PLSC 597: Modern Measurement

Cluster Analysis

February 15, 2018

Cluster Analysis

"...a statistical operation of grouping objects. The resulting groups are clusters. Clusters have the following properties:

- We find them during the operation and their number is also not always fixed in advance.
- They are the combination of objects having similar characteristics."

"...groups objects (observations, events) based on the information found in the data describing the objects or their relationships. The goal is that the objects in a group will be similar (or related) to one other and different from (or unrelated to) the objects in other groups. The greater the similarity (or homogeneity) within a group, and the greater the difference between groups, the 'better' or more distinct the clustering."

Why Cluster?

- Classification / Taxonomy (*description*)
- Data Reduction (*measurement*)
- Identify Relationships (*inductive inference*)
- Prediction (typically out-of-sample)

Clustering: Intuition

Figure 1a: Initial points.

Figure 1b: Two clusters.

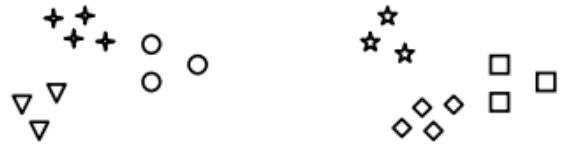


Figure 1c: Six clusters

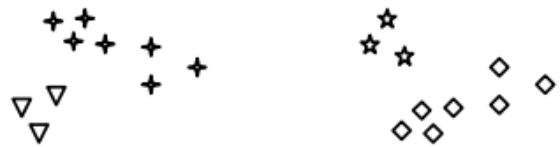
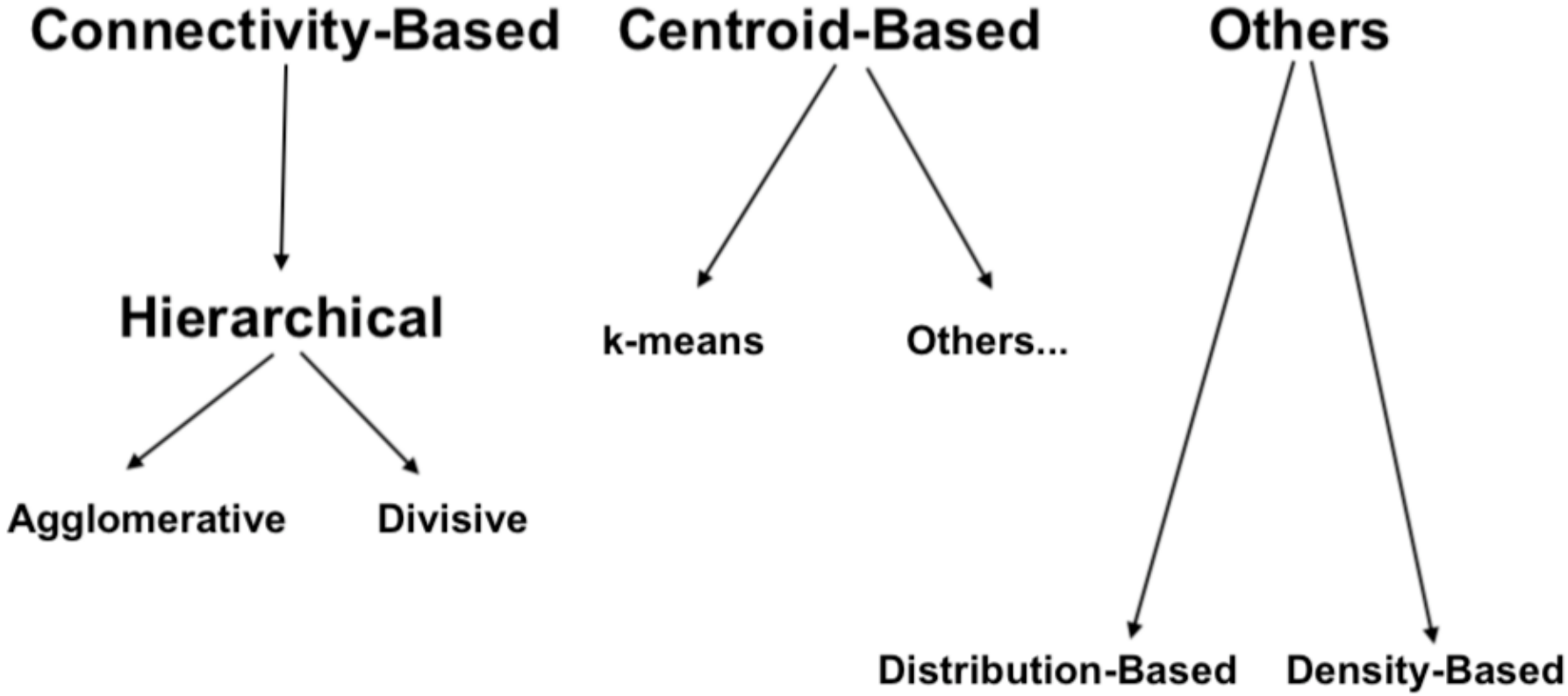


Figure 1d: Four clusters.

(source)

Cluster Analysis: Typology



Euclidean ("L2") Distance:

$$d_{L2}(\mathbf{X}, \mathbf{Y}) = \sqrt{\sum_{i=1}^{K} (X_i - Y_i)^2}.$$

"City-Block" / Manhattan ("L1") Distance:

$$d_{L1}(\mathbf{X}, \mathbf{Y}) \equiv \|\mathbf{X} - \mathbf{Y}\|_1 = \sum_{i=1}^{K} |X_i - Y_i|.$$

Mahalanobis Distance:

$$d_M(\mathbf{X}, \mathbf{Y}) = \sqrt{(\mathbf{X} - \mathbf{Y})' \mathbf{S}^{-1} (\mathbf{X} - \mathbf{Y})}.$$

Distance Example

	X	Y	Z
Tick	1	711	0.08
Arthur	0	588	0.27
Tick - Arthur	1	123	-0.19

Euclidean:

$$\begin{aligned} D_{L2} &= \sqrt{(1-0)^2 + (711-588)^2 + (0.08-0.27)^2} \\ &= \sqrt{1 + 15129 + 0.0361} \\ &= 123.004 \end{aligned}$$

Manhattan:

$$\begin{aligned} D_{L1} &= |1-0| + |711-588| + |0.08-0.27| \\ &= 1 + 123 + 0.19 \\ &= 124.19 \end{aligned}$$

Mahalanobis:

$$\begin{aligned} D_{M} &= \sqrt{(\text{Tick} - \text{Arthur})' \hat{\mathbf{S}}^{-1} (\text{Tick} - \text{Arthur})} \\ &= 1.386 \end{aligned}$$

Defining Intra-Cluster Distances

For two clusters C_A and C_B, the distance between can be defined in terms of:

