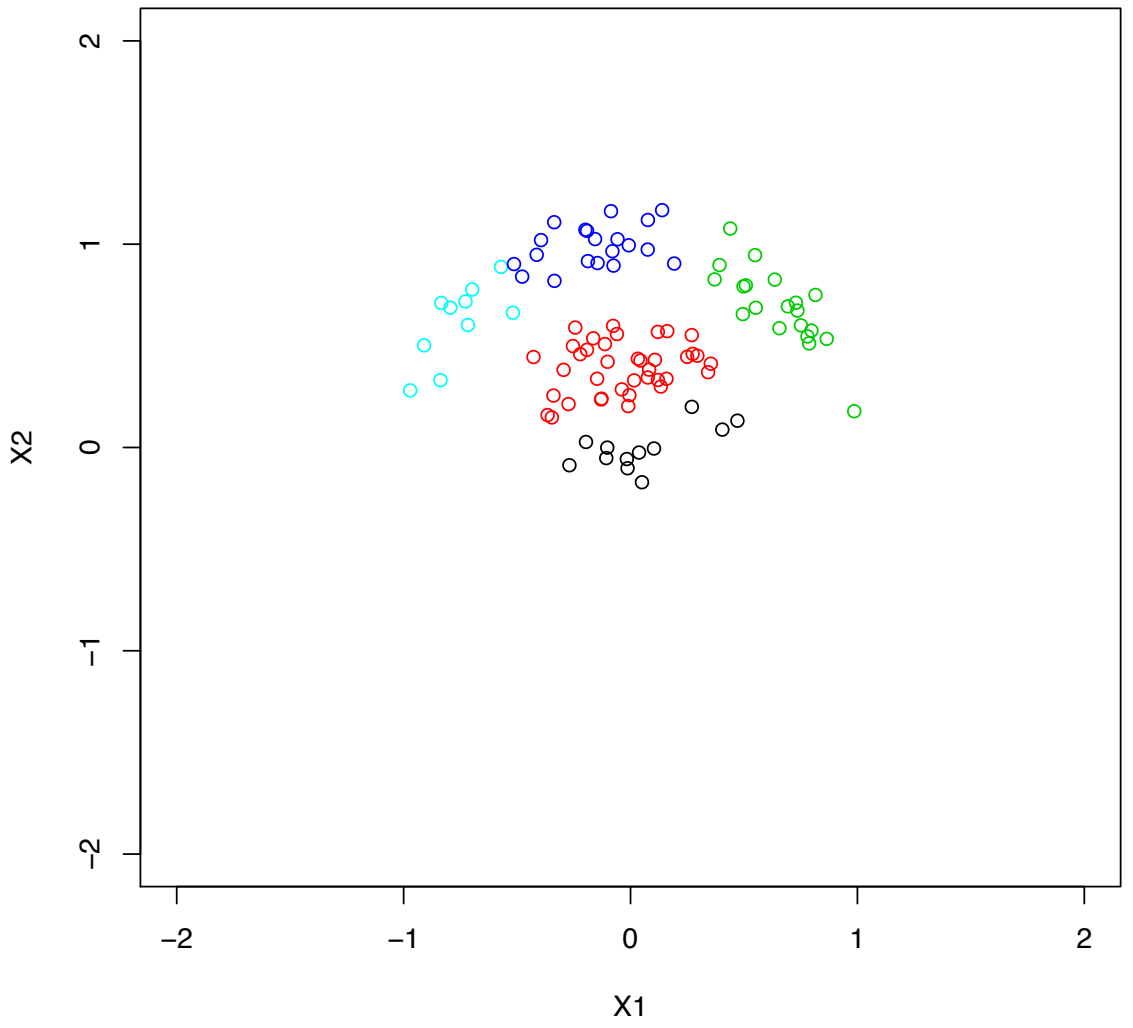
New Data

Fit with K-means:

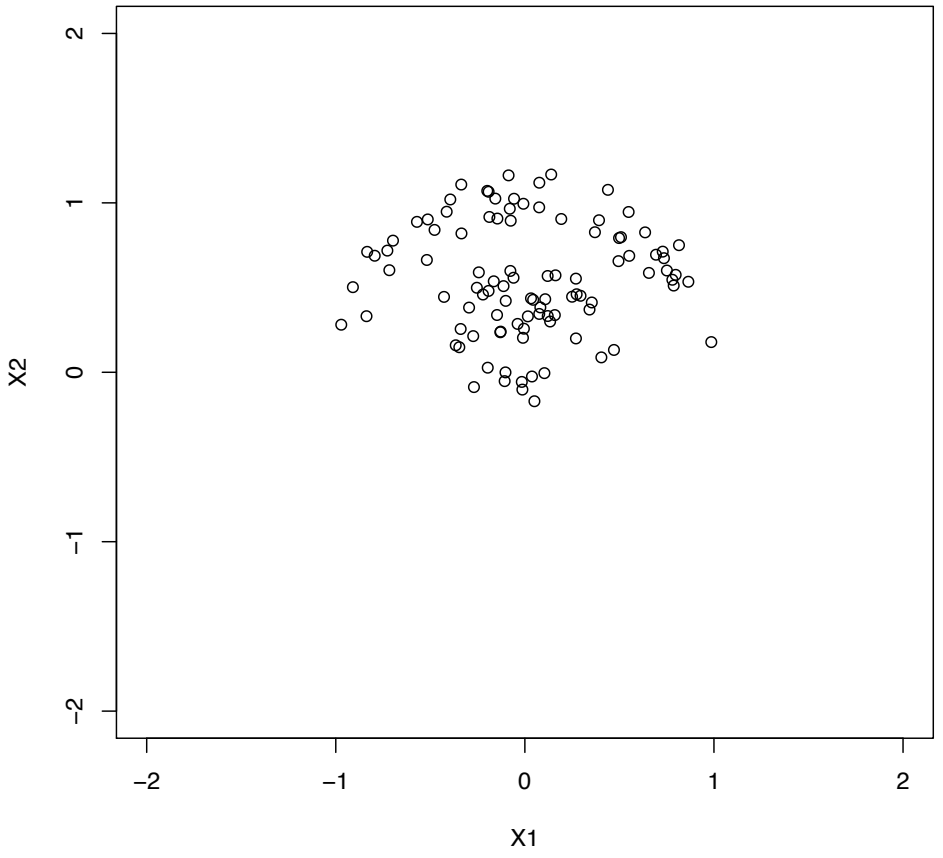


New Data

Fit with a Gaussian mixture model (`Mclust` in the `mclust` package):



New Data



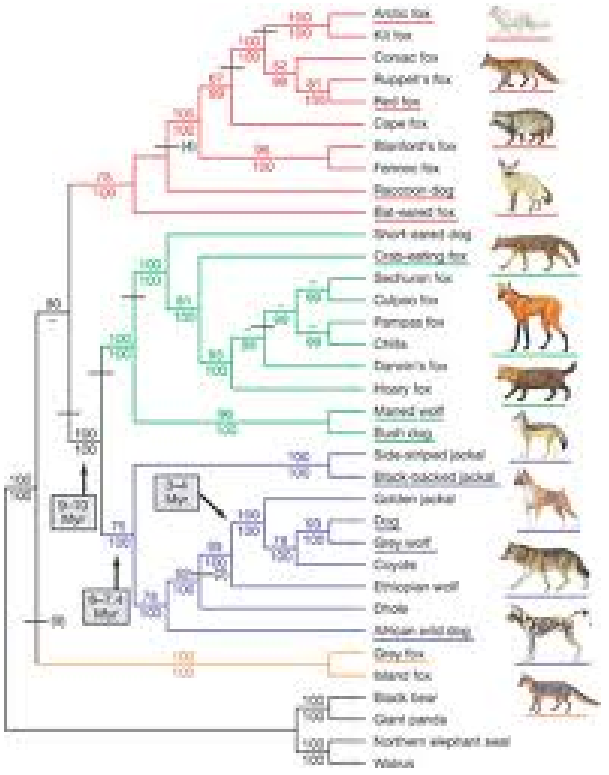
One of the clusters is not well-modeled by a Gaussian distribution...

Outline

Hierarchical Clustering

Idea:

- build a binary tree to represent clustering
- successively merge separate groups
- trees are quite useful for visualizing data



Hierarchical Clustering

What do we need for hierarchical clustering?

K-Means needs:

- a number of clusters K
- an initial clustering
- a distance between points, $d(x_i, x_j)$

Hierarchal clustering needs:

- a distance between *groups of data points*

Outline

Agglomerative Clustering

There are two ways to do hierarchical clustering:

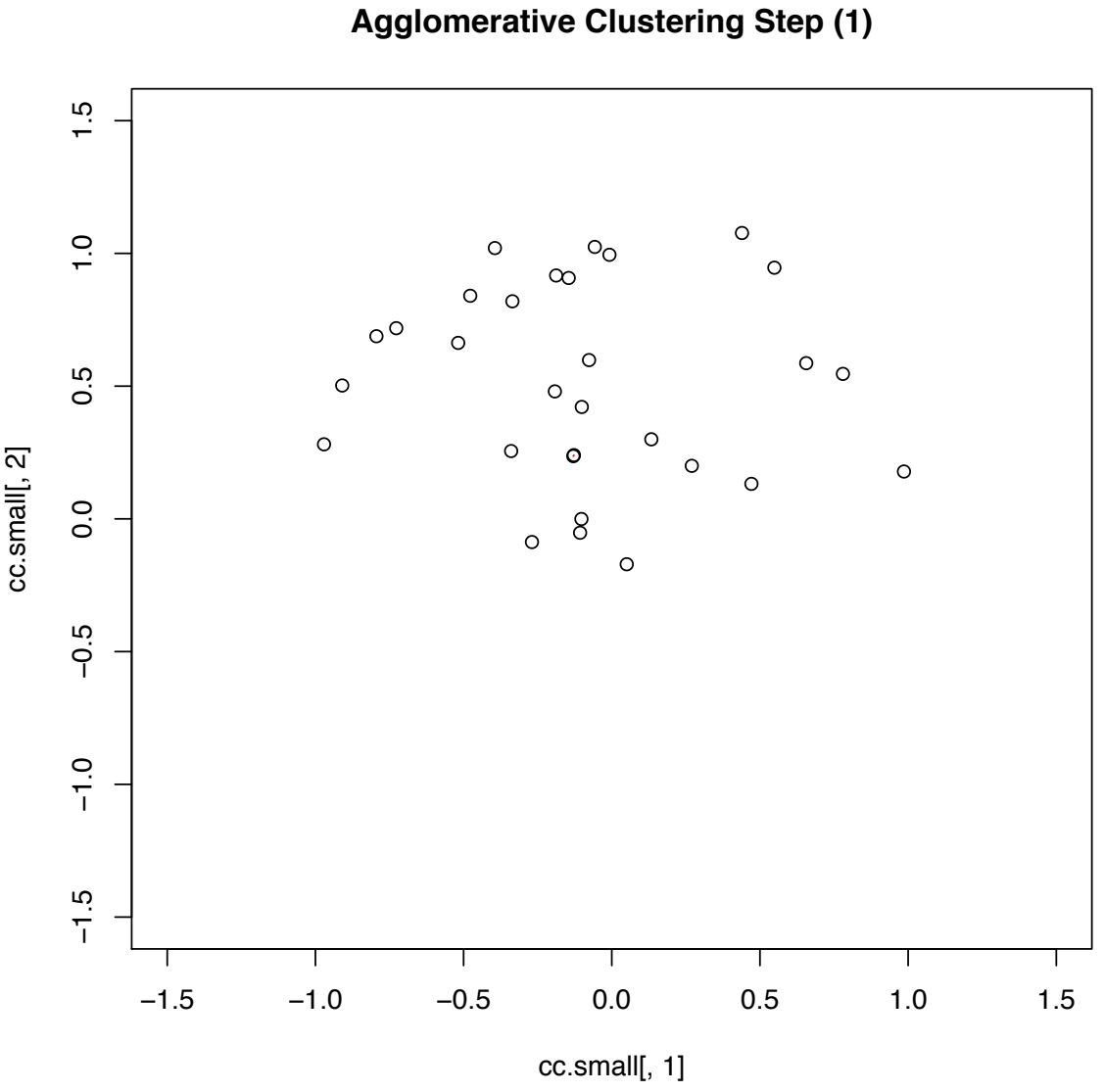
- agglomerative clustering
- divisive clustering

Let's start with *agglomerative clustering*

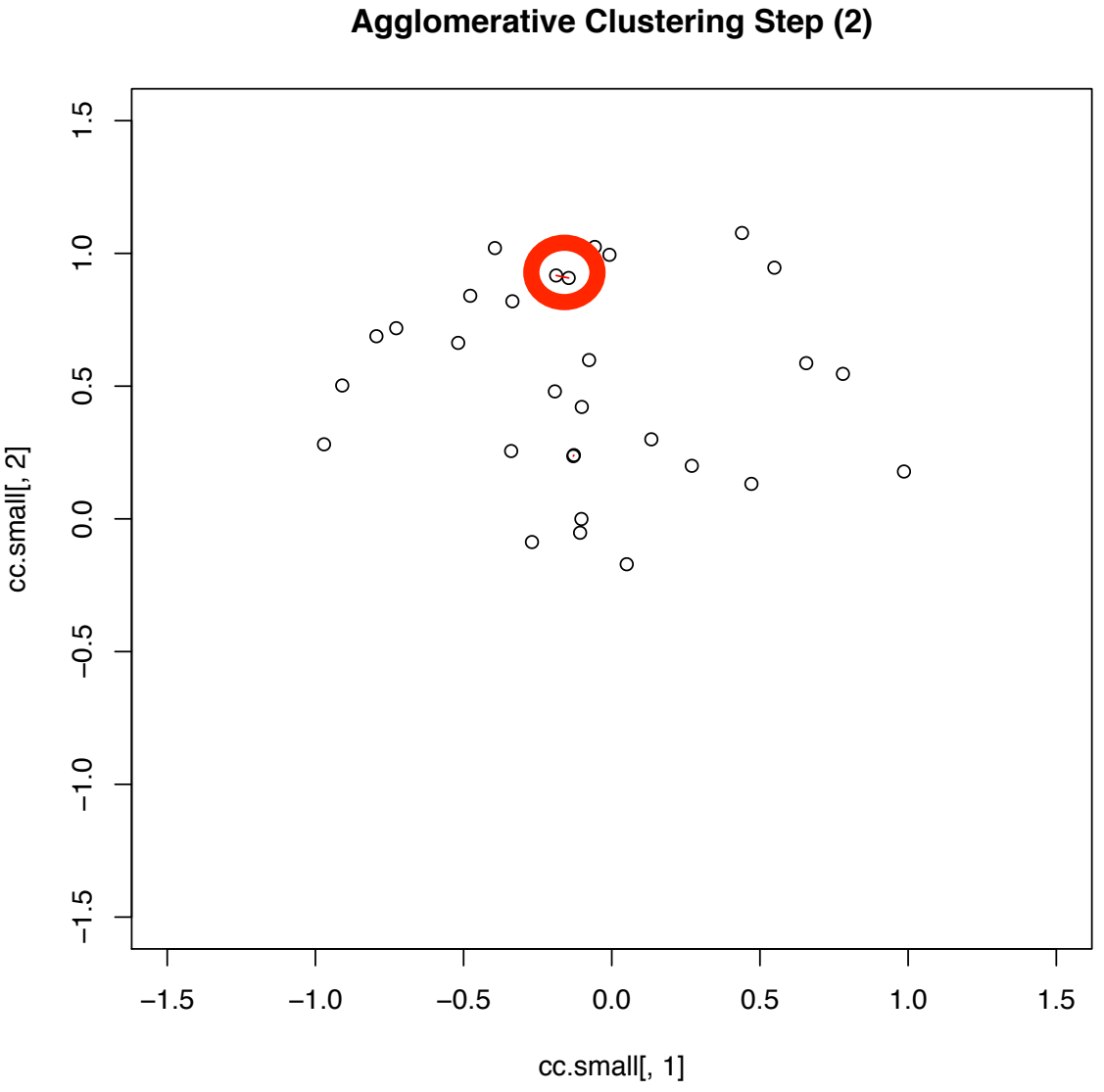
Basic algorithm:

- start with all data points in individual groups
- repeat: merge the two "closest" groups
- stop: when all groups have been merged into a single group

