PLSC 504

Principal Components Analysis, Factor Analysis, and Clustering

October 28, 2020

Measurement: Concepts

- Often: *data reduction* (many $\mathbf{X} \rightarrow$ one X)
- Classification *is* measurement (taxonomy and typology)
- Level and quality of measurement are distinct
- **All measurement implies theory**

Today's Plan

- Principal Components Analysis (+ biplots!)
- Factor Analysis
- Cluster Analysis

Some Basics

```
> X <- data.frame(X1=c(0,1,2),X2=c(6,5,3),X3=c(7,9,10))
> X
  X1 X2 X3
1  0  6  7
2  1  5  9
3  2  3 10

> CX <- sweep(X,2,colMeans(X),"-")  # "centered" X
> CX
  X1       X2      X3
1 -1  1.3333 -1.6667
2  0  0.3333  0.3333
3  1 -1.6667  1.3333
```

```
> Sigma <- cov(CX)
> Sigma
     X1     X2     X3
X1  1.0 -1.500  1.500
X2 -1.5  2.333 -2.167
X3  1.5 -2.167  2.333

> R <- cor(CX)
> R
       X1      X2      X3
X1  1.000 -0.9820  0.9820
X2 -0.982  1.0000 -0.9286
X3  0.982 -0.9286  1.0000
```

Eigenvalues and Eigenvectors

For the variance-covariance matrix Σ of (centered) $\mathbf{X}$, we can diagonalize:

$$\Sigma = \mathbf{VLV}'$$

where

- $\mathbf{V}$ is the matrix of *eigenvectors* ("principal axes"), and
- $\mathbf{L}$ is the (diagonal) matrix of *eigenvalues*.

Things:

- The sum of the eigenvalues equals the trace of Σ
- The product of the eigenvalues is $|\Sigma|$

Eigenvalues and Eigenvectors

```
> E <- eigen(Sigma)
> E
$values
[1] 5.5000000000 0.1666666666666667407 0.0000000000000001776

$vectors
        [,1]   [,2]    [,3]
[1,]  0.4264 0.0000  0.9045
[2,] -0.6396 0.7071  0.3015
[3,]  0.6396 0.7071 -0.3015

> L <- E$values
> V <- E$vectors
>
> sum(E$values)
[1] 5.667
> tr(Sigma)
[1] 5.667
```

Singular Value Decomposition

The *singular value decomposition* (SVD) of $\mathbf{X}$ is:

$$\mathbf{X} = \mathbf{USV}'$$

where $\mathbf{S}$ is the diagonal matrix of *singular values*, $\mathbf{U}$ is a unitary (orthogonal) matrix, and $\mathbf{V}$ is again the matrix of eigenvectors.

Note:

- Elements of $\mathbf{S}$ s_i are related to the eigenvalues v_i according to $v_i = s_i^2/(N-1)$.
- The *principal components* are equal to $\mathbf{US}$ ($\equiv \mathbf{XV}$).

SVD

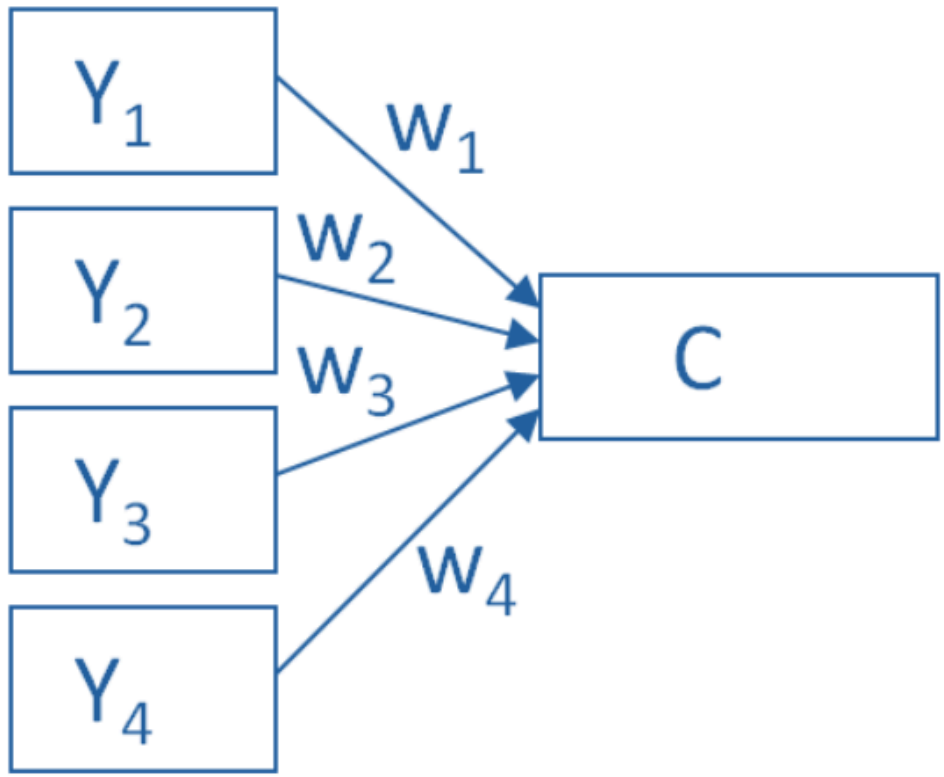
```
> SVD <- svd(CX)
> SVD
$d
[1] 3.3166247903553993659 0.5773502691896256200 0.0000000000000004209

$u
                         [,1]    [,2]   [,3]
[1,] -0.7071067811865470176  0.4082 0.5774
[2,]  0.0000000000000001665 -0.8165 0.5774
[3,]  0.7071067811865475727  0.4082 0.5774

$v
        [,1]        [,2]    [,3]
[1,]  0.4264  3.332e-17 -0.9045
[2,] -0.6396 -7.071e-01 -0.3015
[3,]  0.6396 -7.071e-01  0.3015

> S <- SVD$d
> U <- SVD$u
> otherV <- SVD$v
>
> # Eigenvalues:
>
> (S^2)/(2)
[1] 5.500e+00 1.667e-01 8.858e-32
```

Principal Components (PCA)

PCA is:

- an orthogonal transformation, that
- converts a set of variables $\underset{N \times K}{\mathbf{X}}$ into a set of K linearly-uncorrelated values, where
- the first principal component has the largest possible variance, and
- the second has the second-highest (subject to orthogonality),
- etc.

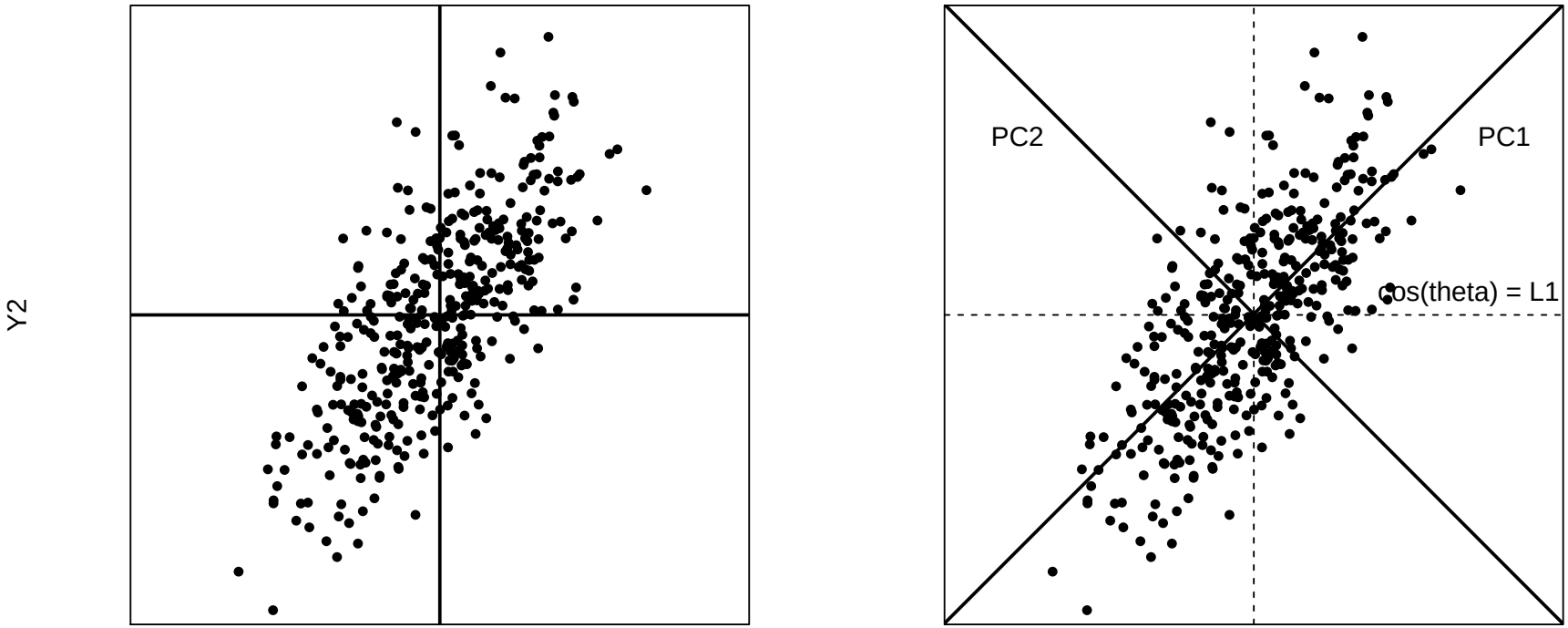
PCA, Conceptually



$$C = w_1 Y_1 + w_2 Y_2 + w_3 Y_3 + w_4 Y_4$$

(Source)

PCA Intuition



"(Principal components) can be considered as a rotation of original variable coordinate system to new (orthogonal) axes... such that the new axes coincide with the directions of maximum variation in the original observations." (Campbell and Atchley 1981)

```
> princomp(CX) # via eigenvalues
Call:
princomp(x = CX)

Standard deviations:
      Comp.1       Comp.2       Comp.3
1.9148542155 0.3333333333 0.0000000365

 3  variables and  3 observations.

> prcomp(CX) # via SVD
Standard deviations:
[1] 2.345e+00 4.082e-01 6.833e-18

Rotation:
       PC1         PC2     PC3
X1  0.4264  1.071e-17  0.9045
X2 -0.6396 -7.071e-01  0.3015
X3  0.6396 -7.071e-01 -0.3015

> otherV # from -svd-
        [,1]       [,2]    [,3]
[1,]  0.4264  3.332e-17 -0.9045
[2,] -0.6396 -7.071e-01 -0.3015
[3,]  0.6396 -7.071e-01  0.3015
```

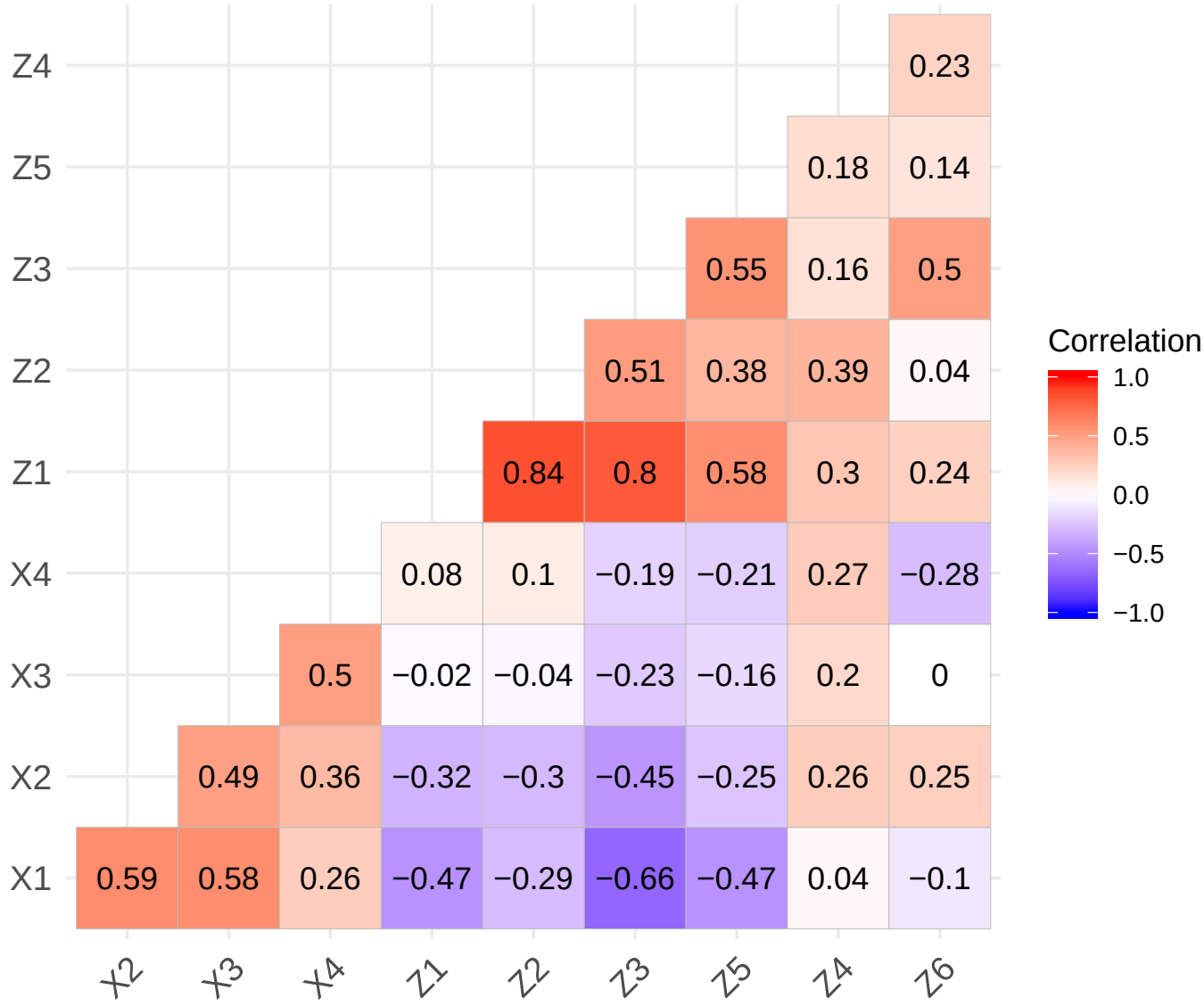
PCA Steps

- *Extract* the principal components
- *Interpret* the components...
- Consider *rotation*
- Choosing the *number of components* (dimensions)
- Generating *scores*

PCA: A Simulation Example

```
> N <- 20
> set.seed(7222009)
> Name <- randomNames(N, which.names="first")
> Z <- rnorm(N)
> Z1 <- Z + 0.2*rnorm(N)
> Z2 <- Z + 0.5*rnorm(N)
> Z3 <- Z + 1*rnorm(N)
> Z4 <- Z + 1.5*rnorm(N)
> Z5 <- Z + 2*rnorm(N)
> Z6 <- Z + 3*rnorm(N)
>
> X <- rnorm(N)
> X1 <- X + rnorm(N)
> X2 <- X + rnorm(N)
> X3 <- X + rt(N,5)
> X4 <- X + rt(N,5)
>
> df <- data.frame(Z1,Z2,Z3,Z4,Z5,Z6,X1,X2,X3,X4)
> rownames(df)<-Name
```

Correlations, Envisioned



Friendly PCA using `principal`

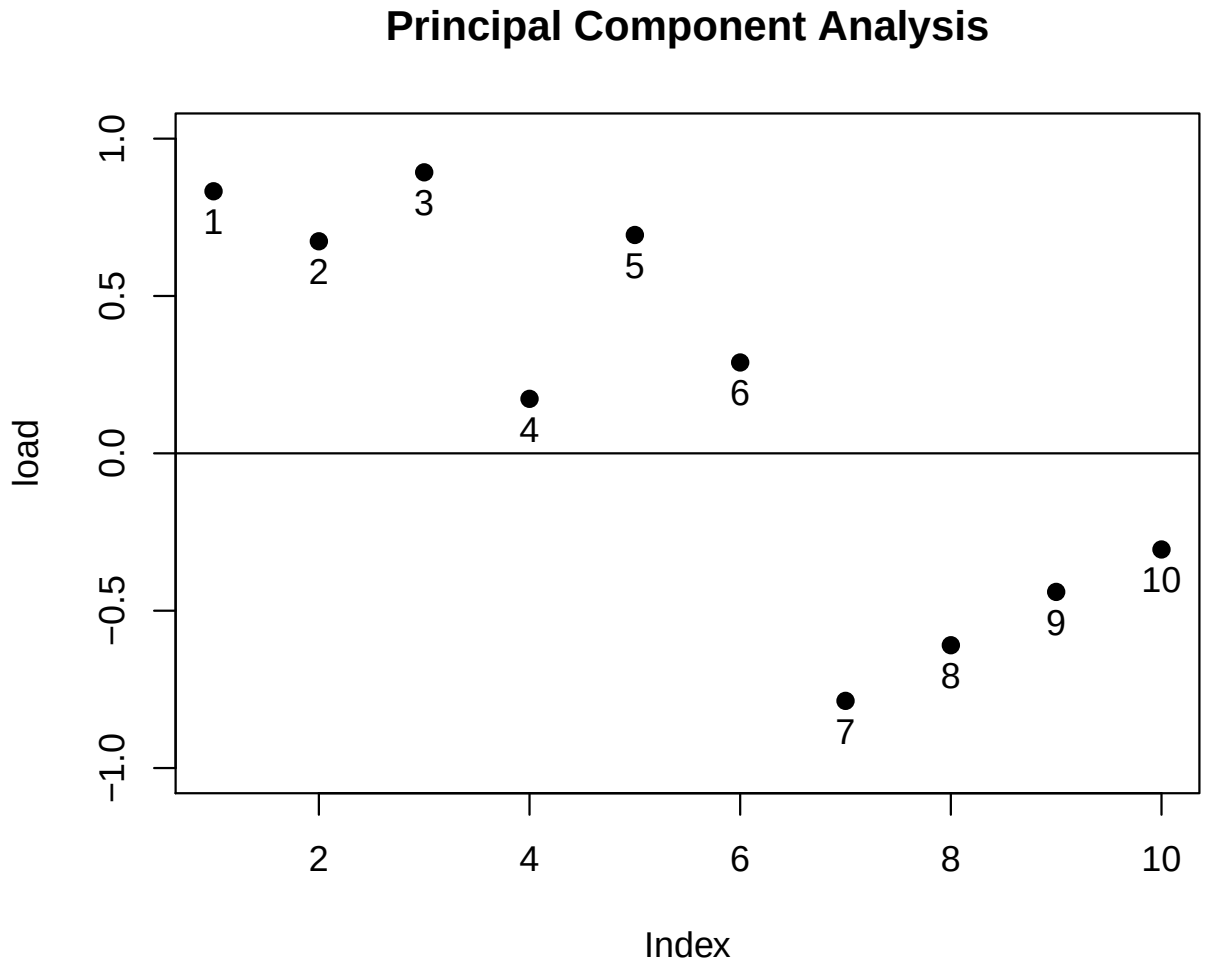
```
> PCSim1 <- principal(df, nfactors=1,rotate="none")
> PCSim1
Principal Components Analysis
Call: principal(r = df, nfactors = 1, rotate = "none")
Standardized loadings (pattern matrix) based upon correlation matrix
     PC1    h2   u2 com
Z1  0.83 0.694 0.31   1
Z2  0.67 0.454 0.55   1
Z3  0.89 0.798 0.20   1
Z4  0.17 0.030 0.97   1
Z5  0.69 0.482 0.52   1
Z6  0.29 0.083 0.92   1
X1 -0.79 0.618 0.38   1
X2 -0.61 0.372 0.63   1
X3 -0.44 0.194 0.81   1
X4 -0.31 0.093 0.91   1

                PC1
SS loadings    3.82
Proportion Var 0.38

Mean item complexity =  1
Test of the hypothesis that 1 component is sufficient.

The root mean square of the residuals (RMSR) is  0.2
 with the empirical chi square  72.9  with prob <  0.00018

Fit based upon off diagonal values = 0.71
```

Let's break that down...