- Single-linkage

$$d_{AB} = \min(d_{a,b})$$

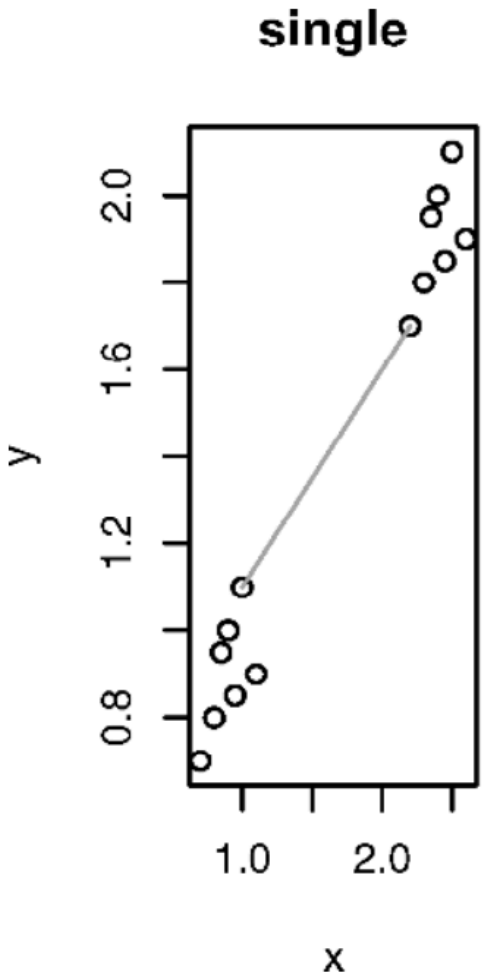
- Complete linkage

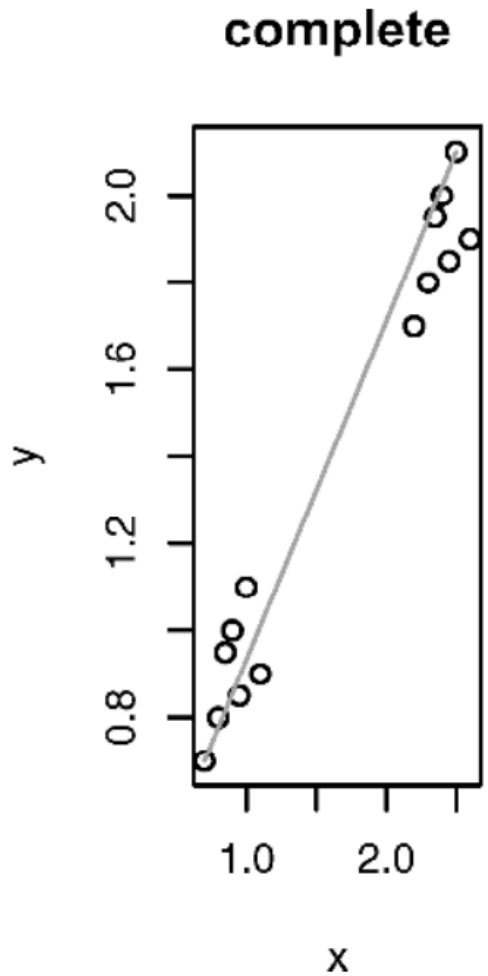
$$d_{AB} = \max(d_{a,b})$$

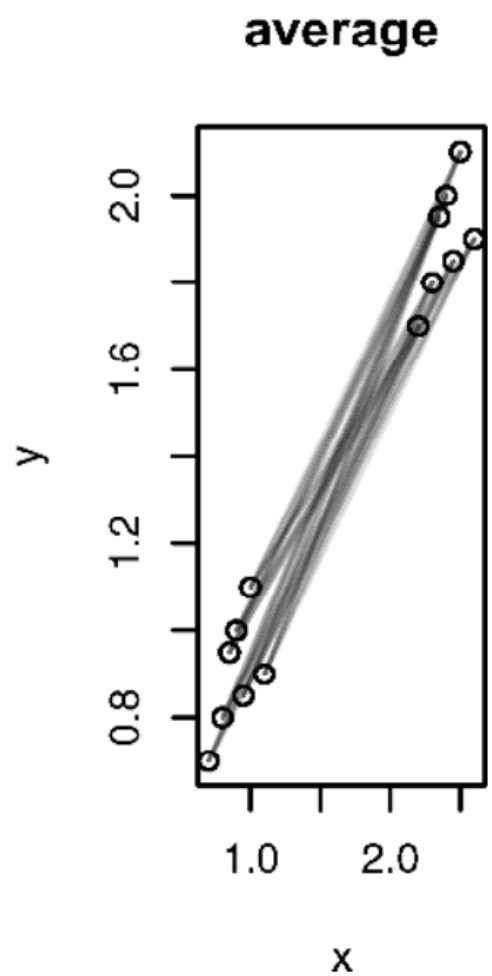
- Group average

$$d_{AB} = \frac{1}{N_A N_B} \sum_{a=1}^{N_A} \sum_{b=1}^{N_b} (d_{a,b})$$

Cluster Linkages







Agglomerative Clustering

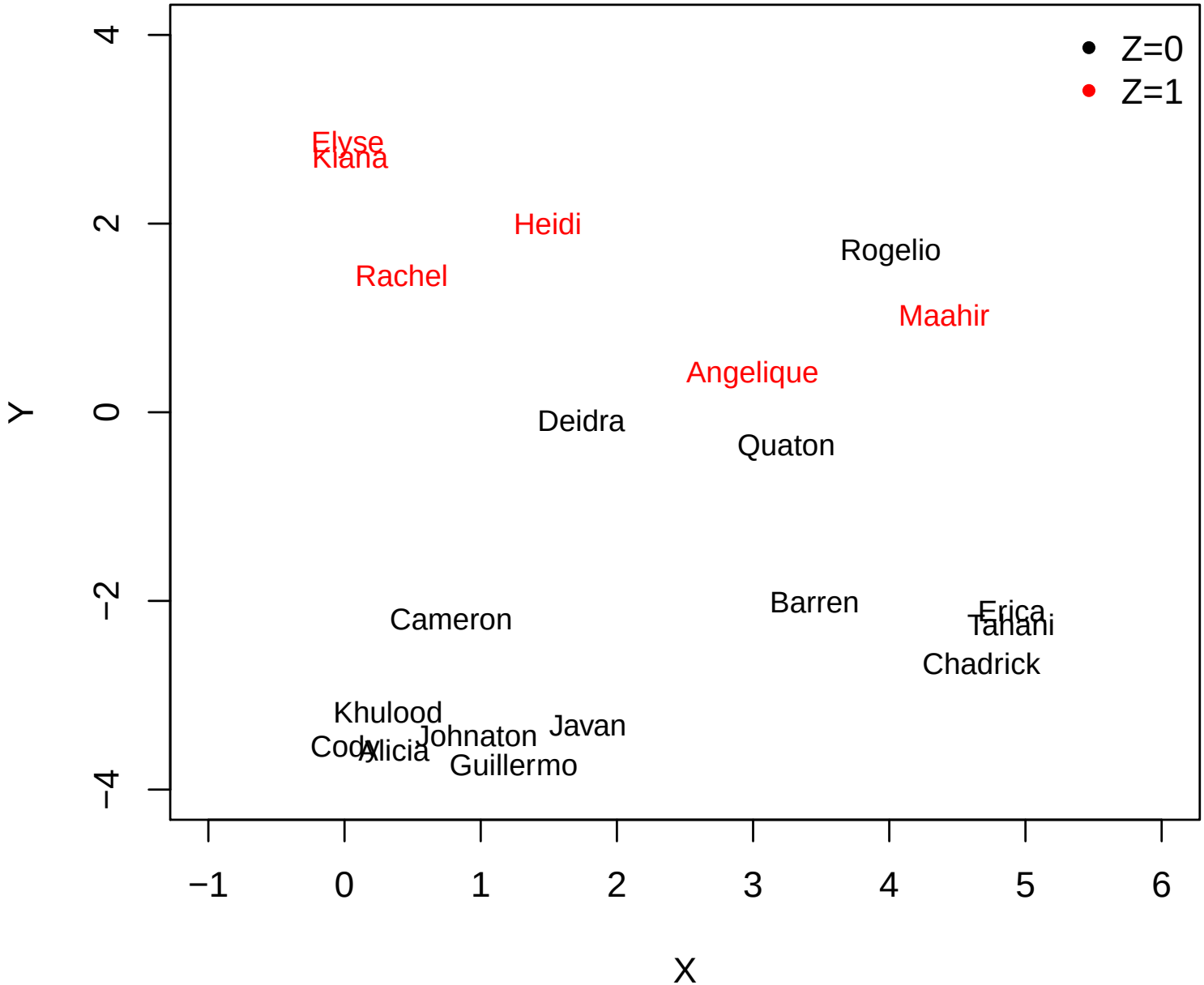
Basic steps:

1. Begin with N observations on K variables in $\mathbf{X}$
2. Define each observation as its own "cluster" C_i
3. Find the two clusters C_ℓ and C_m that are "closest" to each other
4. Merge them into a single cluster, and delete the two component clusters
5. Recalculate the distances between all remaining clusters
6. Repeat steps 3-5 until only one cluster remains

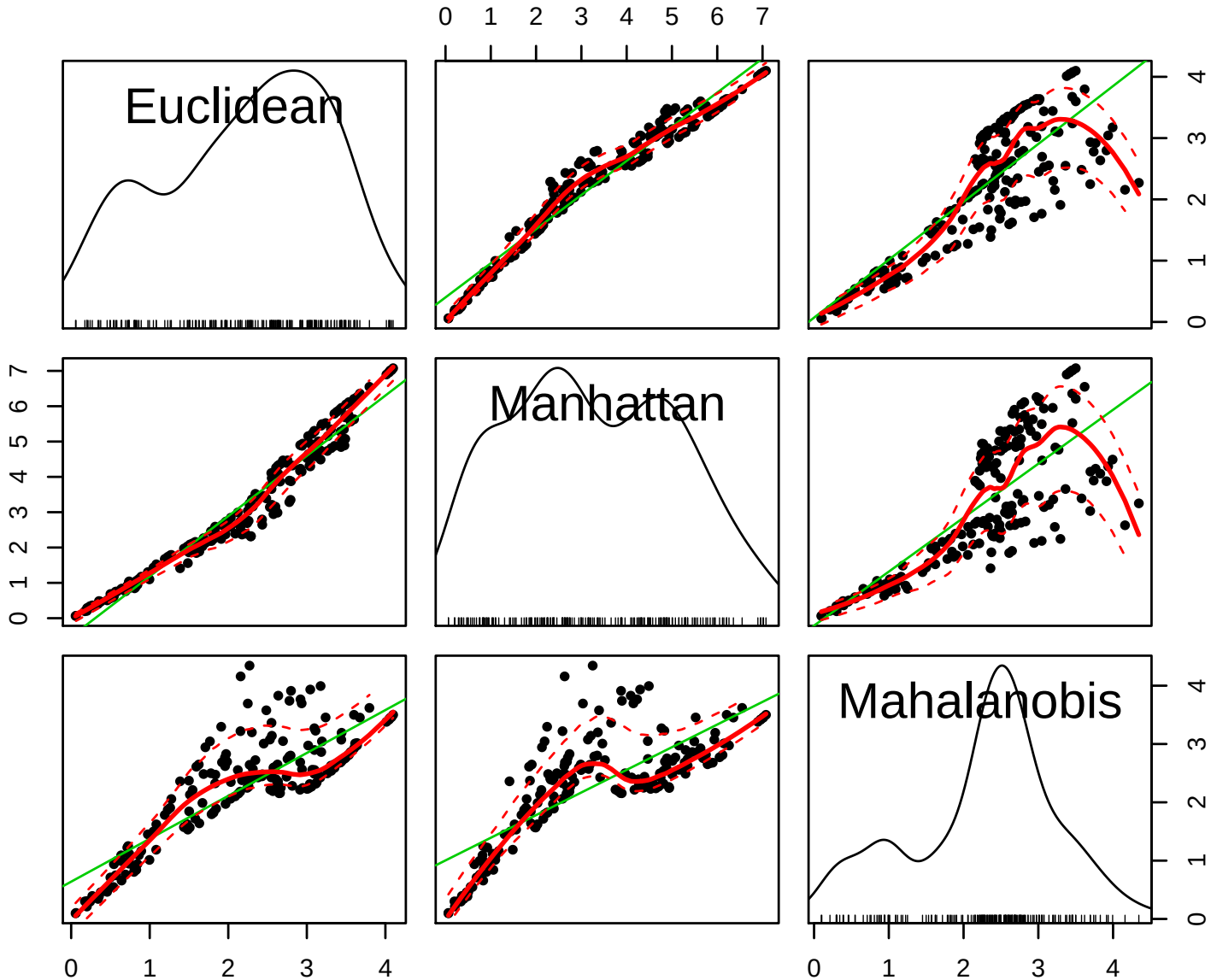
Simulation Example

```
> N <- 20
> set.seed(7222009)
> Name <- randomNames(N, which.names="first")
> X <- 5*rbeta(N,0.5,0.5)
> Y <- runif(N,-4,4)
> Z <- rbinom(N,1,pnorm(Y/2))

> df <- data.frame(Name=Name,X=X,Y=Y,Z=Z)
> rownames(df)<-df$Name
>
> # Distances:
> #
> # CENTER AND RESCALE / STANDARDIZE THE DATA:
>
> ds <- scale(df[,2:4])
>
> DL2 <- dist(ds) # L2 / Euclidean distance
> DL1 <- dist(ds,method="manhattan") # L1 / Manhattan distance
> DM <- sqrt(D2.dist(ds,cov(ds))) # Mahalanobis distances
```