Agglomerative Clustering



Agglomerative Clustering



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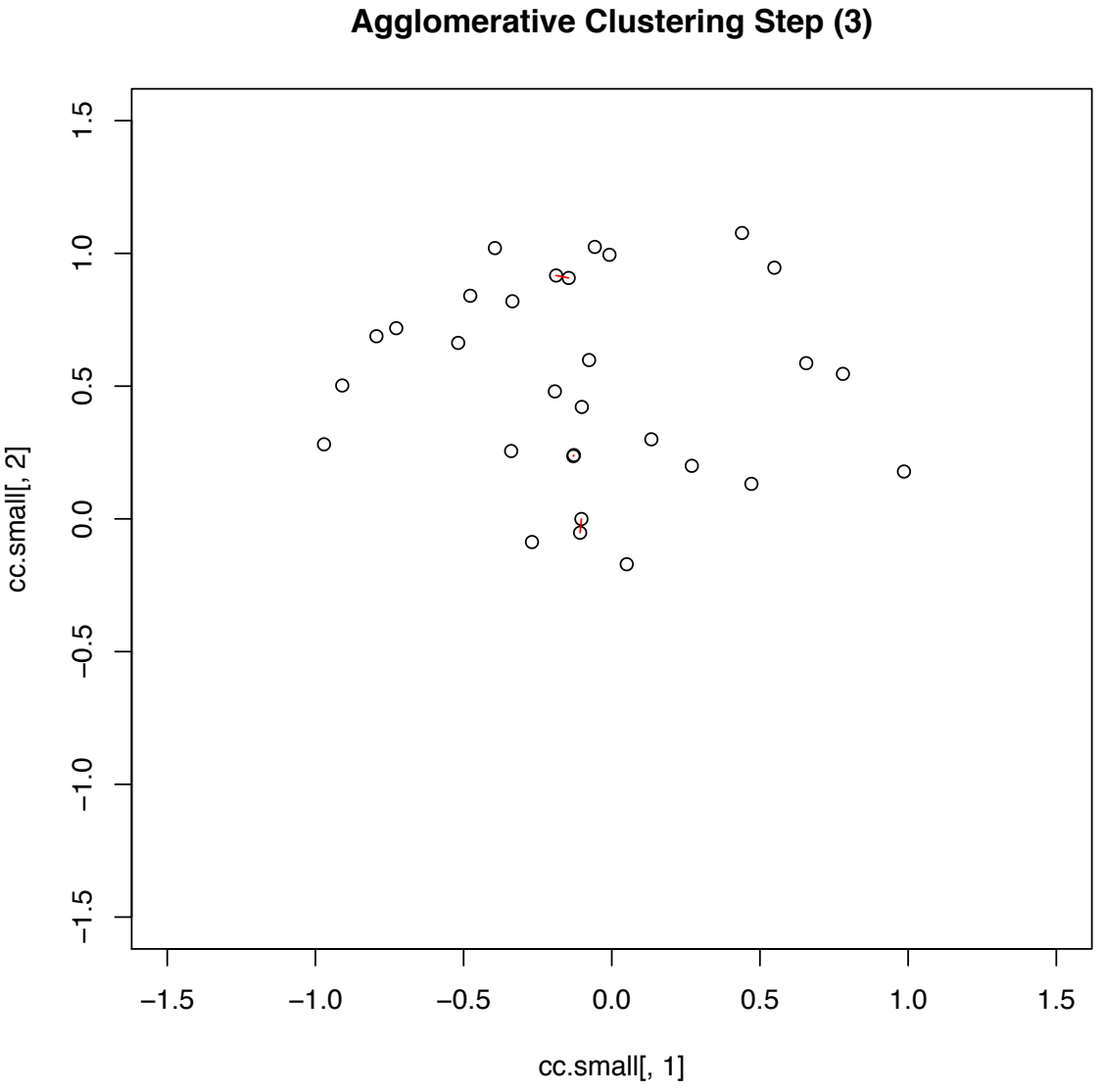
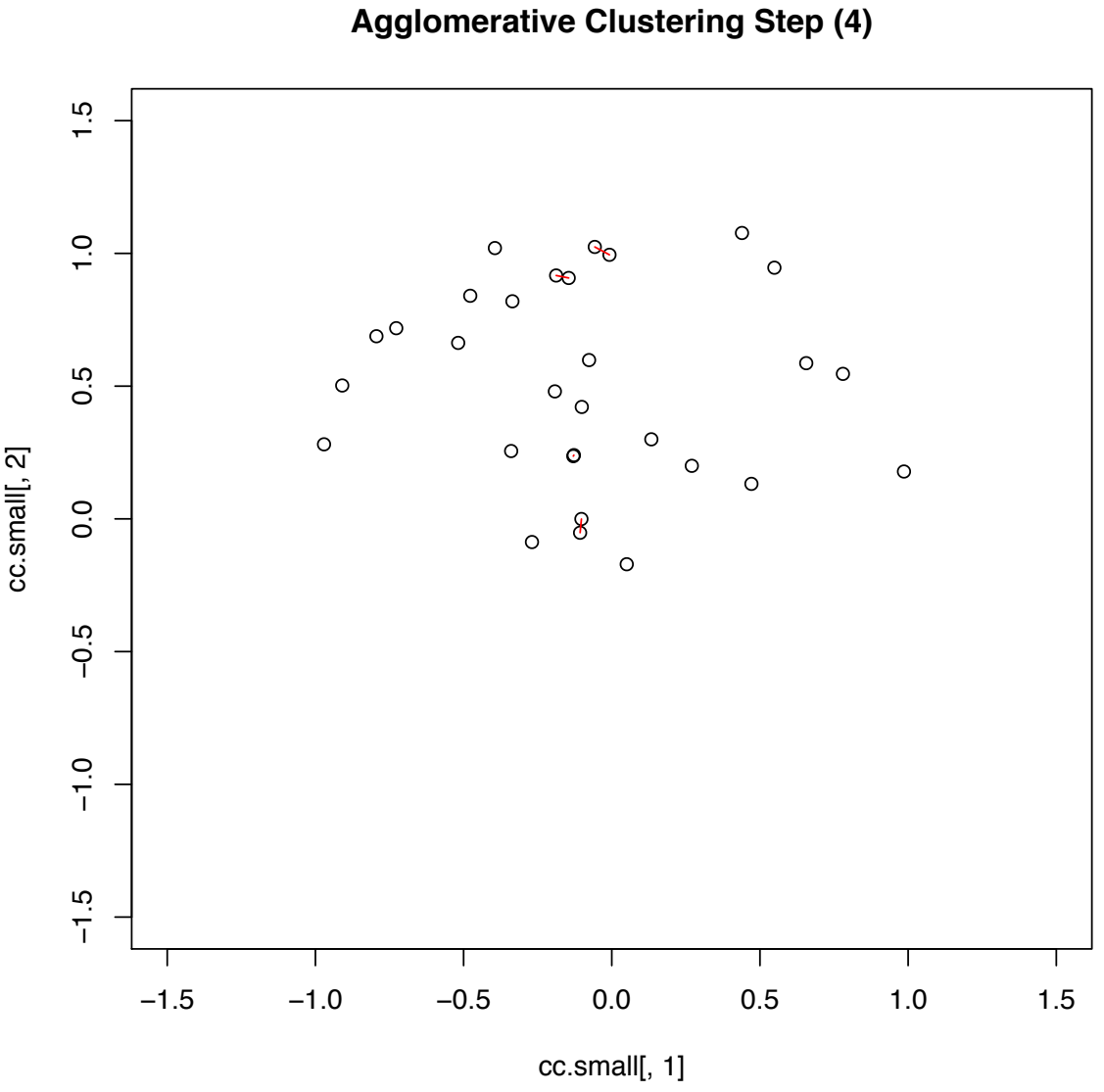
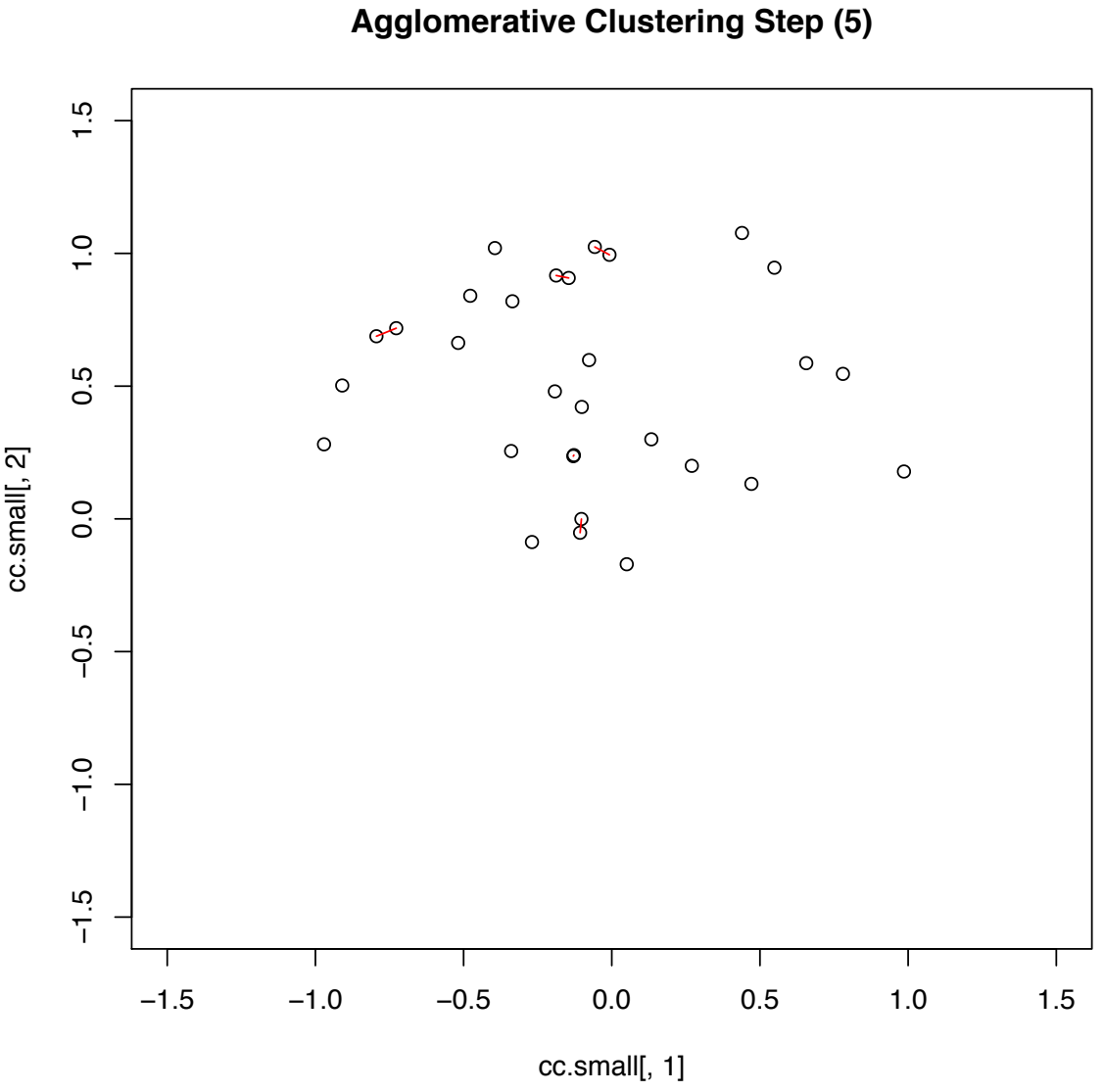


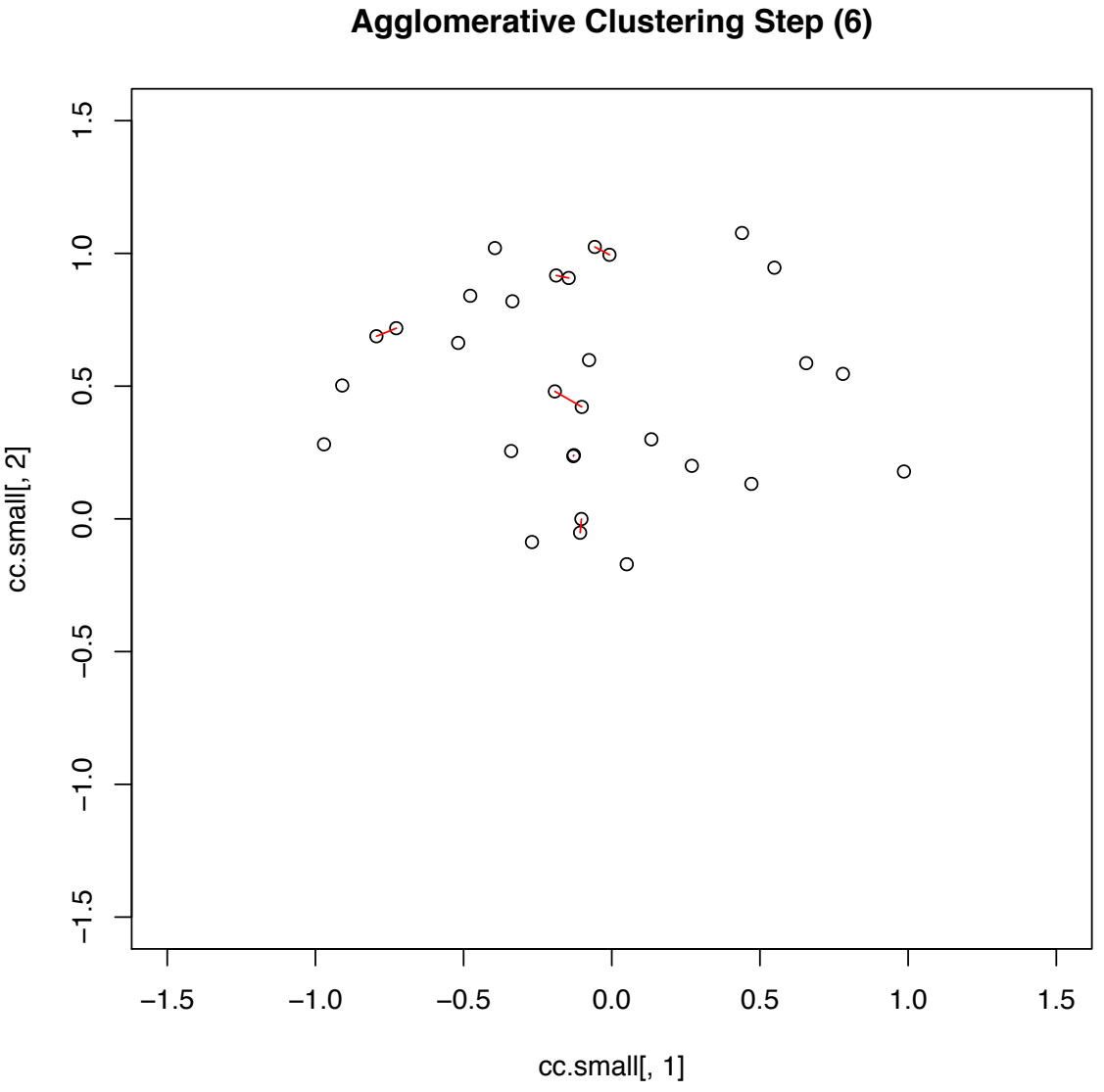
Agglomerative Clustering



Agglomerative Clustering



Agglomerative Clustering



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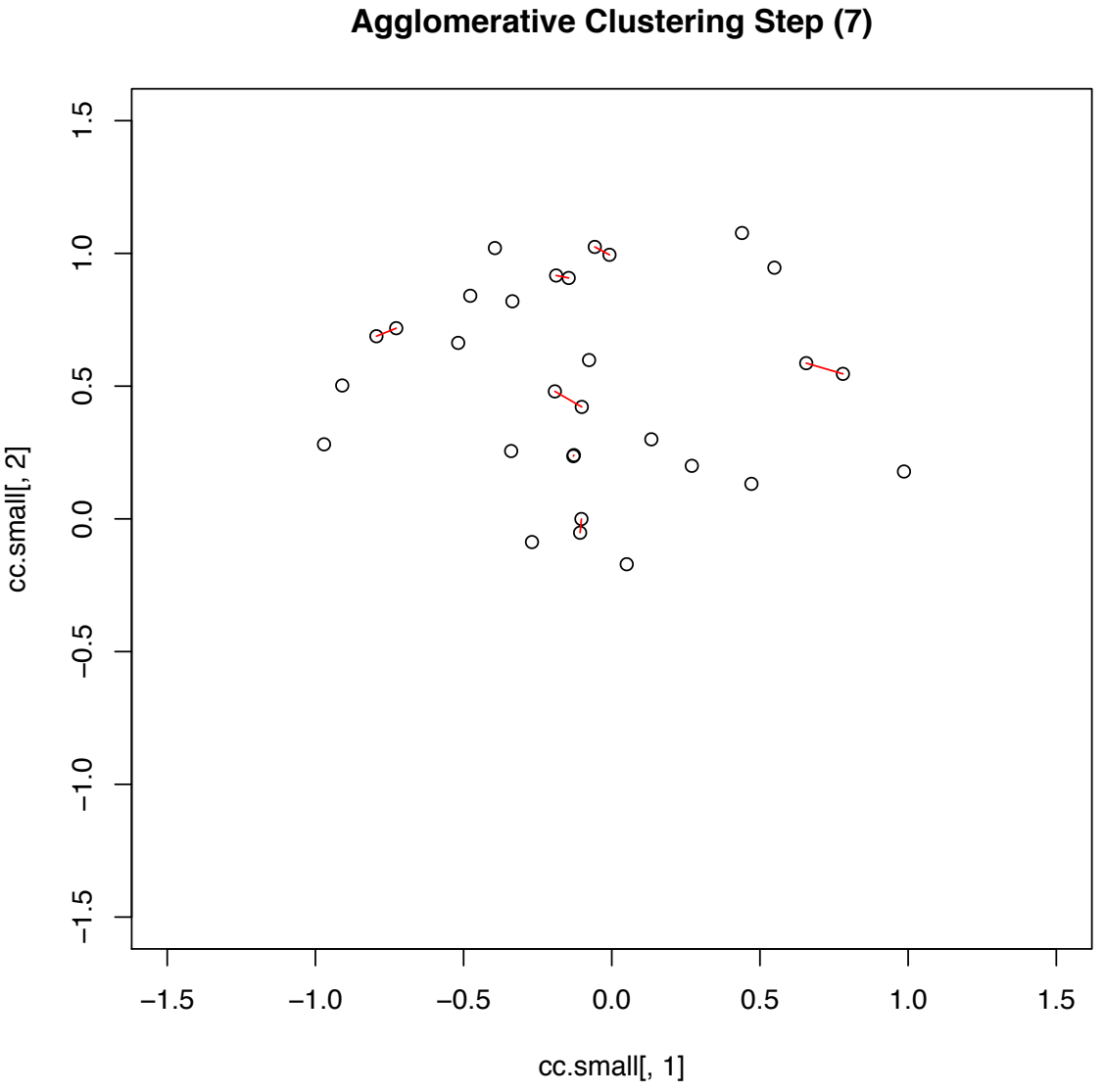

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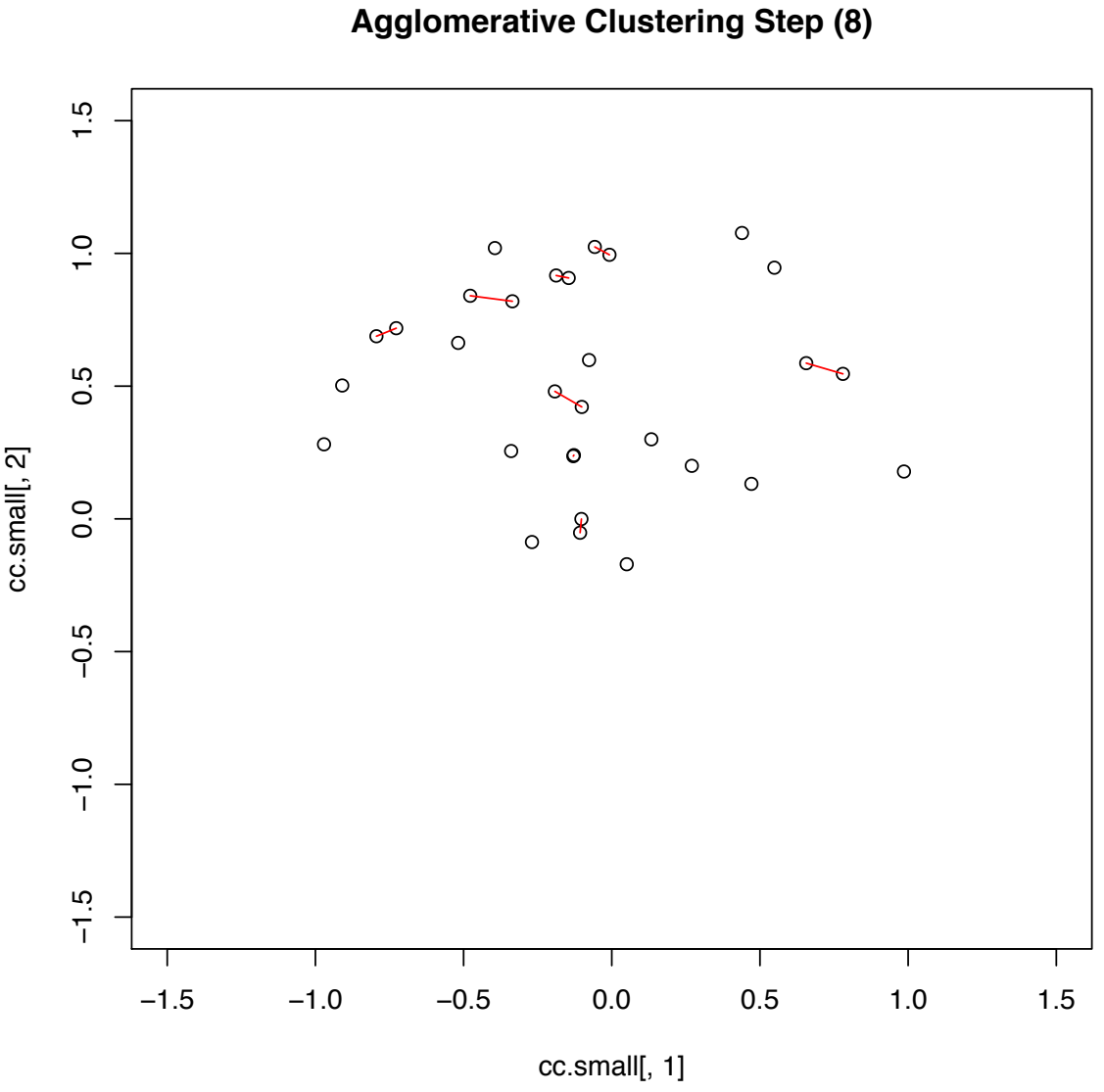

