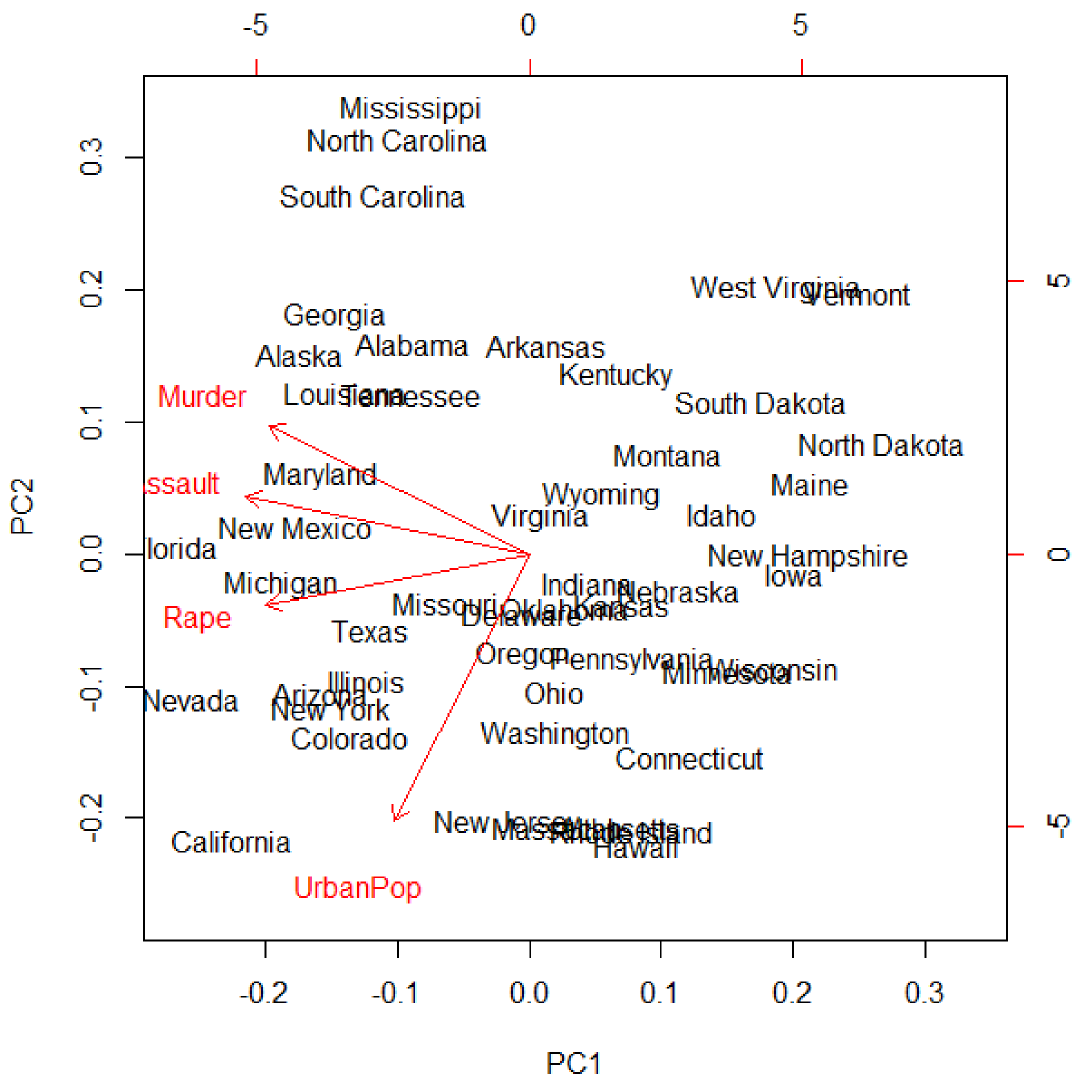
CLUSTERING

0. Review of principal components – another unsupervised learning method

```
> attach(USArrests)
```

This data set contains statistics, in arrests per 100,000 residents for assault, murder, and rape in each of the 50 US states in 1973. Also given is the percent of the population living in urban areas.

```
> names(USArrests)
[1] "Murder"   "Assault"  "UrbanPop" "Rape"

> pc = prcomp(USArrests, scale=TRUE)
> biplot(pc)
```



Red vectors are projections of the original X-variables on the space of the first two principal components. We can see that the first principal component Z_1 mostly represents the combined crime rate, and the second principal component Z_2 mostly represents the level of urbanization.