Simulated Data, Plotted



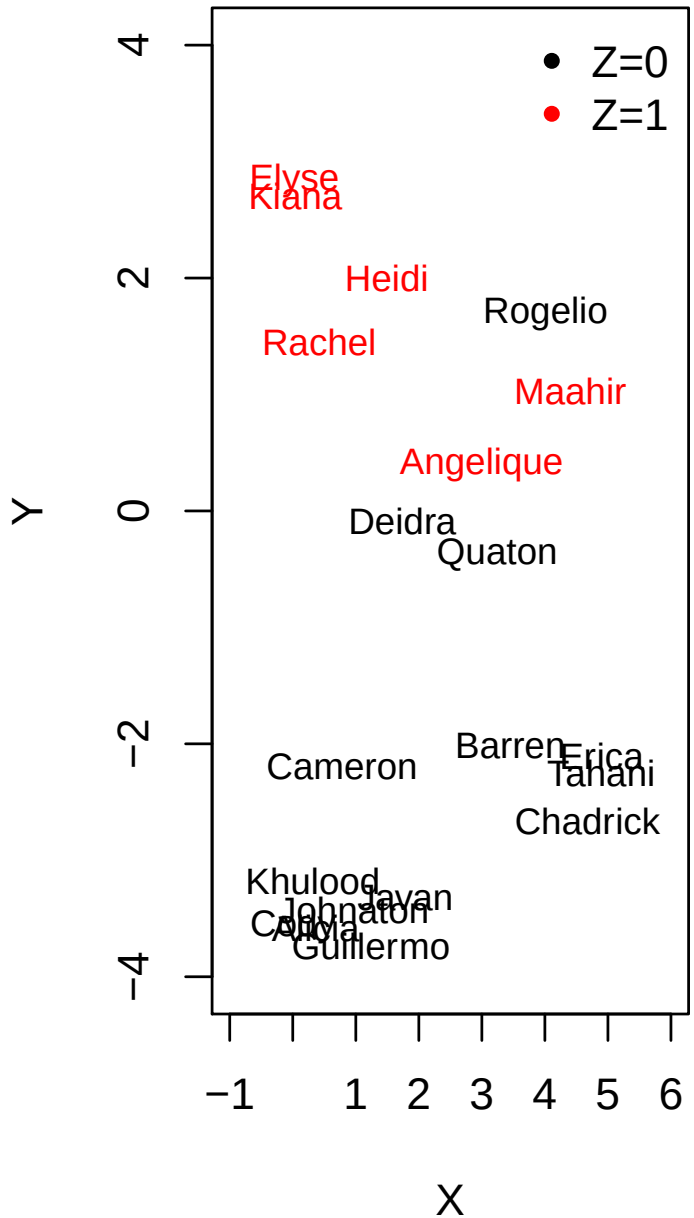
Distance Comparisons

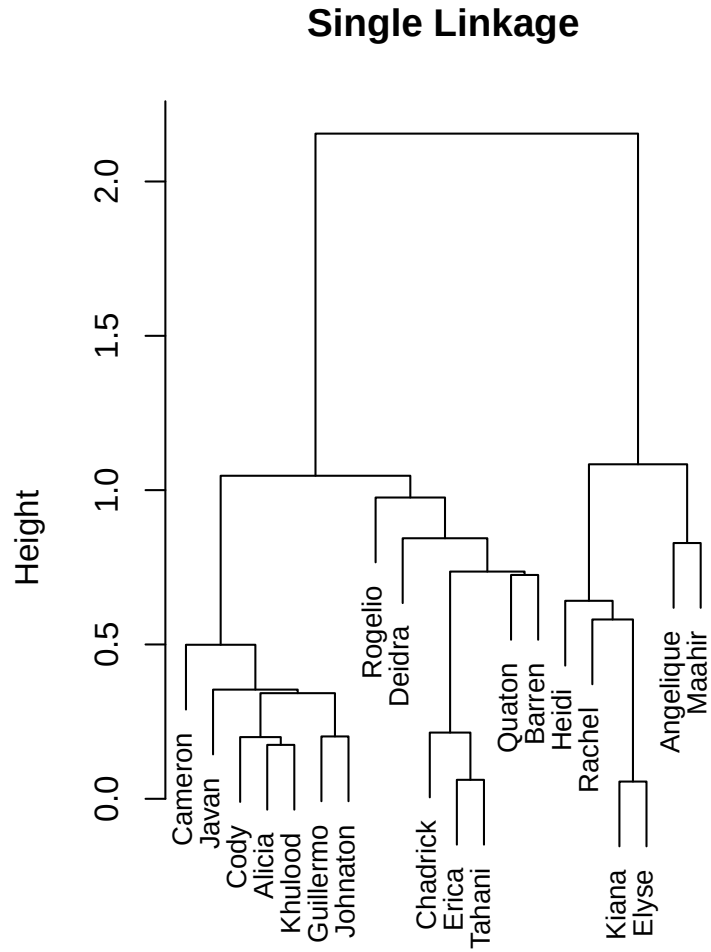


Using hclust (in cluster)

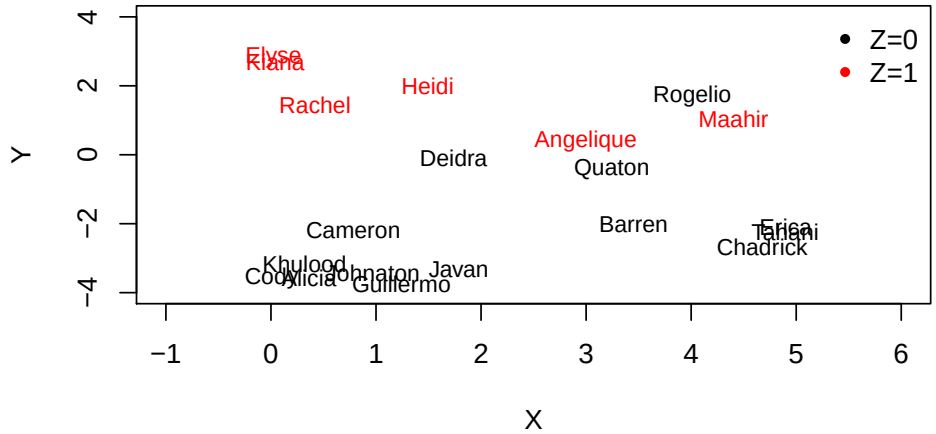
```
> ADL2.s <- hclust(DL2,method="single")
> ADL2.c <- hclust(DL2,method="complete")
> ADL2.a <- hclust(DL2,method="average")

> str(ADL2.s)
List of 7
 $ merge      : int [1:19, 1:2] -17 -15 -5 -9 -1 -19 4 -8 -11 -2 ...
 $ height     : num [1:19] 0.129 0.143 0.36 0.405 0.413 ...
 $ order      : int [1:20] 17 18 2 12 11 8 9 5 10 1 ...
 $ labels     : chr [1:20] "Guillermo" "Rachel" "Deidra" "Quaton" ...
 $ method     : chr "single"
 $ call       : language hclust(d = DL2, method = "single")
 $ dist.method: chr "euclidean"
 - attr(*, "class")= chr "hclust"
```