- It's a PCA, where we're extracting the first principal component (`nfactors = 1`)
- No rotation (`rotate = "none"`)
- `PC1` are the "loadings" of each variable on the first principal component (think of these as the w_k in the conceptual figure)
- `h2` are *communalities*; the sums of the squared loadings (so, here, $\texttt{PC1}^2$)
- `u2` is *uniqueness*; simply $1 - \texttt{h2}$
- `SS Loadings` is the value(s) of the principal component(s)
- `Proportion Var` is the proportion of the total variance in $\mathbf{X}$ that that principal component accounts for
- The model fit statistic suggests that the one-component model doesn't fit the data very well (we can reject the hypothesis that one component is sufficient)

Minimalist PCA Plot

```
> plot(PCSim1,ylim=c(-1,1))
```



PCA Scores

```
> PCSim1$scores

               PC1
Guillermo -2.11824
Rachel     0.78544
Deidra     0.63716
Quaton    -0.92891
Alicia    -0.33762
Angelique  1.10640
Johnaton  -0.49378
Javan      0.23606
Khulood    1.06142
Cody      -0.07695
Cameron   -0.02655
Heidi      1.41409
Maahir     1.57304
Rogelio   -0.15324
Erica     -0.11558
Barren    -1.57311
Kiana      1.04688
Elyse     -1.19026
Chadrick  -0.41816
Tahani    -0.42809
```

PCA with nfactors = 2

```
> PCSim2 <- principal(df, nfactors=2,rotate="none")
> PCSim2
Principal Components Analysis
Call: principal(r = df, nfactors = 2, rotate = "none")
Standardized loadings (pattern matrix) based upon correlation matrix
     PC1  PC2   h2   u2 com
Z1  0.83 0.44 0.89 0.11 1.5
Z2  0.67 0.45 0.66 0.34 1.8
Z3  0.89 0.13 0.81 0.19 1.0
Z4  0.17 0.71 0.53 0.47 1.1
Z5  0.69 0.11 0.49 0.51 1.1
Z6  0.29 0.24 0.14 0.86 1.9
X1 -0.79 0.32 0.72 0.28 1.3
X2 -0.61 0.52 0.64 0.36 1.9
X3 -0.44 0.68 0.65 0.35 1.7
X4 -0.31 0.63 0.49 0.51 1.4

                       PC1  PC2
SS loadings           3.82 2.21
Proportion Var        0.38 0.22
Cumulative Var        0.38 0.60
Proportion Explained  0.63 0.37
Cumulative Proportion 0.63 1.00

Mean item complexity =  1.5
Test of the hypothesis that 2 components are sufficient.

The root mean square of the residuals (RMSR) is  0.12
 with the empirical chi square  25.8  with prob <  0.47

Fit based upon off diagonal values = 0.9
```

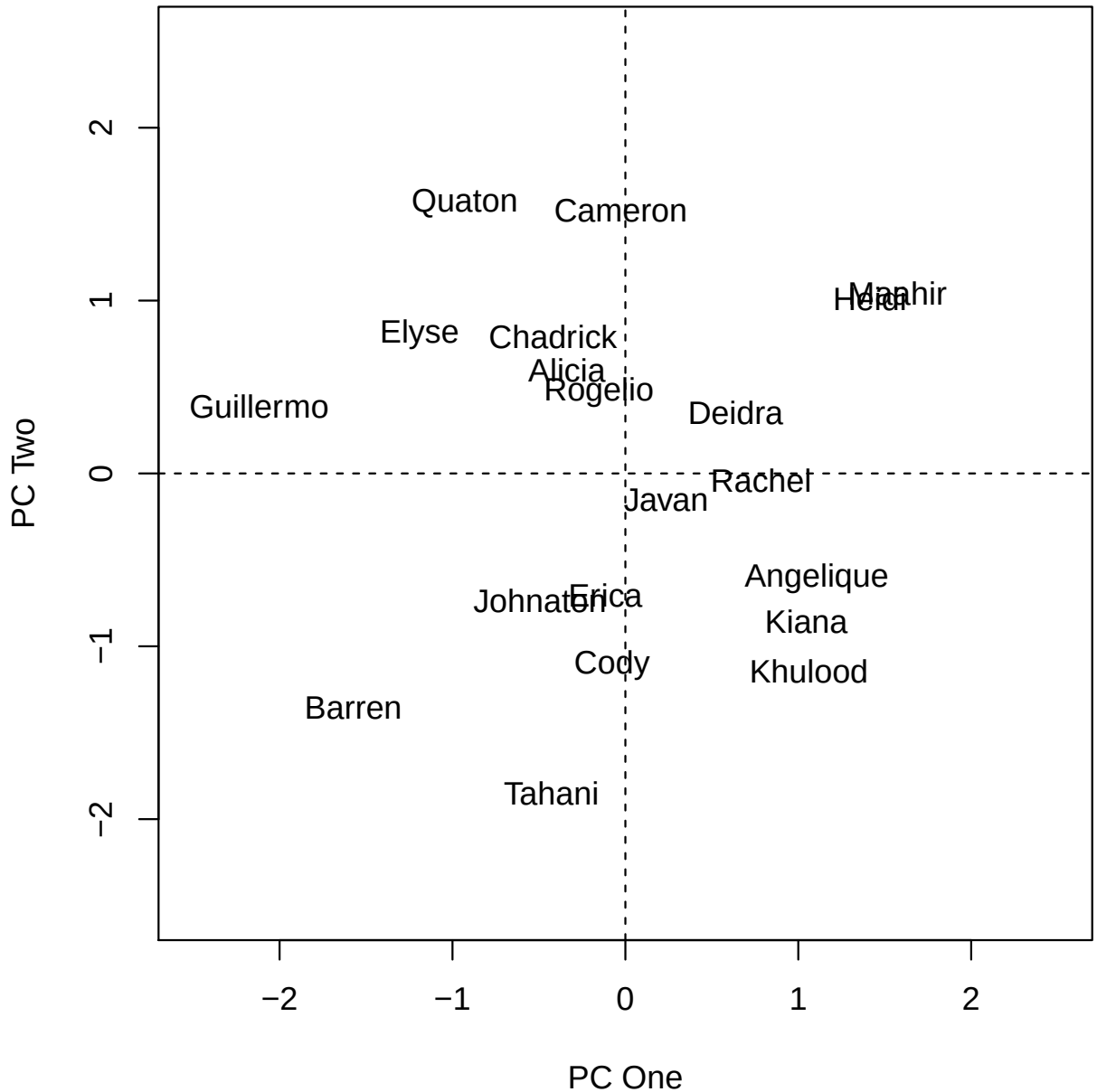
Let's break that down again...

- It's a PCA, where now we're extracting the first two principal components (`nfactors = 2`)
- No rotation (`rotate = "none"`)
- `PC1`, `PC2`, `h2`, and `u2` are the same as above
- `com` is the *complexity* c_k of each measure; $c_k = \frac{(\sum PC_k^2)^2}{\sum PC_k^4}$
- `SS Loadings` are again the value(s) of the principal component(s)
- There are now both total and cumulative variance explained statistics
- The model fit statistic now suggests that the model fits well (we cannot reject the hypothesis that two components are sufficient)

Scores, Redux

```
> PCSim2$scores
                PC1     PC2
Guillermo -2.11824  0.3897
Rachel     0.78544 -0.0387
Deidra     0.63716  0.3501
Quaton    -0.92891  1.5769
Alicia    -0.33762  0.5989
Angelique  1.10640 -0.6102
Johnaton  -0.49378 -0.7382
Javan      0.23606 -0.1504
Khulood    1.06142 -1.1449
Cody      -0.07695 -1.1076
Cameron   -0.02655  1.5239
Heidi      1.41409  1.0112
Maahir     1.57304  1.0410
Rogelio   -0.15324  0.4666
Erica     -0.11558 -0.7050
Barren    -1.57311 -1.3553
Kiana      1.04688 -0.8571
Elyse     -1.19026  0.8022
Chadrick  -0.41816  0.7941
Tahani    -0.42809 -1.8473
```

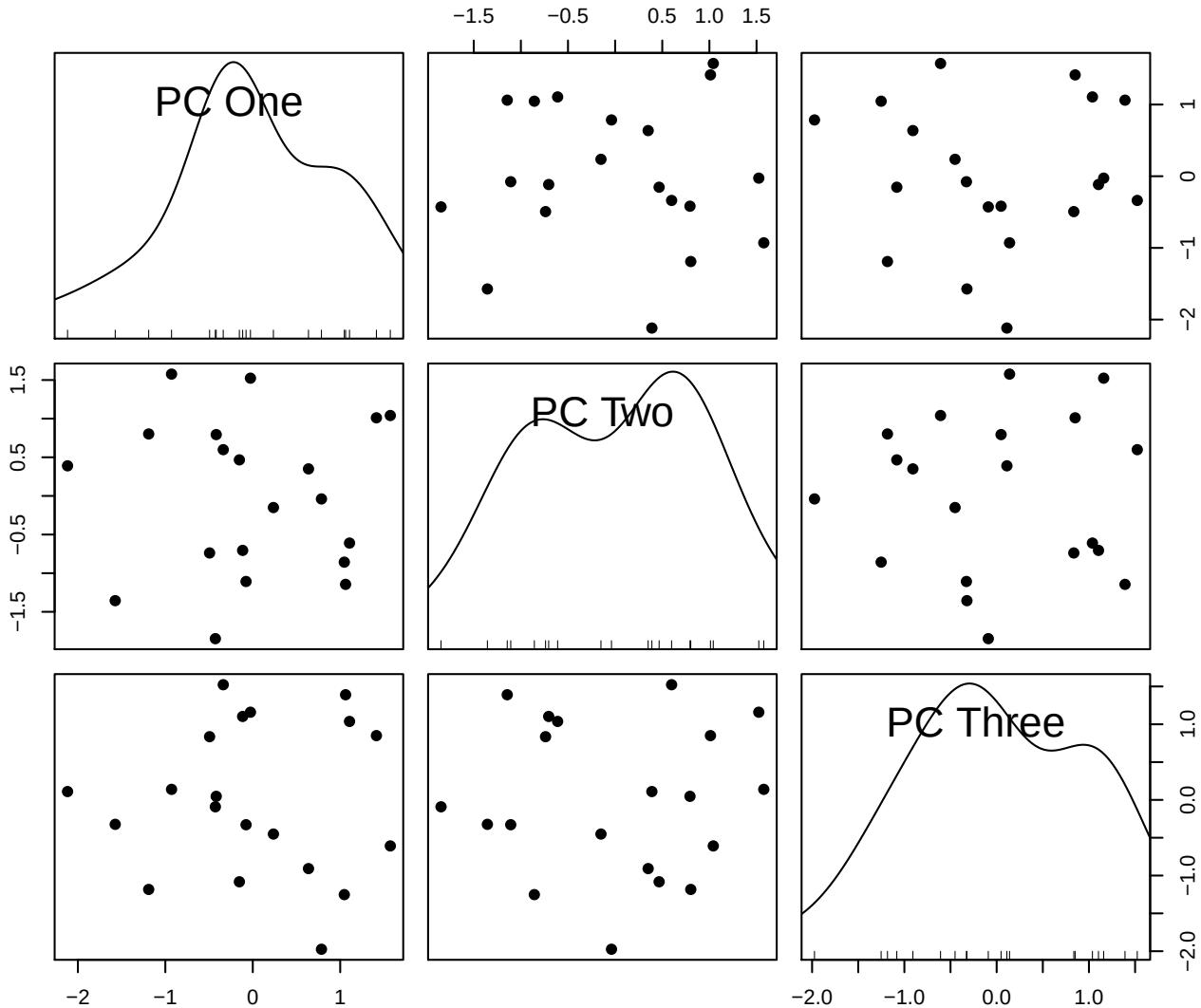
PCA Scores


Quaton
Cameron
Manhir
Heidi
Elyse
Chadrick
Alicia
Rogelio
Guillermo
Deidra
Rachel
Javan
Angelique
Johnatan
Erica
Kiana
Cody
Khulood
Barren
Tahani
PC Two
PC One
2
1
0
−1
−2
−2
−1
0
1
2

PCA with `nfactors = 3`

```
> PCSim3 <- principal(df, nfactors=3,rotate="none")
> PCSim3
Principal Components Analysis
Call: principal(r = df, nfactors = 3, rotate = "none")
Standardized loadings (pattern matrix) based upon correlation matrix
     PC1  PC2   PC3   h2   u2 com
Z1  0.83 0.44 -0.15 0.91 0.09 1.6
Z2  0.67 0.45 -0.33 0.77 0.23 2.3
Z3  0.89 0.13  0.19 0.85 0.15 1.1
Z4  0.17 0.71  0.11 0.54 0.46 1.2
Z5  0.69 0.11  0.05 0.50 0.50 1.1
Z6  0.29 0.24  0.88 0.91 0.09 1.4
X1 -0.79 0.32  0.07 0.73 0.27 1.3
X2 -0.61 0.52  0.40 0.80 0.20 2.7
X3 -0.44 0.68 -0.05 0.65 0.35 1.7
X4 -0.31 0.63 -0.48 0.72 0.28 2.4

                       PC1  PC2  PC3
SS loadings           3.82 2.21 1.35
Proportion Var        0.38 0.22 0.14
Cumulative Var        0.38 0.60 0.74
Proportion Explained  0.52 0.30 0.18
Cumulative Proportion 0.52 0.82 1.00

Mean item complexity =  1.7
Test of the hypothesis that 3 components are sufficient.

The root mean square of the residuals (RMSR) is  0.08
 with the empirical chi square  11.12  with prob <  0.89

Fit based upon off diagonal values = 0.96
```

PCA Scores, Again



Biplots!

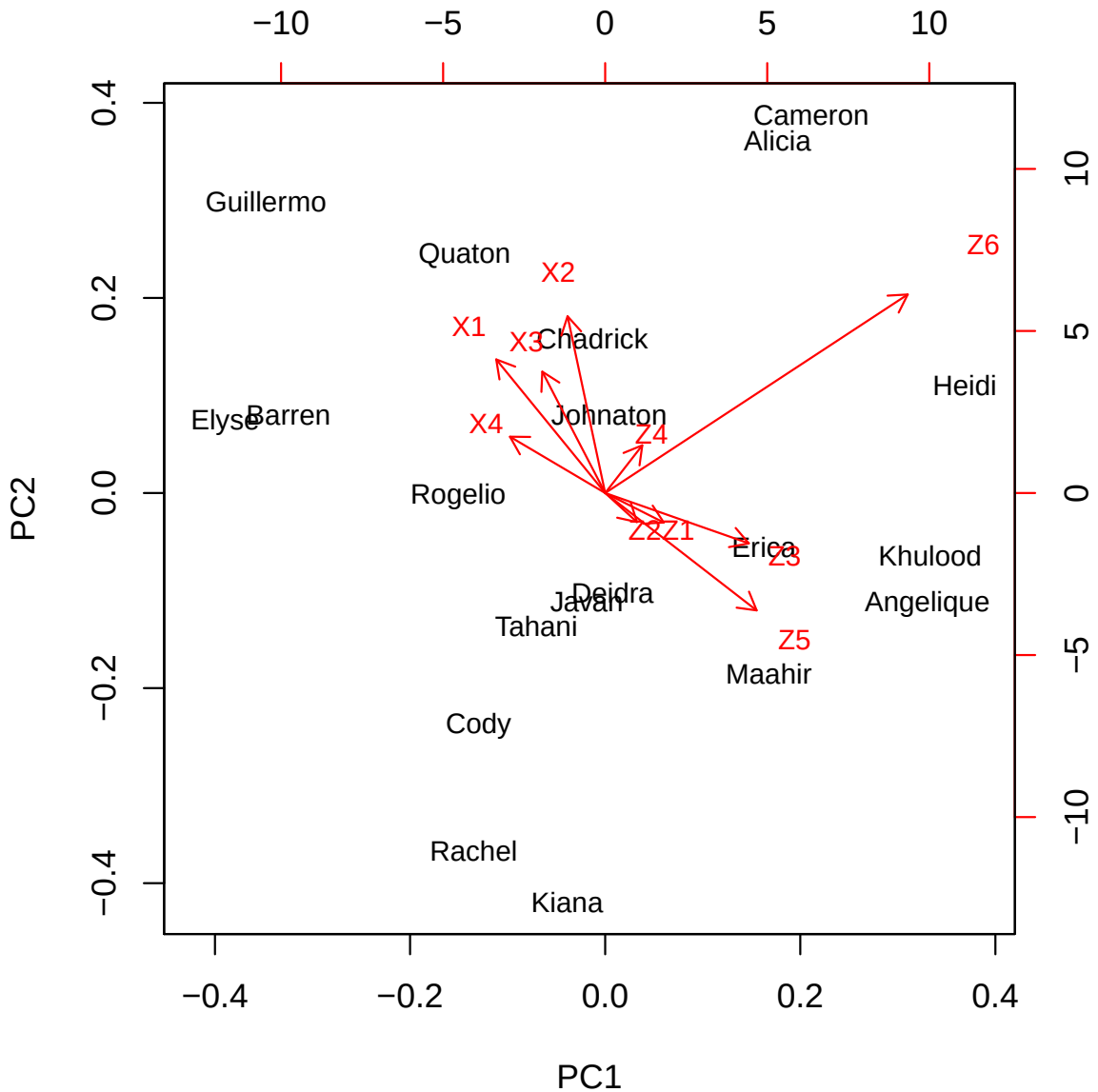
A *biplot* is a graphical representation of a two-axis PCA.