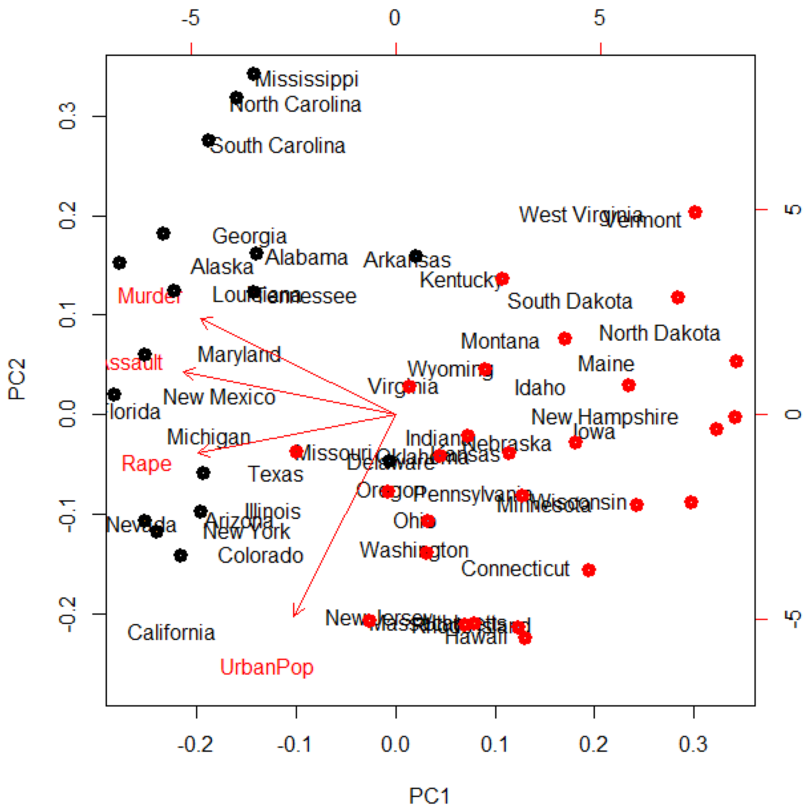
1. K-means method

Now we use K-means clustering to find more homogeneous groups among the states.
Let's start with K=2 clusters. The 50 states are partitioned into 2 groups, Cluster 1 with 21 and Cluster 2 with 29 states.

```
> KM2 = kmeans(X,2)
> KM2
K-means clustering with 2 clusters of sizes 21, 29

Cluster means:
    Murder  Assault UrbanPop     Rape
1 11.857143 255.0000 67.61905 28.11429
2  4.841379 109.7586 64.03448 16.24828

Clustering vector:
     Alabama       Alaska      Arizona     Arkansas   California
           1            1            1            1            1
    Colorado  Connecticut     Delaware      Florida      Georgia
           1            2            1            1            1
      Hawaii        Idaho     Illinois      Indiana         Iowa
           2            2            1            2            2
      Kansas     Kentucky    Louisiana        Maine     Maryland
           2            2            1            2            1
Massachusetts     Michigan    Minnesota  Mississippi     Missouri
           2            1            2            1            2
     Montana     Nebraska       Nevada New Hampshire   New Jersey
           2            2            1            2            2
  New Mexico     New York North Carolina North Dakota         Ohio
           1            1            1            2            2
    Oklahoma       Oregon Pennsylvania Rhode Island South Carolina
           2            2            2            2            1
South Dakota    Tennessee        Texas         Utah      Vermont
           2            1            1            2            2
    Virginia   Washington West Virginia   Wisconsin      Wyoming
           2            2            2            2            2

Within cluster sum of squares by cluster:
[1] 41636.73 54762.30
 (between_SS / total_SS =  72.9 %)
```