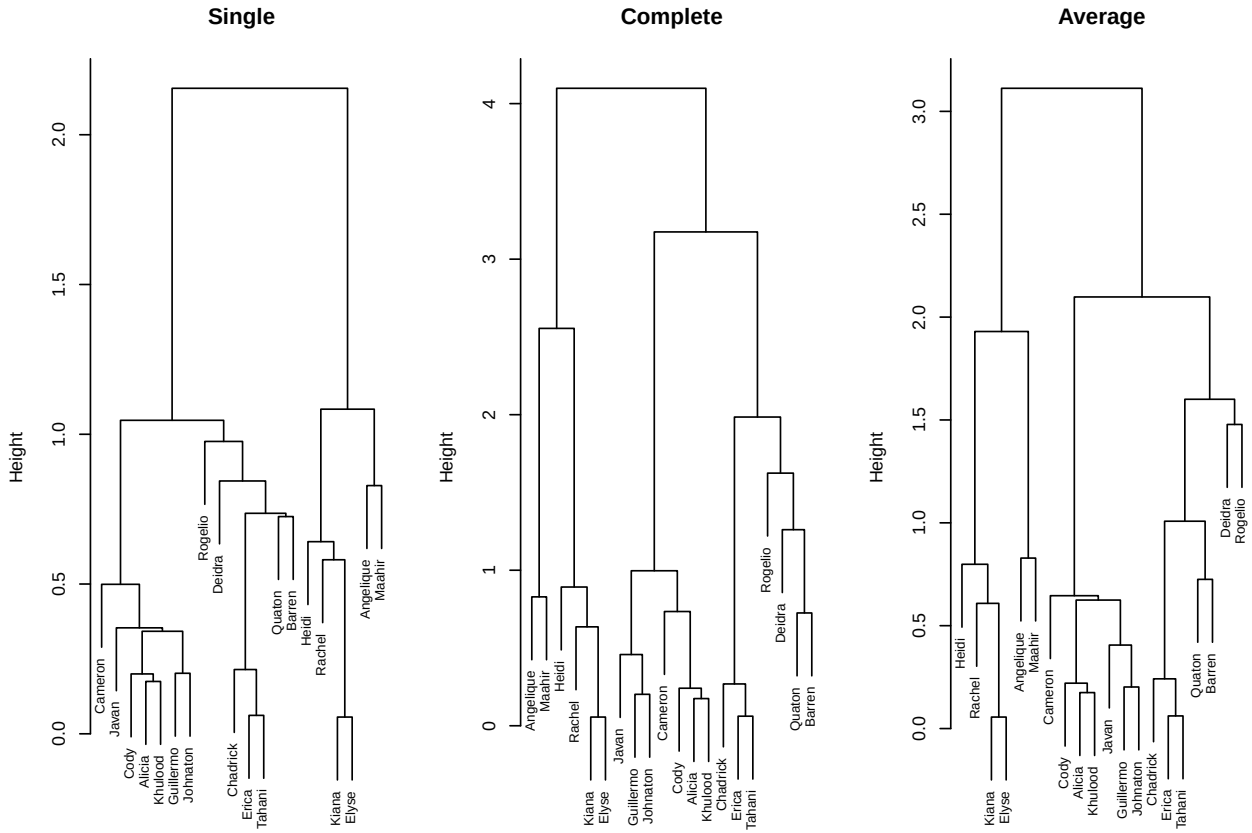
The Dendrogram



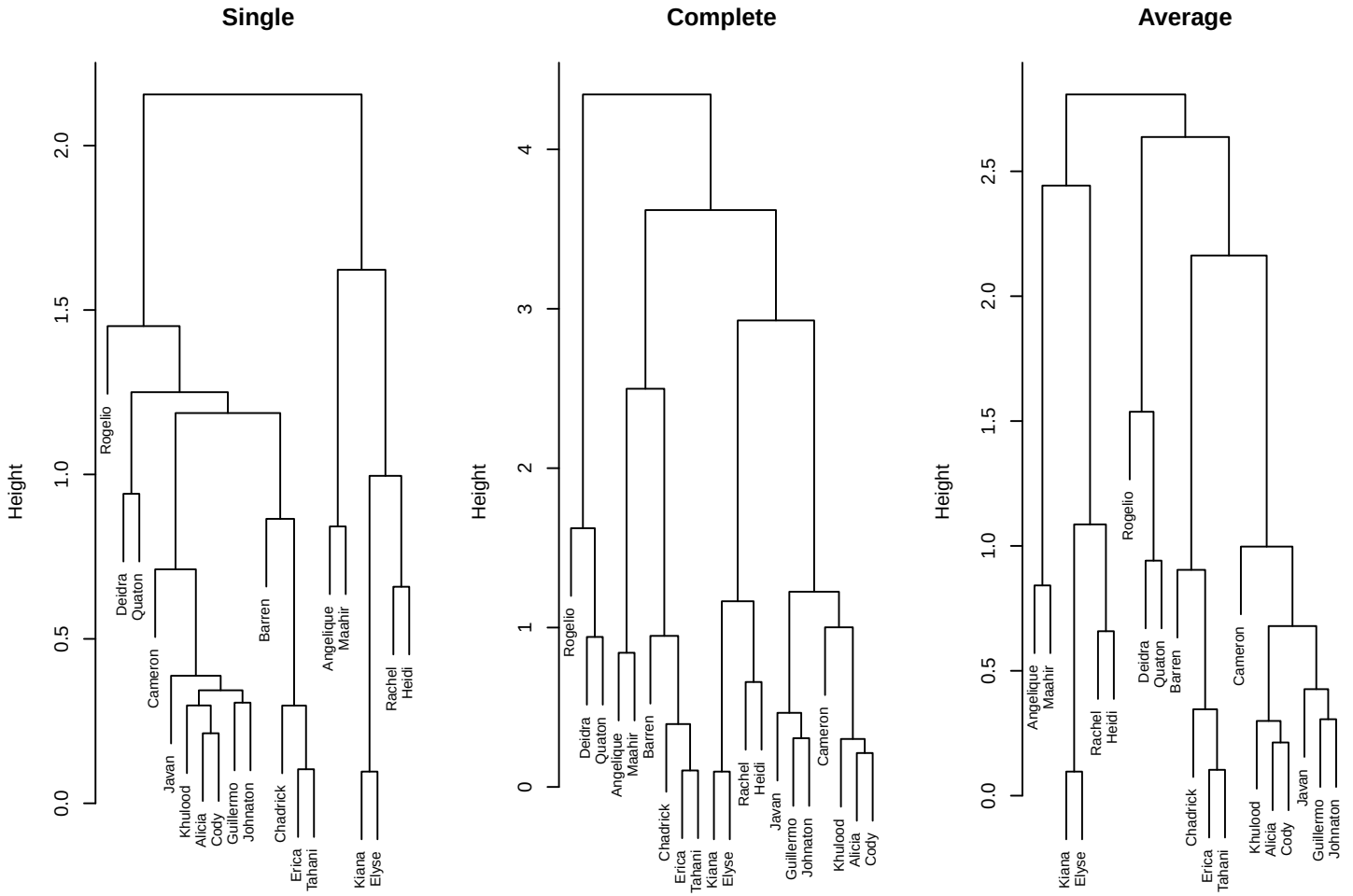


Comparing Linkages





Using Mahalanobis Distance

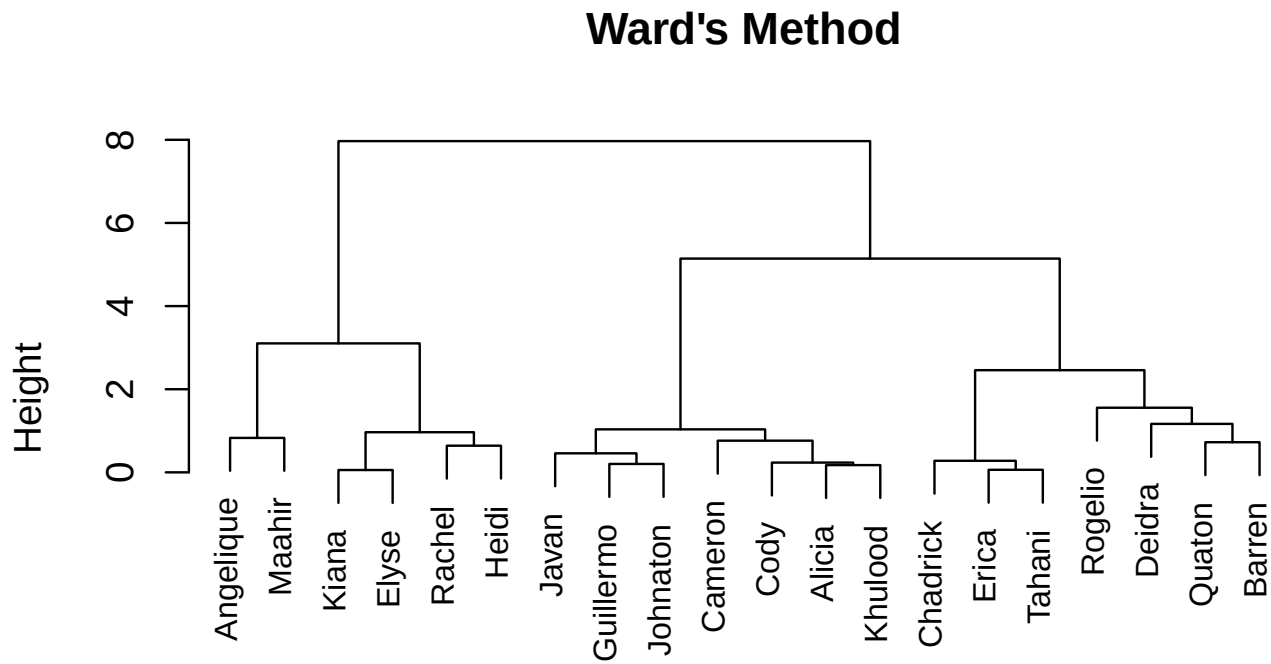


An Alternative: Ward's Method

- "Ward's minimum variance method."
- Creates clusters by minimizing the total within-cluster variance
- Begins with a Euclidean distance matrix
- Implemented via the Lance-Williams algorithm (see link for details)

Ward's Method Illustrated

```
> ADL2.w <- hclust(DL2,method="ward.D2")
```



The Agglomeration Coefficient

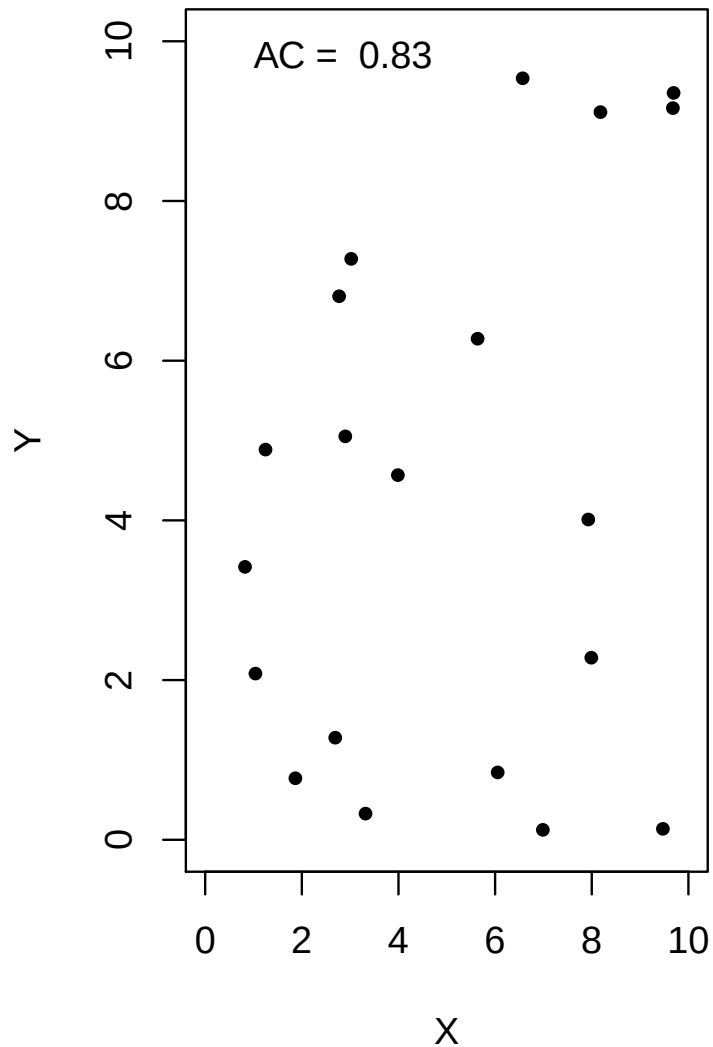
The *agglomeration coefficient* AC measures the clustering structure of the data. For each observation i, define m_i as the dissimilarity of observation i with the first cluster with which it is merged, divided by the dissimilarity in the final iteration (i.e., the greatest dissimilarity). The coefficient is then:

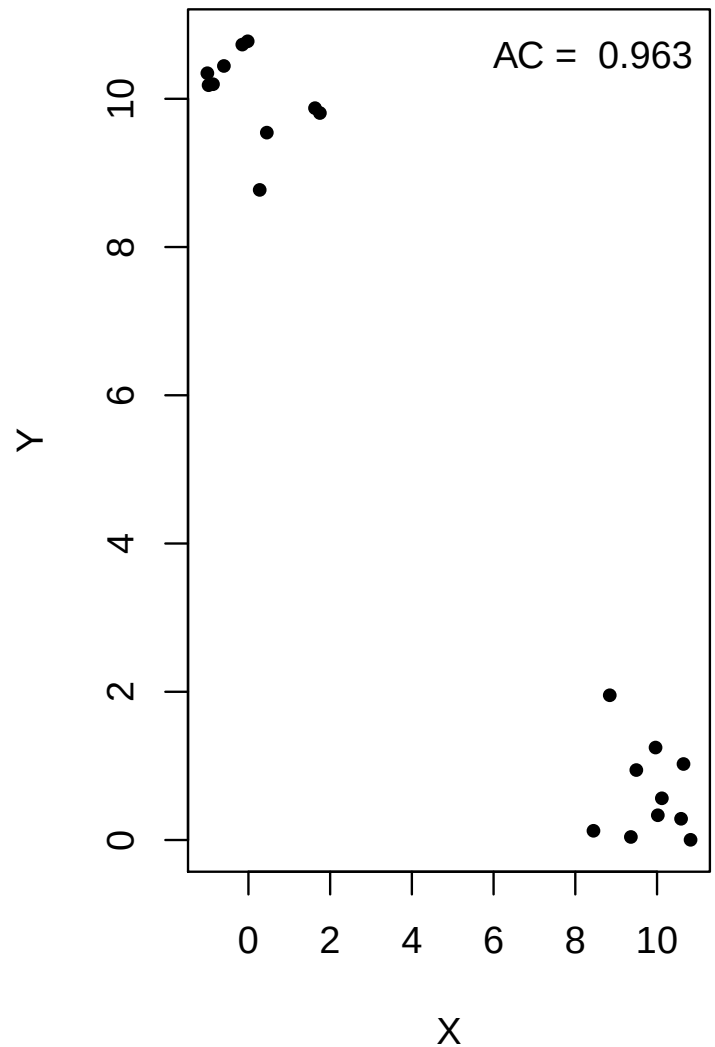
$$AC = \frac{1}{N-1} \sum_{i=1}^{N-1} 1 - m_i$$

Notes:

- Higher values correspond to greater clustering in the data.
- AC increases with N so should not be used to compare datasets of very different sizes

Example AC Values





Example *AC*s: Simulated Data

```
> Agnes.s <- agnes(ds, metric="euclidean",method="single")
> Agnes.s$ac
[1] 0.805

> Agnes.c <- agnes(ds, metric="euclidean",method="complete")
> Agnes.c$ac
[1] 0.8754

> Agnes.a <- agnes(ds, metric="euclidean",method="average")
> Agnes.a$ac
[1] 0.8398

> # Using Mahalanobis distance:
> Agnes.M <- agnes(DM, diss=TRUE, method="average")
> Agnes.M$ac
[1] 0.8071
```