- It plots both loadings (of variables) and scores (of observations)
- It represents the former as vectors from the origin, and the latter as points in the (transformed) space
- Interpretation:
    - Angles between item vectors represent degrees of correlation/covariance
    - Distances between points reflect dissimilarities between those observations
- Details are in Gower and Hand (1996) and Jacoby (1998, Chapter 7)

Biplot Basics (Simulation Data)

```
> foo<-prcomp(df)

> foo$rotation[,1:2]
        PC1      PC2
Z1  0.14329 -0.08291
Z2  0.07769 -0.08154
Z3  0.35128 -0.14139
Z4  0.09075  0.13402
Z5  0.37041 -0.32978
Z6  0.73986  0.55782
X1 -0.26633  0.37528
X2 -0.09196  0.49655
X3 -0.15372  0.34087
X4 -0.23278  0.15817
```

A Biplot...

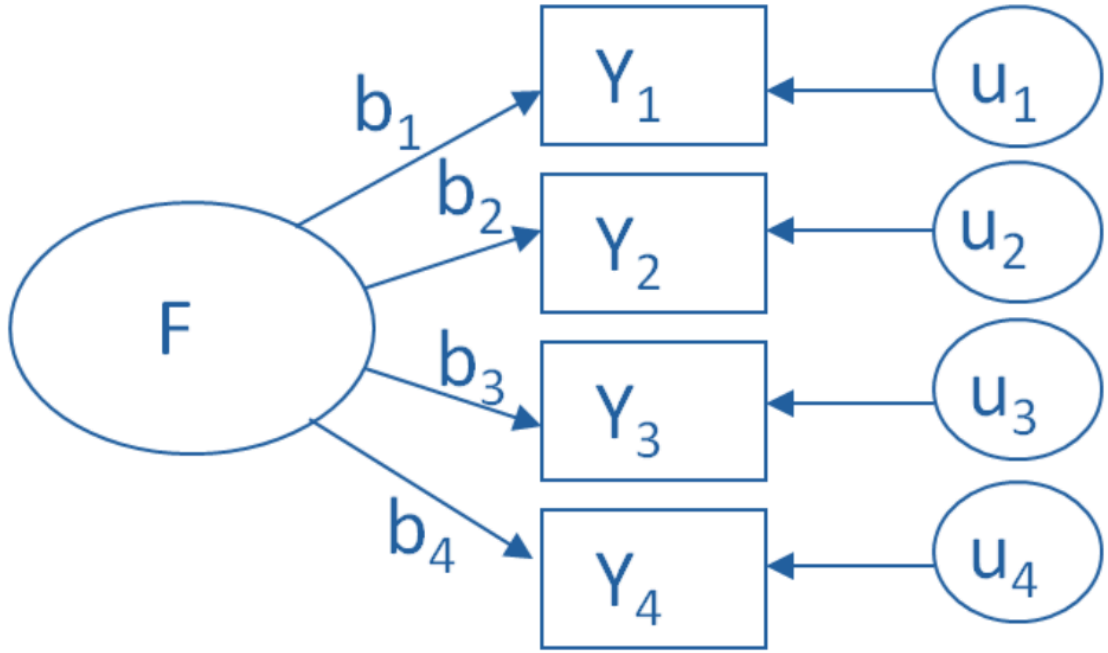

−10
−5
0
5
10
0.4
0.2
0.0
−0.2
−0.4
PC2
PC1
10
5
0
−5
−10
Cameron
Alicia
Guillermo
Quaton
X2
X1
X3
Chadrick
Z6
Heidi
Elyse
Barren
X4
Johnaton
Z4
Rogelio
Z2
Z1
Erica
Z3
Khulood
Deidra
Javan
Angelique
Tahani
Z5
Maahir
Cody
Rachel
Kiana

(Exploratory) Factor Analysis

Factor analysis (FA) is a model for the measurement of a latent variable using manifest / observable indicators.

- Observable indicators are manifestations of one or more latent / unobservable *factors*
- Extant indicators are differentially caused by the latent factor(s), and are observed with error
- The goal of FA is to derive measures of the latent factor from the observed data, by estimating factor *loadings* (associations between latent factors and observable variables)

Factor Analysis, Conceptually



$$
\begin{aligned}
Y_1 &= b_1 F + u_1 \\
Y_2 &= b_2 F + u_2 \\
Y_3 &= b_3 F + u_3 \\
Y_4 &= b_4 F + u_4
\end{aligned}
$$

(Source)

Formally:

$$\mathbf{Y} = \Lambda\mathbf{F} + \mathbf{U}$$

This implies that the observed covariance matrix Σ can be written:

$$\Sigma = \Lambda\Lambda' + \Psi$$

where

$$\Psi = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_K^2 \end{bmatrix}$$

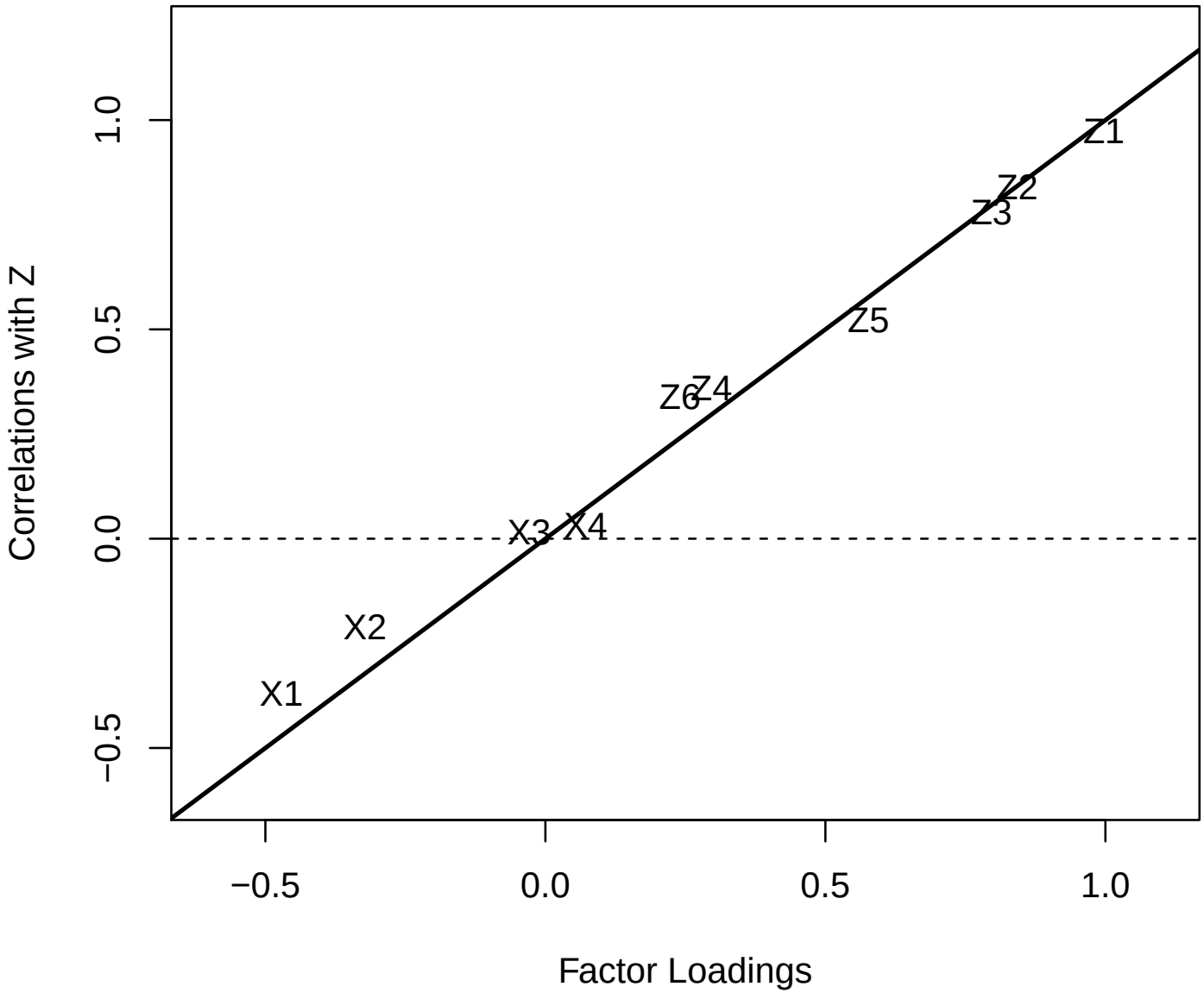
Practical Factor Analysis

- Choose the *number of factors* (dimensions)
- Consider *rotation*
- *Estimate* the factor loadings $\hat{\Lambda}$
- *Interpret* the factors...
- Generate *factor scores*

Factor Analysis Simulation

```
> FASim1 <- factanal(df,factors=1,scores="regression",
+                    rotation="none")
> print(FASim1,cutoff=0)

Call:
factanal(x = df, factors = 1, scores = "regression", rotation = "none")

Uniquenesses:
   Z1    Z2    Z3    Z4    Z5    Z6    X1    X2    X3    X4
0.005 0.290 0.365 0.912 0.667 0.942 0.778 0.896 0.999 0.995

Loadings:
   Factor1
Z1  0.998
Z2  0.843
Z3  0.797
Z4  0.297
Z5  0.577
Z6  0.240
X1 -0.471
X2 -0.322
X3 -0.029
X4  0.072

               Factor1
SS loadings      3.150
Proportion Var   0.315

Test of the hypothesis that 1 factor is sufficient.
The chi square statistic is 57.3 on 35 degrees of freedom.
The p-value is 0.0101
```

Factor Loadings vs. Correlations with Z



Factor Analysis Simulation: Two Factors

```
> FASim2 <- factanal(df,factors=2,scores="regression",
+                    rotation="none")
> print(FASim2,cutoff=0)

Call:
factanal(x = df, factors = 2, scores = "regression", rotation = "none")

Uniquenesses:
   Z1    Z2    Z3    Z4    Z5    Z6    X1    X2    X3    X4
0.005 0.276 0.226 0.810 0.608 0.938 0.271 0.525 0.444 0.667

Loadings:
   Factor1 Factor2
Z1  0.997   0.013
Z2  0.841   0.129
Z3  0.801  -0.364
Z4  0.295   0.320
Z5  0.579  -0.238
Z6  0.242  -0.060
X1 -0.478   0.707
X2 -0.327   0.607
X3 -0.034   0.745
X4  0.068   0.573

               Factor1 Factor2
SS loadings      3.166   2.064
Proportion Var   0.317   0.206
Cumulative Var   0.317   0.523

Test of the hypothesis that 2 factors are sufficient.
The chi square statistic is 31.42 on 26 degrees of freedom.
The p-value is 0.213
```

Factor Analysis Simulation: Three Factors

```
> FASim3 <- factanal(df,factors=3,scores="regression",
+                    rotation="none")
> print(FASim3,cutoff=0)

Call:
factanal(x = df, factors = 3, scores = "regression", rotation = "none")

Uniquenesses:
   Z1    Z2    Z3    Z4    Z5    Z6    X1    X2    X3    X4
0.005 0.246 0.111 0.758 0.621 0.005 0.312 0.276 0.518 0.582

Loadings:
   Factor1 Factor2 Factor3
Z1  0.809   0.021   0.583
Z2  0.582   0.136   0.629
Z3  0.836  -0.379   0.216
Z4  0.334   0.359   0.036
Z5  0.475  -0.207   0.333
Z6  0.761   0.002  -0.645
X1 -0.382   0.674  -0.297
X2 -0.071   0.704  -0.473
X3 -0.024   0.693  -0.032
X4 -0.125   0.567   0.285

                Factor1 Factor2 Factor3
SS loadings       2.775   2.086   1.706
Proportion Var    0.277   0.209   0.171
Cumulative Var    0.277   0.486   0.657

Test of the hypothesis that 3 factors are sufficient.
The chi square statistic is 15.13 on 18 degrees of freedom.
The p-value is 0.653
```

Real Data: ANES 2016 Feeling Thermometers

```
> describe(Therms,range=FALSE)
                           vars    n  mean    sd  skew kurtosis   se
Asian-Americans               1 2387 70.17 20.20 -0.38     0.02 0.41
Hispanics                     2 2387 69.35 20.91 -0.41     0.01 0.43
Blacks                        3 2387 69.00 21.19 -0.35    -0.24 0.43
Illegal Immigrants            4 2387 42.54 27.31  0.13    -0.71 0.56
Whites                        5 2387 71.63 19.40 -0.46     0.08 0.40
Dem. Pres. Candidate          6 2387 44.12 34.91  0.12    -1.42 0.71
GOP Pres. Candidate           7 2387 40.53 35.65  0.23    -1.43 0.73
Libertarian Pres. Candidate   8 2387 43.61 19.92 -0.58     0.25 0.41
Green Pres. Candidate         9 2387 43.20 20.87 -0.54     0.22 0.43
Dem. VP                      10 2387 48.24 25.91 -0.22    -0.44 0.53
GOP VP                       11 2387 49.59 33.42 -0.10    -1.21 0.68
John Roberts                 12 2387 53.75 18.39 -0.41     1.44 0.38
Pope Francis                 13 2387 69.55 25.17 -0.73     0.14 0.52
Christian Fundamentalists    14 2387 48.59 28.48 -0.07    -0.72 0.58
Feminists                    15 2387 56.94 26.65 -0.24    -0.47 0.55
Liberals                     16 2387 52.27 27.35 -0.24    -0.67 0.56
Labor Unions                 17 2387 56.70 24.74 -0.27    -0.29 0.51
Poor People                  18 2387 72.20 19.63 -0.36    -0.06 0.40
Big Business                 19 2387 49.34 22.52 -0.15    -0.18 0.46
Conservatives                20 2387 55.22 25.91 -0.24    -0.45 0.53
SCOTUS                       21 2387 59.34 19.38 -0.32     0.54 0.40
Gays & Lesbians              22 2387 62.83 26.86 -0.46    -0.20 0.55
Congress                     23 2387 41.17 22.32  0.02    -0.34 0.46
Rich People                  24 2387 53.53 20.69 -0.13     0.52 0.42
Muslims                      25 2387 55.80 25.64 -0.29    -0.23 0.52
Christians                   26 2387 74.40 23.80 -0.87     0.35 0.49
Jews                         27 2387 72.20 21.19 -0.45    -0.14 0.43
Tea Party                    28 2387 42.97 27.08 -0.06    -0.70 0.55
Police                       29 2387 75.57 22.50 -1.15     1.13 0.46
Transgender People           30 2387 57.29 26.88 -0.28    -0.31 0.55
Scientists                   31 2387 77.74 19.23 -0.77     0.39 0.39
BLM                          32 2387 48.26 32.66 -0.06    -1.15 0.67
```

Factor Analysis: One Factor

```
> FTFA1 <- fa(Therms,nfactors=1,fm="ml",rotate="none")
> print(FTFA1)
Factor Analysis using method =  ml
Call: fa(r = Therms, nfactors = 1, rotate = "none", fm = "ml")
Standardized loadings (pattern matrix) based upon correlation matrix
                             ML1      h2   u2 com
Asian-Americans             0.29 0.08306 0.92   1
Hispanics                   0.37 0.13456 0.87   1
Blacks                      0.39 0.15227 0.85   1
Illegal Immigrants          0.61 0.37552 0.62   1
Whites                     -0.03 0.00066 1.00   1
Dem. Pres. Candidate        0.79 0.62770 0.37   1
GOP Pres. Candidate        -0.81 0.65791 0.34   1
Libertarian Pres. Candidate -0.07 0.00476 1.00   1
Green Pres. Candidate       0.22 0.05026 0.95   1
Dem. VP                     0.65 0.42135 0.58   1
GOP VP                     -0.80 0.64779 0.35   1
John Roberts               -0.24 0.05942 0.94   1
Pope Francis                0.27 0.07253 0.93   1
Christian Fundamentalists  -0.49 0.23650 0.76   1
Feminists                   0.69 0.47926 0.52   1
Liberals                    0.80 0.63513 0.36   1
Labor Unions                0.49 0.24414 0.76   1
Poor People                 0.25 0.06198 0.94   1
Big Business               -0.31 0.09877 0.90   1
Conservatives              -0.65 0.42099 0.58   1
SCOTUS                      0.11 0.01287 0.99   1
Gays & Lesbians             0.62 0.38096 0.62   1
Congress                   -0.20 0.04024 0.96   1
Rich People                -0.18 0.03379 0.97   1
Muslims                     0.63 0.39894 0.60   1
Christians                 -0.32 0.10381 0.90   1
Jews                        0.23 0.05481 0.95   1
Tea Party                  -0.62 0.38321 0.62   1
Police                     -0.31 0.09796 0.90   1
Transgender People          0.65 0.42375 0.58   1
Scientists                  0.39 0.15438 0.85   1
BLM                         0.73 0.53747 0.46   1
.
.
.
```