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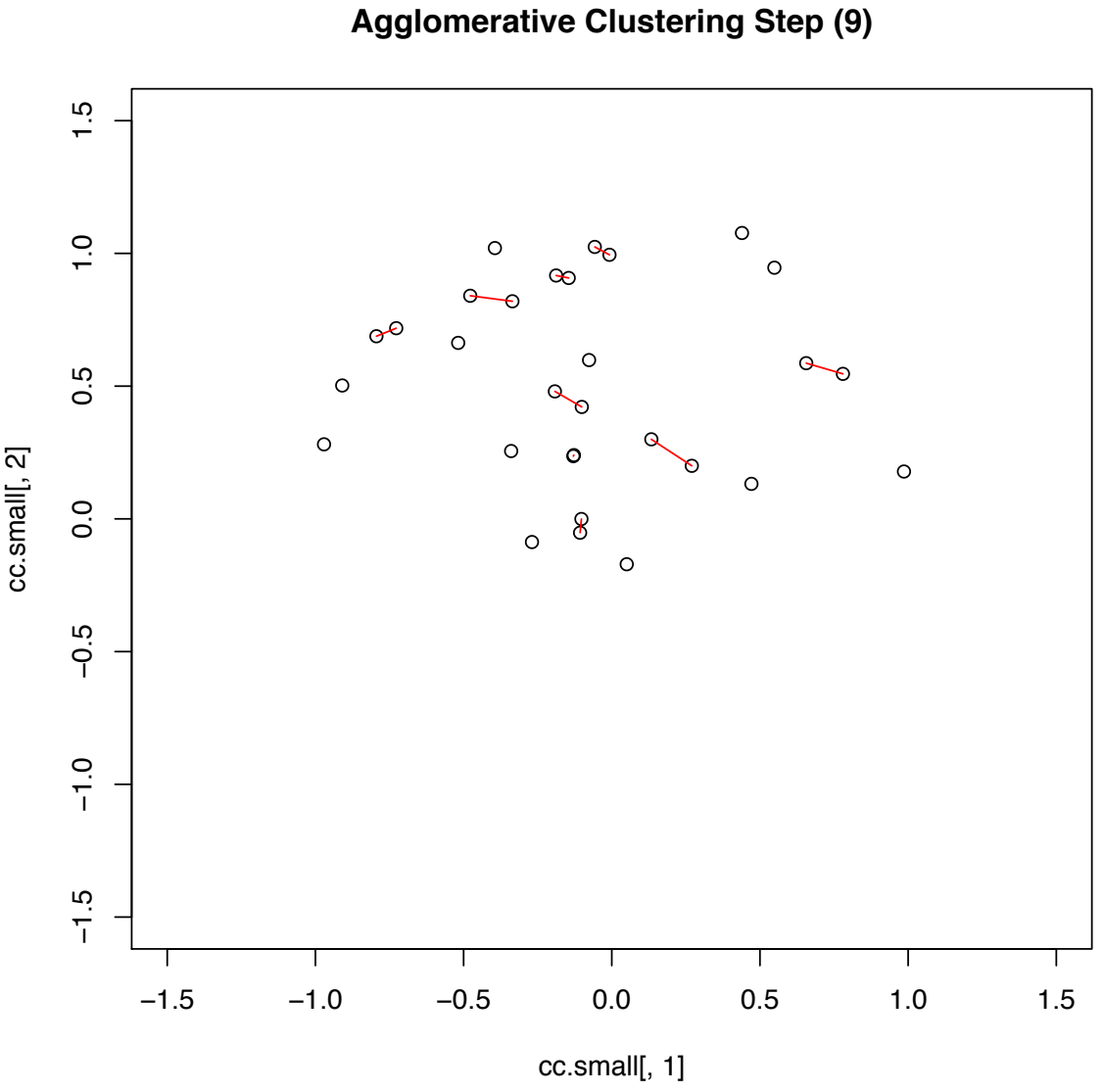
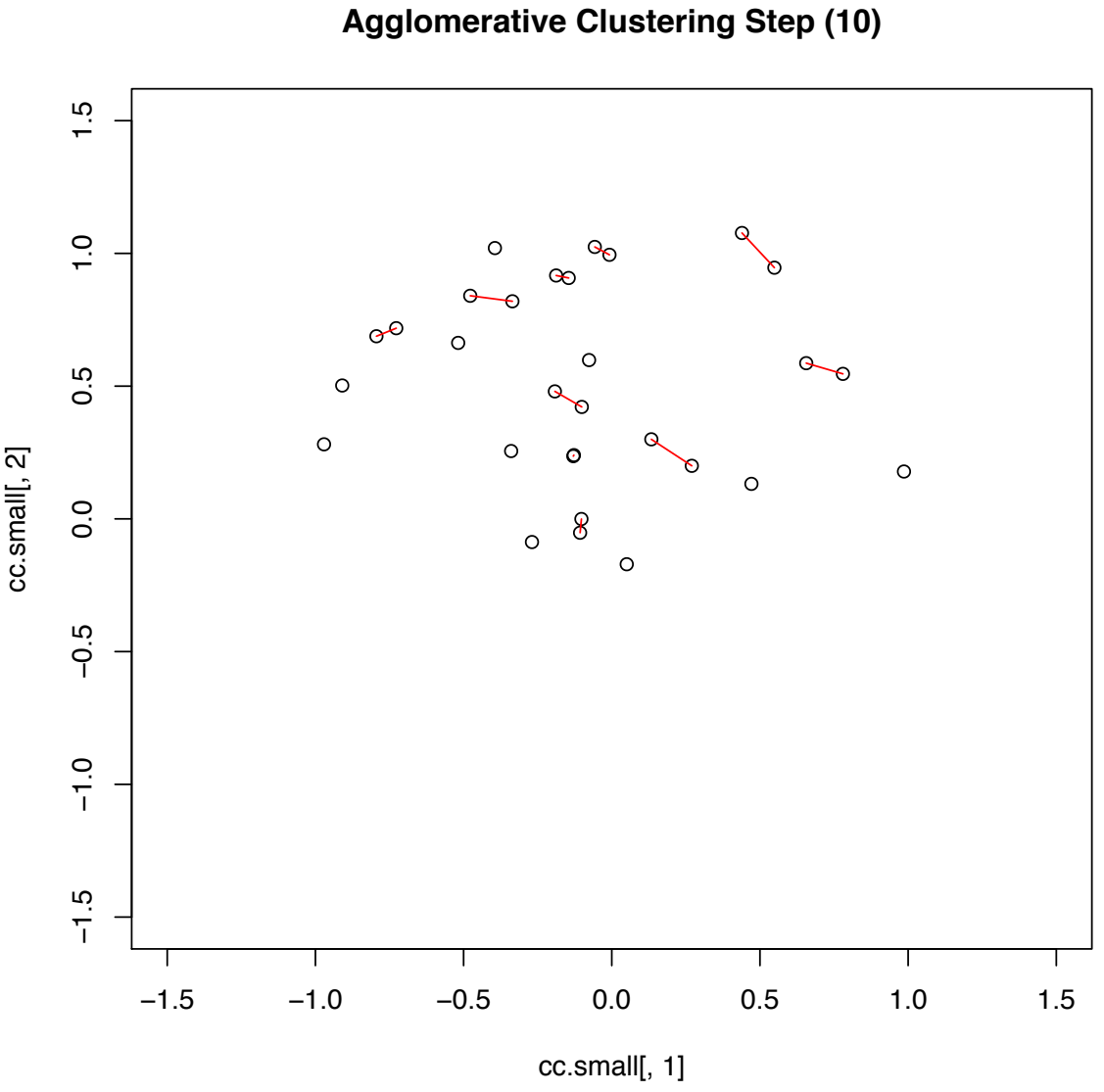


Agglomerative Clustering



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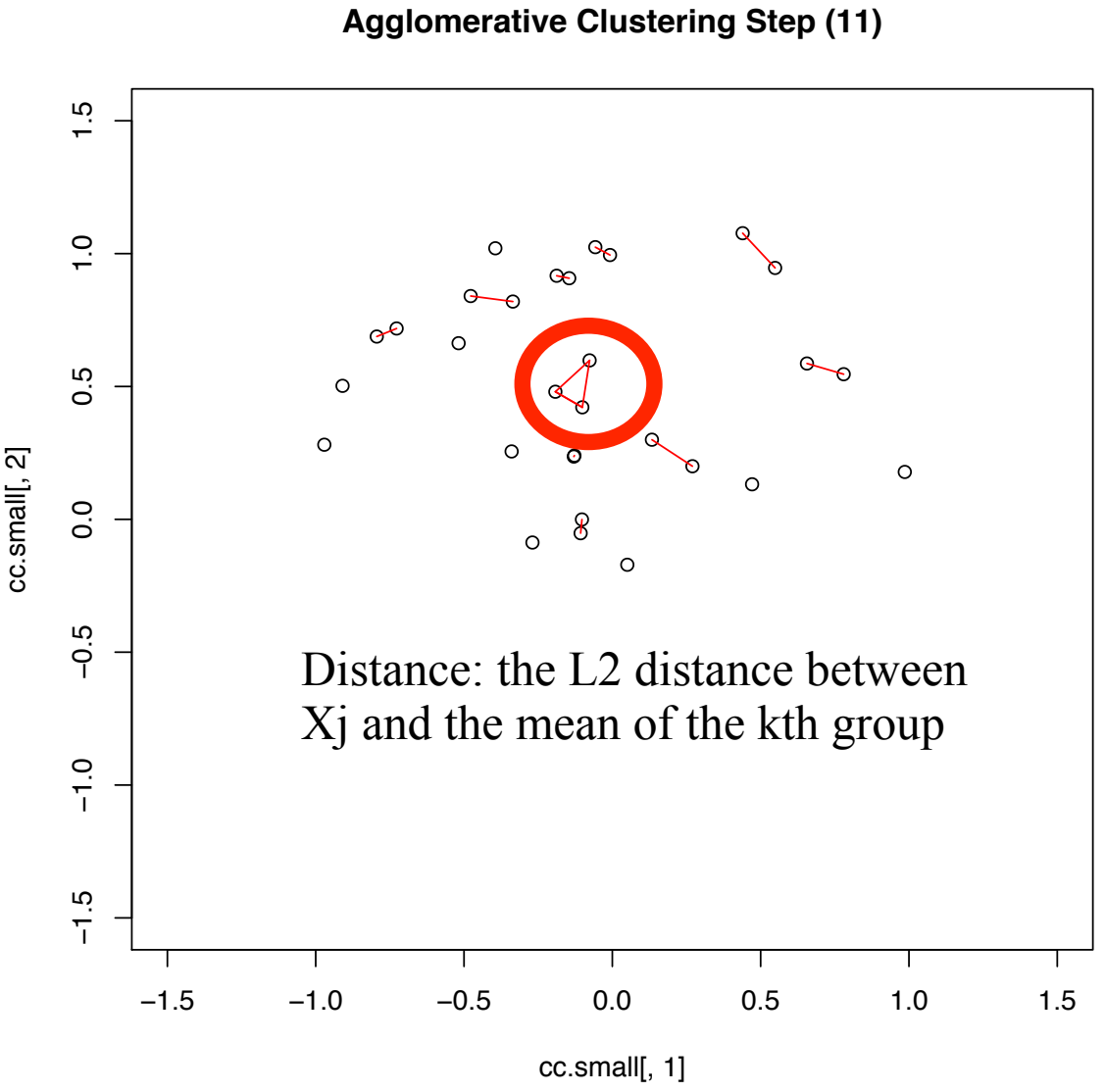

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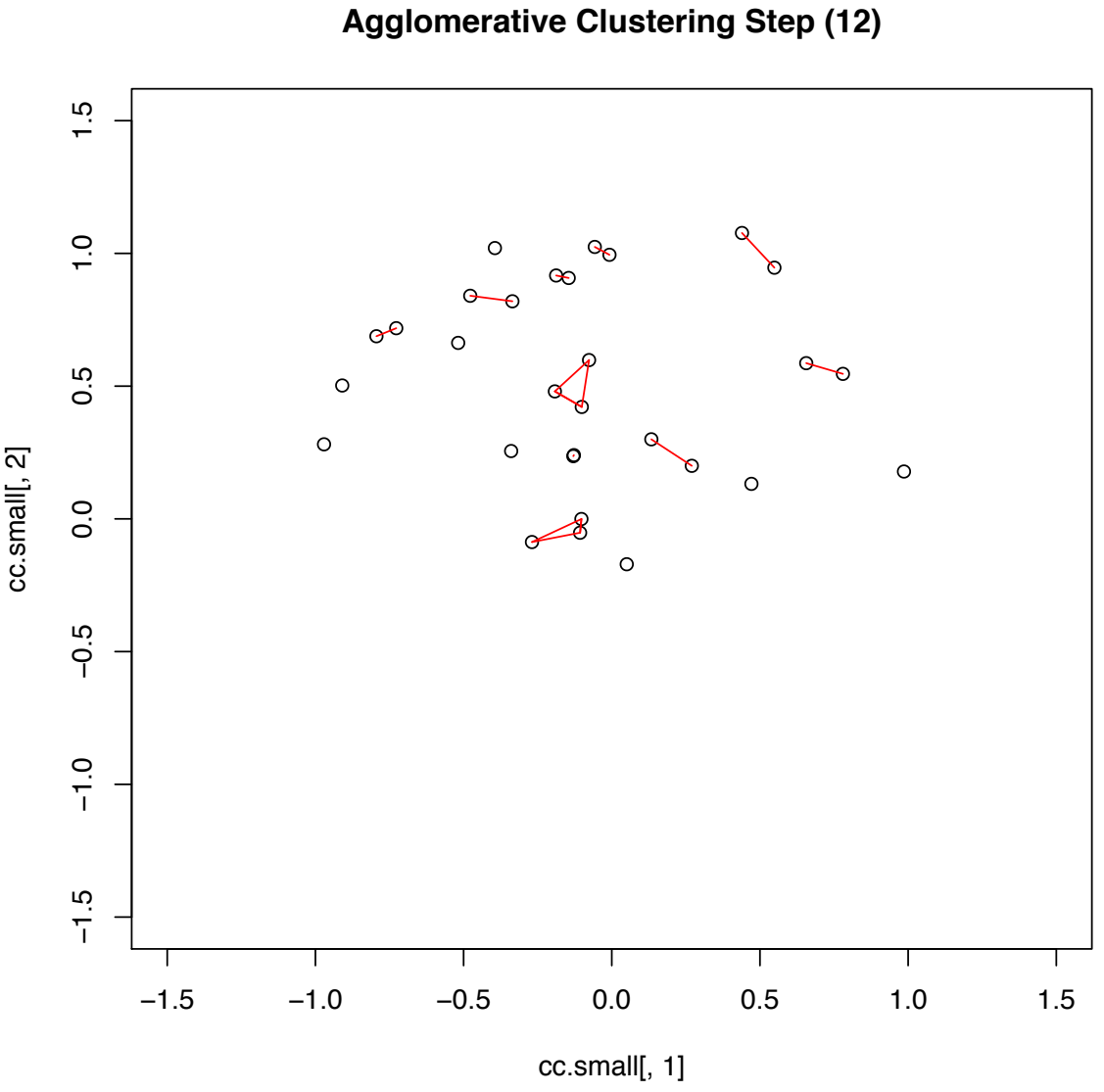

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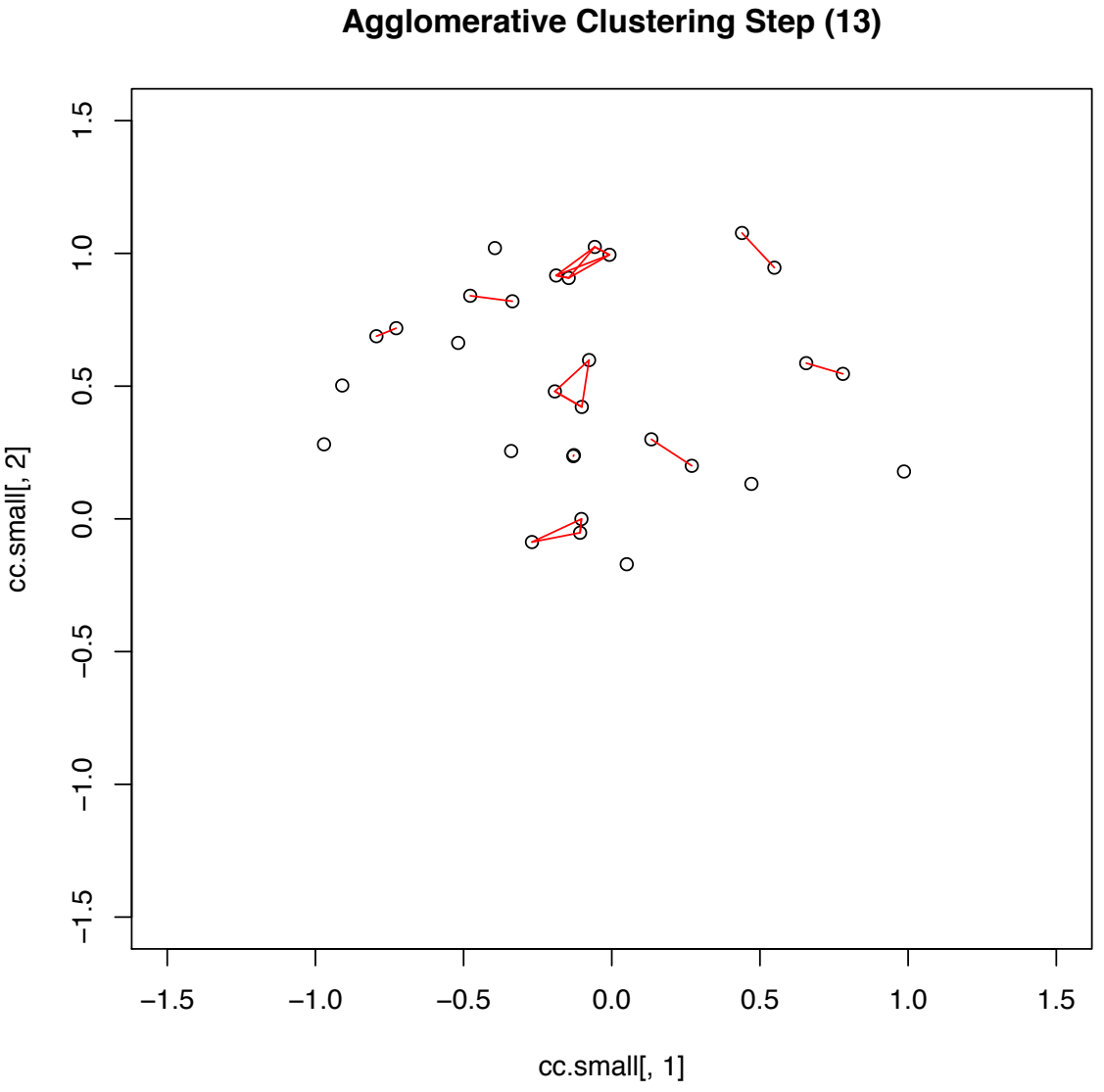

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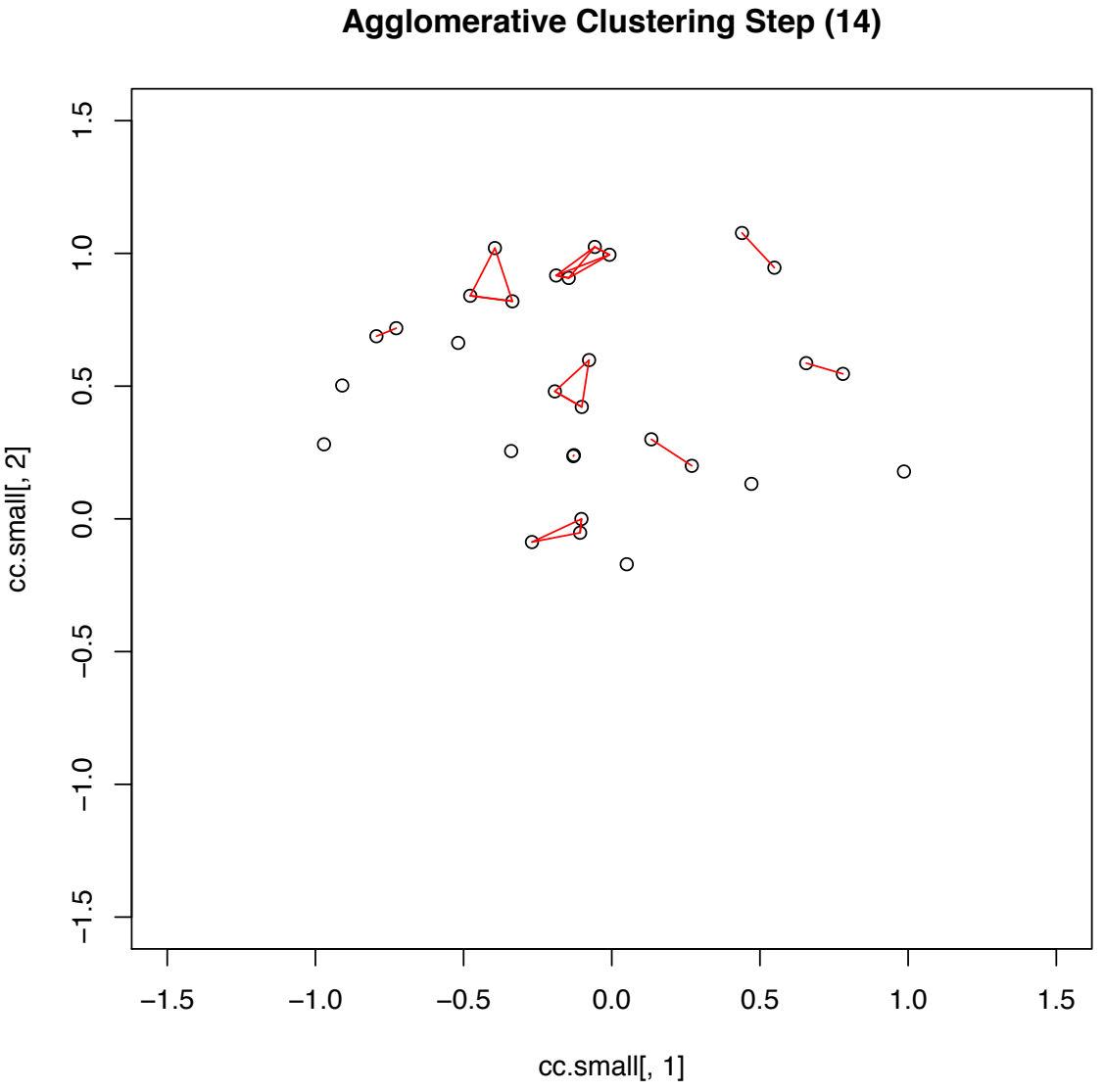