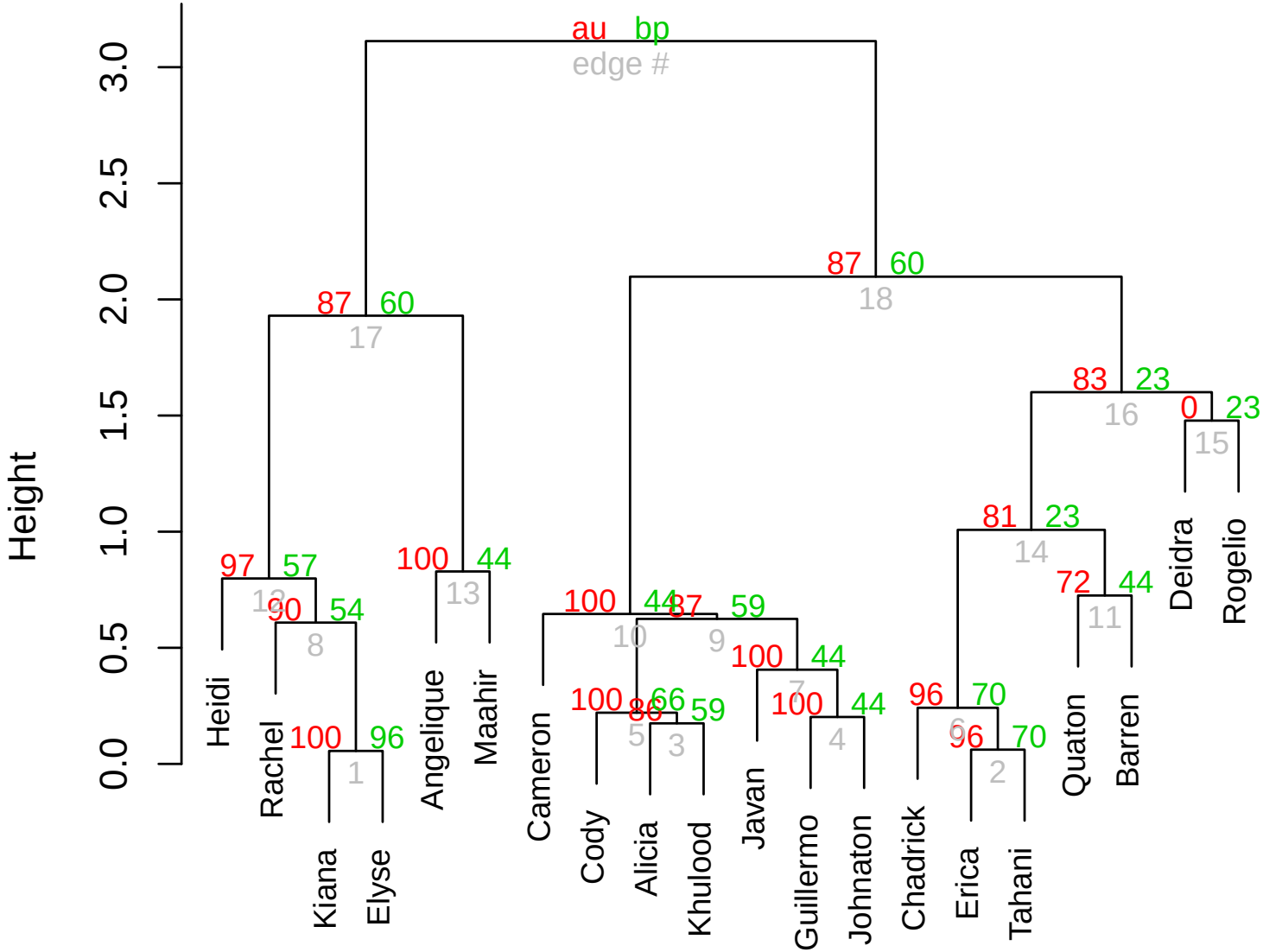
P-Values via Bootstrap

- Can calculate *P*-values for each cluster (at each agglomeration stage) via multiscale bootstrap resampling
- Reference: Suzuki, R., and H. Shimodaira. 2006. "pvclust: An R package for assessing the uncertainty in hierarchical clustering." *Bioinformatics* 22:1540-1542.
- The R package is `pvclust`
- Reports "approximately unbiased" and "bootstrap probability" *P*-values (use the former)
- "Clusters with high values... are strongly supported by the data."

P-Values...

```
dst<-data.frame(t(ds))
PVDL2.s <- pvclust(dst,method.hclust="single",
                   method.dist="euclidean",nboot=1001)
                   > PVDL2.s

Cluster method: average
Distance      : euclidean

Estimates on edges:

      au    bp se.au se.bp      v      c  pchi
1  0.997 0.957 0.001 0.003 -2.222  0.501 0.607
2  0.963 0.695 0.005 0.006 -1.147  0.636 0.022
3  0.856 0.593 0.013 0.006 -0.648  0.413 0.000
4  0.999 0.445 0.000 0.006 -1.482  1.621 0.105
5  0.997 0.656 0.001 0.006 -1.599  1.198 0.002
6  0.963 0.695 0.005 0.006 -1.147  0.636 0.022
7  0.999 0.445 0.000 0.006 -1.482  1.621 0.105
8  0.902 0.543 0.020 0.006 -0.701  0.592 0.000
9  0.869 0.594 0.012 0.006 -0.681  0.442 0.000
10 0.999 0.445 0.000 0.006 -1.482  1.621 0.105
11 0.721 0.445 0.019 0.006 -0.223  0.362 0.000
12 0.970 0.569 0.008 0.006 -1.028  0.853 0.065
13 0.999 0.439 0.001 0.006 -1.434  1.589 0.095
14 0.807 0.233 0.091 0.007 -0.069  0.797 0.607
15 0.002 0.233 0.002 0.007  1.837 -1.109 0.607
16 0.834 0.233 0.082 0.007 -0.121  0.849 0.607
17 0.866 0.601 0.012 0.006 -0.682  0.427 0.000
18 0.866 0.601 0.012 0.006 -0.682  0.427 0.000
19 1.000 1.000 0.000 0.000  0.000  0.000 0.000
```

Dendrogram with P-Values...



Divisive Clustering (`diana`)

Basic steps:

1. Begin with N observations on K variables in $\mathbf{X}$
2. Select the cluster C_{maxD} with the largest *diameter* (defined as the cluster with the largest dissimilarity between any two of its observations)
3. Select the observation j in C_{maxD} that has the highest average dissimilarity to the other observations in the cluster); this is the "seed" of the "splinter group" $C_{splinter}$
4. Iteratively assign observations to either the splinter group $C_{splinter}$ or the parent cluster C_{parent}, based on their dissimilarity to each.
5. Repeat step 4 until each observation in C_{maxD} is reassigned to either C_{parent} or $C_{splinter}$
6. Iterate steps 2-5 until each observation is its own cluster

Divisive Clustering Example

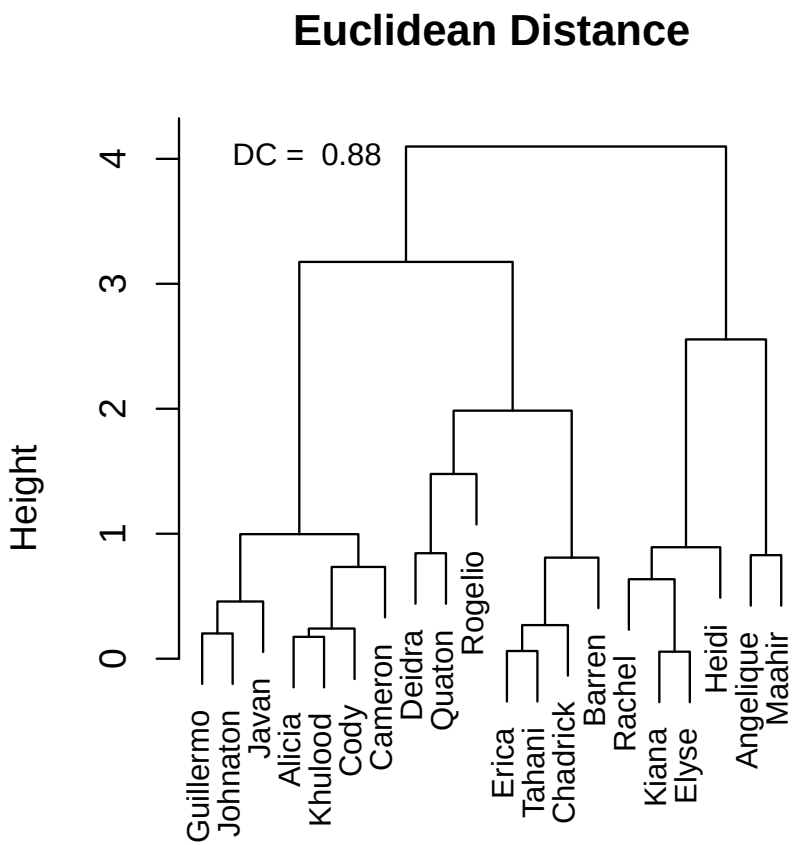
```
> Diana.L2 <- diana(ds,metric="euclidean")
> Diana.L2
Merge:
      [,1] [,2]
 [1,]  -17  -18
 [2,]  -15  -20
 [3,]   -5   -9
 [4,]   -1   -7
 [5,]    3  -10
 [6,]    2  -19
 [7,]    4   -8
 [8,]   -2    1
 [9,]    5  -11
[10,]    6  -16
[11,]   -6  -13
[12,]   -3   -4
[13,]    8  -12
[14,]    7    9
[15,]   12  -14
[16,]   15   10
[17,]   13   11
[18,]   14   16
[19,]   18   17
Order of objects:
 [1] Guillermo Johnaton  Javan     Alicia    Khulood   Cody
 [7] Cameron   Deidra    Quaton    Rogelio   Erica     Tahani
[13] Chadrick  Barren    Rachel    Kiana     Elyse     Heidi
[19] Angelique Maahir
Height:
 [1] 0.20204 0.45777 0.99653 0.17474 0.24121 0.73438 3.17509 0.84410
 [9] 1.47820 1.98490 0.06146 0.26884 0.80881 4.09856 0.63594 0.05589
[17] 0.89190 2.55486 0.82867
Divisive coefficient:
[1] 0.8798
Available components:
[1] "order"     "height"    "dc"        "merge"     "diss"
[6] "call"      "order.lab" "data"
```

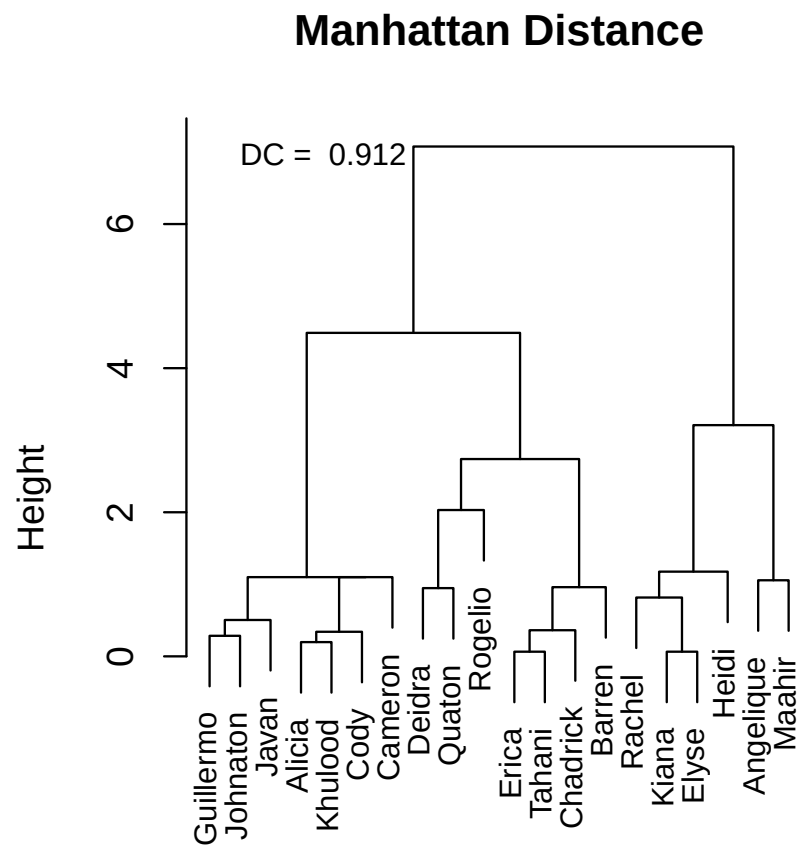
Practical Agglomerative Clustering: Linkages

> *"The performances of traditional hierarchical clustering methods have been evaluated for a variety of simulated situations. Single linkage clustering is simple to understand and compute, but has the tendency to build unphysical elongated chains of clusters joined by a single point, especially when unclustered noise is present. Figure 12.4 of Izenman (2008) illustrates how a single linkage dendrogram can differ considerably from the average linkage, complete linkage and divisive dendrograms, which can be quite similar to each other. Kaufman and Rosseeuw (1990, Section 5.2) report that "Virtually all authors agreed that single linkage was least successful in their [simulation] studies." Everitt et al. (2001, Section 4.2) report that "Single linkage, which has satisfactory mathematical properties and is also easy to program and apply to large data sets, tends to be less satisfactory than other methods because of 'chaining'." Ward's method is successful with clusters of similar populations, but tends to misclassify objects when the clusters are elongated or have very different diameters. Average linkage is generally found to be an effective technique in simulations, although its results depend on the cluster size. Average linkage also has better consistency properties than single or complete linkage as the sample size increases towards infinity (Hastie et al. 2009, Section 14.3)."*

– Eric D. Feigelson and G. Jogesh Babu. 2012. *Modern Statistical Methods for Astronomy: With R Applications*. New York: Cambridge University Press, p. 228.