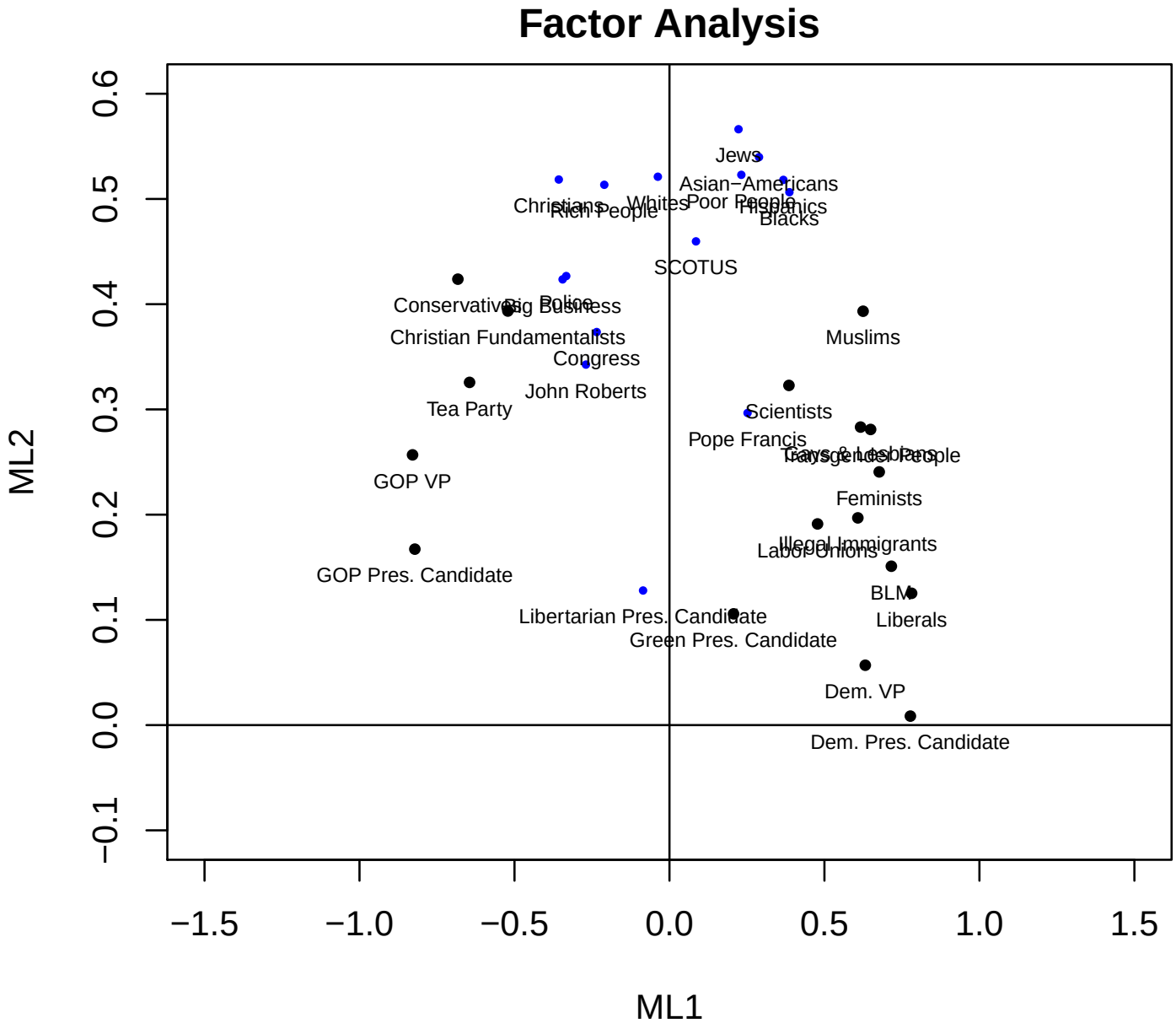
Factor Analysis: One Factor

```
(...continued)

                ML1
SS loadings    8.09
Proportion Var 0.25

Mean item complexity =  1
Test of the hypothesis that 1 factor is sufficient.

The degrees of freedom for the null model are 496 and the objective function was 16.99 with
    Chi Square of 40352
The degrees of freedom for the model are 464 and the objective function was 8.87

The root mean square of the residuals (RMSR) is  0.15
The df corrected root mean square of the residuals is  0.16

The harmonic number of observations is  2387 with the empirical chi square  53448  with prob <  0
The total number of observations was  2387  with MLE Chi Square =  21052  with prob <  0

Tucker Lewis Index of factoring reliability =  0.448
RMSEA index =  0.137  and the 90 % confidence intervals are  0.135 0.138
BIC =  17443
Fit based upon off diagonal values = 0.74
Measures of factor score adequacy
                                                ML1
Correlation of scores with factors             0.97
Multiple R square of scores with factors       0.94
Minimum correlation of possible factor scores  0.88
```

Factor Analysis: Two Factors

```
> FTFA2 <- fa(Therms,nfactors=2,fm="ml", rotate="none")
> print(FTFA2)
Factor Analysis using method =  ml
Call: fa(r = Therms, nfactors = 2, rotate = "none", fm = "ml")
Standardized loadings (pattern matrix) based upon correlation matrix
                             ML1  ML2    h2   u2 com
Asian-Americans             0.29 0.54 0.375 0.63 1.5
Hispanics                   0.37 0.52 0.404 0.60 1.8
Blacks                      0.39 0.51 0.406 0.59 1.9
Illegal Immigrants          0.61 0.20 0.408 0.59 1.2
Whites                     -0.04 0.52 0.273 0.73 1.0
Dem. Pres. Candidate        0.78 0.01 0.604 0.40 1.0
GOP Pres. Candidate        -0.82 0.17 0.703 0.30 1.1
Libertarian Pres. Candidate -0.09 0.13 0.024 0.98 1.7
Green Pres. Candidate       0.21 0.11 0.054 0.95 1.5
Dem. VP                     0.63 0.06 0.402 0.60 1.0
GOP VP                     -0.83 0.26 0.753 0.25 1.2
.
.
.
Police                     -0.33 0.43 0.293 0.71 1.9
Transgender People          0.65 0.28 0.500 0.50 1.4
Scientists                  0.39 0.32 0.253 0.75 1.9
BLM                         0.72 0.15 0.535 0.46 1.1

                       ML1  ML2
SS loadings           8.16 4.29
Proportion Var        0.26 0.13
Cumulative Var        0.26 0.39
Proportion Explained  0.66 0.34
Cumulative Proportion 0.66 1.00

Mean item complexity =  1.5
.
.
```

Factor Analysis: Two Factors



Topic: Rotation

PCA / FA are *data reduction* techniques...

- Rotation is exactly that: Rotation of the axes in the transformed space to make the results more interpretable.
- Two broad types:
  - *Orthogonal* rotation (maintains orthogonality of the axes)
  - *Oblique* rotation (allows components / factors to be correlated)
- **The goal of rotation is to improve the interpretability of the PCA/FA results (that is, to reveal "simple structure")**

Rotation Methods

Orthogonal rotations:

- **Varimax** (minimizes the number of variables that have high loadings on each factor.)
- **Quartimax** (minimizes the number of factors needed to explain each variable)
- **Equamax** (a combination of varimax and quartimax)
- Others...

Oblique rotations (less easily interpretable):

- **Direct Oblimin** (the de facto standard for oblique rotation)
- **Promax** (simpler / faster than oblimin)
- Others...

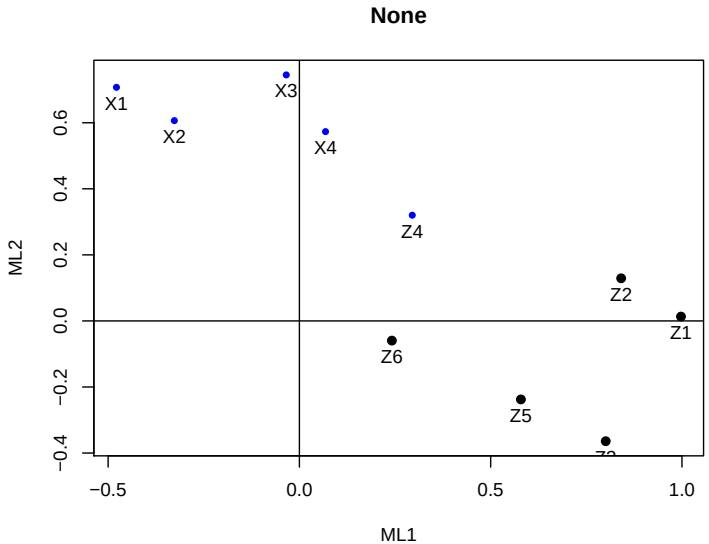
Rotation: Considerations

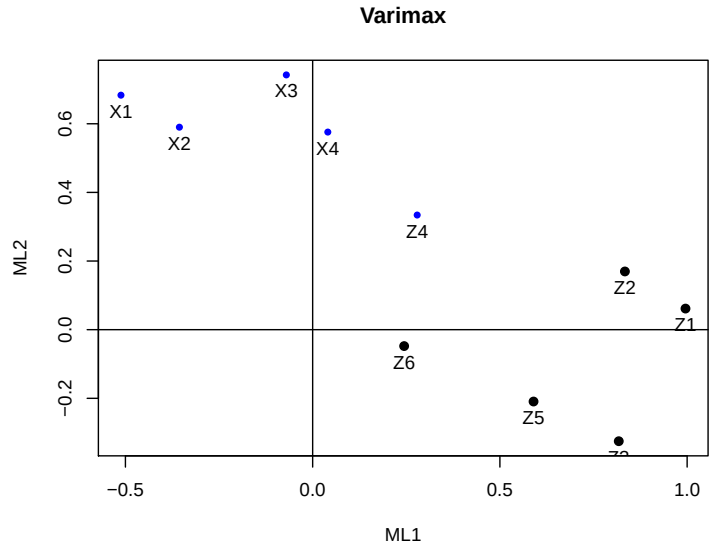
"Simple structure": "A condition in which variables load at near 1 (in absolute value) or at near 0 on an eigenvector (factor). Variables that load near 1 are clearly important in the interpretation of the factor, and variables that load near 0 are clearly unimportant." (Bryant and Yarnold 1995)

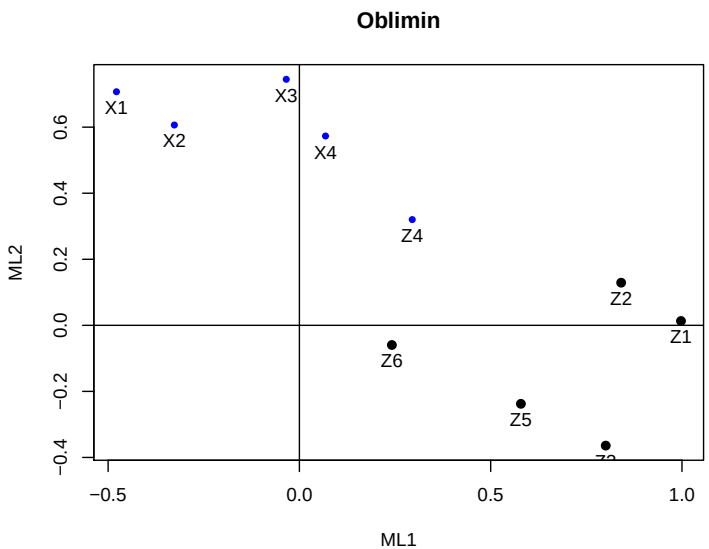
Factor Loading ℓ Guidelines:

- $0.10 < \ell < -0.10$ are unimportant
- $|\ell| > 0.30$ are important with $N \geq 100$
- Variables with $\ell > 0.30$ on more than one factor are *complex*

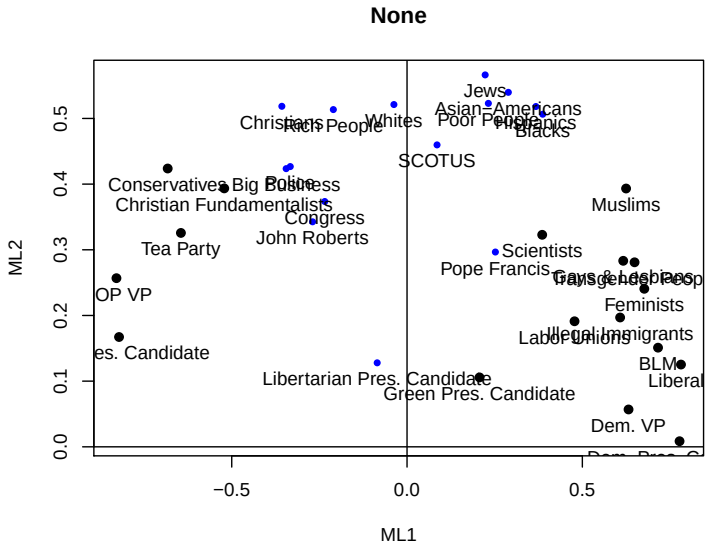
Rotation: Simulated Data

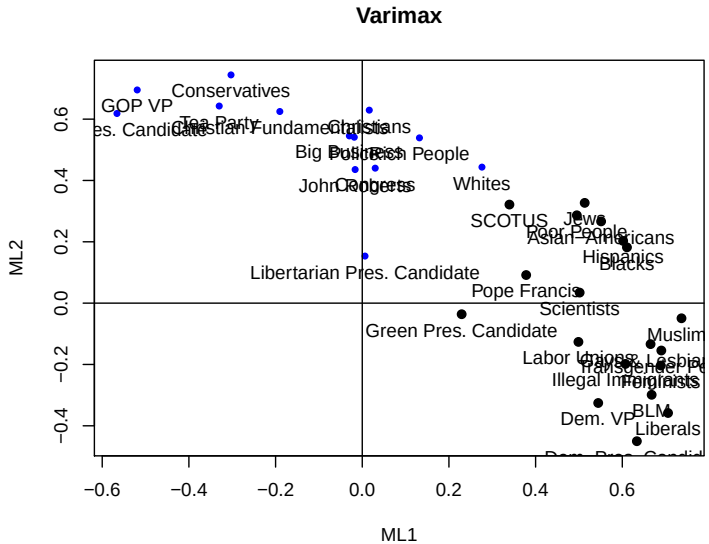


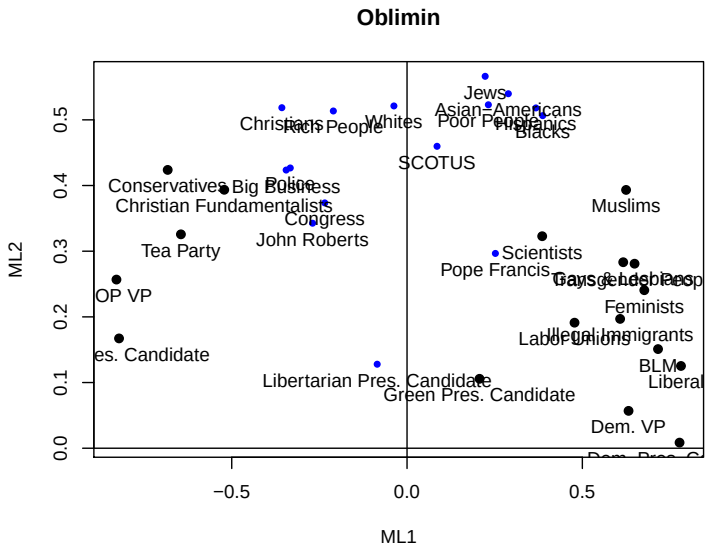




Rotation: Feeling Thermometers







Topic: Dimensionality

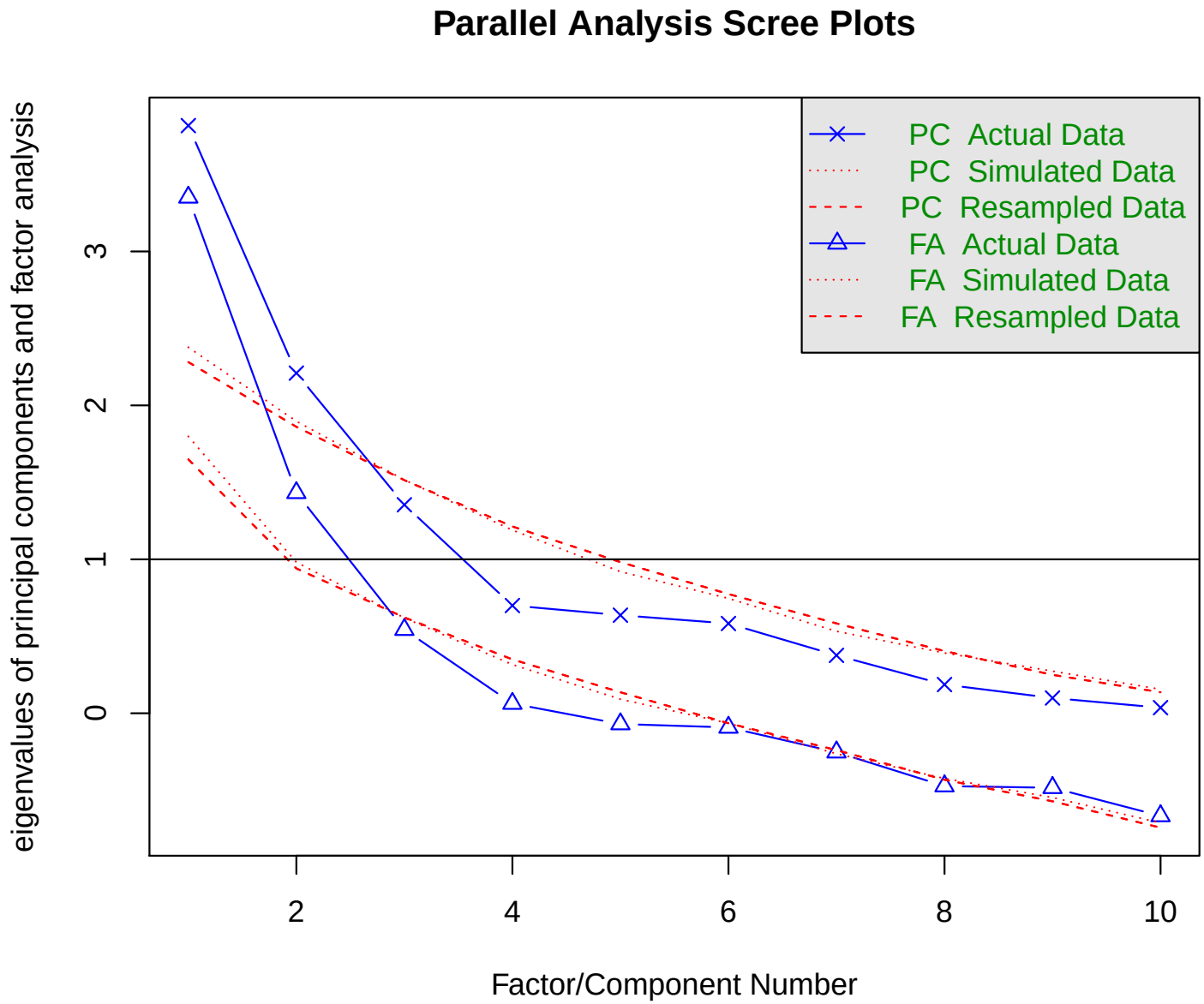
PCA/FA are *data reduction* techniques...