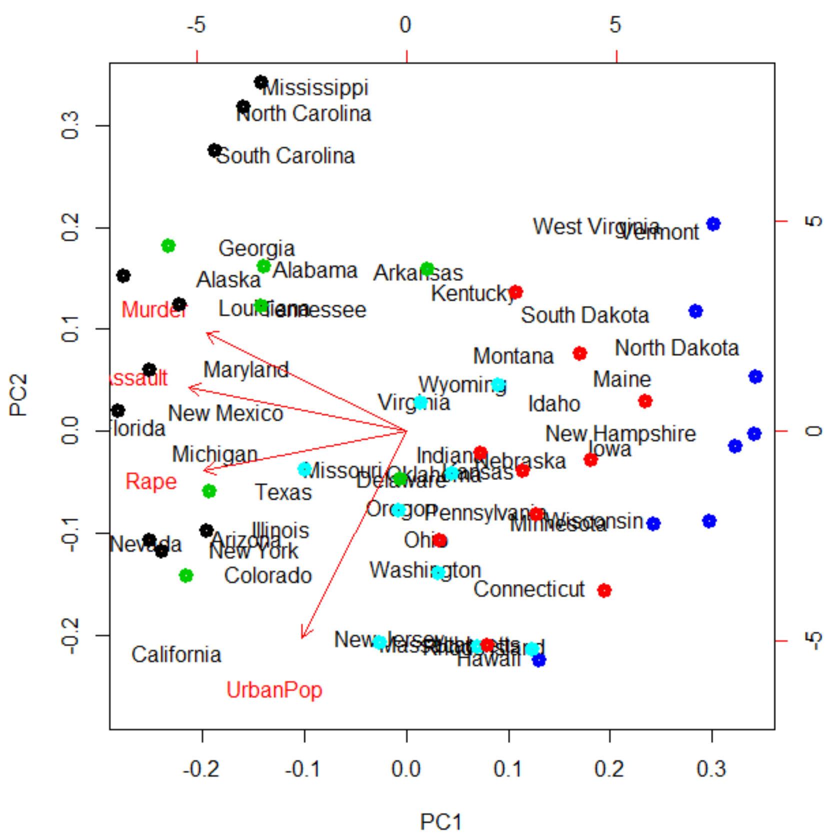
Let's look at the position of these clusters on our biplot. There is a discrepancy of scales in biplot, so I am using a coefficient 3.5, to match points to state names.

```
> points(3.5*pc$x[,1], 3.5*pc$x[,2], col=KM2$cluster, lwd=5)
```



Use more clusters?

```
> KM5 = kmeans(X,5)
> points(3.5*pc$x[,1], 3.5*pc$x[,2], col=KM5$cluster, lwd=5)
```



2. Hierarchical Clustering and Dendrogram

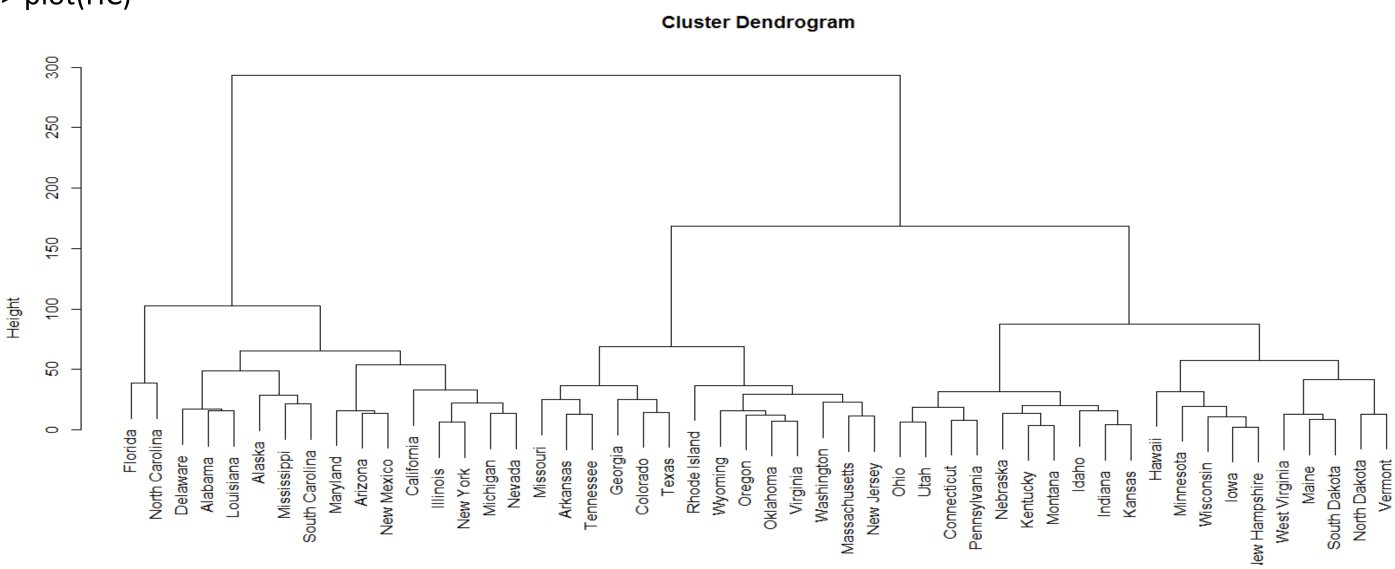
So, how many clusters should be used? We can apply the hierarchical clustering algorithm, which does not require to pre-specify the number of clusters.