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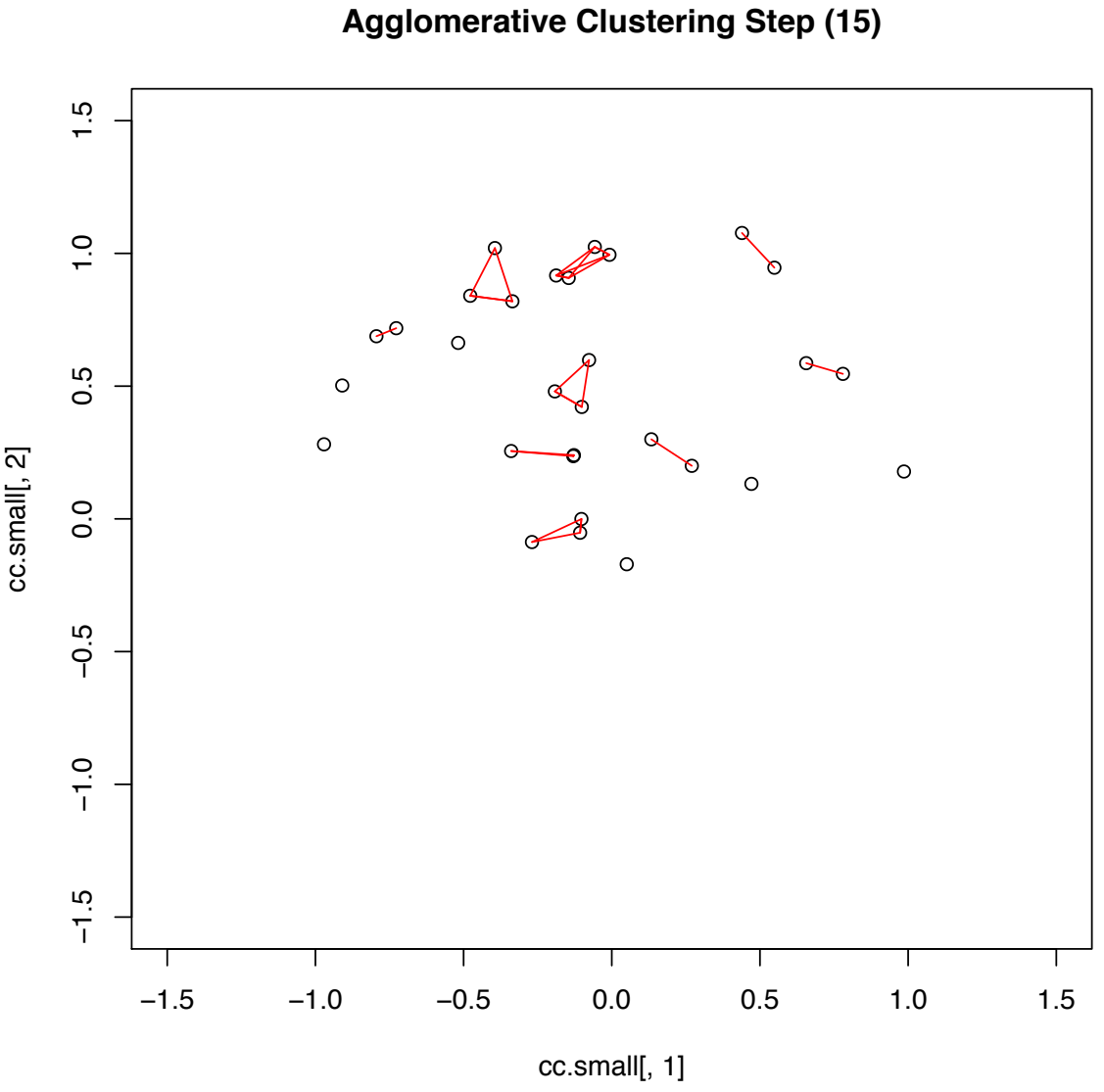

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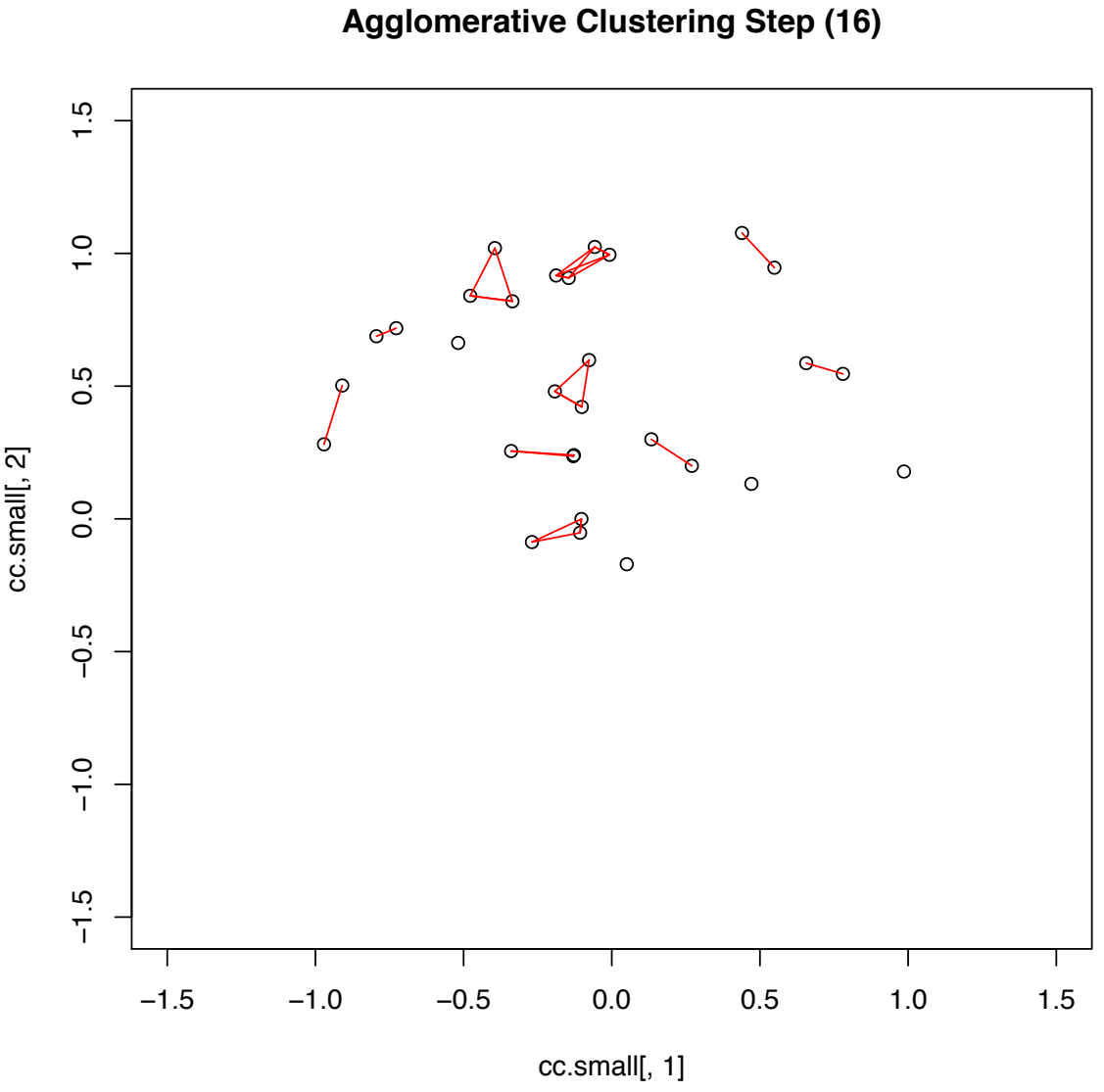

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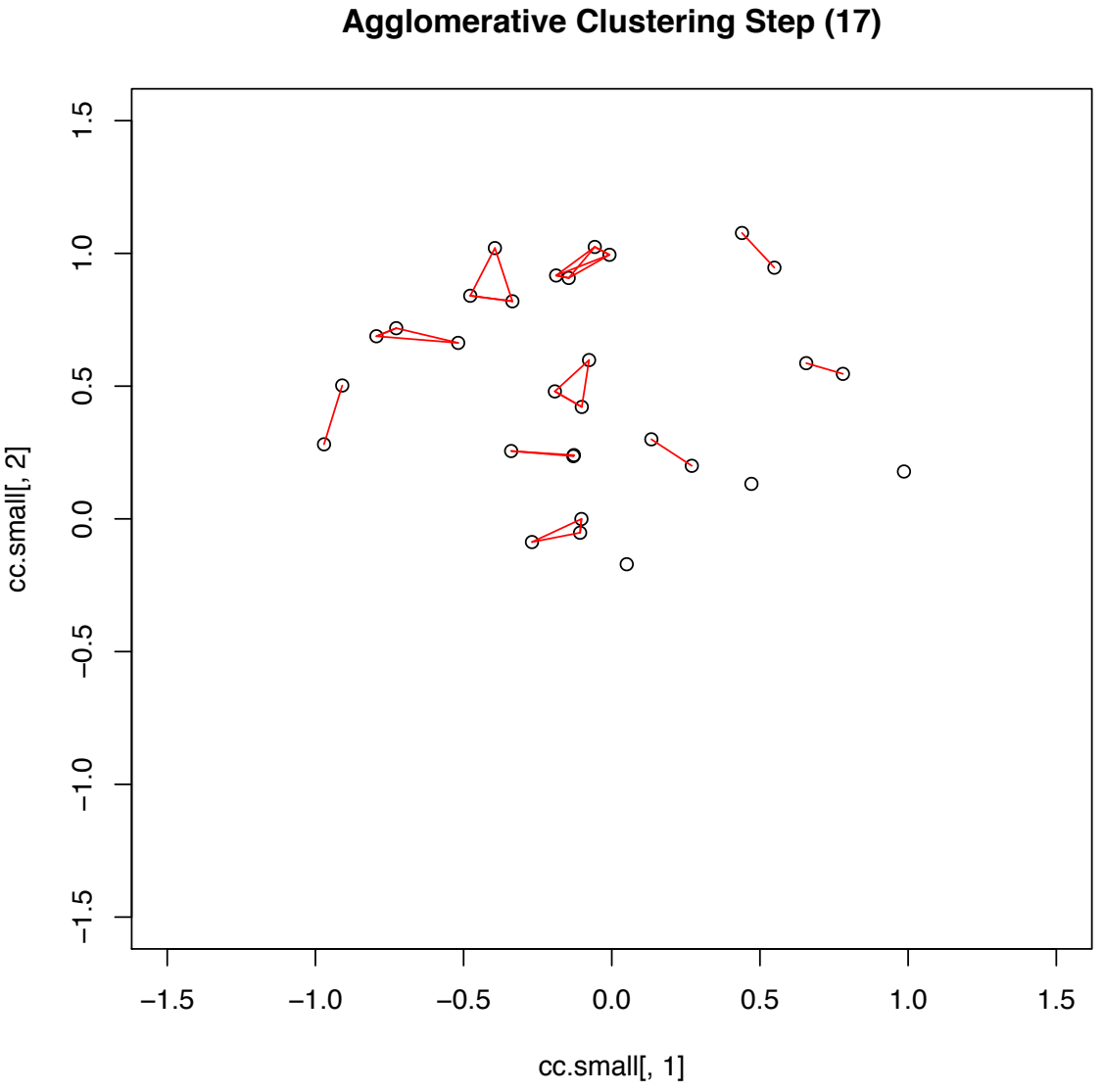

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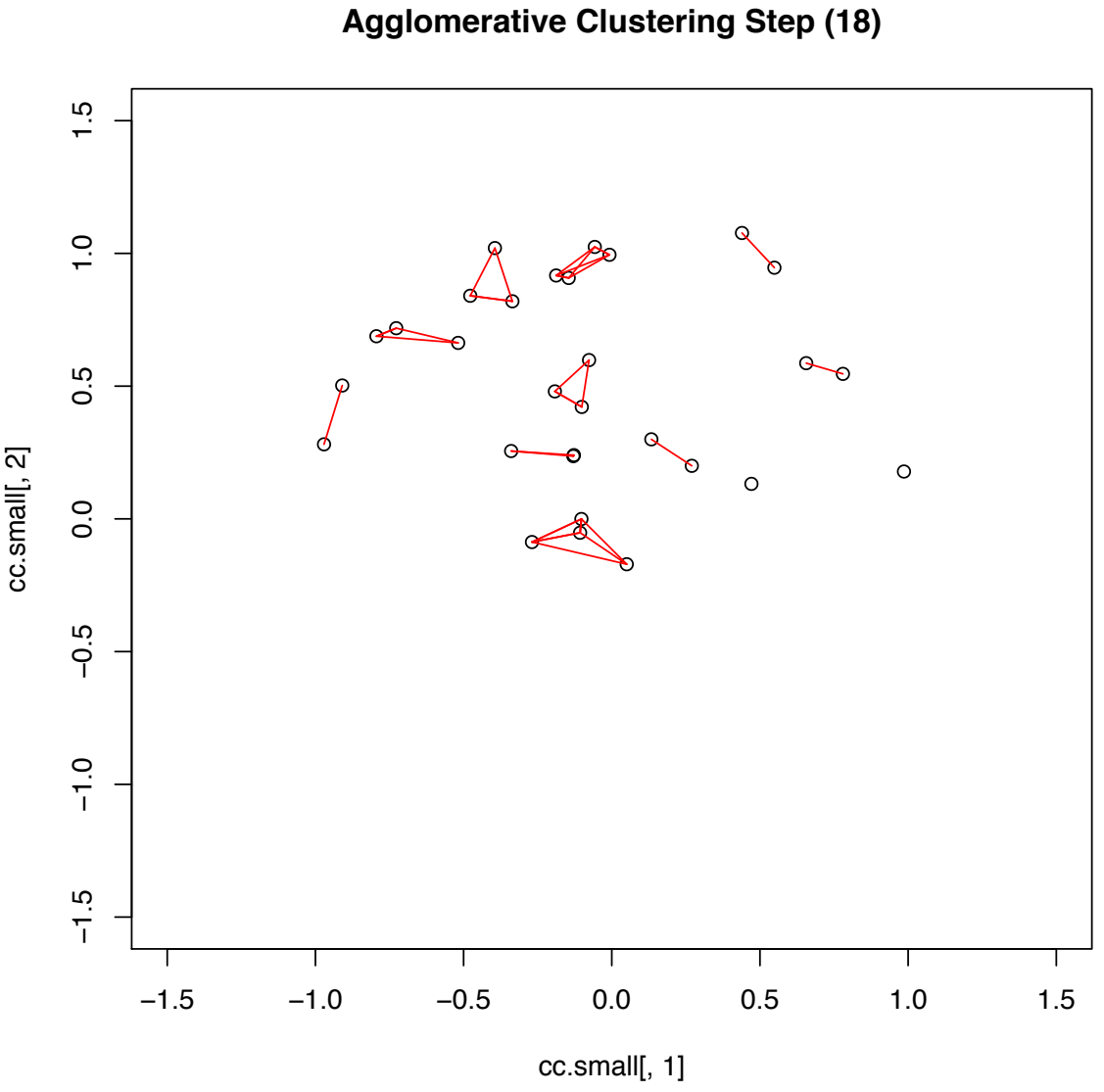

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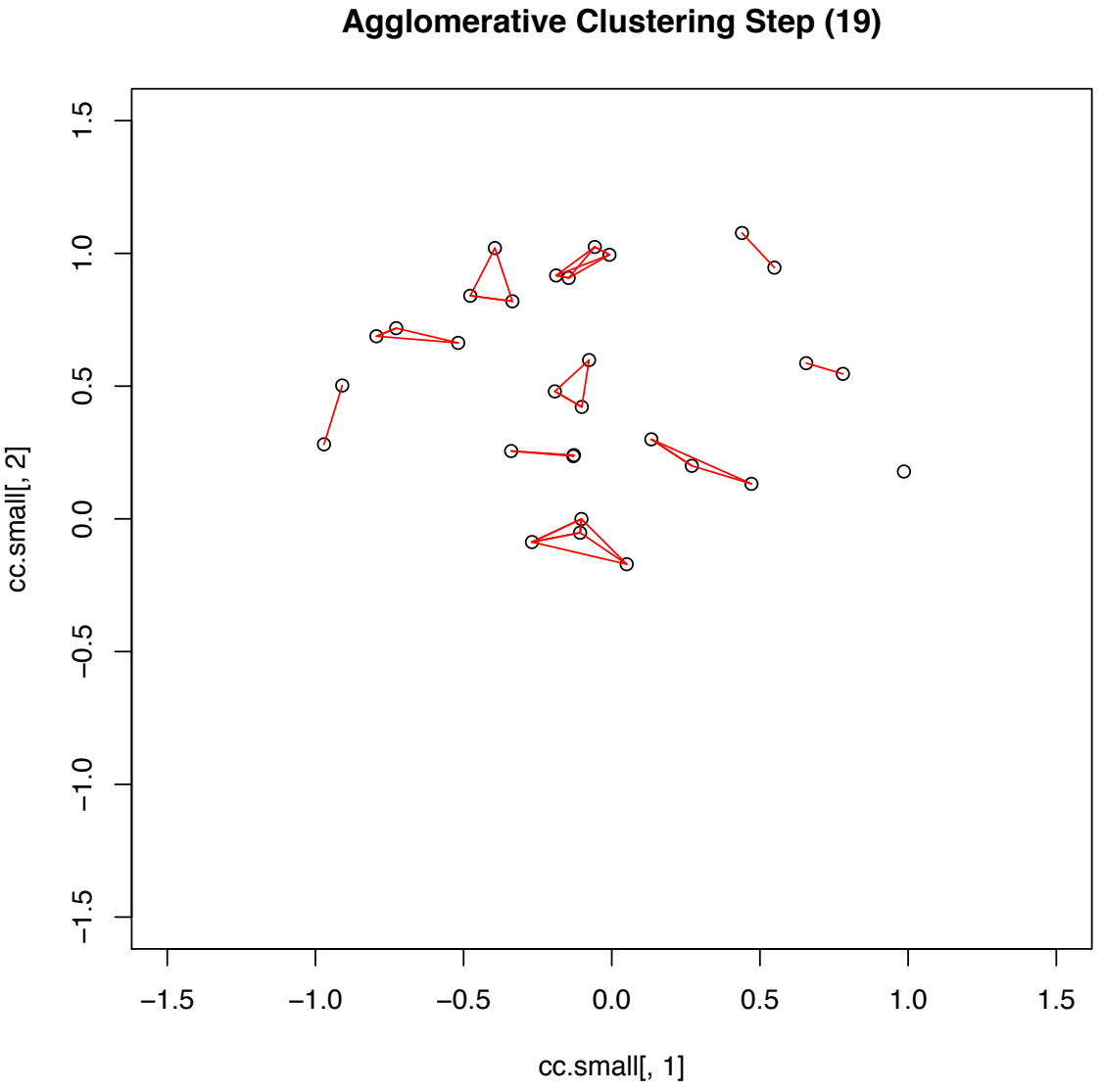