- The sum of the eigenvalues equals K; so...
- A factor / component with an eigenvalue less than 1.0 isn't even "explaining itself"
- "Kaiser criterion"

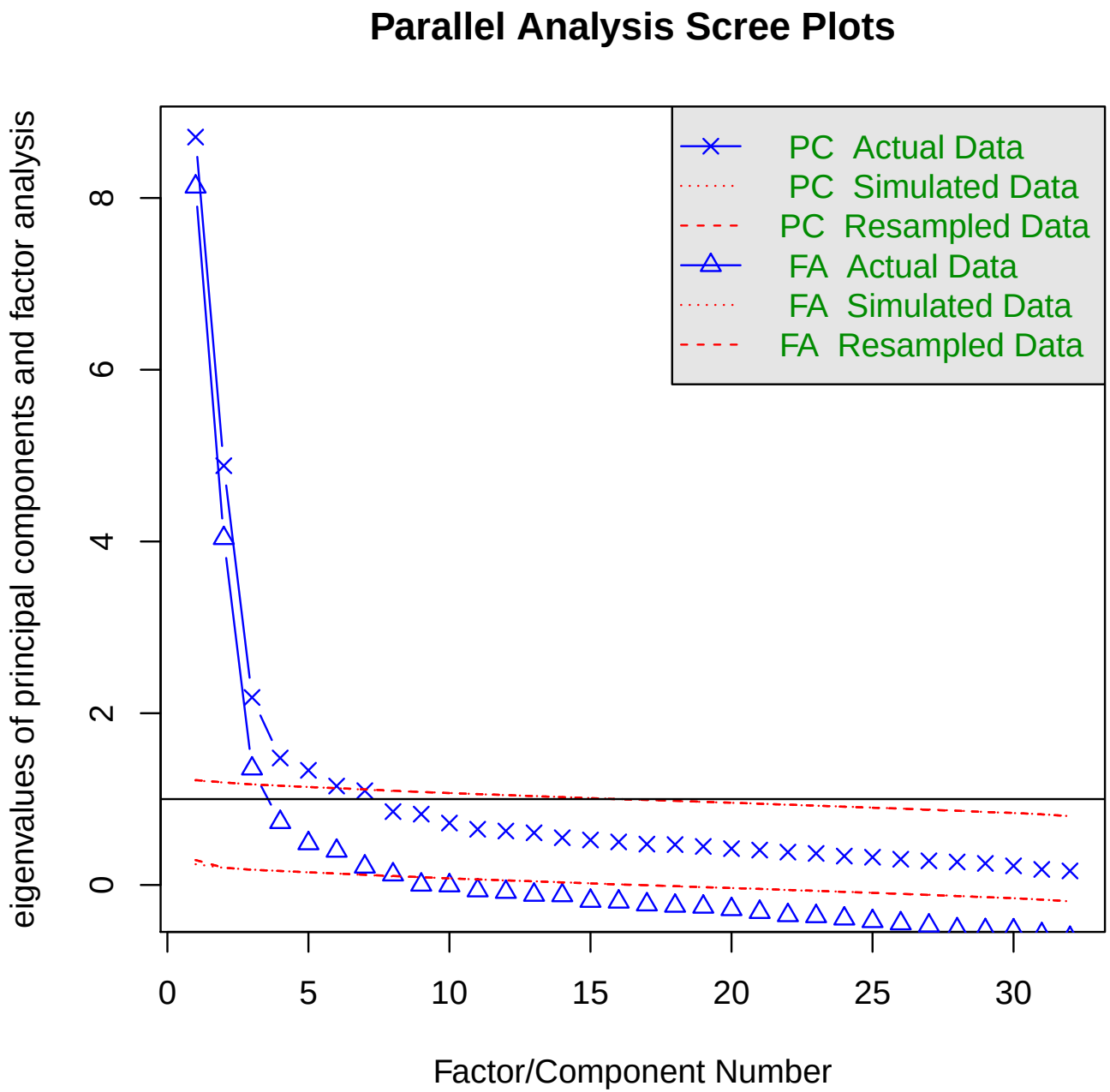
Other approaches:

- *Theory*...
- "Scree plot" (look for the "elbow")
- Target variance explained
- Others...

"Parallel" Scree Plot (Simulated Data)



"Parallel" Scree Plot (Feeling Thermometer Data)



Useful References

- Gorsuch, Richard L. 1983. *Factor Analysis*, 2nd Ed. NJ: Lawrence Erlbaum.

- Cudek, Robert and Robert C. MacCallum, Eds. 2007. *Factor Analysis at 100*. NJ: Lawrence Erlbaum.

- Mulaik, Stanley A. 2010. *Foundations of Factor Analysis*, 2nd Ed. Boca Raton, FL: CRC Press.

- Fabrigar, Leandre R., and Duane T. Wegener. 2014. *Exploratory Factor Analysis*. New York: Oxford University Press.

Useful R Packages and Routines

PCA and Biplots

- `stats::prcomp` (principal components via SVD)
- `biplot` (biplots)
- `psych::principal` (User-friendly PCA routine)
- Others...

Factor Analysis

- `nFactors` (Routines for assessing dimensionality / number of factors)
- `FactoMineR` (Hugely expanded FA package...)
- `GPARotation` (Many, many rotation options)

Cluster Analysis

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.

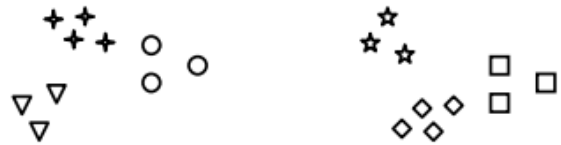


Figure 1c: Six clusters

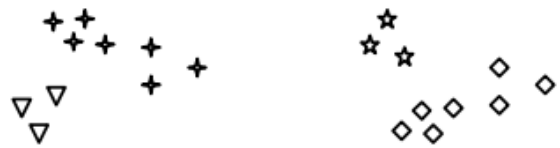
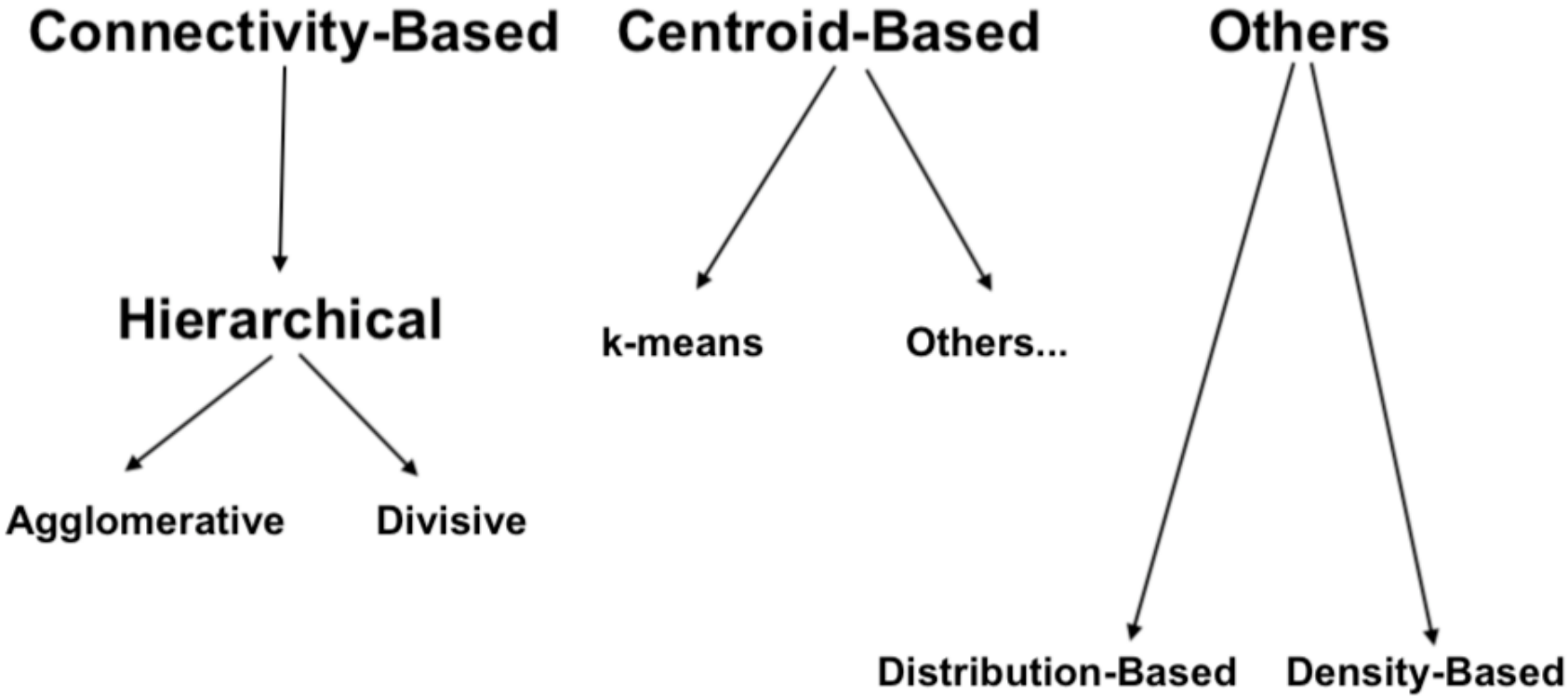


Figure 1d: Four clusters.

(source)

Cluster Analysis: Typology



Distances...

Euclidean ("L2") Distance:

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

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

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

Mahalanobis Distance:

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

Distance Example

Data ($N = 2$):

	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:

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

Lesson: Standardize variables!

Defining Intra-Cluster Distances

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

- Single-linkage

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

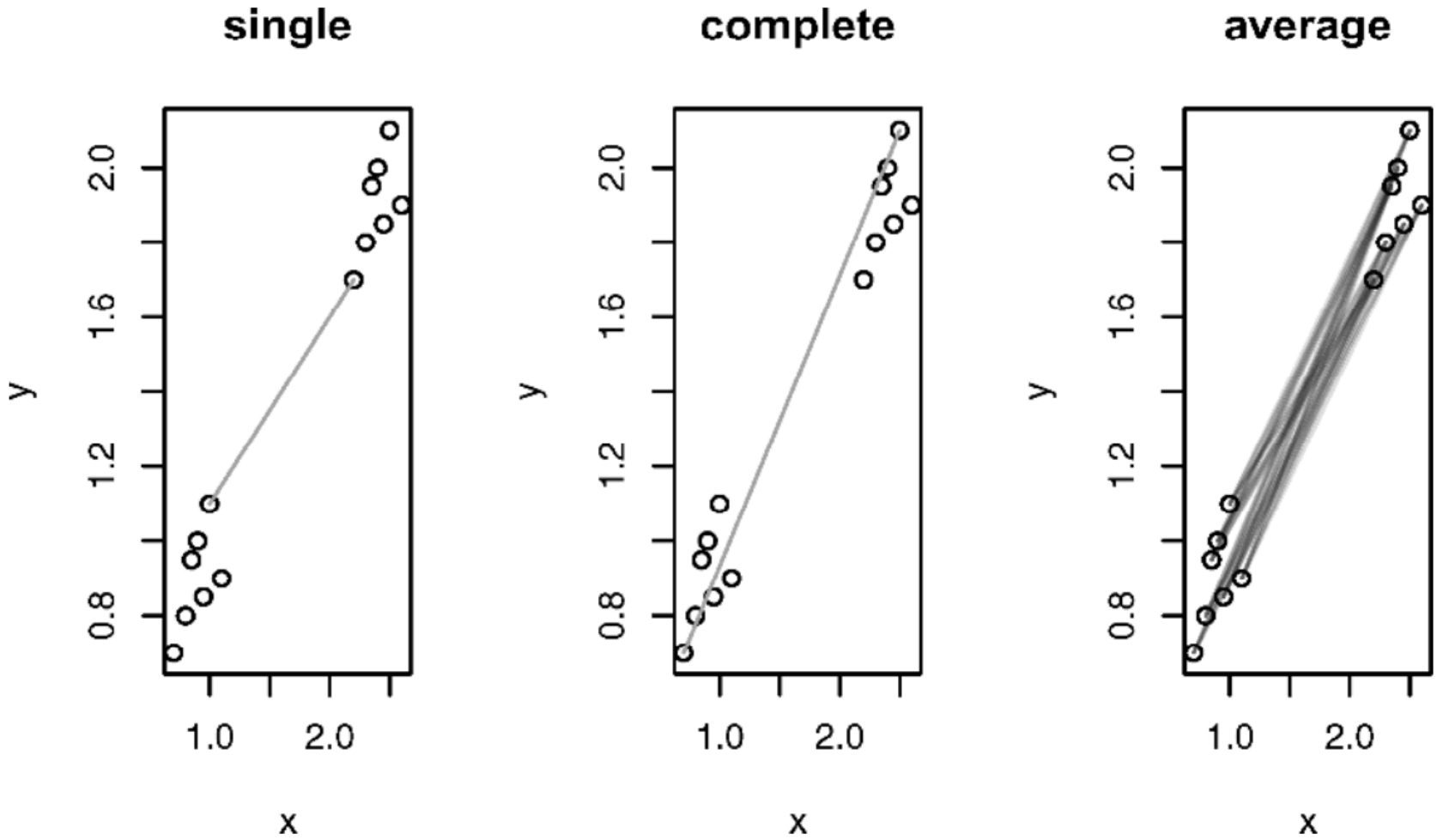
- Complete linkage

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

- 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

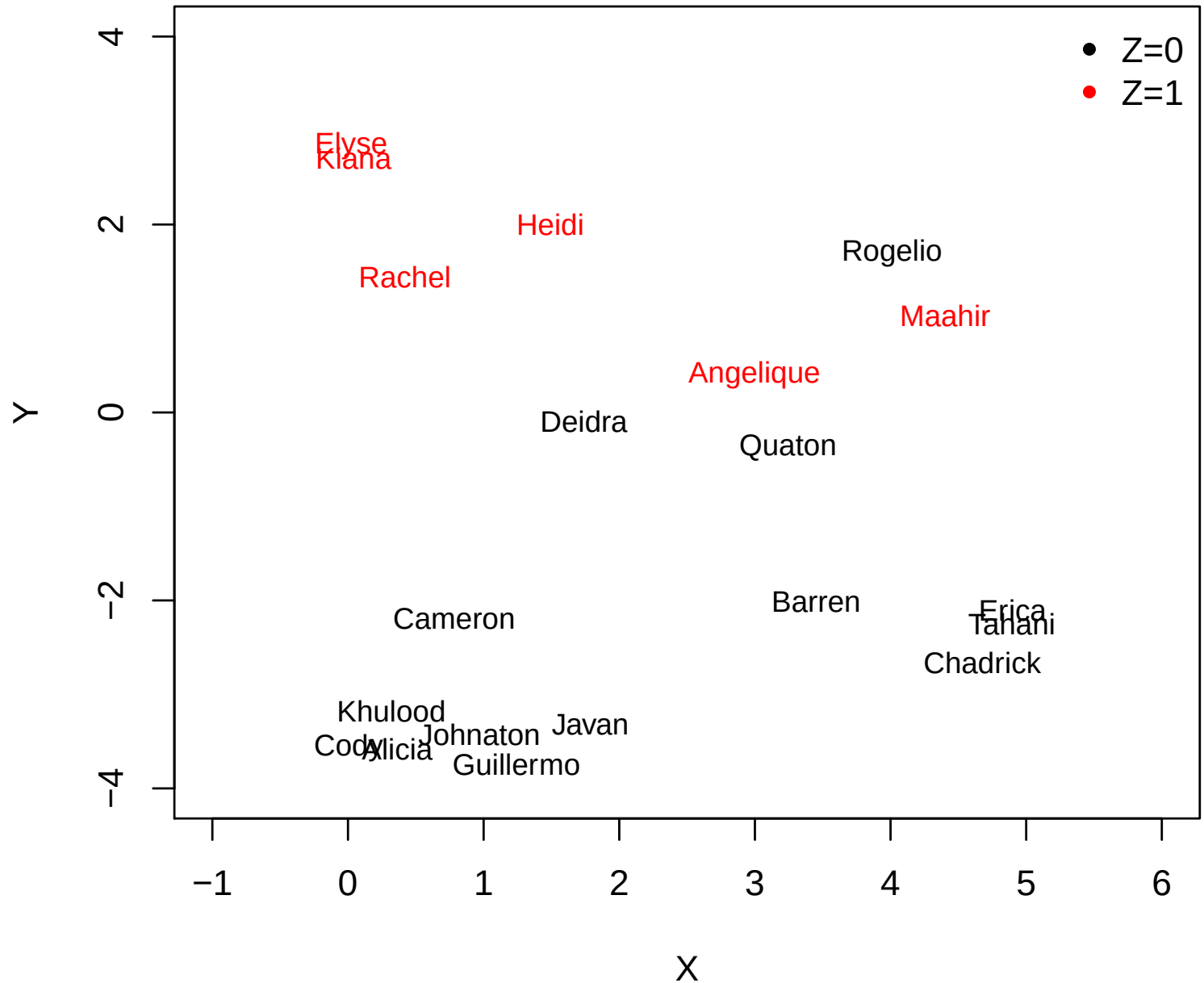
Basic steps:

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

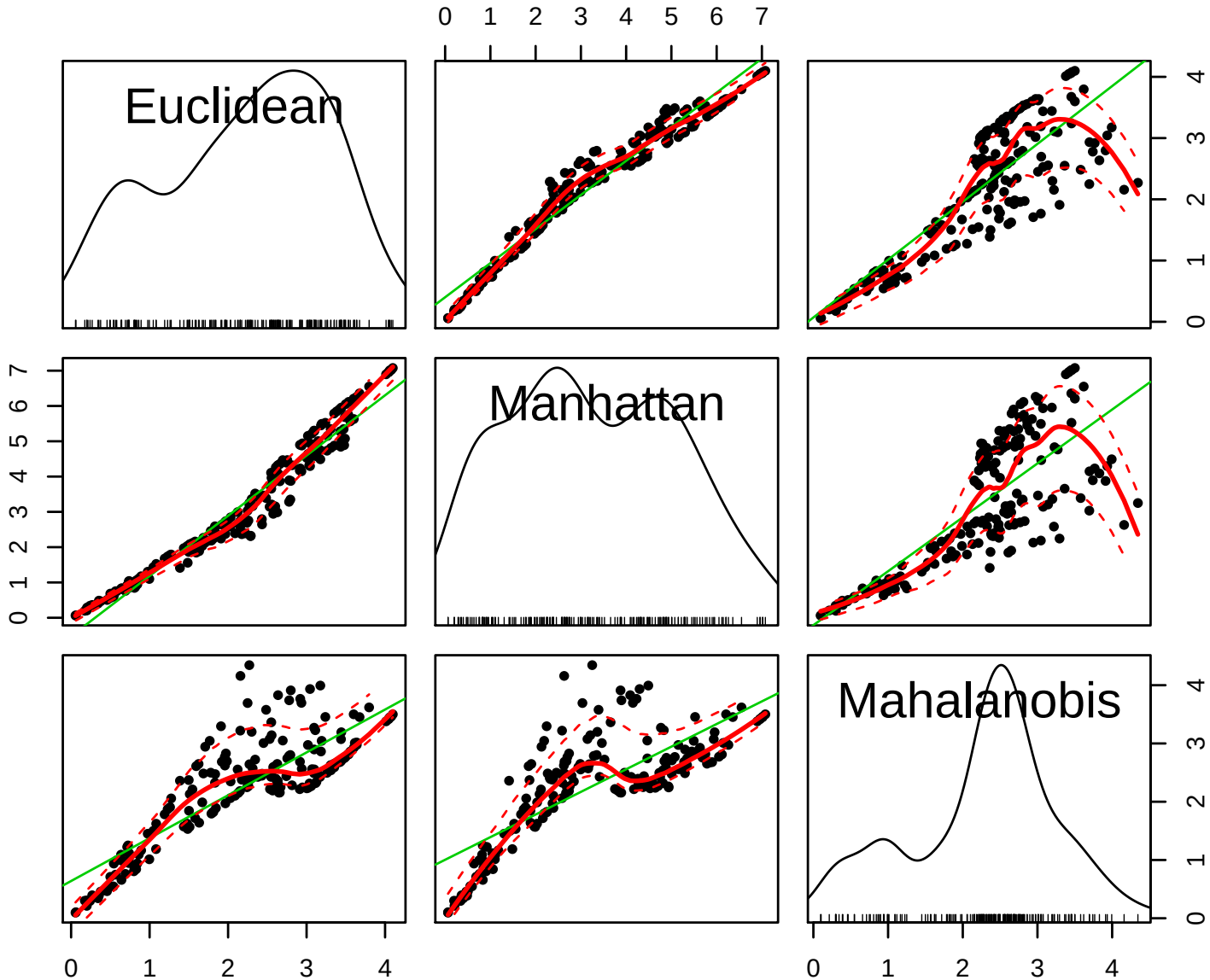
Simulation Example

```
> 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



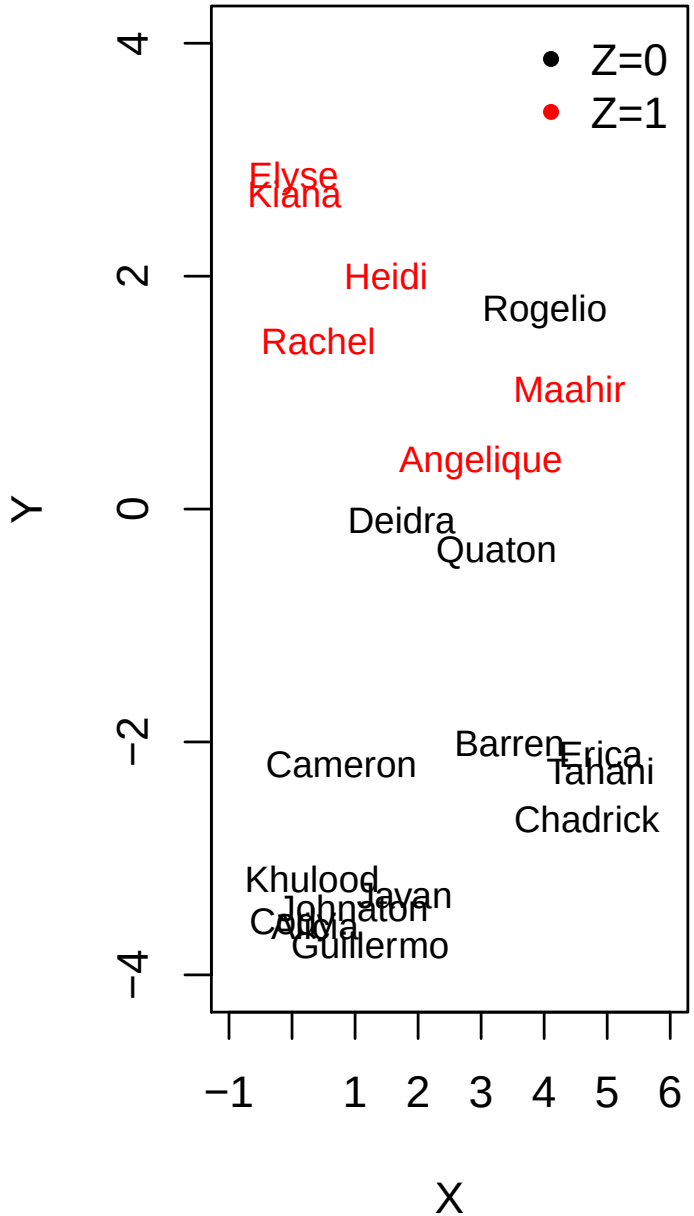
Distance Comparisons

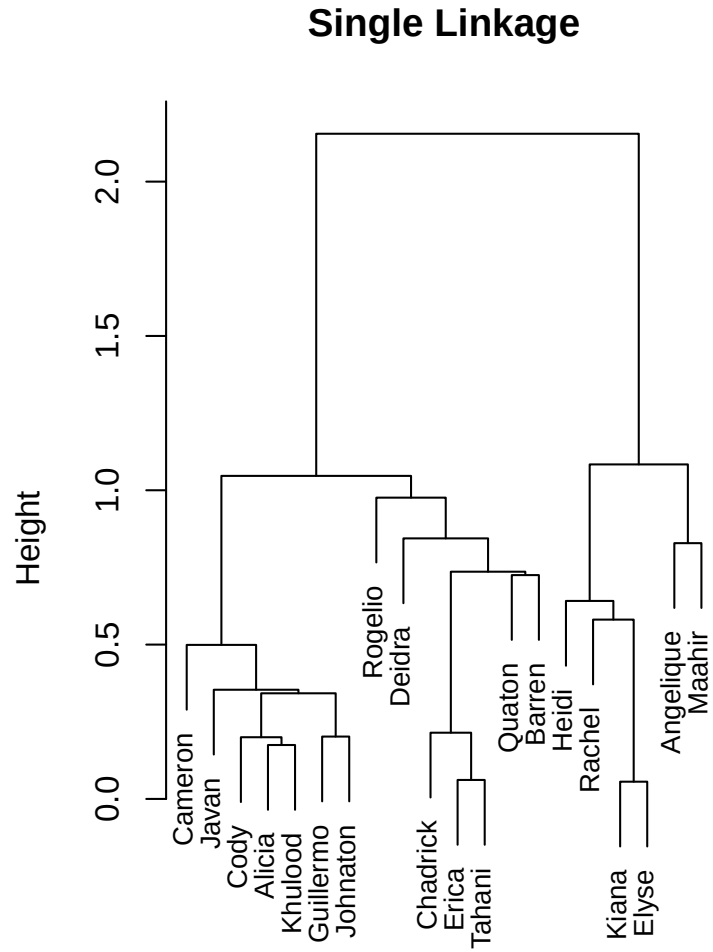


Using hclust (in cluster)

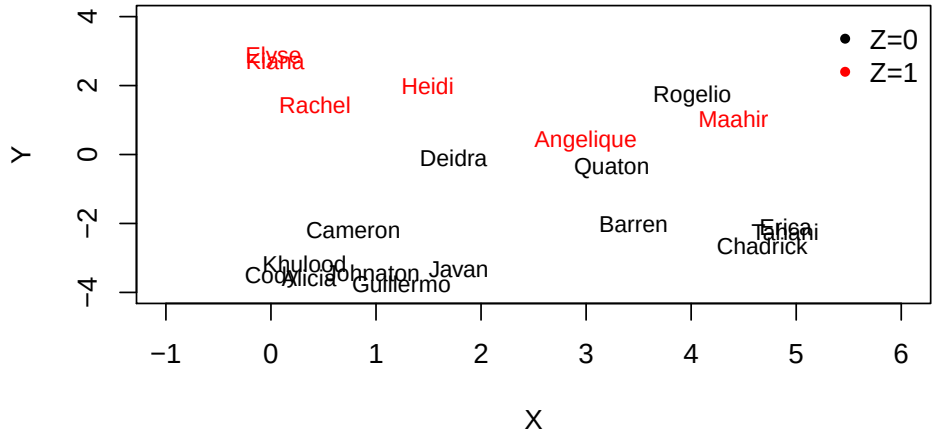
```
> ADL2.s <- hclust(DL2,method="single")
> ADL2.c <- hclust(DL2,method="complete")
> ADL2.a <- hclust(DL2,method="average")

> 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"
```

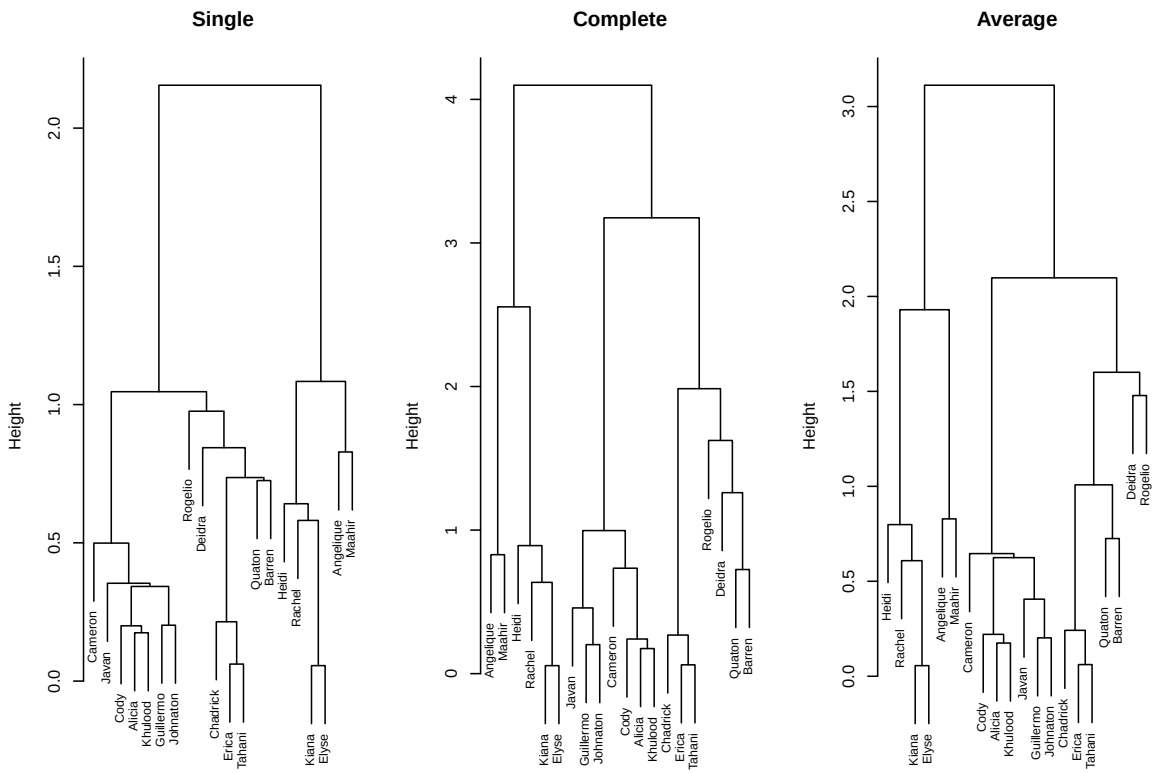
The Dendrogram



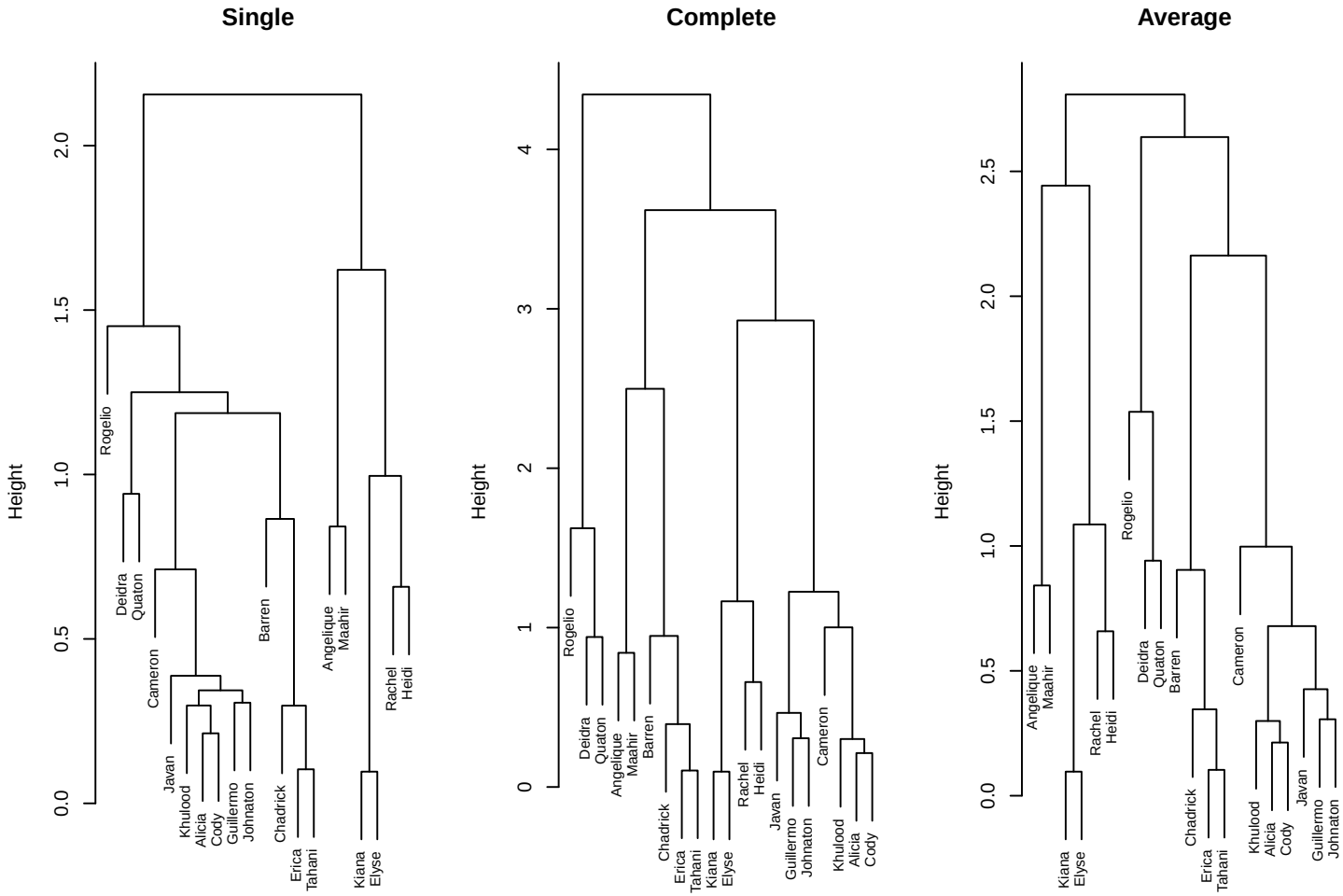


Comparing Linkages





Using Mahalanobis Distance



The Agglomeration Coefficient

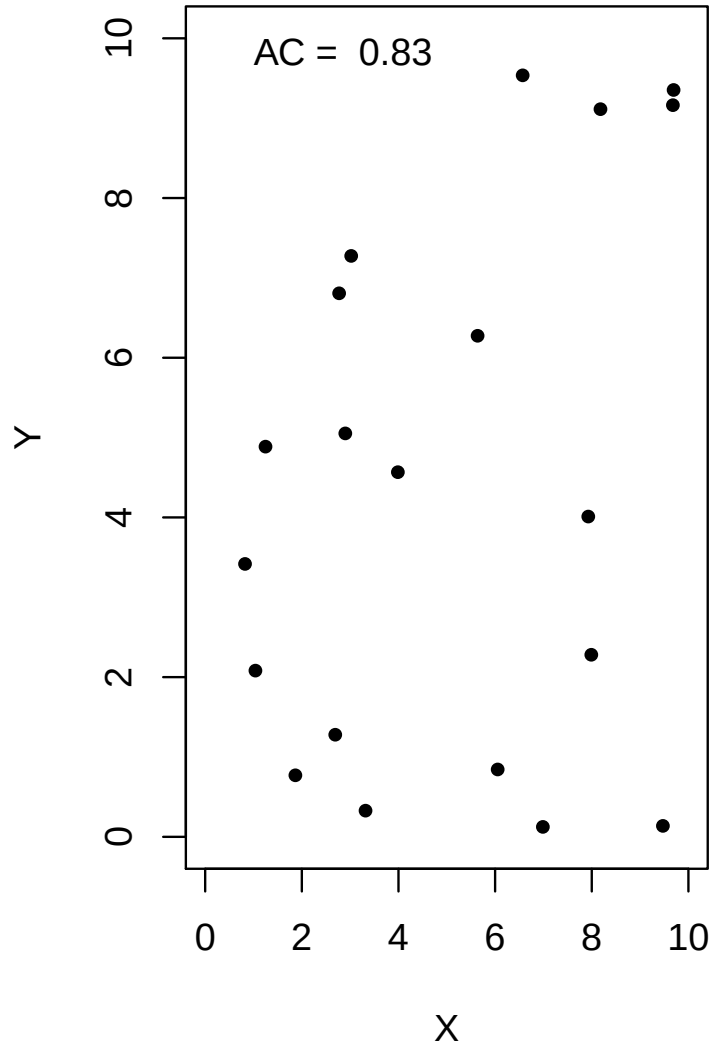
The *agglomeration coefficient* AC measures the clustering structure of the data. For each observation i, define m_i as the dissimilarity of observation i with the first cluster with which it is merged, divided by the dissimilarity in the final iteration (i.e., the greatest dissimilarity). The coefficient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

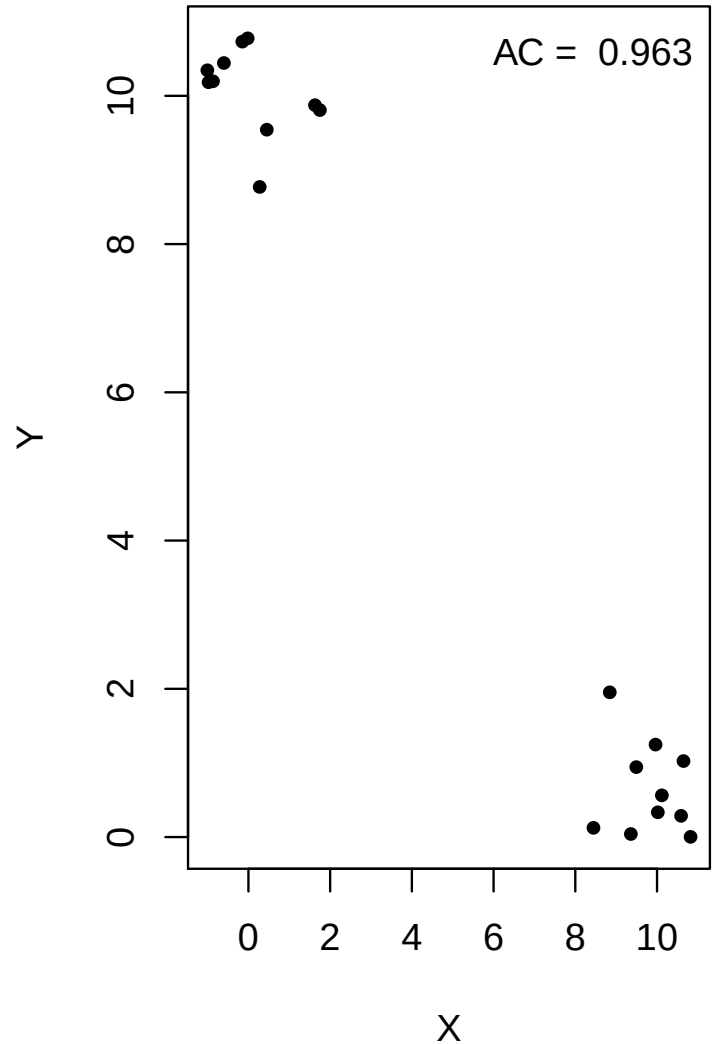
$$AC = \frac{1}{N-1} \sum_{i=1}^{N-1} 1 - m_i$$

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
```