Divisive Clustering: Dendrograms





Non-Hierarchical Clustering

k-means clustering "aims to partition the points into k groups such that the sum of squares from points to the assigned cluster centers is minimized."

- Formally, find:

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2 = \arg\min_{\mathbf{S}} \sum_{i=1}^{k} |S_i| \operatorname{Var} S_i$$

  for the set of k clusters $S_1 \ldots S_k$ in $\mathbf{S}$.

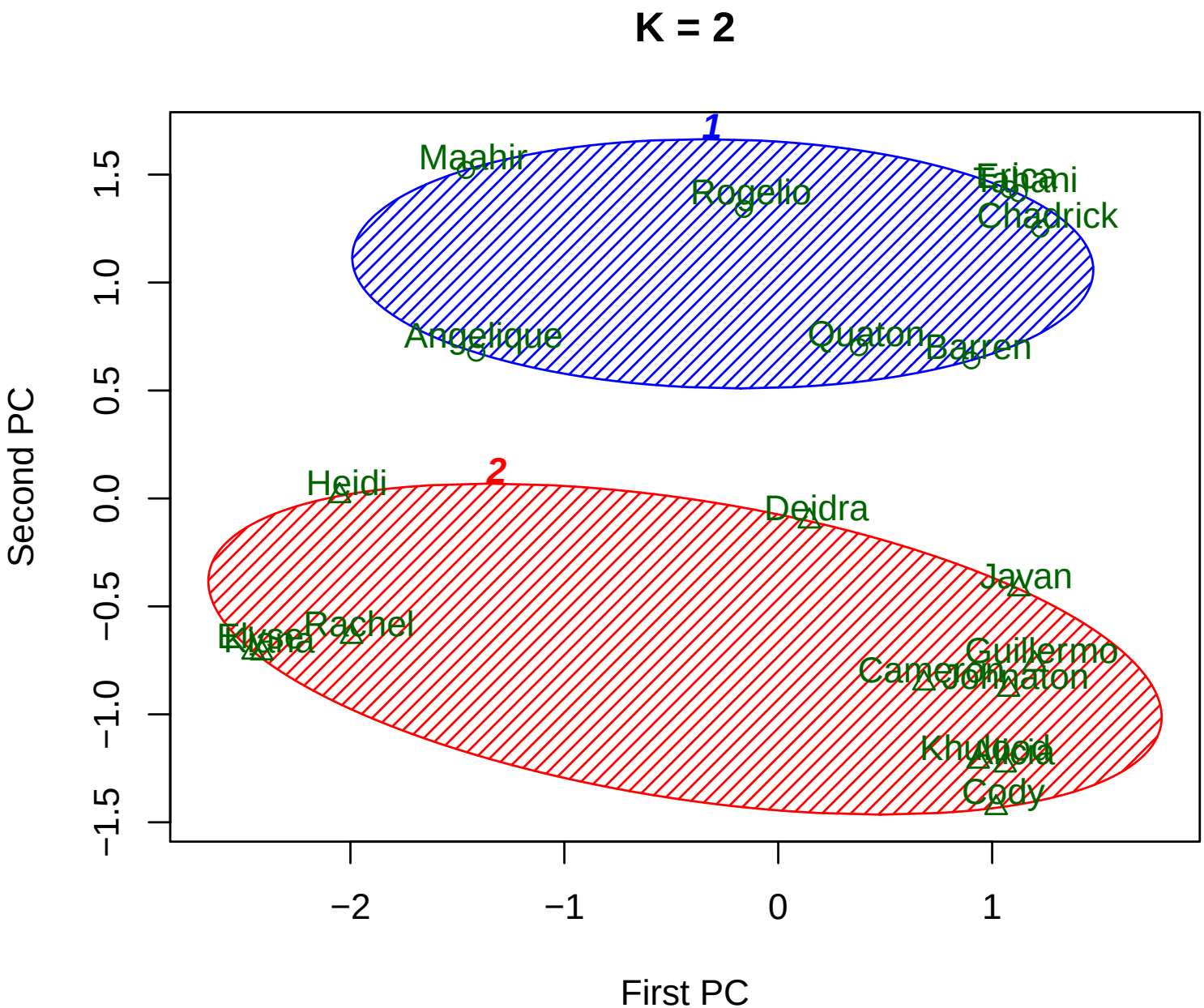
- Requires the analyst to designate the number of clusters desired k *a priori*.

- Standard algorithm:
  0. Initialize a set of k clusters.
  1. Assign each observation to the cluster whose mean is the least "distant" from it
  2. Calculate the new means as the centroids of the resulting clusters
  3. Repeat steps 1-2 until convergence.

k-means Clustering: Example ($k = 2$)

```
> KM2 <- kmeans(ds,2)
> KM2
K-means clustering with 2 clusters of sizes 7, 13

Cluster means:
        X       Y       Z
1 -0.7265 -0.9753 -0.6381
2  0.3912  0.5252  0.3436

Clustering vector:
Guillermo    Rachel    Deidra    Quaton    Alicia Angelique  Johnaton
        1         2         2         2         1         2         1
    Javan   Khulood      Cody   Cameron     Heidi    Maahir   Rogelio
        1         1         1         1         2         2         2
    Erica    Barren     Kiana     Elyse  Chadrick    Tahani
        2         2         2         2         2         2

Within cluster sum of squares by cluster:
[1]  0.9928 35.6954
 (between_SS / total_SS =  35.6 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"
[5] "tot.withinss" "betweenss"    "size"         "iter"
[9] "ifault"
```

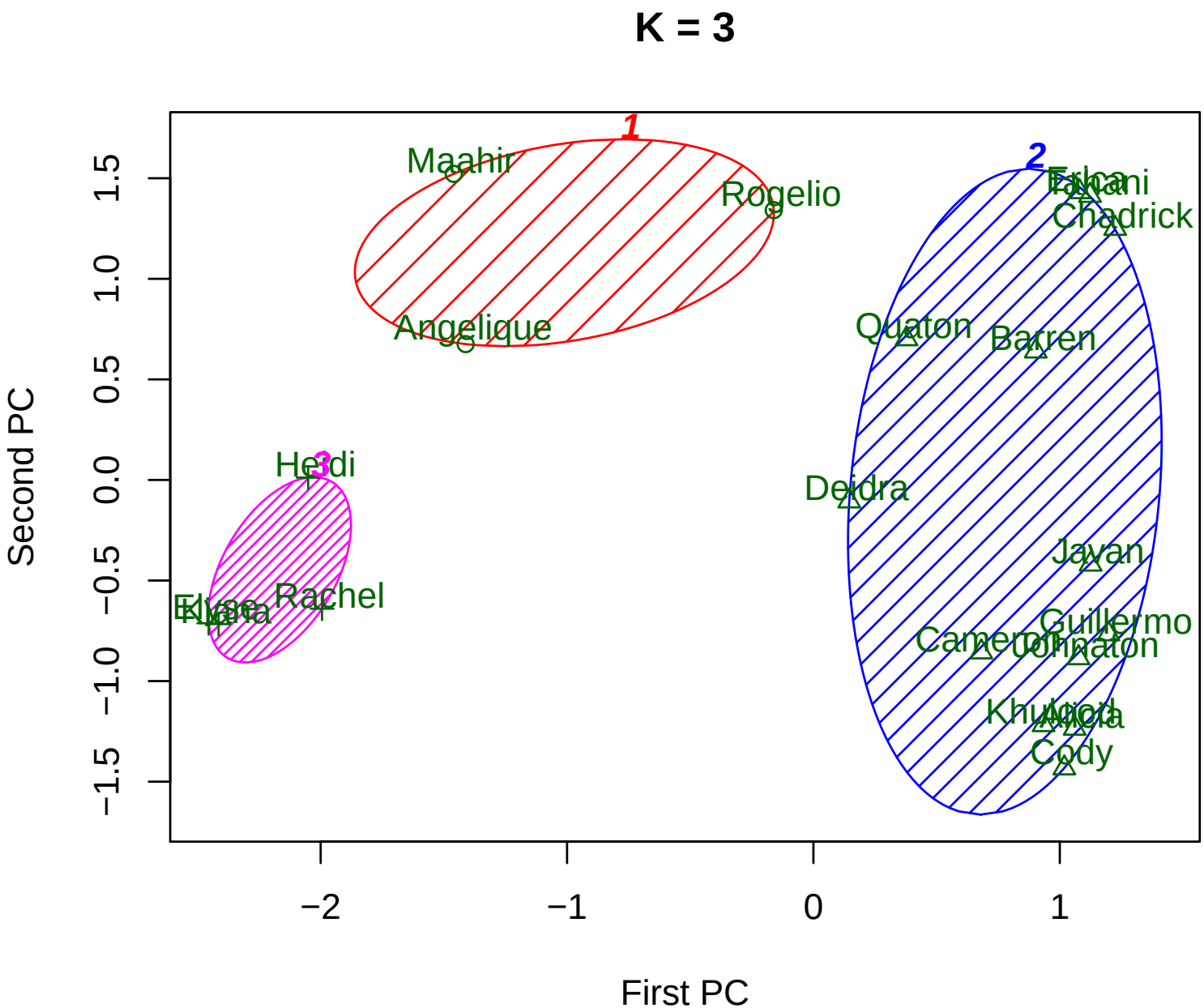
K-Means Clusters vs. Principal Components ($k = 2$)



k-means Clustering: Example ($k = 3$)

```
> KM3 <- kmeans(ds,3)
> KM3
K-means clustering with 3 clusters of sizes 7, 7, 6

Cluster means:
        X        Y       Z
1 -0.7265 -0.97528 -0.6381
2  0.9769 -0.03947 -0.6381
3 -0.2921  1.18387  1.4888

Clustering vector:
Guillermo    Rachel    Deidra    Quaton    Alicia Angelique  Johnaton
        1         3         2         2         1         3         1
    Javan   Khulood      Cody   Cameron     Heidi    Maahir   Rogelio
        1         1         1         1         3         3         2
    Erica    Barren     Kiana     Elyse  Chadrick    Tahani
        2         2         3         3         2         2

Within cluster sum of squares by cluster:
[1] 0.9928 5.2115 5.8304
 (between_SS / total_SS =  78.9 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"
[5] "tot.withinss" "betweenss"    "size"         "iter"
[9] "ifault"
```