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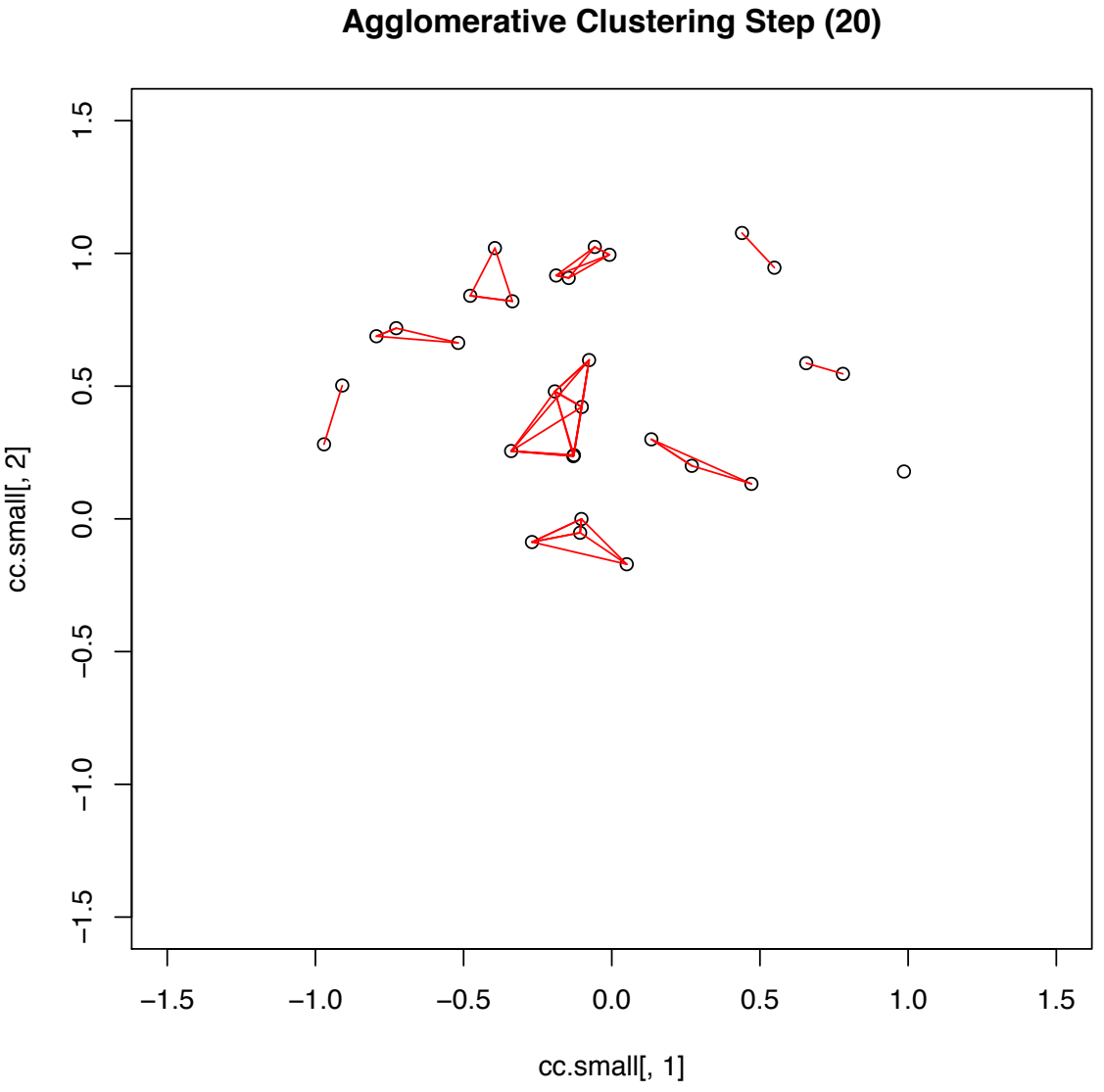

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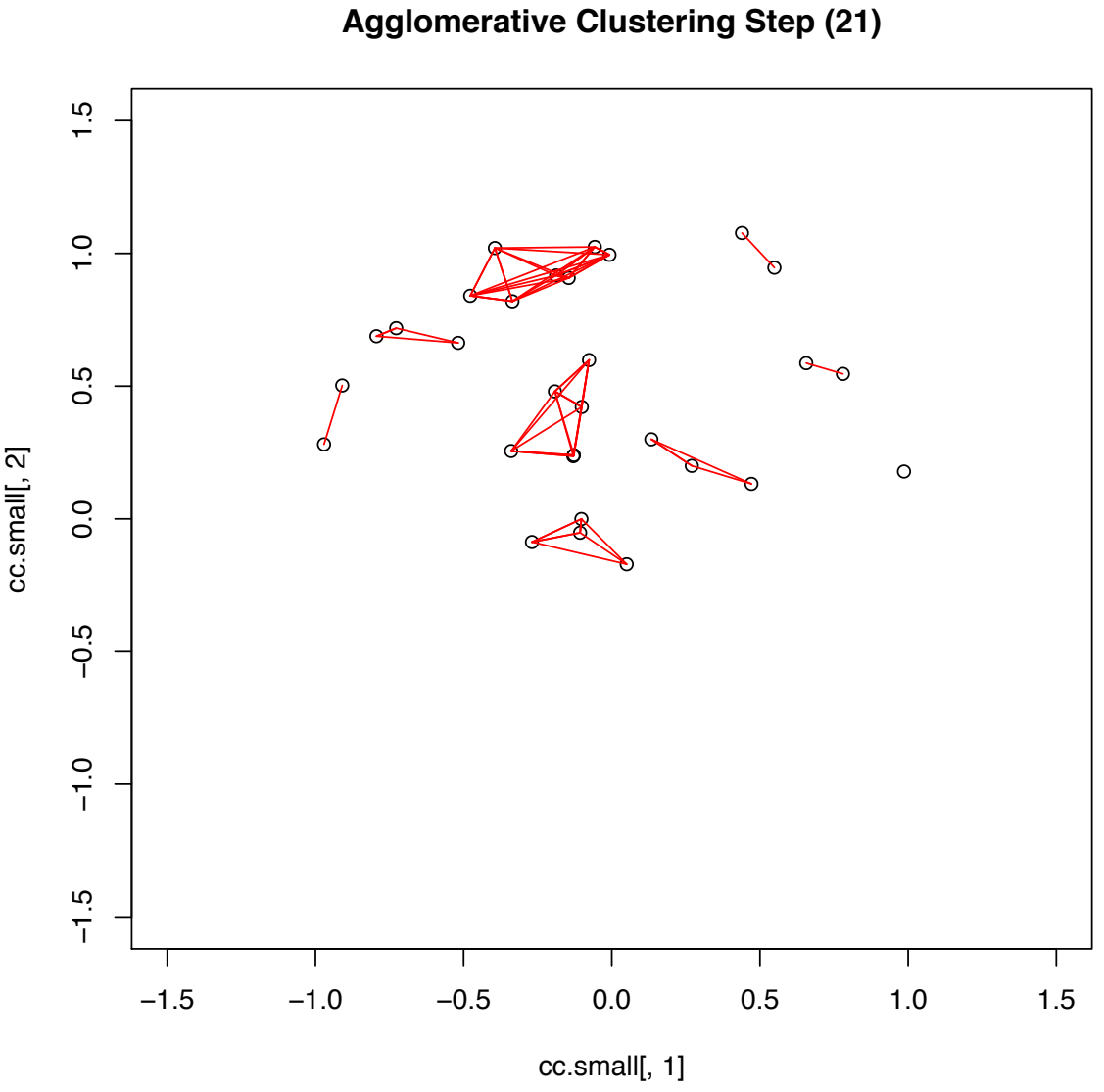

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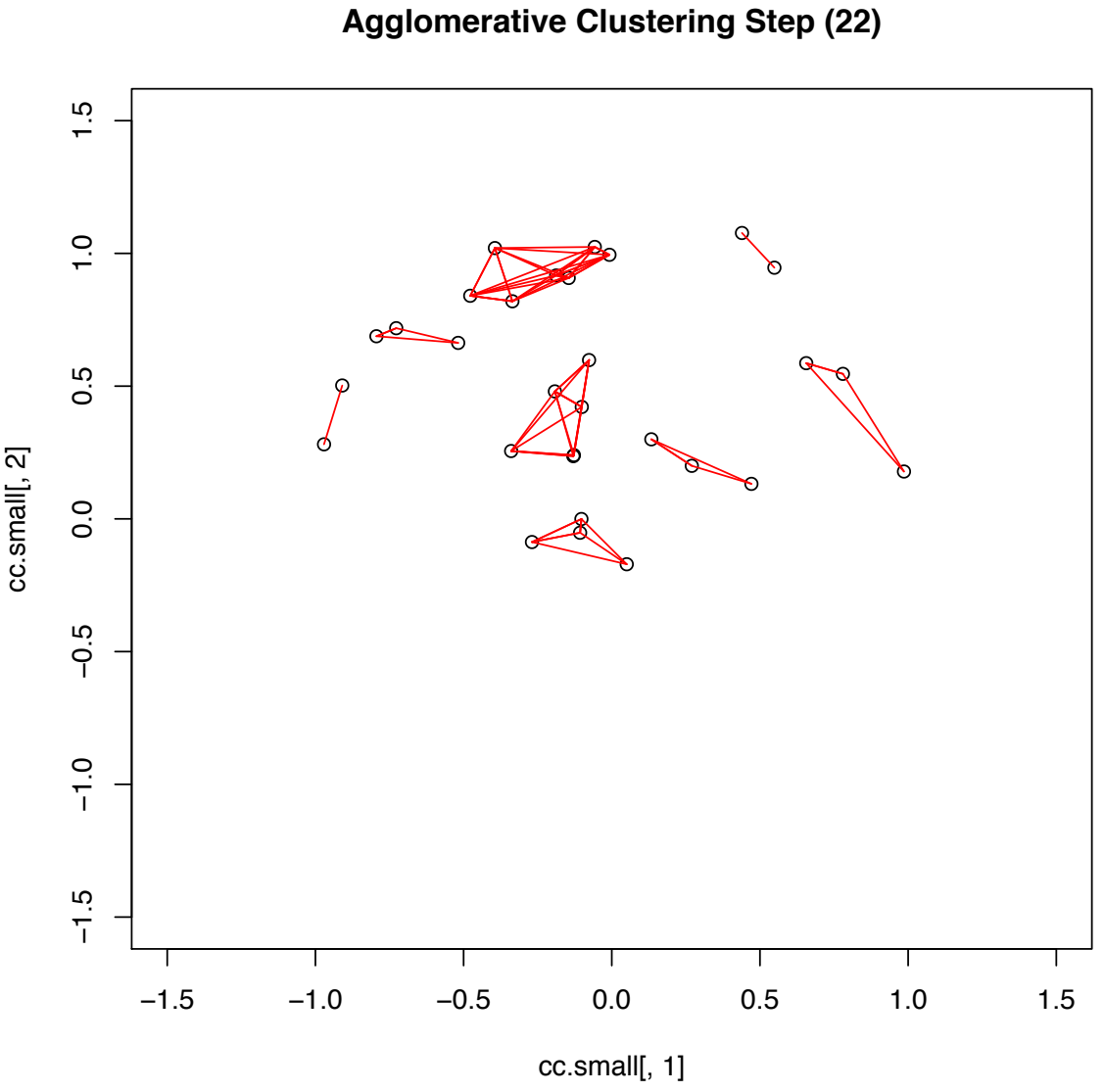

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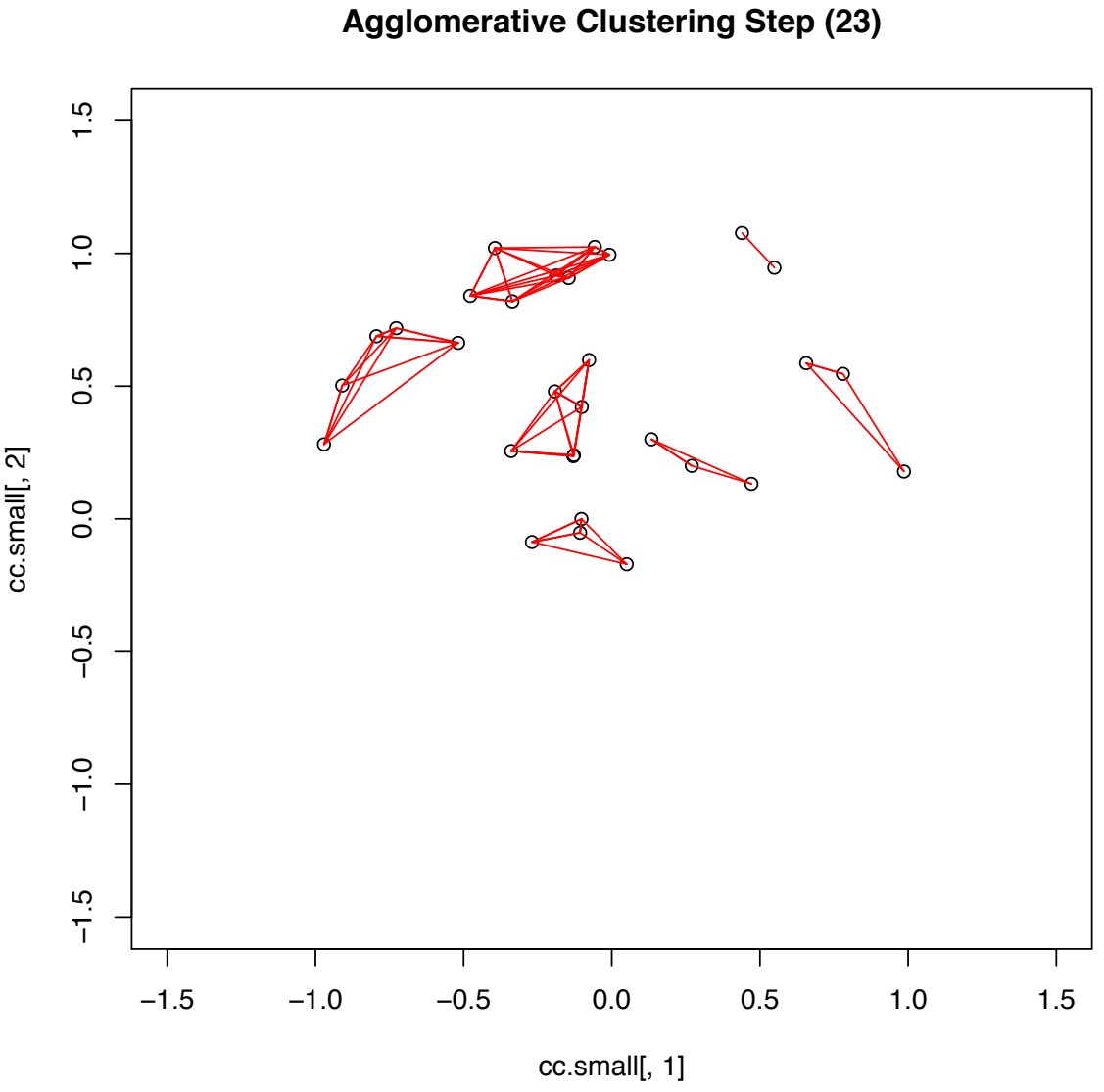

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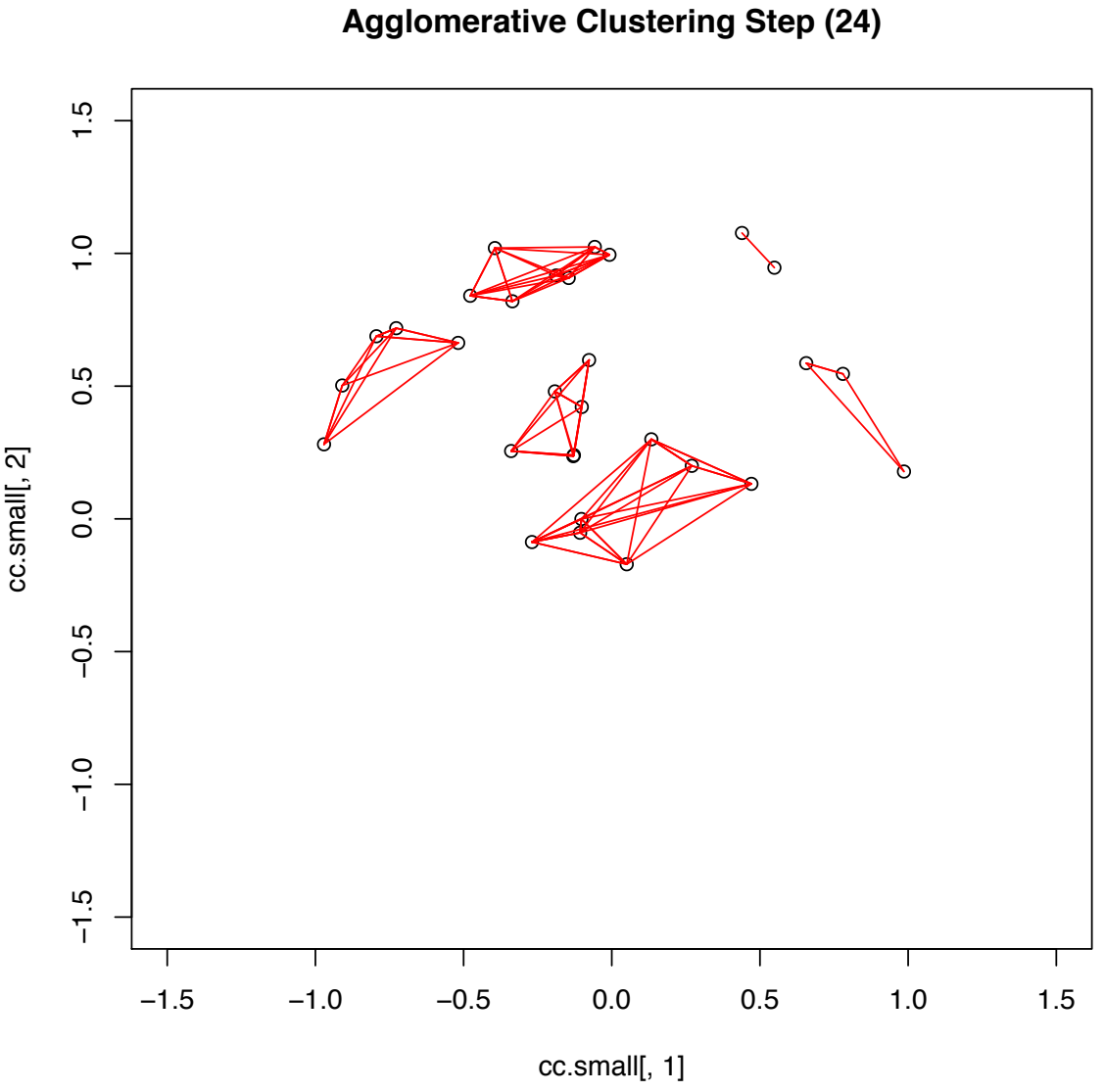

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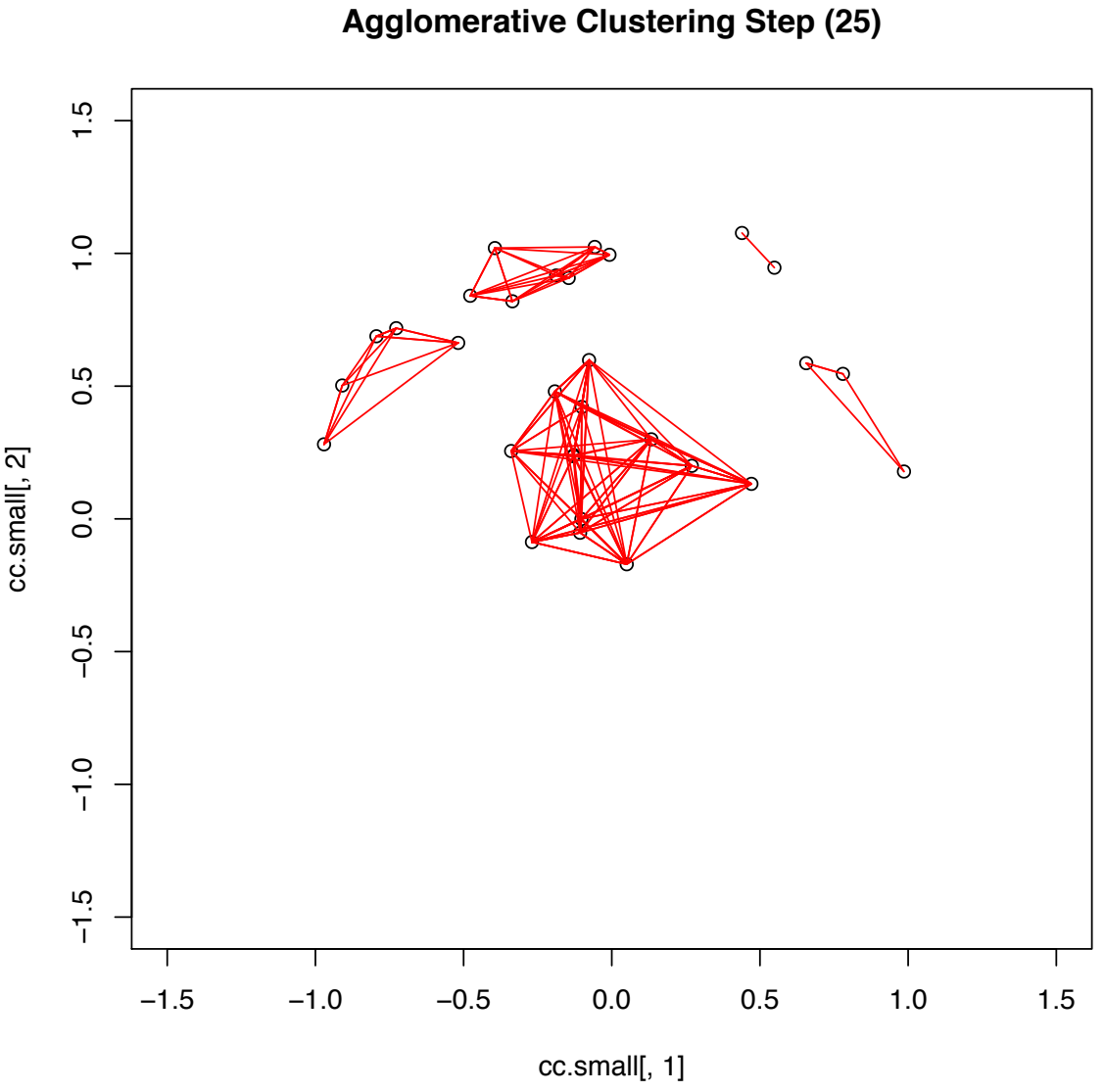