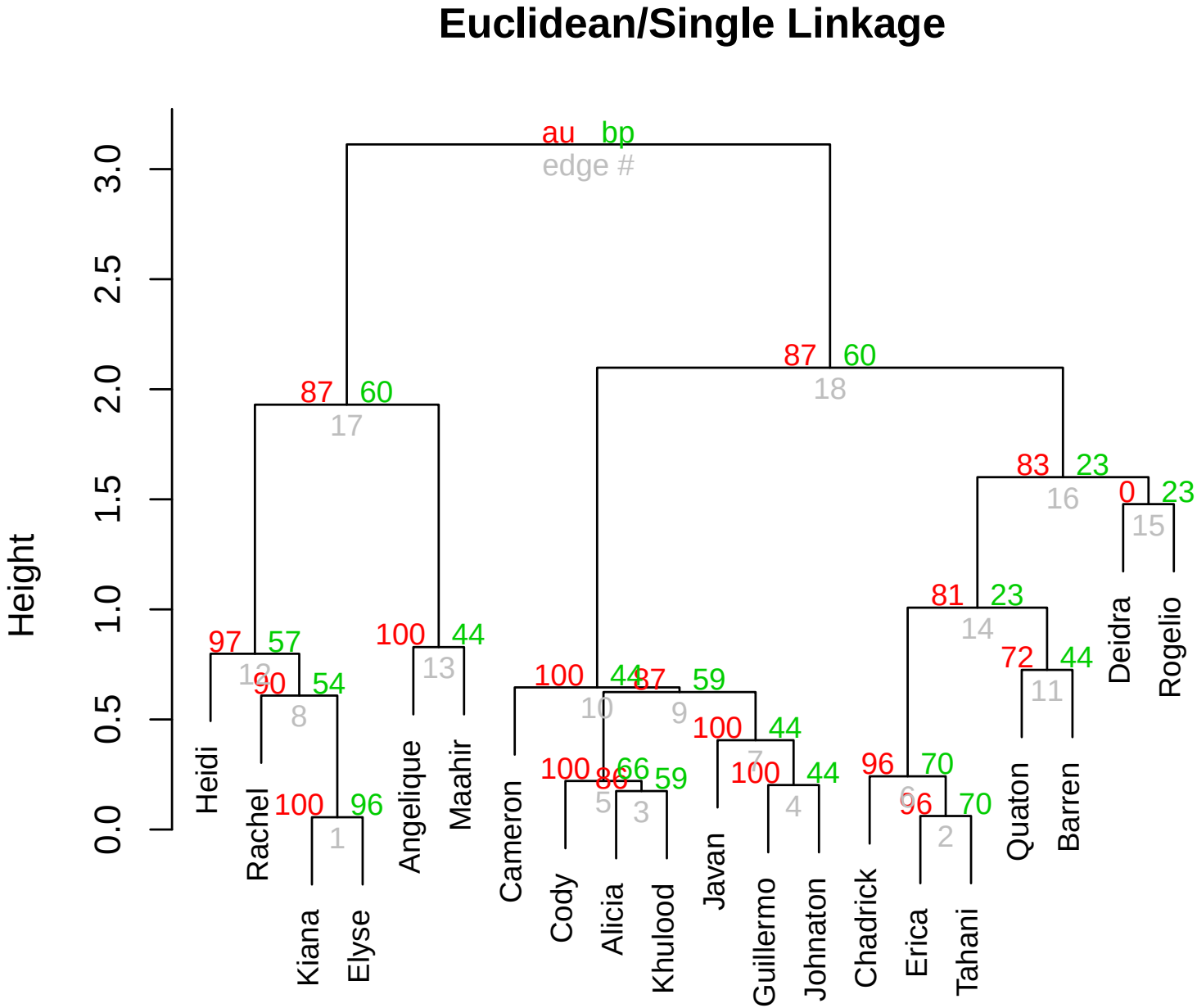
P-Values via Bootstrap

- 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...



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 (`diana`)

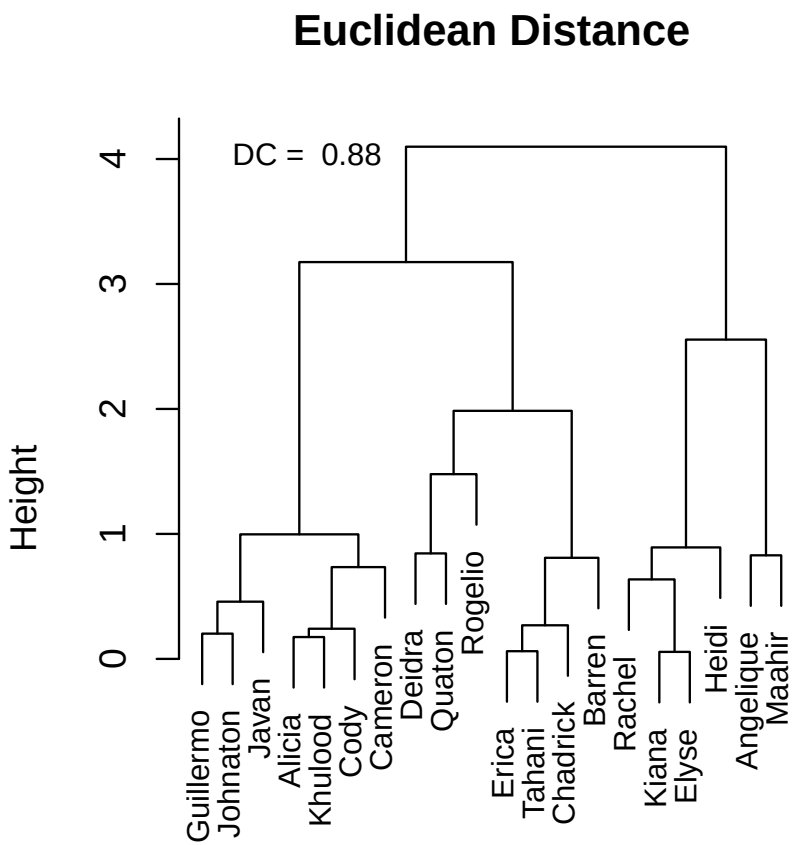
Basic steps:

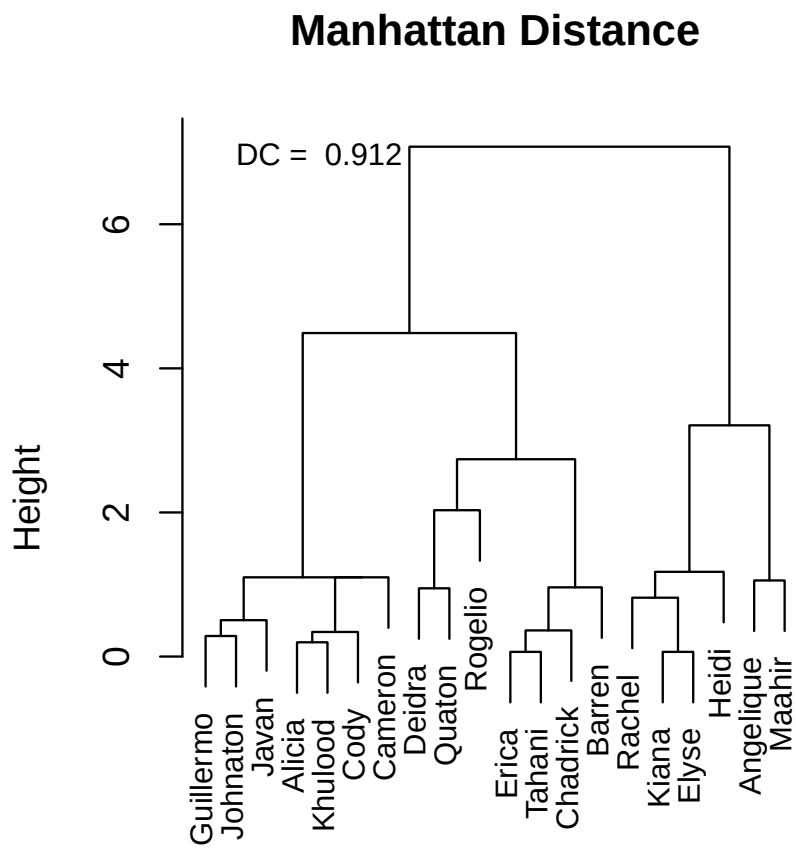
1. Begin with N observations on K variables in $\mathbf{X}$
2. Select the cluster C_{maxD} with the largest *diameter* (defined as the cluster with the largest dissimilarity between any two of its observations)
3. Select the observation j in C_{maxD} that has the highest average dissimilarity to the 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"
```

Divisive Clustering: Dendrograms





Non-Hierarchical Clustering: k-Means

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 $S_1 ... S_k$ in $\mathbf{S}$.

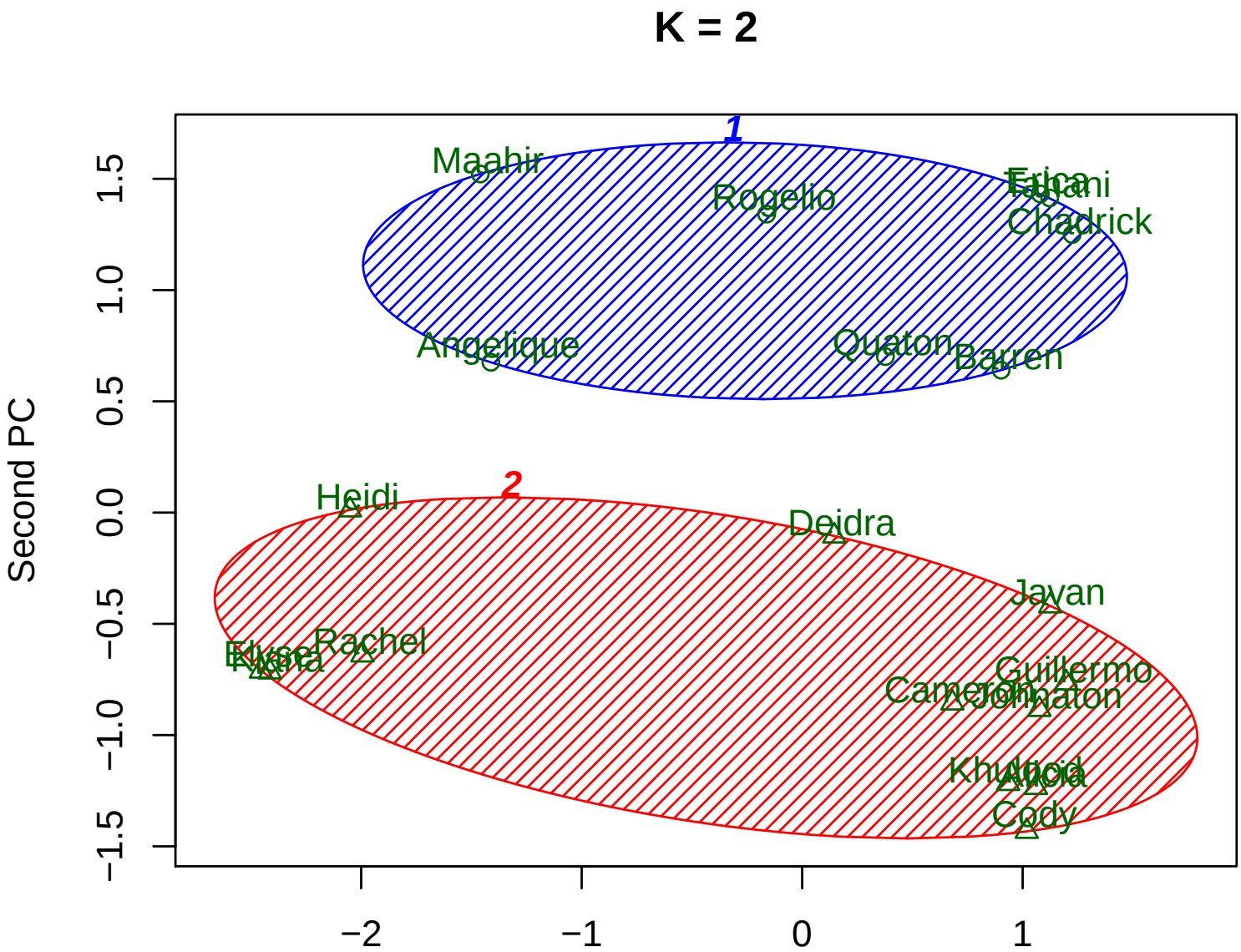
- Requires the analyst to designate the number of clusters desired k *a priori*.

- 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"
```

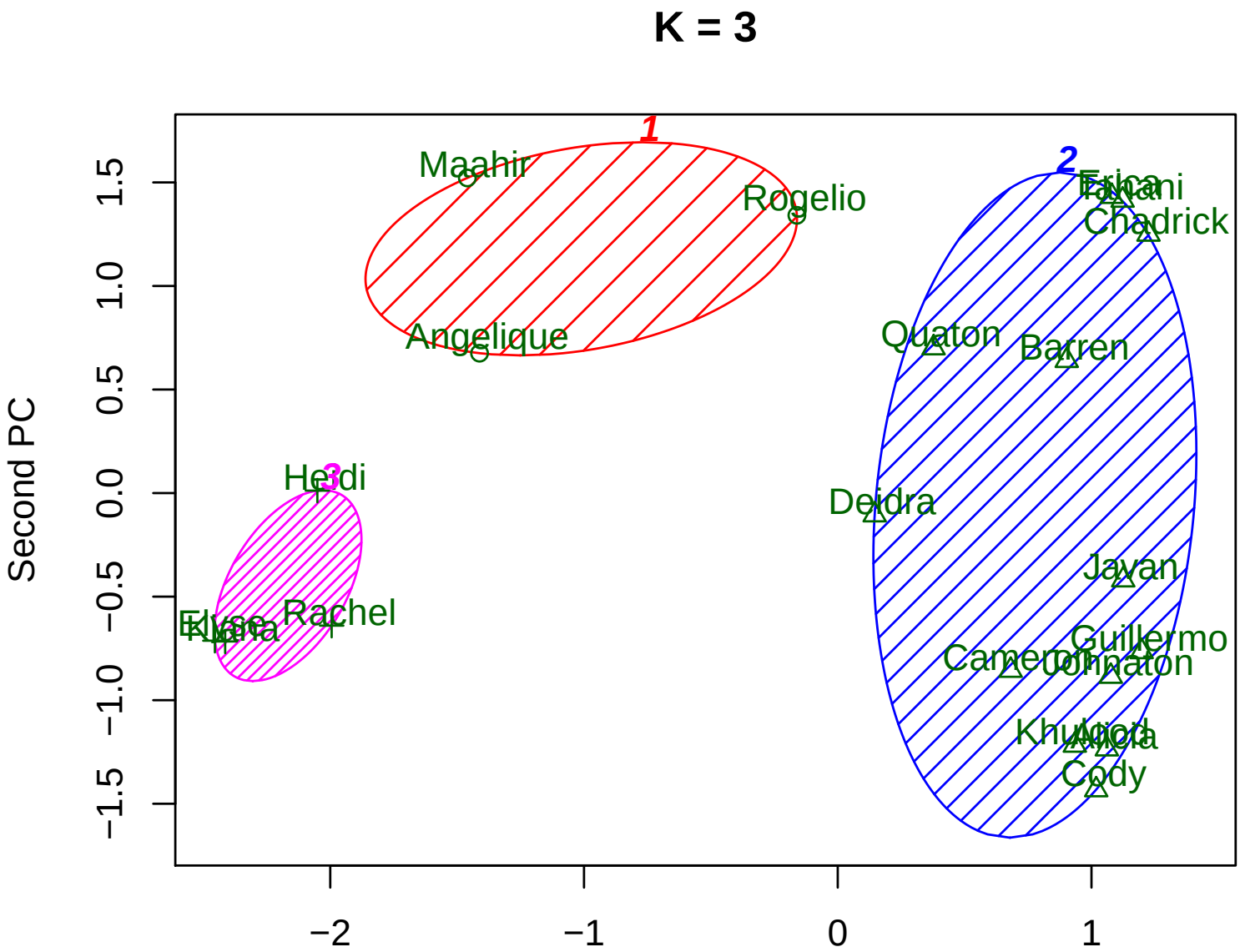
K-Means Clusters vs. Principal Components ($k = 2$)