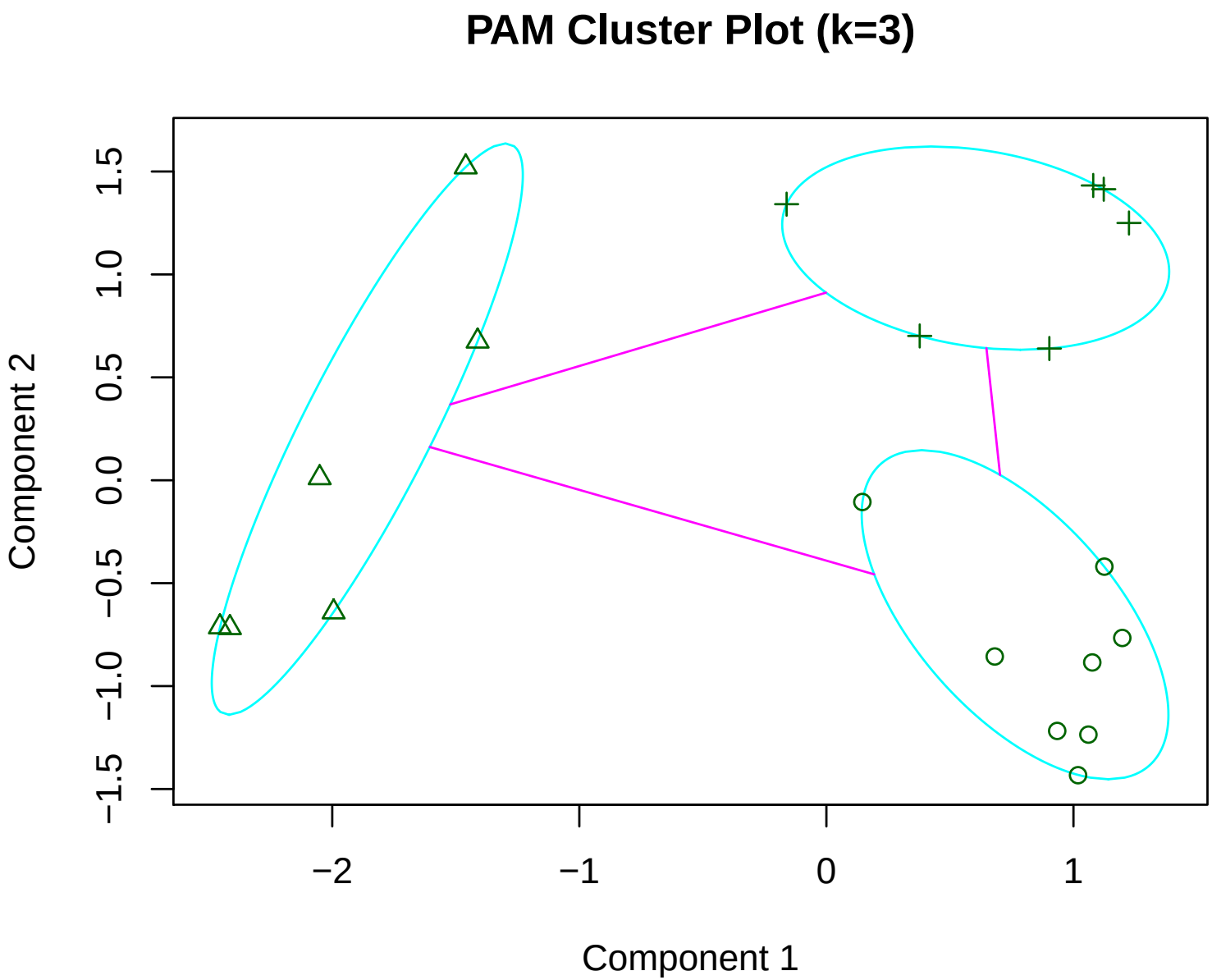
K-Means Clusters vs. Principal Components ($k = 3$)



Alternative: "Partitioning Around Medoids" ($k = 3$)

```
> PAM3 <- pam(ds,3)
> PAM3
Medoids:
         ID       X      Y       Z
Johnaton  7 -0.6226 -1.037 -0.6381
Heidi    12 -0.3315  1.297  1.4888
Erica    15  1.5634 -0.468 -0.6381
Clustering vector:
Guillermo    Rachel    Deidra    Quaton    Alicia Angelique  Johnaton
        1         2         1         3         1         2         1
    Javan   Khulood      Cody   Cameron     Heidi    Maahir   Rogelio
        1         1         1         1         2         2         3
    Erica    Barren     Kiana     Elyse  Chadrick    Tahani
        3         3         2         2         3         3
Objective function:
 build   swap
0.7054 0.6573

Available components:
 [1] "medoids"    "id.med"     "clustering" "objective"  "isolation"
 [6] "clusinfo"   "silinfo"    "diss"       "call"       "data"
```