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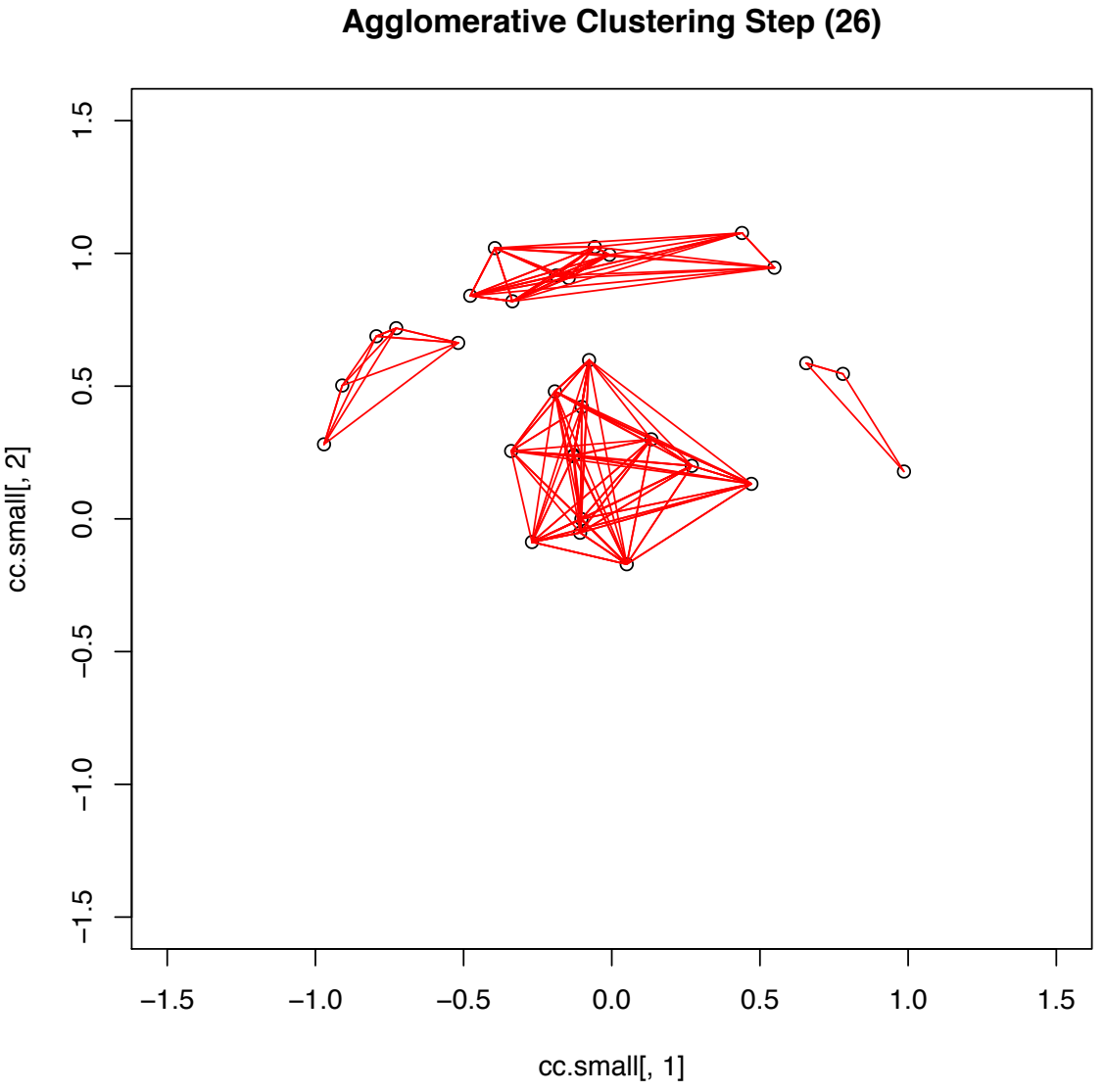

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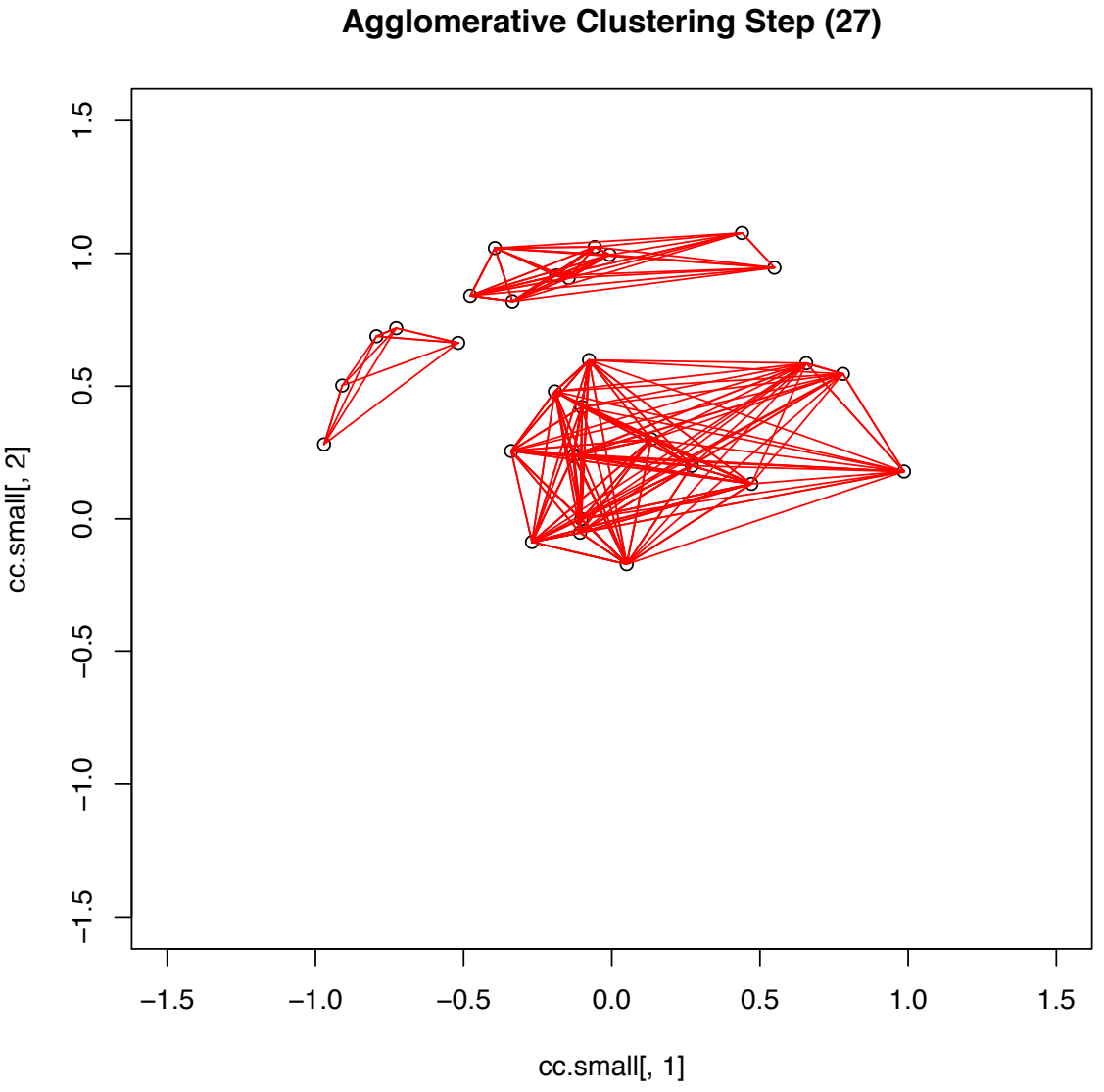
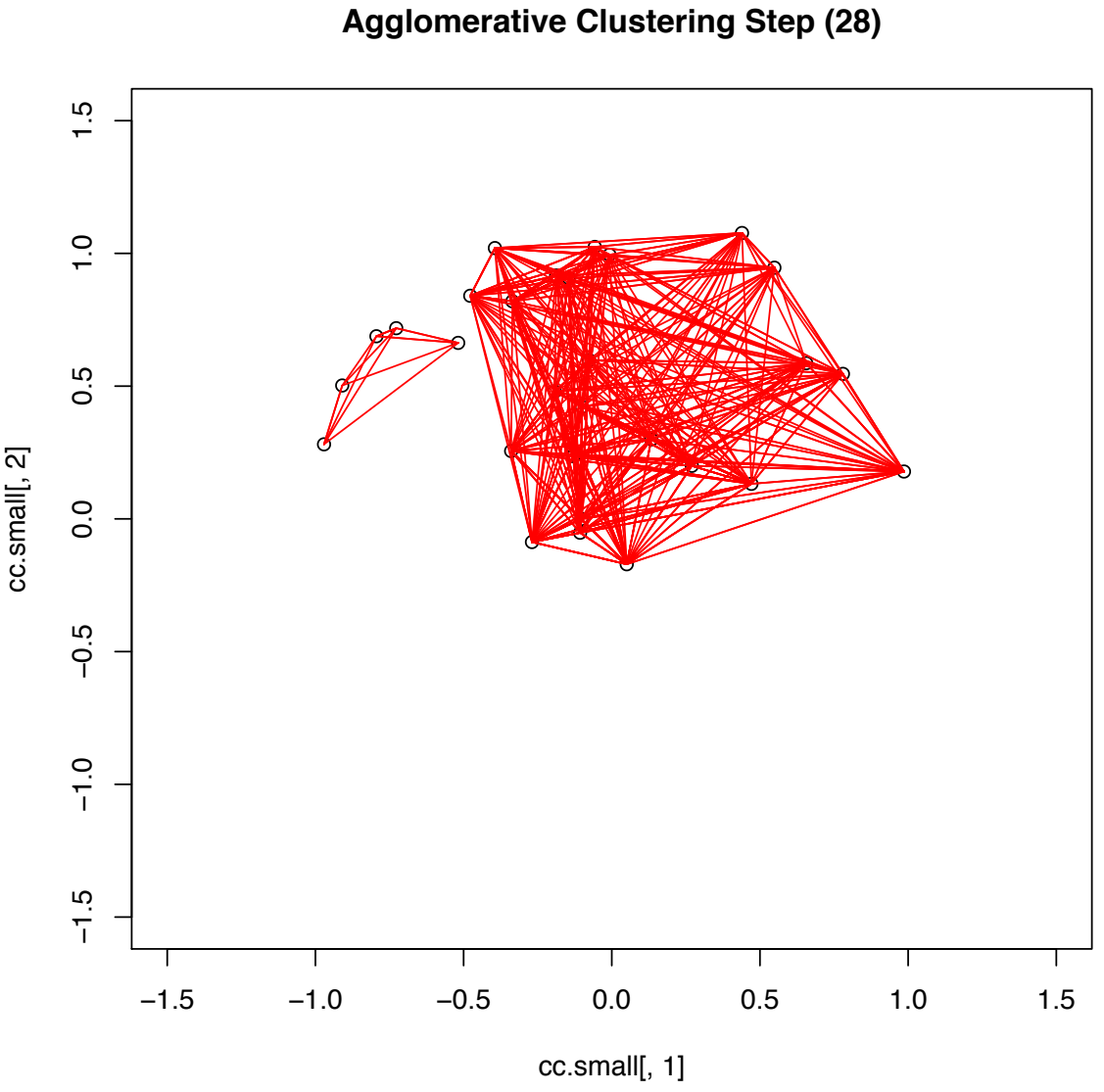


Agglomerative Clustering



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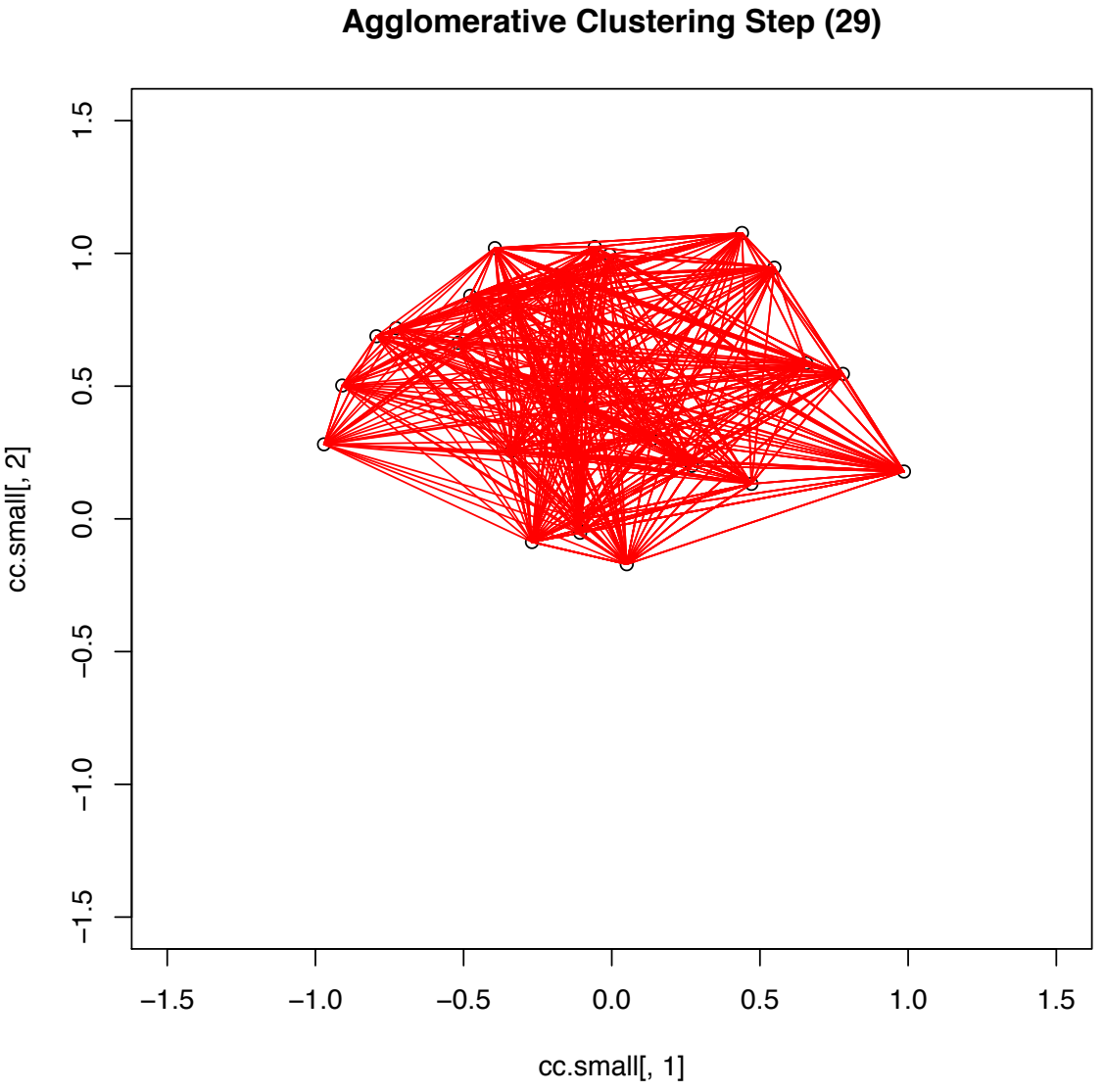
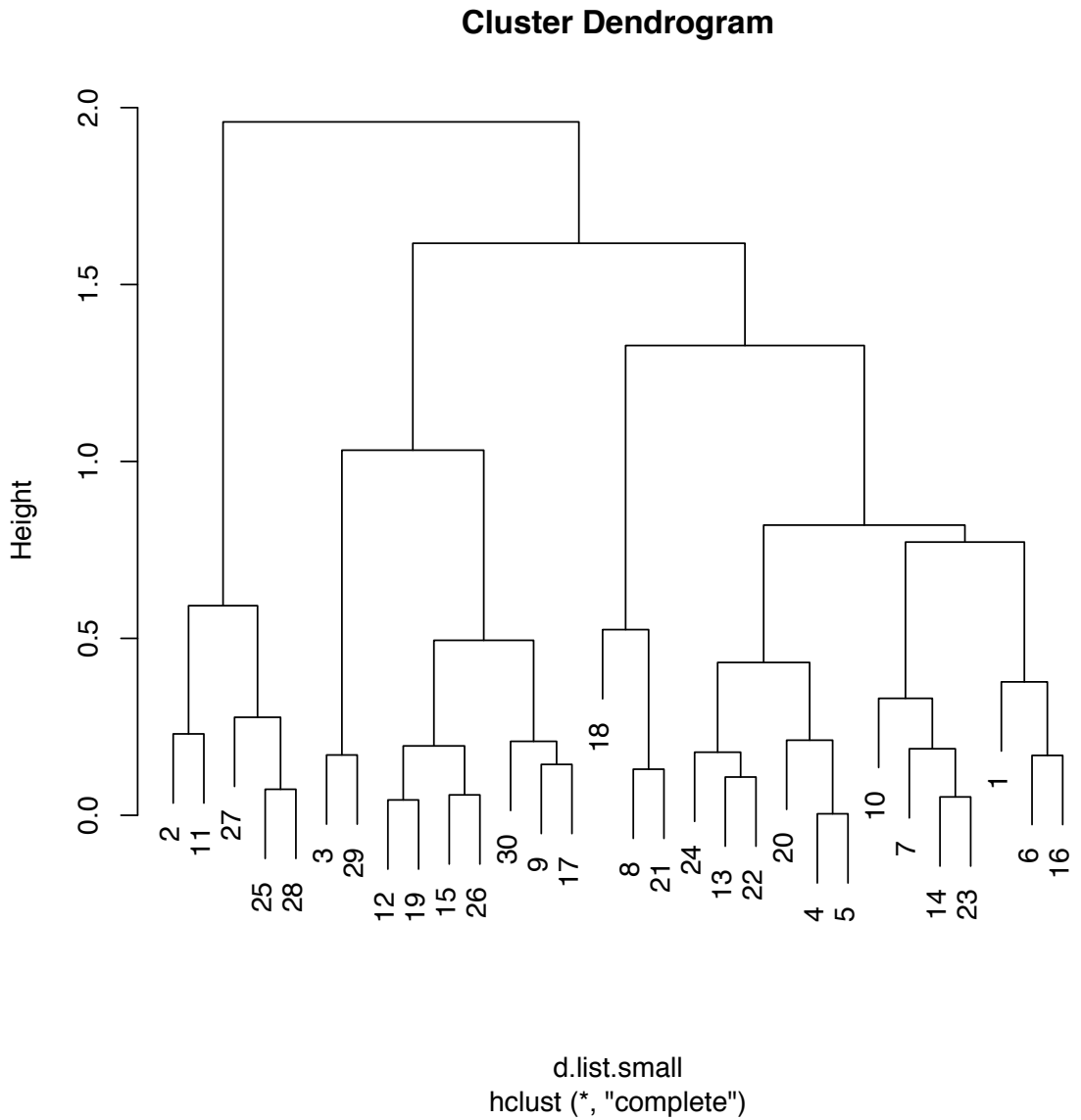


Agglomerative Clustering

This can be viewed as a tree:

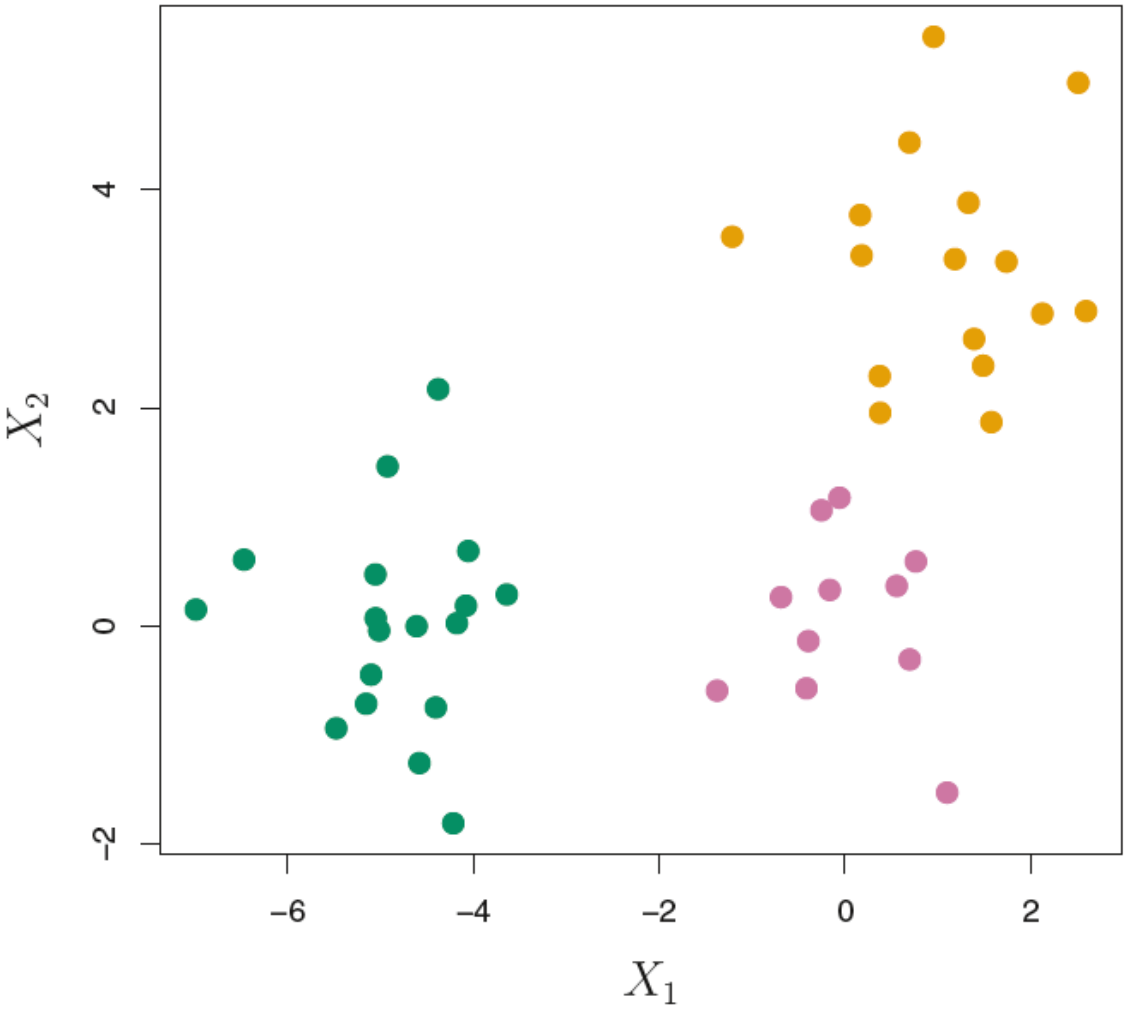


Agglomerative Clustering

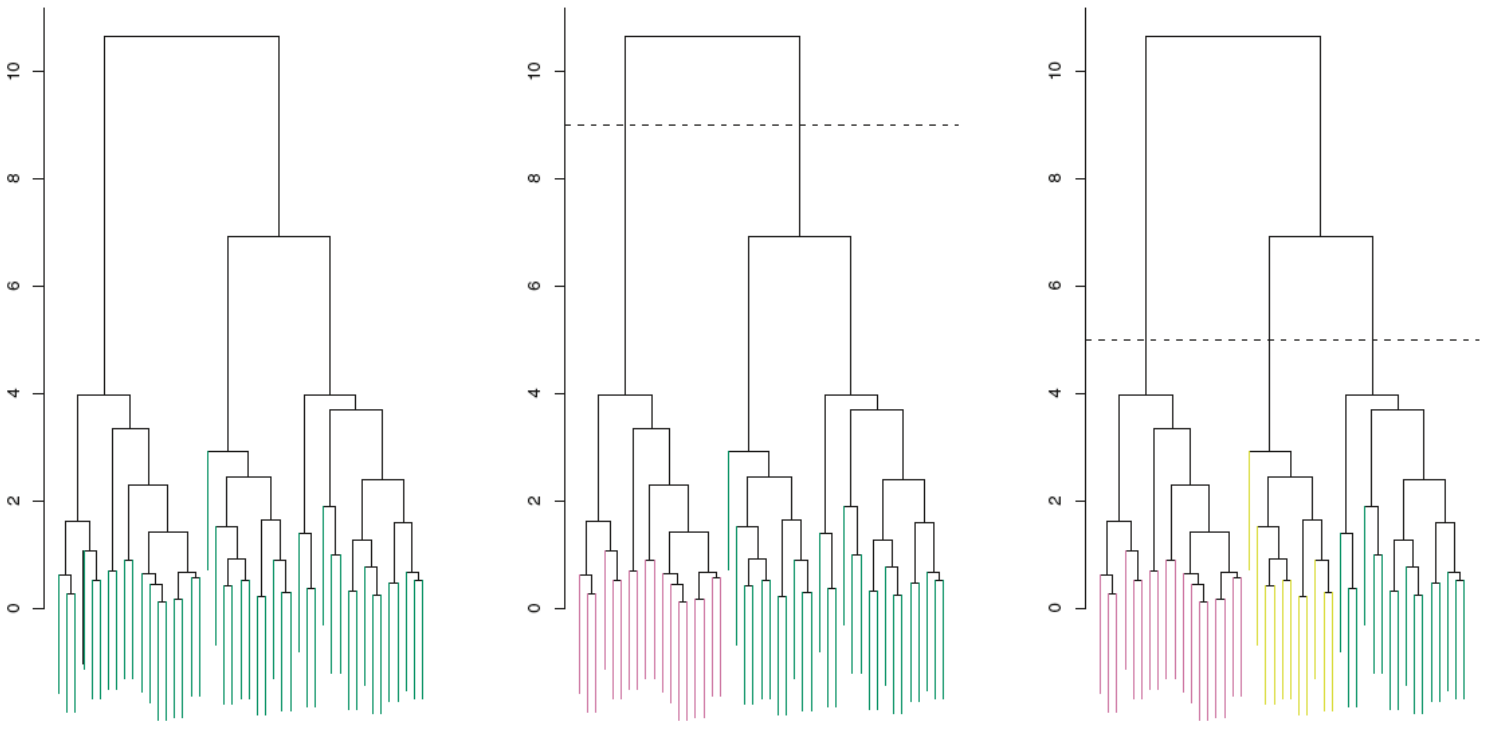
Representing clustering with a tree:

- each level represents a segmentation of the data
- the tree represents a sequence of clusterings
- height represents the negative similarity between merged groups
- user must choose best grouping
- great for summarizing algorithm and data

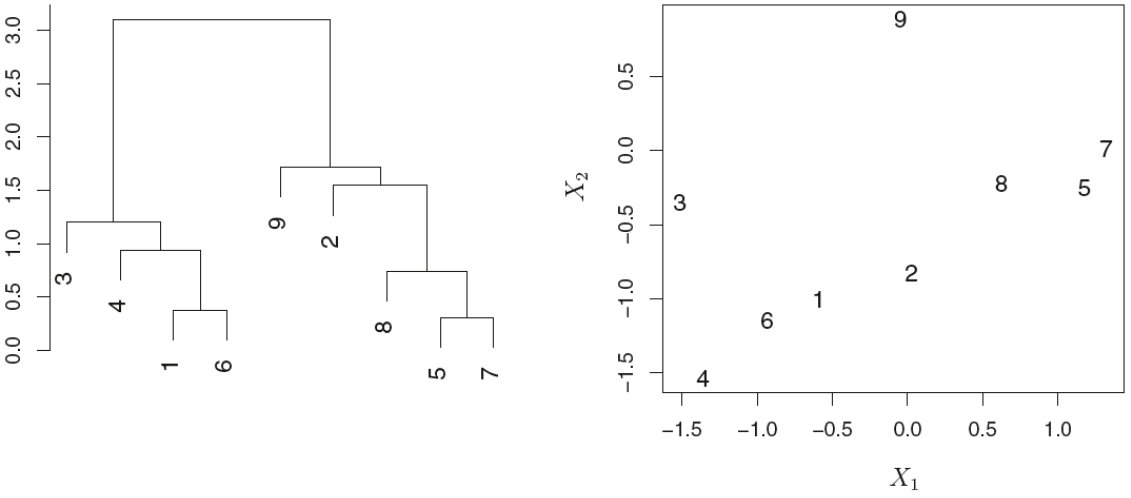
Agglomerative Clustering: data simulated from a 3-class model



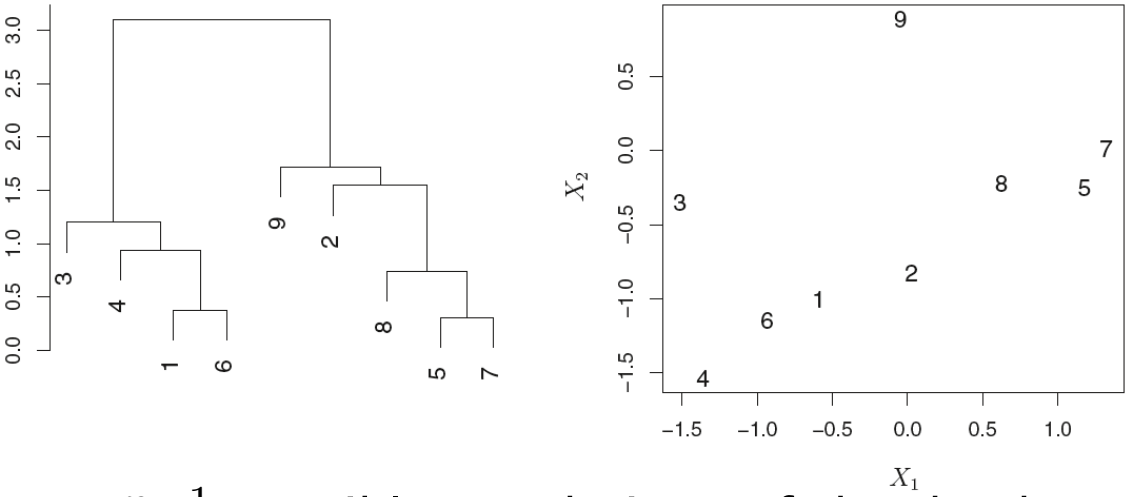
Dendogram obtained from hierarchical clustering



Agglomerative Clustering: interpretation of a dendogram



Agglomerative Clustering: interpretation of a dendogram



- There are 2^{n-1} possible reorderings of the dendrogram, where n is the number of leaves.
- At each of the $n-1$ points where fusions occur, the positions of the two fused branches could be swapped without affecting the meaning of the dendrogram.
- DO NOT draw conclusions about the similarity of two obs based on their proximity along the *horizontal* axis.
- Draw conclusions about the similarity of two observations based on the location on the *vertical* axis where branches containing those two observations first are fused.

Outline

Group Similarity

How do we define similarity between groups?

The most popular choices:

- *Single-linkage*: the distance between the closest pair

$$d_{SL}(G, H) = \min_{i \in G, j \in H} d(x_i, x_j)$$

- *Complete-linkage*: the distance of the furthest pair

$$d_{CL}(G, H) = \max_{i \in G, j \in H} d(x_i, x_j)$$

- *Group-average*: the average distance between groups

$$d_{GA}(G, H) = \frac{1}{N_G N_H} \sum_{i \in G,\, j \in H} d(x_i, x_j)$$

- *Metroid:* the distance between the means or metroids of groups

$$d_{ME}(G, H) = d(\mu_G, \mu_H)$$

Group Similarity

- single linkage can produce "chaining", where a few close observations can cause early merger of two groups
- complete linkage can cause groups not to merge if there are a few distant observations
- group averaging is a compromise, although it can require scaling of the data/similarities
- Metroids are similar to k-means. Major drawback that an *inversion* can occur: two clusters are fused at a height **below** either of the individual clusters in the dendrogram. This can lead to difficulties in visualization as well as in interpretation of the dendrogram.

Agglomerative Clustering: interpretation of a dendogram

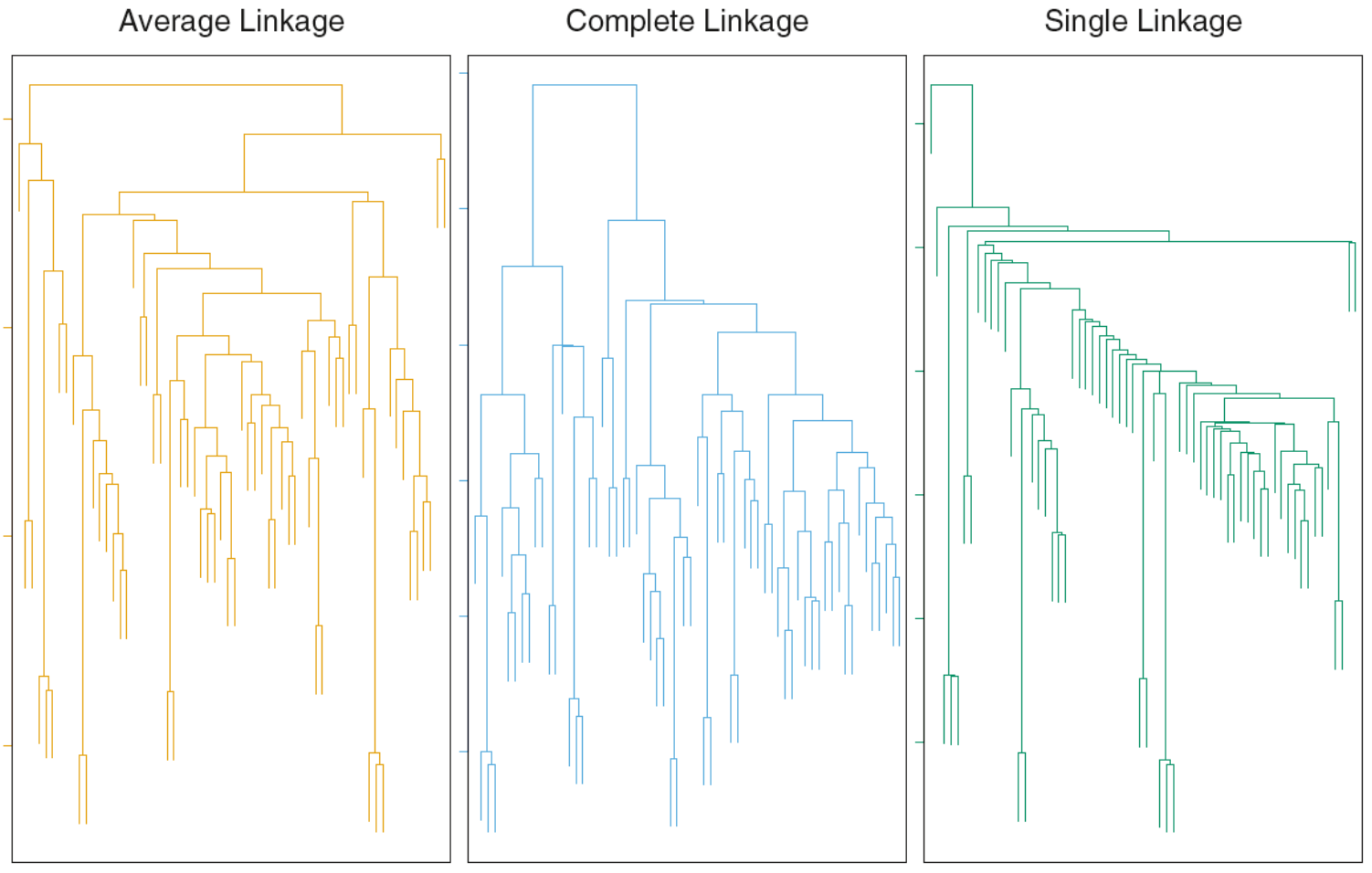
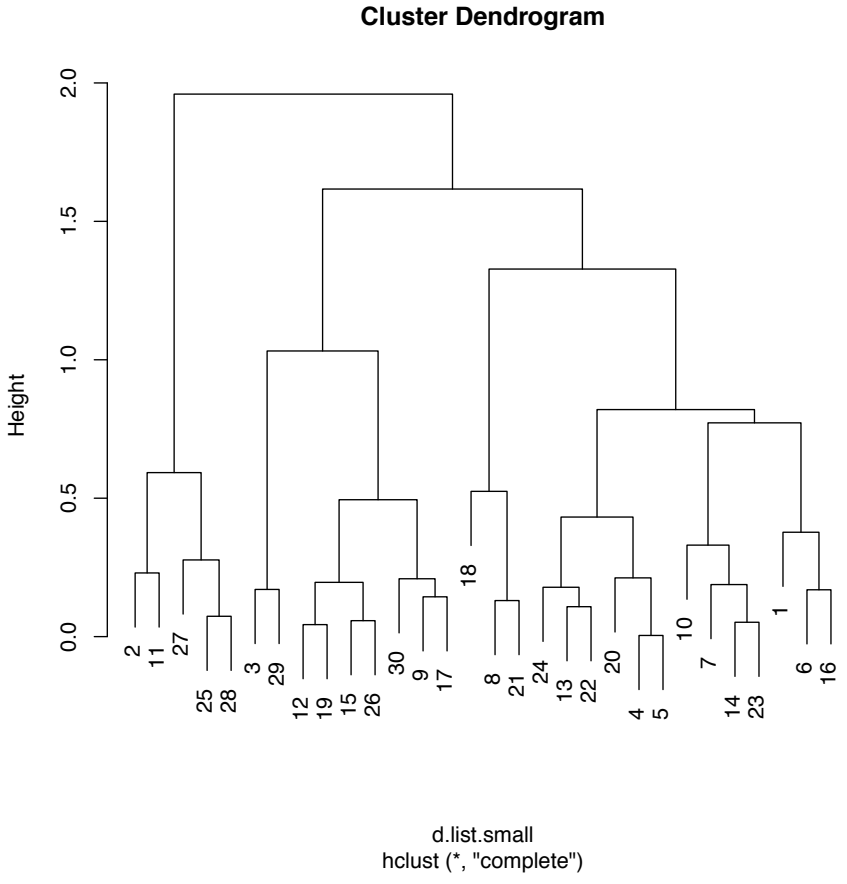
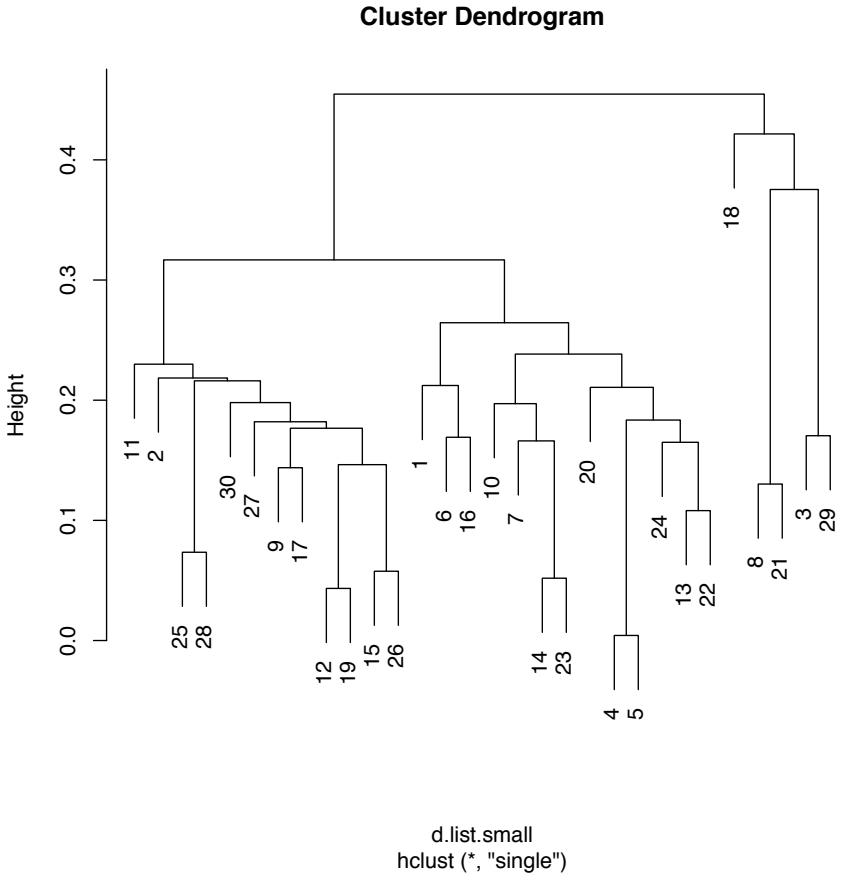