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"
```

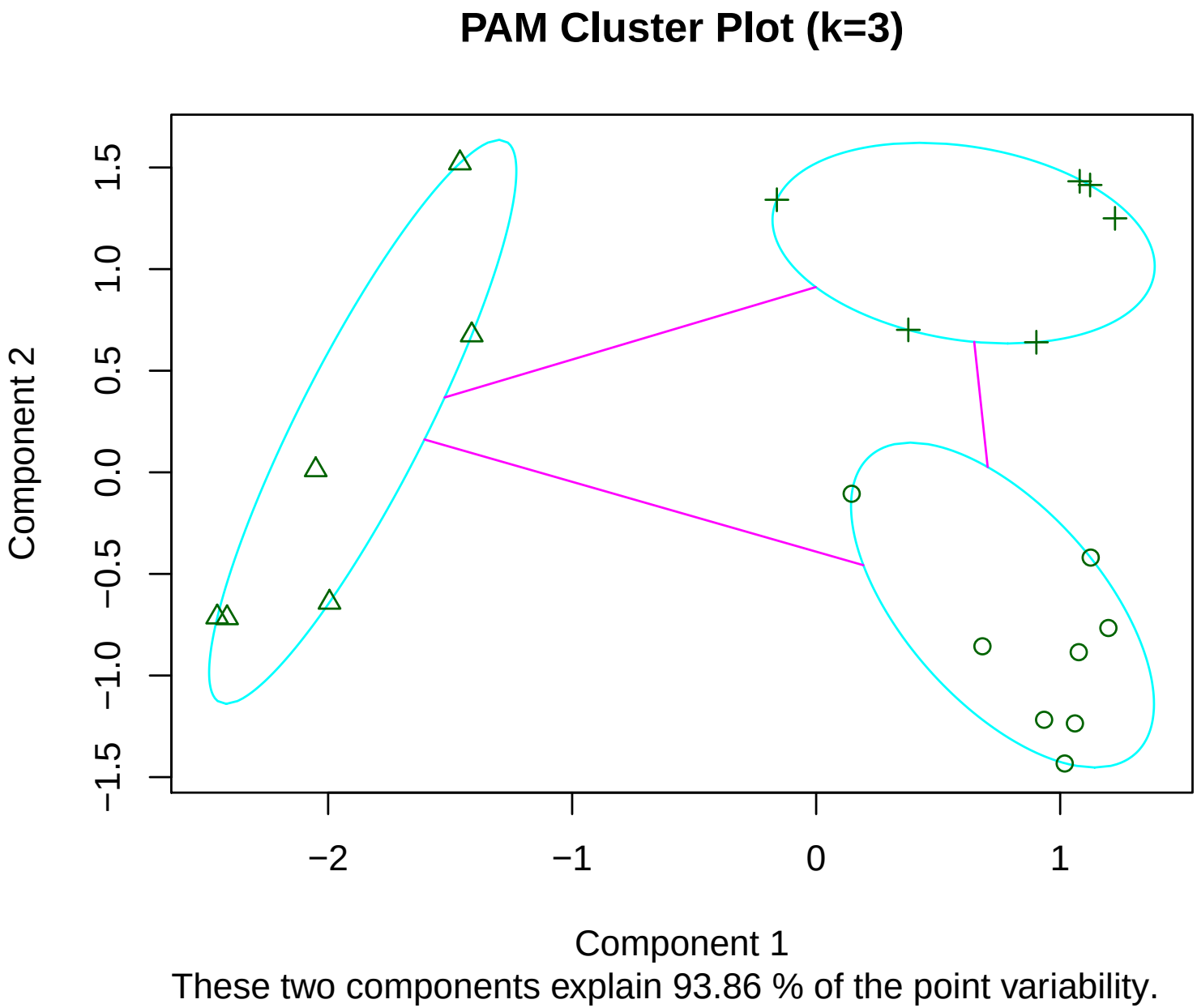
K-Means Clusters vs. Principal Components ($k = 3$)



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"
```

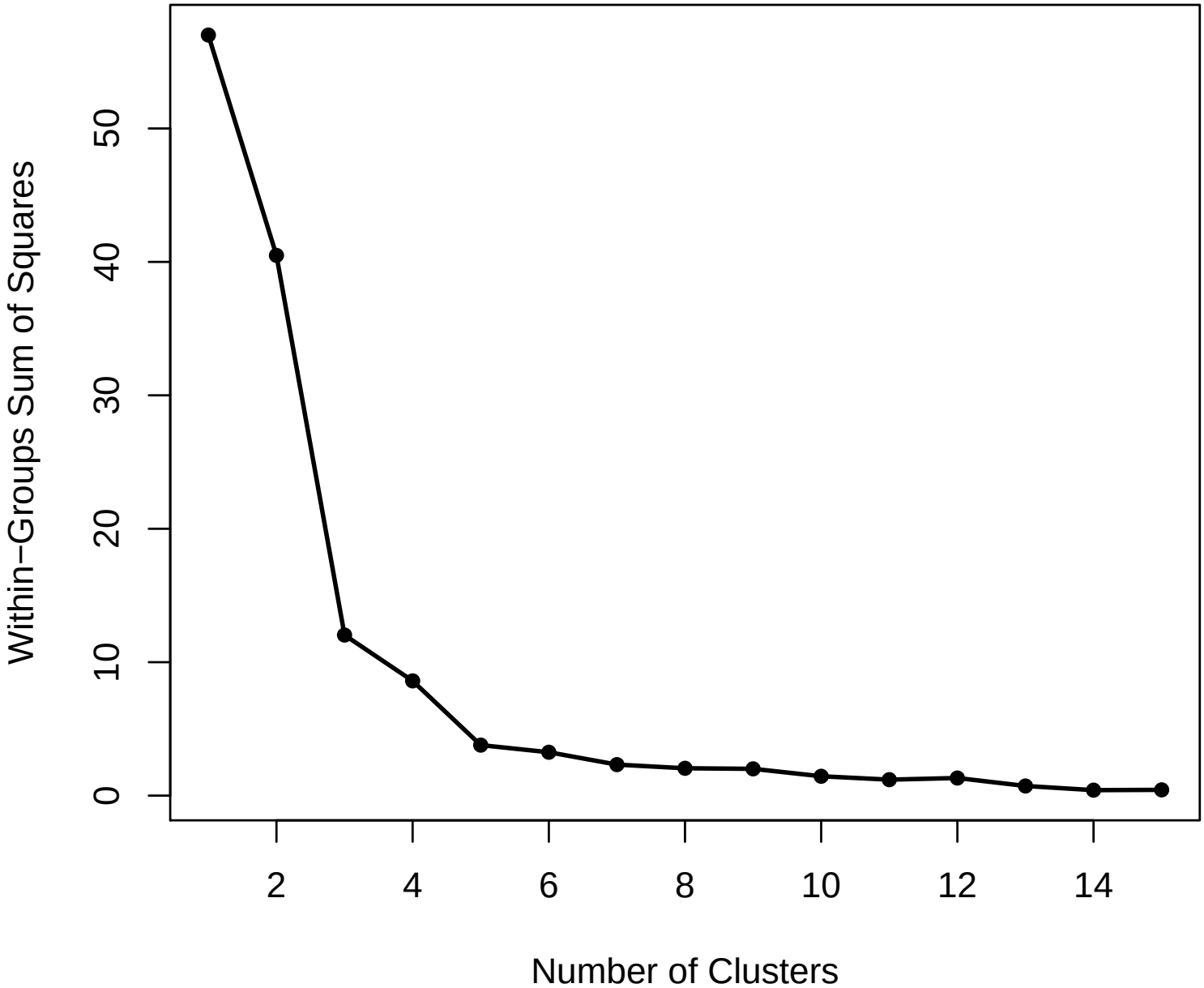
PAM, Illustrated



Practical k-Means: Choosing k

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

Choosing k: Scree Plot



Other Non-Hierarchical Methods

DBSCAN (Density-Based Spatial Clustering of Applications with Noise)

- *Density-based* method...
- Does not require prespecification of k
- Also does not (necessarily) assign "outlying" observations to clusters
- R packages: `dbscan`, others

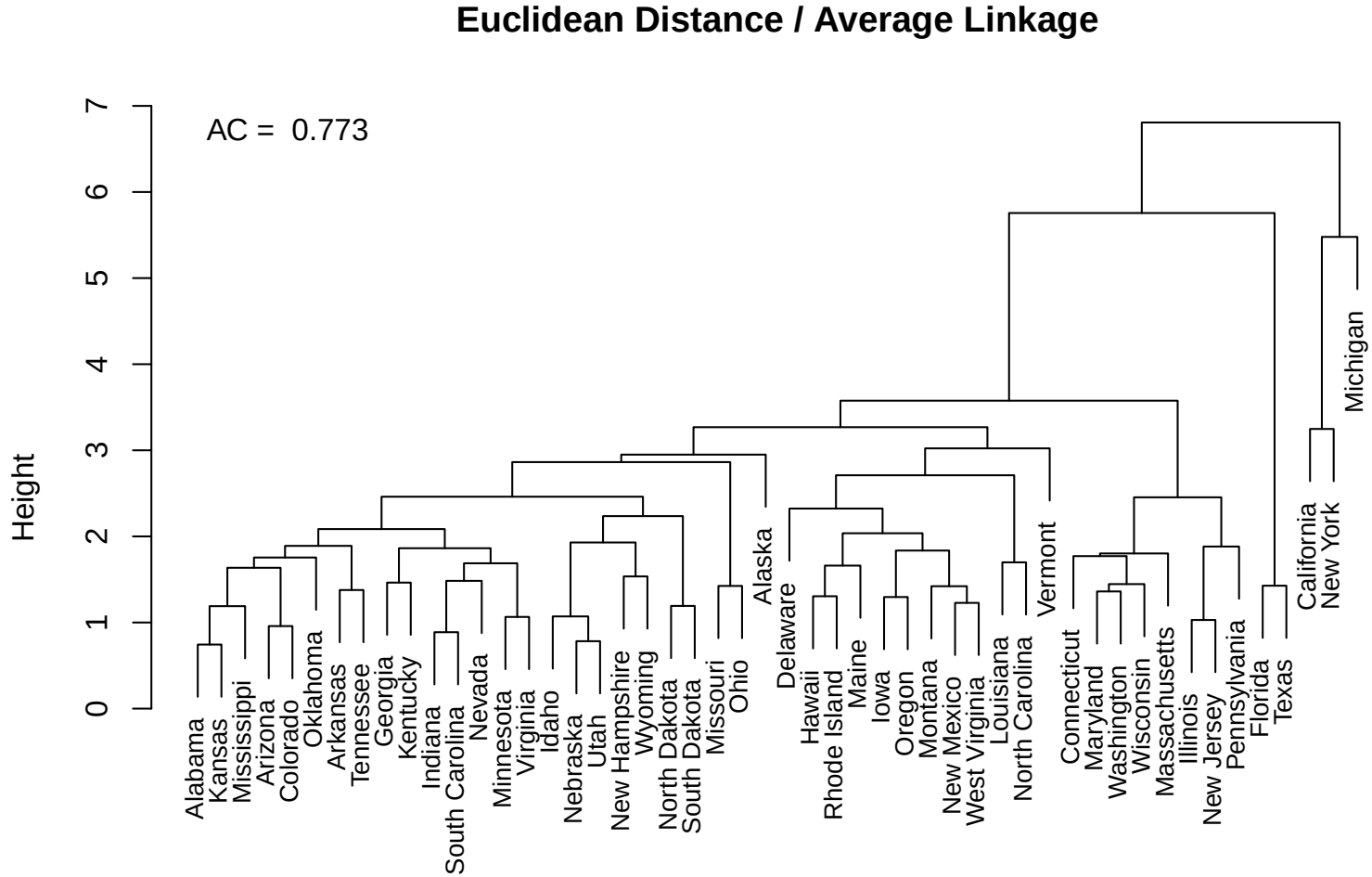
Mean-Shift Clustering

- Operationally similar to DBSCAN
- IME works well with "non-spherical" cluster shapes
- R packages: `meanShiftR`, `LPCM`, etc.

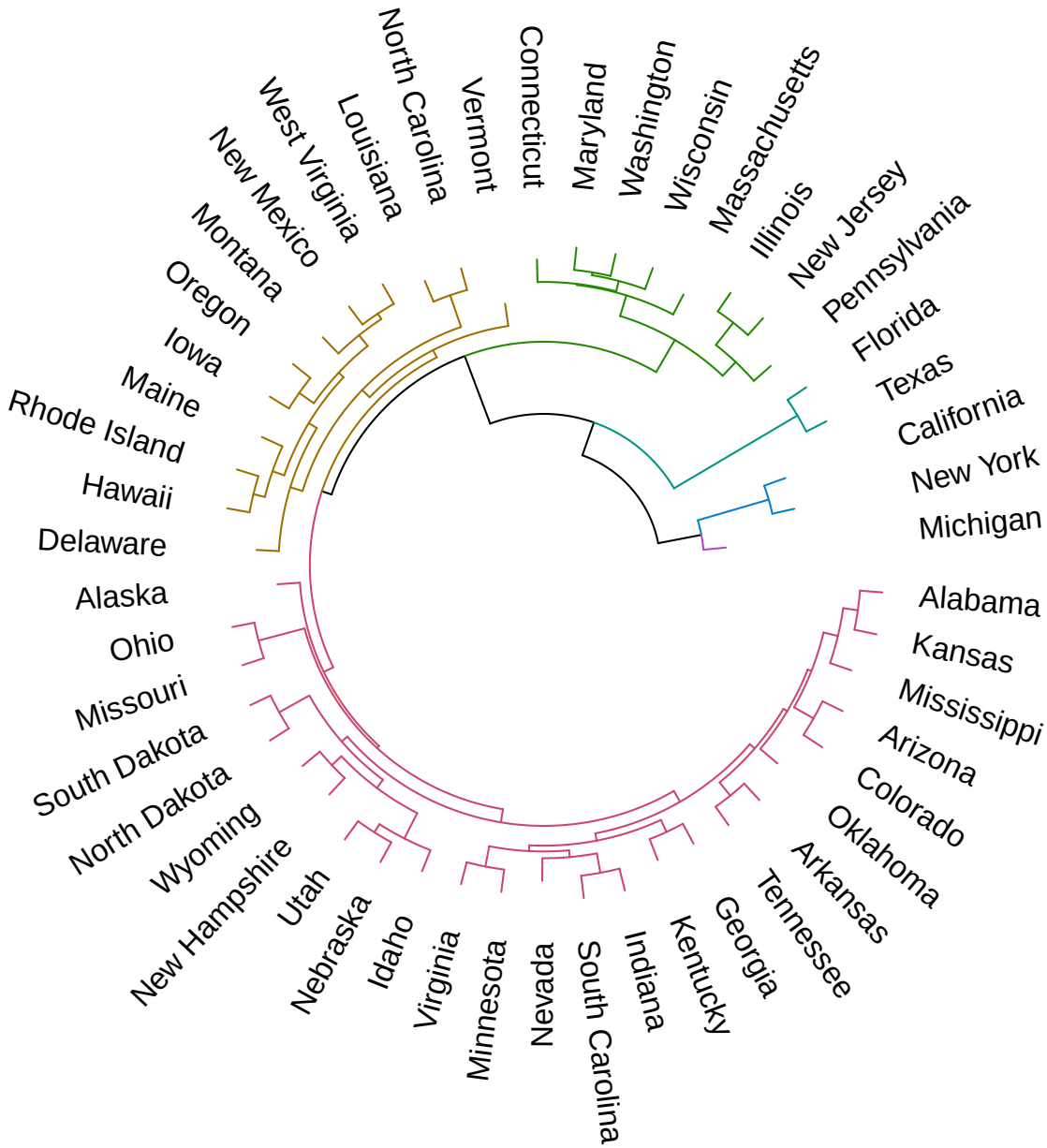
Real-Data Example: U.S. States

```
> url <- getURL("https://raw.githubusercontent.com/PrisonRodeo/
                 PLSC504-2020-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
```

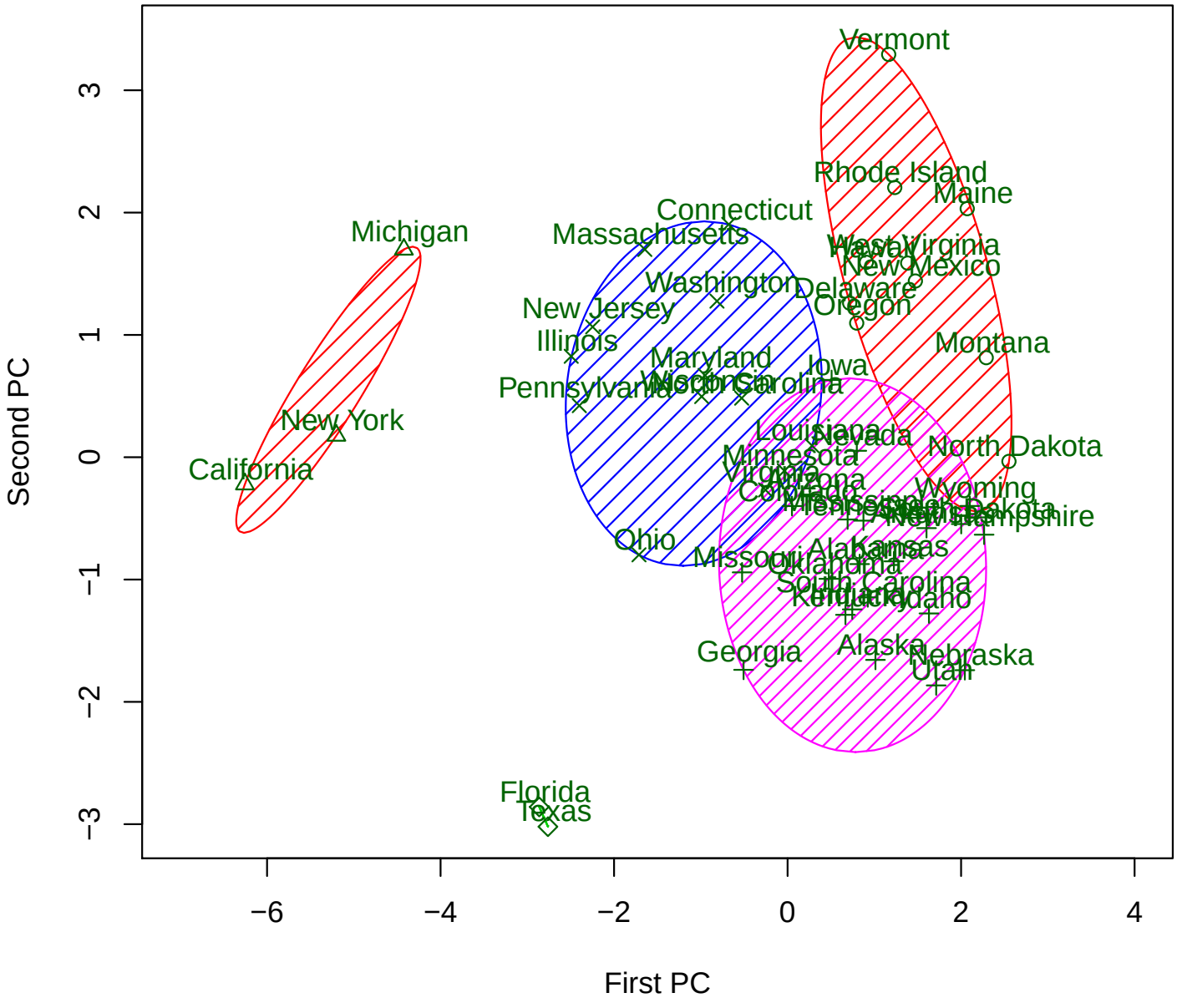
State Data: Agglomerative Dendrogram



State Data: Cooler Agglomerative 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