> HC = hclust(dist(X), method="complete")

Here, "dist" stays for distance between multivariate observations, and method can be "complete", "single", "average", "median", etc. – it is a method of determining similarity with clusters and dissimilarity between clusters.

We can see the *dendrogram* that this method has created.

> plot(HC)



We then cut the tree at some level and create clusters.

> cutree(HC,5)

```
   Alabama       Alaska      Arizona     Arkansas    California
        1            1            1            2            1
  Colorado   Connecticut     Delaware      Florida       Georgia
        2            3            1            4            2
    Hawaii        Idaho     Illinois      Indiana          Iowa
        5            3            1            3            5
    Kansas     Kentucky    Louisiana        Maine      Maryland
        3            3            1            5            1
Massachusetts   Michigan    Minnesota  Mississippi     Missouri
        2            1            5            1            2
   Montana     Nebraska       Nevada  New Hampshire   New Jersey
        3            3            1            5            2
 New Mexico     New York North Carolina  North Dakota       Ohio
        1            1            4            5            3
  Oklahoma       Oregon  Pennsylvania  Rhode Island South Carolina
        2            2            3            2            1
South Dakota   Tennessee       Texas         Utah       Vermont
        5            2            2            3            5
  Virginia   Washington  West Virginia   Wisconsin      Wyoming
        2            2            5            5            2
```

3. College data - K-means method

Our task will be to cluster Colleges into more homogeneous groups.

```
> attach(College);   names(College)
 [1] "Private"     "Apps"        "Accept"      "Enroll"      "Top10perc"   "Top25perc"   "F.Undergrad" "P.Undergrad" "Outstate"
"Room.Board"
[11] "Books"       "Personal"    "PhD"         "Terminal"    "S.F.Ratio"   "perc.alumni" "Expend"      "Grad.Rate"
```

We need to create a matrix of numeric variables. We've used this command to prepare data for LASSO.

```
> X = model.matrix( Private ~ . + as.numeric(Private), data=College )
> dim(X)
[1] 777  19
> head(X)
```

Instead of printing the entire matrix, "head" only shows the first few rows

```
                             (Intercept) Apps Accept Enroll Top10perc Top25perc F.Undergrad P.Undergrad Outstate
Room.Board Books Personal PhD
Abilene Christian University           1 1660   1232    721        23        52        2885         537     7440
3300    450      2200  70
Adelphi University                     1 2186   1924    512        16        29        2683        1227    12280
6450    750      1500  29
Adrian College                         1 1428   1097    336        22        50        1036          99    11250
3750    400      1165  53
Agnes Scott College                    1  417    349    137        60        89         510          63    12960
5450    450       875  92
Alaska Pacific University              1  193    146     55        16        44         249         869     7560
4120    800      1500  76
Albertson College                      1  587    479    158        38        62         678          41    13500
3335    500       675  67
                             Terminal S.F.Ratio perc.alumni Expend Grad.Rate as.numeric(Private)
Abilene Christian University       78      18.1          12   7041        60                   2
Adelphi University                 30      12.2          16  10527        56                   2
Adrian College                     66      12.9          30   8735        54                   2
Agnes Scott College                97       7.7          37  19016        59                   2
Alaska Pacific University          72      11.9           2  10922        15                   2
Albertson College                  73       9.4          11   9727        55                   2
```