FIGURE 10.12. *Average, complete, and single linkage applied to an example data set. Average and complete linkage tend to yield more balanced clusters.*

Caveats





(Left) Complete linkage dendrogram, (Right) Single linkage

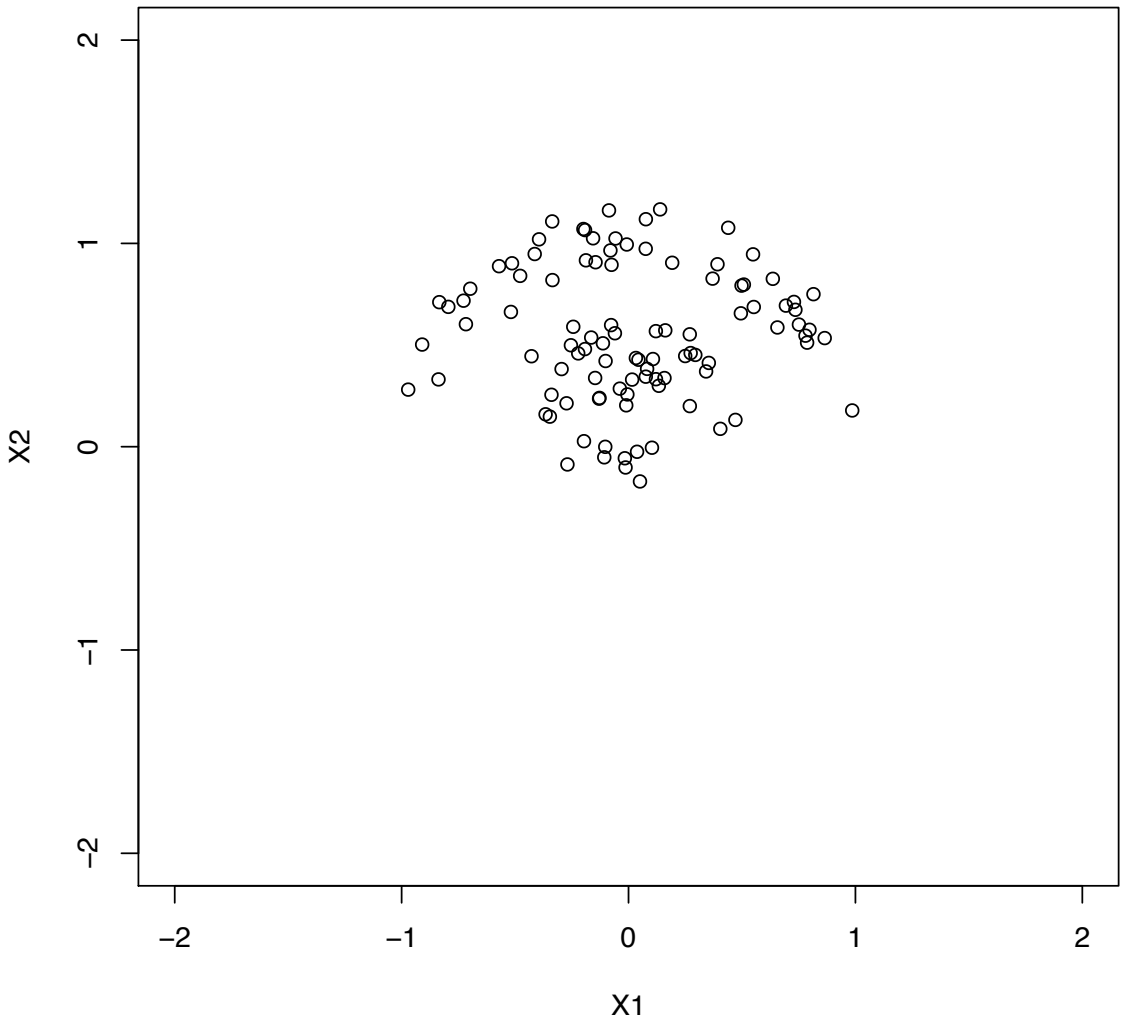
Caveats

Hierarchical clustering has a few issues:

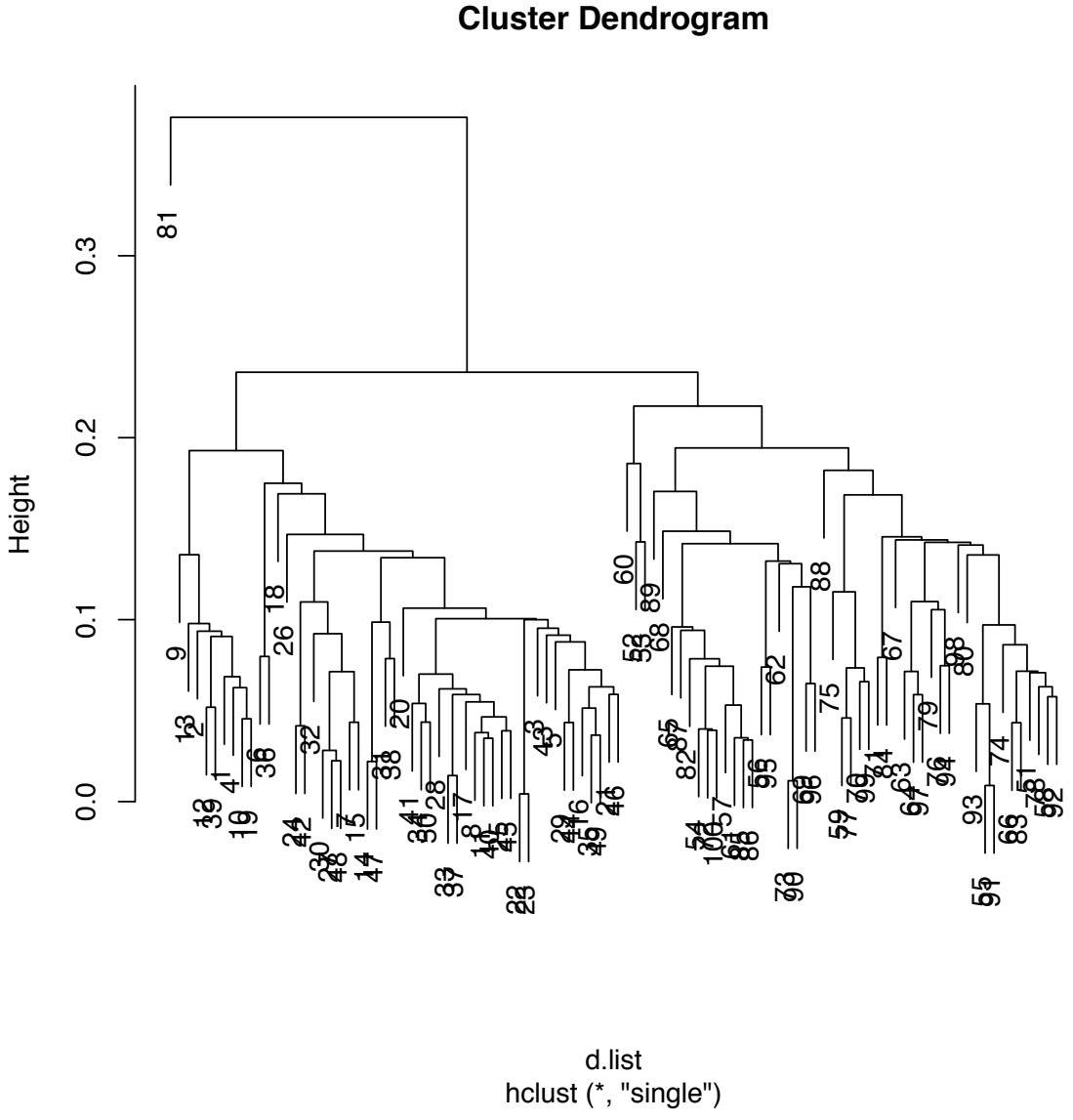
- different similarity metrics can make very different dendrograms (remind you of anything?)
- this method imposes a hierarchical structure on data, even if it does not exist
- minimal complexity is $\mathcal{O}(n^2)$, not good for large datasets

Back to Original Problem

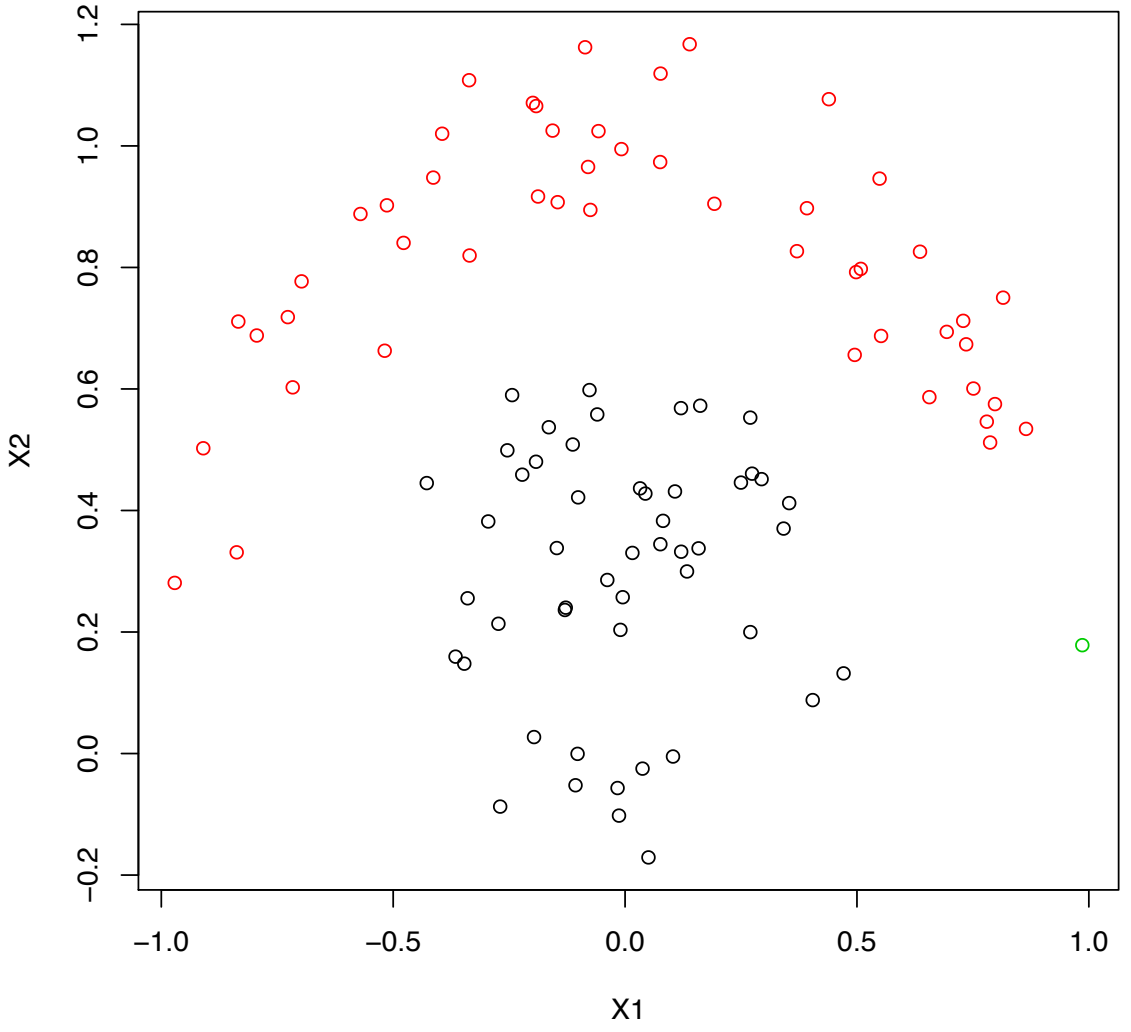
What sort of clustering should we use?



Back to Original Problem



Back to Original Problem



Outline

Divisive Clustering

Now on to *divisive clustering*

Basic algorithm:

- start with all data points in one single group
- repeat: split one cluster
- stop: when all groups only contain individuals

Divisive Clustering

How can we split groups?

Use cuts!

There are many cut-based algorithms, but we will look at one.

Cuts are not the only way to divide data, but they are the simplest.

Divisive Clustering

Inter/Intra Cluster Costs:

Given:

- $U = \{x_1, \ldots, x_n\}$ set of all observations
- A partitioning $C_1, \ldots, C_k$ of the objects

Set:

- $cutcost(C_p) = \sum_{i \in C_p,\ j \notin C_p} d(x_i, x_j)$
- $intracost(C_p) = \sum_{i,j \in C_p} d(x_i, x_j)$
- the contribution of each cluster is the ratio of external similarity to internal similarity

$$cost(C_1, \ldots, C_k) = \sum_{p=1}^{k} \frac{cutcost(C_p)}{intracost(C_p)}$$

Want to find clustering $C_1, \ldots, C_k$ that minimizes $cost(C_1, \ldots, C_k)$

Divisive Clustering

Heuristic way to find $\min cost(C_1, \ldots, C_k)$

1. choose initial partition $C_1, \ldots, C_k$
2. do until change in cost is less than ϵ for outer loop:
   - active set is $\{1, \ldots, n\}$
   - for $i = 1, \ldots, n$:
     - sample j from active set; remove j
     - move x_j into cluster that minimizes cost

Note: more computationally demanding than agglomerative clustering

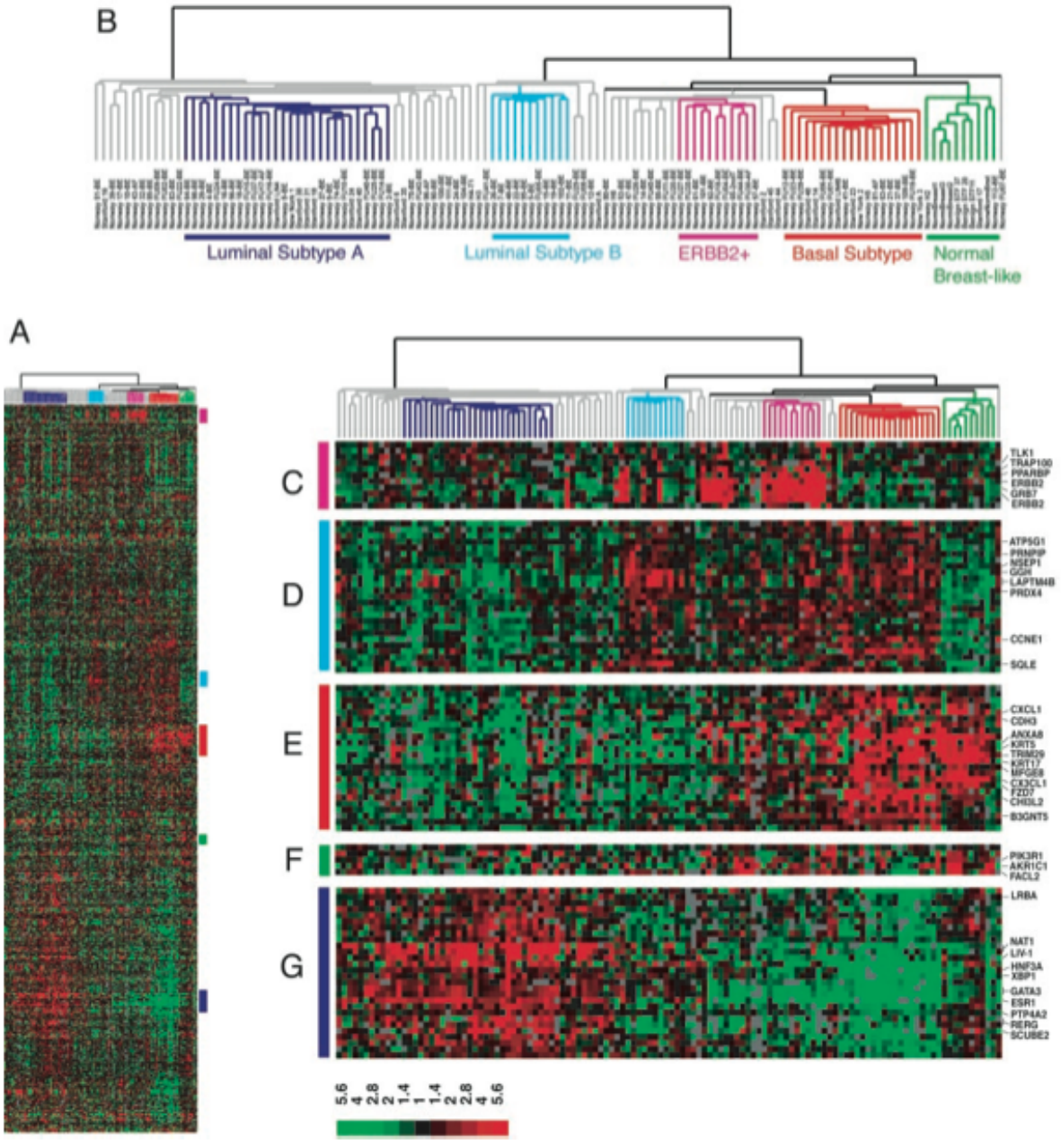
Outline

Applications of Hierarchical Clustering

Microarray gene expression data:

- "Repeated Observation of Breast Tumor Subtypes in Independent Gene Expression Data Sets" (Sorlie et al., 2003)
- hierarchical clustering is used to create new theories (discover tumor subtypes)
- ...which are then tested in the lab
- hypothesis: "breast tumor subtypes represent biologically distinct disease entities"

Applications of Hierarchical Clustering



Outline

Hierarchical Clustering in R

We will use the `hclust` function in the `stats` package (which is likely automatically loaded)

- let's make a function that plots the clusters as connections between points
- (the output of the following code is precisely the set of agglomerative clustering plots we previously viewed)

```
> # Get data
> library(datasets)
> n.faithful <- length(faithful[,1])
> cc.small <- faithful[sample(1:n.faithful,30),]
> n.small <- length(cc.small[,1])
> d.list.small <- dist(cc.small)
> h.list.small <- hclust(d.list.small, method="single")
> plot(h.list.small)
```

Hierarchical Clustering in R

```
> # Make clusters
> cluster.list <- list()
> merge <- h.list.small$merge
> for (i in 1:(n.small-1)){
   temp.vals <- merge[i,]
   if (i==1){
   cluster.list[[i]] <- c(-temp.vals)}
   else{
    # Check to see if negative or positive
    c.temp.1 <- mat.or.vec(1,1)
    if (temp.vals[1] < 0){
      # if neg, include positive version of index
      c.temp.1 <- -temp.vals[1]}
    else{
      # if positive, include indices from cluster
      c.temp.1 <- cluster.list[[temp.vals[1]]]}
    c.temp.2 <- mat.or.vec(1,1)
    if (temp.vals[2] < 0){
      c.temp.2 <- -temp.vals[2]}
    else{
      c.temp.2 <- cluster.list[[temp.vals[2]]]}
    cluster.list[[i]] <- c(c.temp.1,c.temp.2)}}
```

Hierarchical Clustering in R

Plot the results:

```
for (i in 1:(n.small-1)){
  pdf(paste("AgClustS",i,".pdf",sep=""))
  plot(cc.small[,1],cc.small[,2],ylim=c(-1.5,1.5),xlim=c(-1.5,1.5),
      main=paste("Agglomerative Clustering Step (",i,")",sep=""))
  for (j in 1:i){# plot lines
    temp.vec <- cluster.list[[j]]
    temp.n <- length(temp.vec)
    for (k in 1:(temp.n-1)){
      ind.1 <- temp.vec[k]
      for (ell in (k+1):temp.n){
        ind.2 <- temp.vec[ell]
        lines(c(cc.small[ind.1,1],cc.small[ind.2,1]),c(cc.small[ind.1,2],
          cc.small[ind.2,2]),col=3,xlab="X1",ylab="X2")
      }
    }
  }
dev.off()
}
```

Final-esque question

Use hierarchical agglomerative clustering to cluster the following data points with (a) single linkage, then (b) average linkage, and then (c) complete linkage:

x_1	x_2
-1.0	-1.2
-1.2	-1.8
-2.1	-2.4
1.1	1.5
1.5	1.6
1.3	0.7