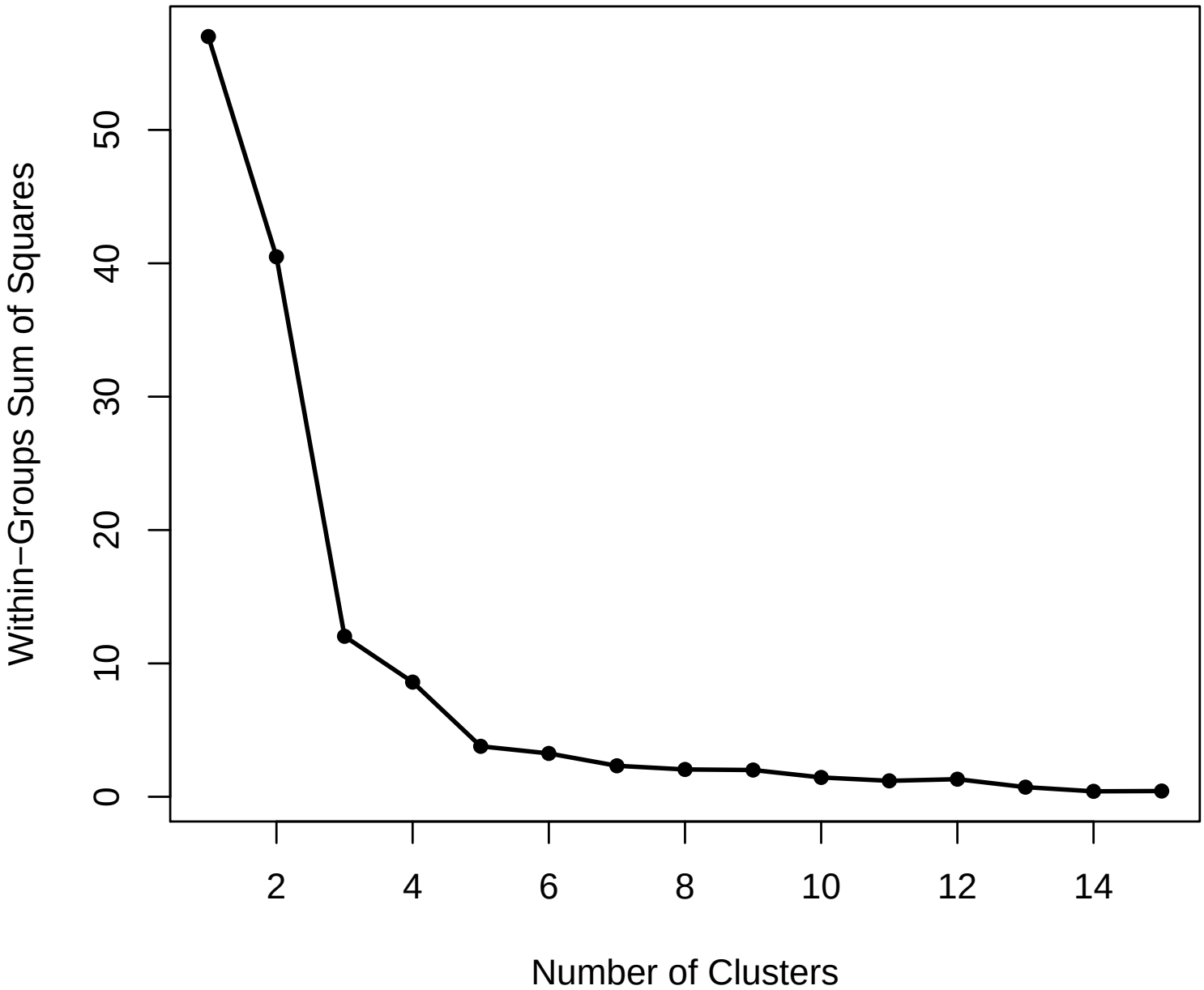
PAM, Illustrated



Practical k-Means: Choosing k

- Theory
- Scree plot of WCSS
- "Model-based" approaches

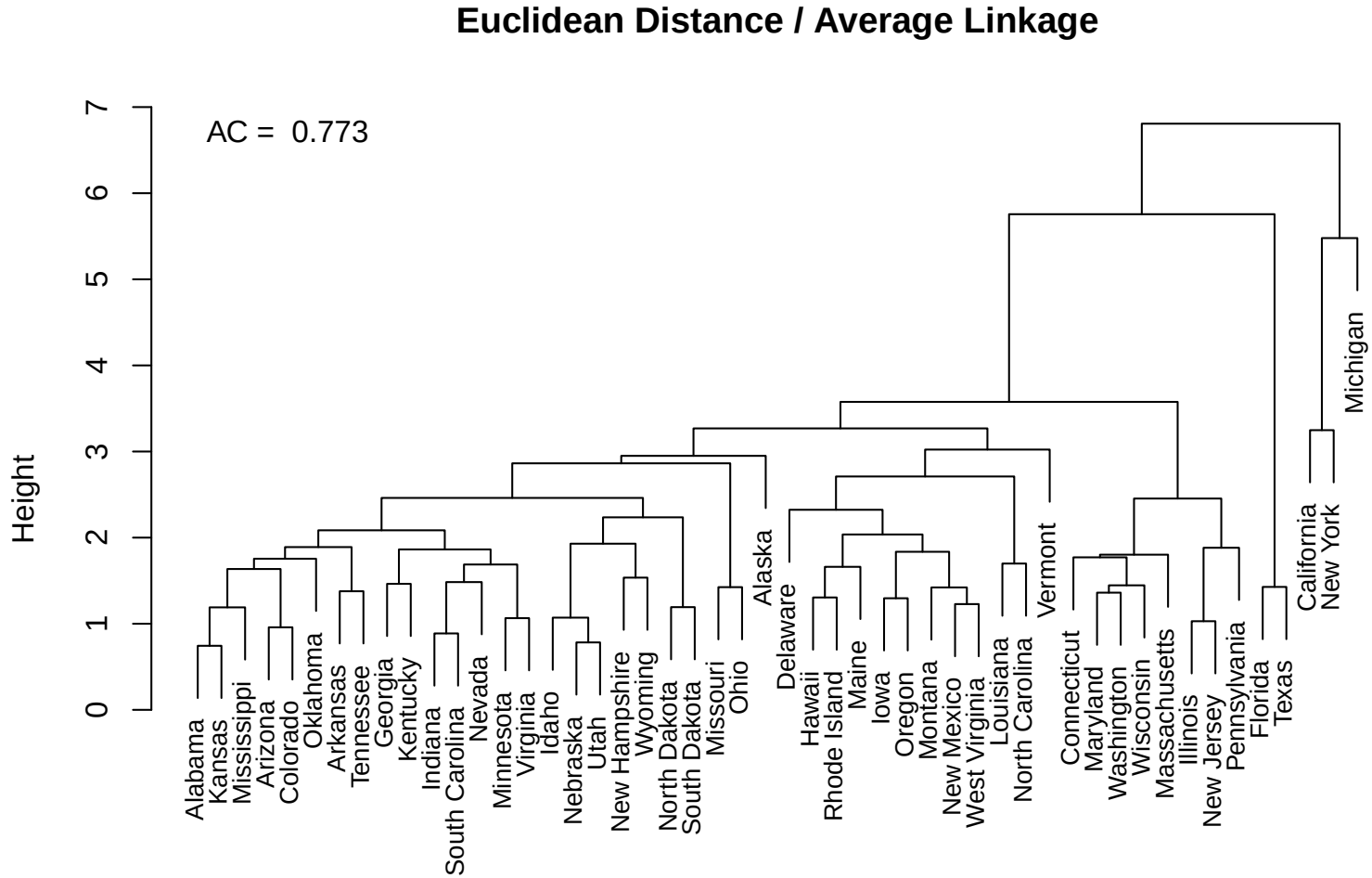
Choosing k: Scree Plot



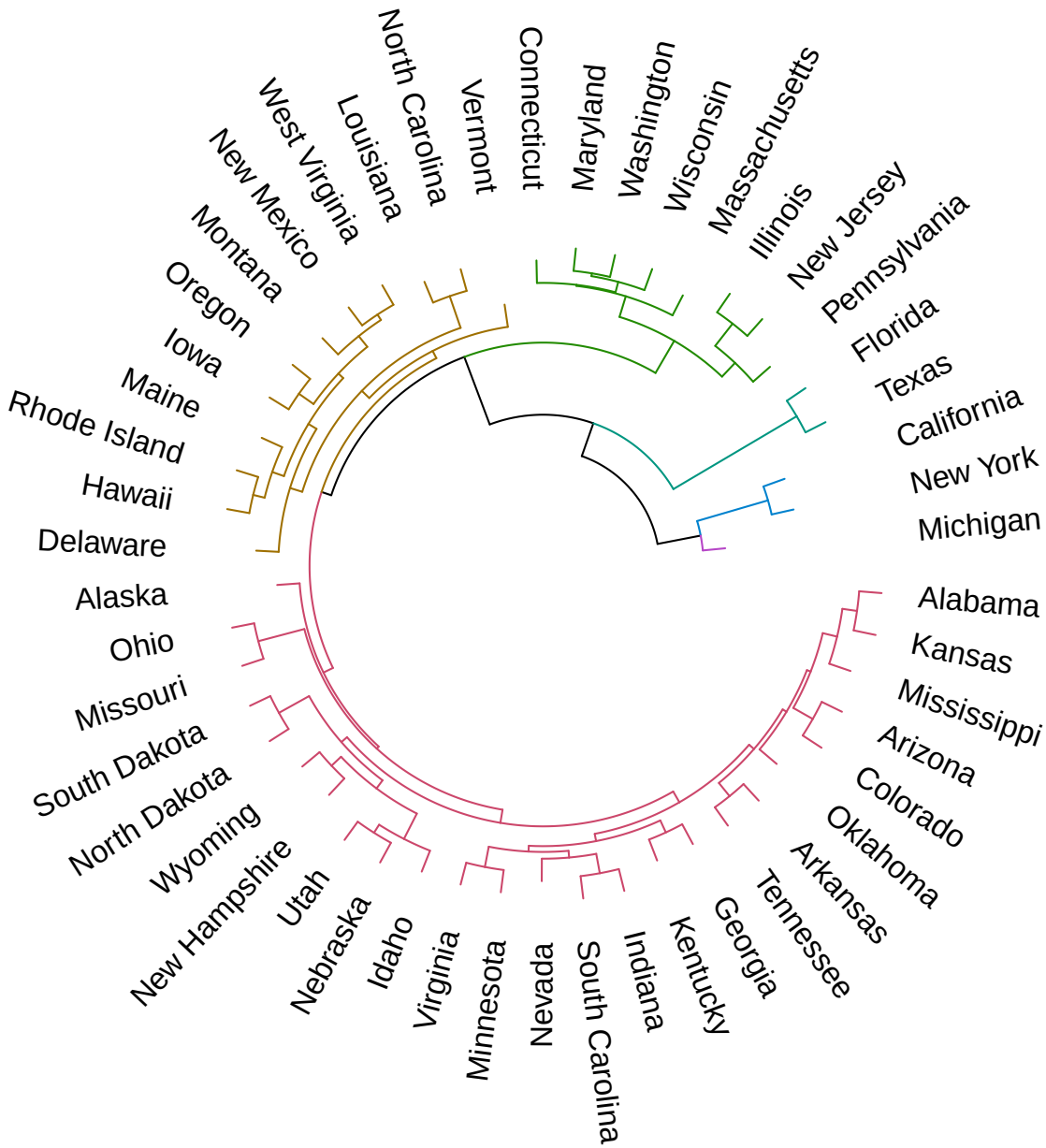
Real-Data Example: U.S. States

```
> url <- getURL("https://raw.githubusercontent.com/PrisonRodeo/MM-git/master/Data/States2005.csv")
> States <- read.csv(text = url)
>
> summary(States)
      statename       Year      CitizenIdeology GovernmentIdeology    govstaff
 Alabama   : 1   Min.   :2005   Min.   :28.2    Min.   :10.1       Min.   :  8.0
 Alaska    : 1   1st Qu.:2005   1st Qu.:43.5    1st Qu.:21.9       1st Qu.: 24.0
 Arizona   : 1   Median :2005   Median :53.1    Median :47.9       Median : 39.0
 Arkansas  : 1   Mean   :2005   Mean   :53.2    Mean   :49.9       Mean   : 59.1
 California: 1   3rd Qu.:2005   3rd Qu.:61.3    3rd Qu.:71.8       3rd Qu.: 69.5
 Colorado  : 1   Max.   :2005   Max.   :91.2    Max.   :92.0       Max.   :310.0
 (Other)   :44
   govsalary         legcomp         legsession         pop            lnGDP
 Min.   : 70000   Min.   :   200   Min.   : 25.0   Min.   :  501   Min.   :10.0
 1st Qu.: 95000   1st Qu.: 15876   1st Qu.: 45.0   1st Qu.: 1772   1st Qu.:11.0
 Median :112822   Median : 23696   Median : 67.5   Median : 4210   Median :11.9
 Mean   :115778   Mean   : 31932   Mean   : 79.0   Mean   : 5918   Mean   :11.9
 3rd Qu.:131326   3rd Qu.: 41709   3rd Qu.: 99.2   3rd Qu.: 6398   3rd Qu.:12.6
 Max.   :179000   Max.   :118600   Max.   :352.0   Max.   :36154   Max.   :14.3

> StS <- data.frame(scale(States[,3:10]))
> rownames(StS)<-States$statename
```

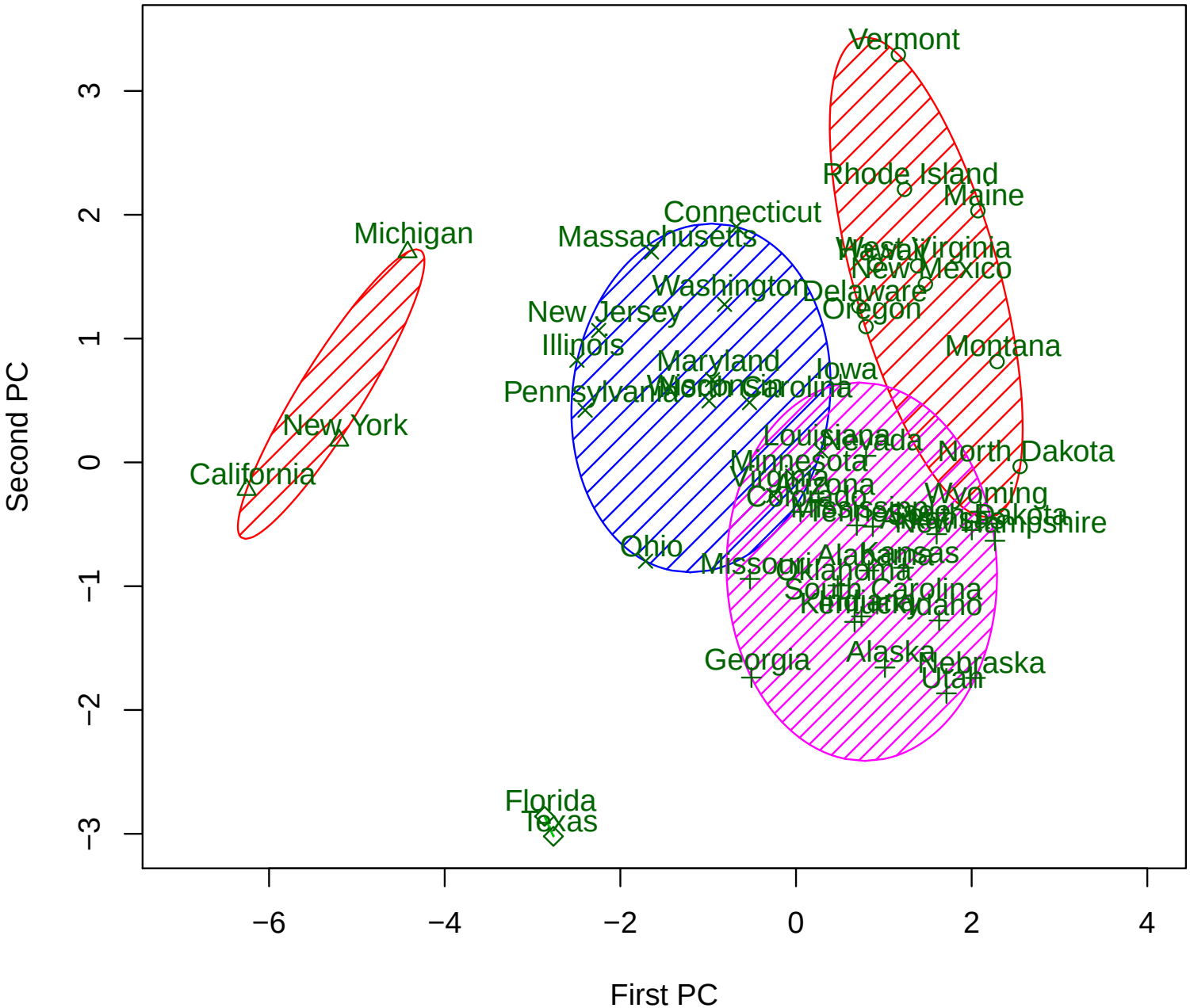
State Data: Dendrogram



State Data: Cooler Dendrogram



State Data: K-Means Results



Useful References

- Johnson, S.C. 1967. "Hierarchical Clustering Schemes." *Psychometrika* 32:241-254.

- Reynolds, A., Richards, G., de la Iglesia, B. and Rayward-Smith, V. 1992. "Clustering Rules: A Comparison of Partitioning and Hierarchical Clustering Algorithms." *Journal of Mathematical Modelling and Algorithms* 5:475-504.

- Kaufman, Leonard, and Peter J. Rousseeuw. 2005. *Finding Groups in Data: An Introduction to Cluster Analysis.* New York: Wiley.

- Hennig, Christian, Marina Meila, Fionn Murtagh, and Roberto Rocci, eds. 2015. *Handbook of Cluster Analysis*. New York: Chapman & Hall.

- Everitt, Brian S., Sabine Landau, Morven Leese, and Daniel Stahl. 2011. *Cluster Analysis*, 5th Ed. New York: Wiley.

- Kassambara, Alboukadel. 2017. *Practical Guide to Cluster Analysis in R.* Createspace.

Useful R Packages and Routines

- `hclust` and `kmeans` (in `stats`)
- `agnes` and `diana` and `pam` (in `cluster`)
- `amap` (alternative agglomerative and k-means clustering)
- `dendextend` (additional functionality for dendograms; e.g., comparisons)
- `mclust` (model-based clustering via MLE)
- `FactoClass` (combinations of factorial and clustering methods)

... and many more.

Useful Links

- The Cluster Analysis R Task View: `http://cran.cnr.berkeley.edu/web/views/Cluster.html`
- The Data Flair R Clustering tutorial: `https://data-flair.training/blogs/r-clustering-tutorial/`
- The `dendextend` vignette: `https://cran.r-project.org/web/packages/dendextend/vignettes/Cluster_Analysis.html`