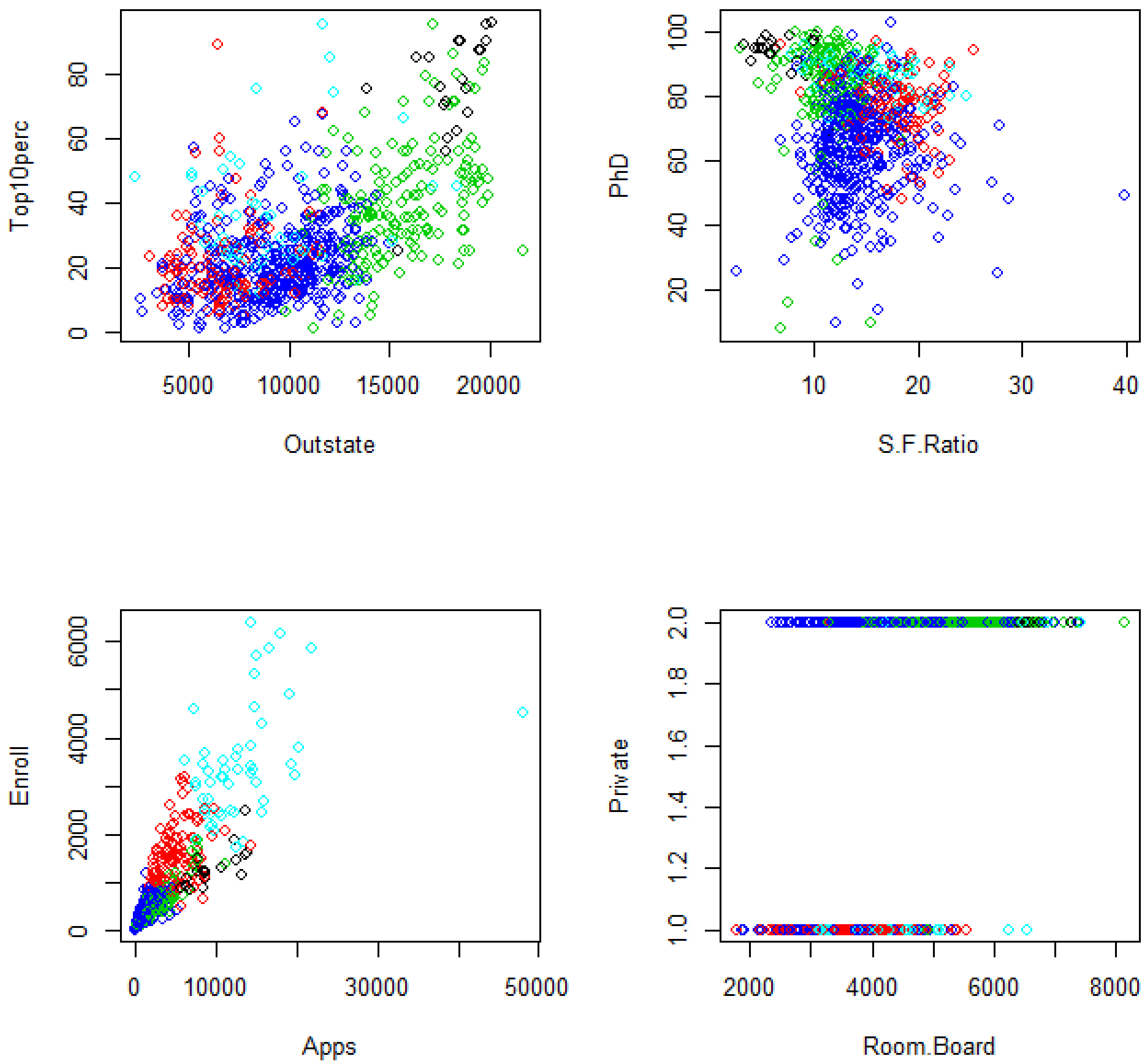
Now, let's create K=5 clusters by the K-means method. No new library is needed, this command comes with basic R.

```
> KM5 = kmeans( X, 5 )

>  KM5
K-means clustering with 5 clusters of sizes 20, 113, 162, 431, 51

Cluster means:
  (Intercept)      Apps    Accept    Enroll Top10perc Top25perc F.Undergrad P.Undergrad
Outstate Room.Board    Books Personal      PhD Terminal
1           1  9341.750 3606.2500 1321.9500  76.05000  91.70000    5283.200    427.2000
18119.750   6042.750 576.6000 1255.550 93.30000 96.80000
2           1  5012.602 3410.1150 1526.5310  21.56637  52.28319    8021.566   2111.3097
6709.283   3703.912 557.1416 1727.186 77.01770 83.65487
3           1  2566.364 1712.7901  521.5123  39.83333  68.96914    2067.241    282.4444
15732.512   5257.864 578.0926 1042.772 83.31481 90.24074
4           1  1140.610  869.9258  341.7007  21.40371  48.75638    1434.332    475.6450
9263.759   4110.290 530.1206 1299.220 65.03016 72.61717
5           1 13169.804 8994.7647 3438.1176  34.84314  67.15686   17836.020   3268.3529
8833.510   4374.353 593.0784 1813.784 85.54902 90.64706

  S.F.Ratio perc.alumni    Expend Grad.Rate as.numeric(Private)
1   6.61500    35.35000 32347.900  88.95000            2.000000
2  17.46903    14.02655  7067.257  54.91150            1.079646
3  11.43333    32.76543 13728.735  76.64198            1.993827
4  14.32343    21.36659  7677.035  63.13225            1.856148
```

```
5  15.99608    16.92157 10343.882  63.82353           1.117647

Clustering vector:
                 Abilene Christian University                            Adelphi
University                                Adrian College
                                            4
3                                             4
                          Agnes Scott College                     Alaska Pacific
University                             Albertson College
                                            3
4                                             4
                      Albertus Magnus College                              Albion
College                              Albright College
                                            4
3                                             3
                    Alderson-Broaddus College                              Alfred
University                             Allegheny College
                                            4
3                                             3

<truncated>

Within cluster sum of squares by cluster:
[1] 2115931982 3262290091 3917614114 5524699694 5934672728
 (between_SS / total_SS =  71.2 %)

Available components:

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

We can see the cluster assignment (truncated), multivariate cluster means (centroids), within and between sums of squares as measures of cluster purity. To explore the obtained clusters, we can plot some pairs of variables along with the assigned clusters:

```
> par(mfrow=c(2,2))
> plot( Outstate, Top10perc, col=KM5$cluster )
> plot( S.F.Ratio, PhD, col=KM5$cluster )
> plot( Apps, Enroll, col=KM5$cluster )
> plot( Room.Board, Private, col=KM5$cluster )
```



For example, we can see here that the green cluster consists of rather expensive and relatively small private colleges with a high percent of PhD degrees among faculty and small class sizes because of a low student-to-faculty ratio.

4. College data - Hierarchical Clustering

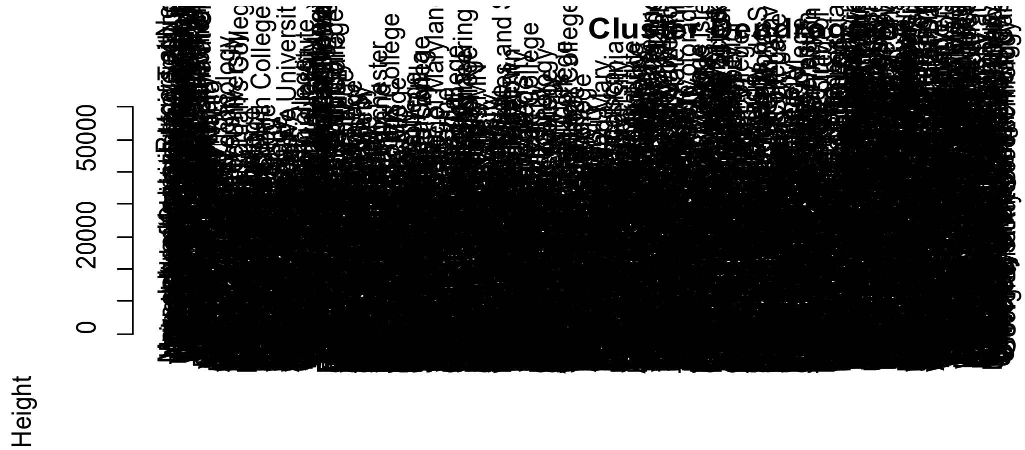
Without specifying the number K of clusters, apply hierarchical clustering algorithm to the College data.

> HC = hclust(dist(X), method="complete")

Here, "dist" stays for distance between multivariate observations, and method can be "complete", "single", "average", "median", etc. – it is a method of determining similarity with clusters and dissimilarity between clusters.

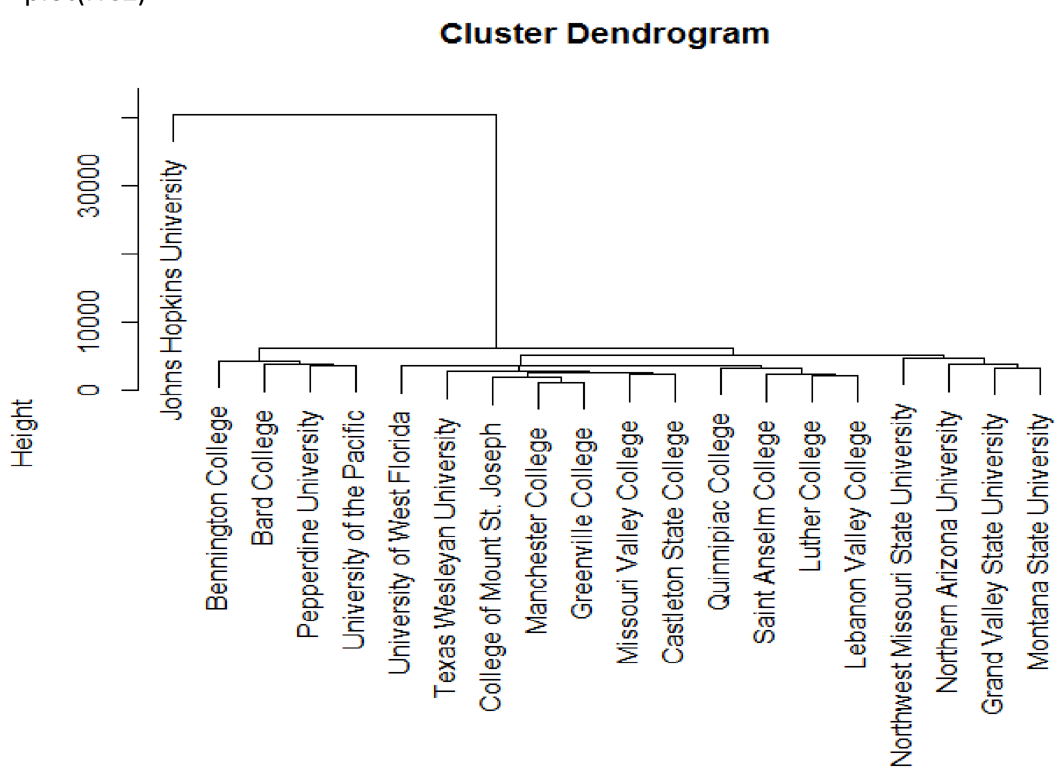
The full dendrogram with so many leafs would not be legible.

> plot(HC)



To illustrate the method, let's take a small random sample of colleges and cluster them hierarchically.

```
> Z = sample(n,20)
> Y = X[Z,]
> HCZ = hclust( dist(Y), method="complete" )
> plot(HCZ)
```



We can choose where to "cut" this tree to create clusters. For example, we let's create 4 clusters.

```
> HC4 = cutree(HC, k = 4)
> HC4
   Christian Brothers University      Nazareth College of Rochester
                               1                                  1
             Sweet Briar College                  Dartmouth College
                               1                                  2
                  Eckerd College      Appalachian State University
                               1                                  3
```

< truncated >

So, we get assignments of colleges into clusters.