Unsupersived Learning

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R Markdown

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When you click the **Knit** button a document will be generated that includes both content as well as the output of any embedded R code chunks within the document. You can embed an R code chunk like this:

```r
states <- row.names(USArrests)
states
```

```
##  [1] "Alabama"        "Alaska"         "Arizona"        "Arkansas"
##  [5] "California"     "Colorado"       "Connecticut"    "Delaware"
##  [9] "Florida"        "Georgia"        "Hawaii"         "Idaho"
## [13] "Illinois"       "Indiana"        "Iowa"           "Kansas"
## [17] "Kentucky"       "Louisiana"      "Maine"          "Maryland"
## [21] "Massachusetts"  "Michigan"       "Minnesota"      "Mississippi"
## [25] "Missouri"       "Montana"        "Nebraska"       "Nevada"
## [29] "New Hampshire"  "New Jersey"     "New Mexico"     "New York"
## [33] "North Carolina" "North Dakota"   "Ohio"           "Oklahoma"
## [37] "Oregon"         "Pennsylvania"   "Rhode Island"   "South Carolina"
## [41] "South Dakota"   "Tennessee"      "Texas"          "Utah"
## [45] "Vermont"        "Virginia"       "Washington"     "West Virginia"
## [49] "Wisconsin"      "Wyoming"
```

```r
names(USArrests)
```

```
## [1] "Murder"   "Assault"  "UrbanPop" "Rape"
```

```r
apply(USArrests, 2, mean)
```

```
##   Murder  Assault UrbanPop     Rape
##    7.788  170.760   65.540   21.232
```

```r
apply(USArrests, 2, var)
```

```
##     Murder    Assault   UrbanPop       Rape
##   18.97047 6945.16571  209.51878   87.72916
```

We run PCA on our dataset using the prcomp() function.

```
pr.out <- prcomp(USArrests, scale = TRUE)
```

Now lets examing the results from The prcomp() function.

```
names(pr.out)
```

```
## [1] "sdev"     "rotation" "center"   "scale"    "x"
```

The center and scale components contain the mean and standard deviations prior to scaling.

```
pr.out$center
```

```
##   Murder  Assault UrbanPop     Rape 
##    7.788  170.760   65.540   21.232
```

```
pr.out$scale
```

```
##    Murder   Assault  UrbanPop      Rape 
##  4.355510 83.337661 14.474763  9.366385
```

The rotation component correspondes to the rotation matrix whose columns contain the eigenvectors.

```
pr.out$rotation
```

```
##                 PC1        PC2        PC3         PC4
## Murder   -0.5358995  0.4181809 -0.3412327  0.64922780
## Assault  -0.5831836  0.1879856 -0.2681484 -0.74340748
## UrbanPop -0.2781909 -0.8728062 -0.3780158  0.13387773
## Rape     -0.5434321 -0.1673186  0.8177779  0.08902432
```

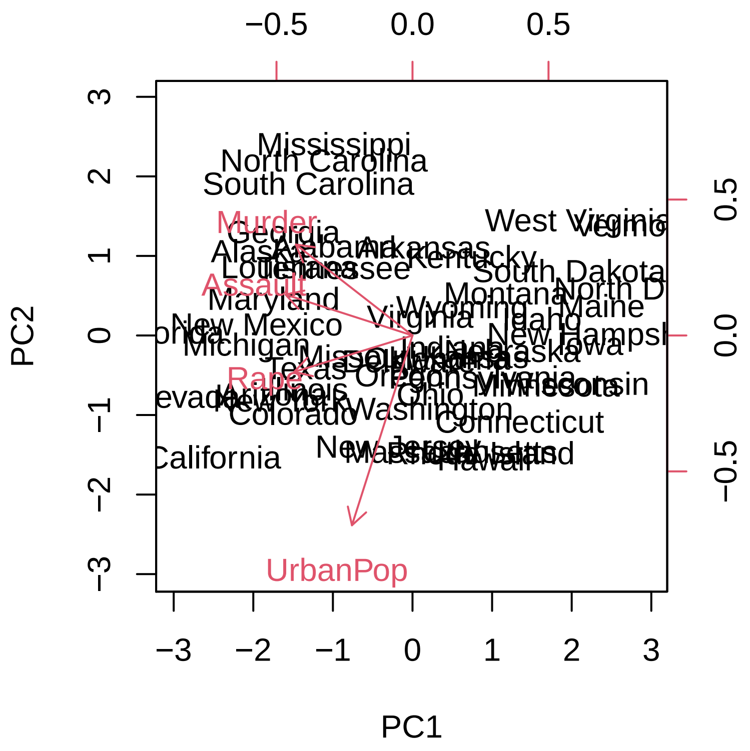
Let's check the dimentions of x component which returns the rotated data.

```
dim(pr.out$x)
```

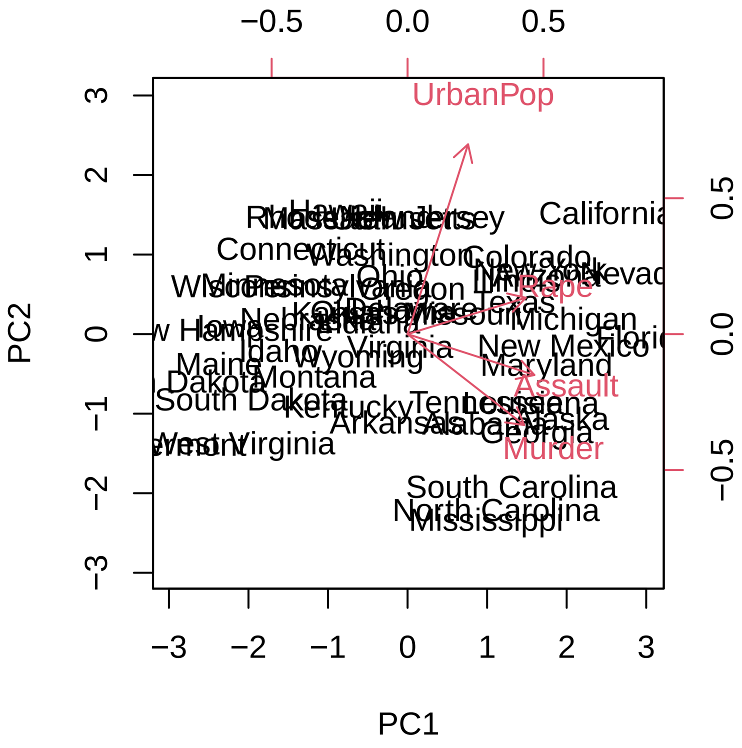
```
## [1] 50  4
```

We then plot the first two principal components using biplot().

```
biplot(pr.out, scale = 0)
```



```
pr.out$rotation <- -pr.out$rotation
pr.out$x <- -pr.out$x
biplot(pr.out, scale = 0)
```



We can compute the variance associated with each principal component from the standard deviation returned by prcomp().

```
pr.out$sdev
```

```
## [1] 1.5748783 0.9948694 0.5971291 0.4164494
```

```
pr.var <- pr.out$sdev^2
pr.var
```

```
## [1] 2.4802416 0.9897652 0.3565632 0.1734301
```

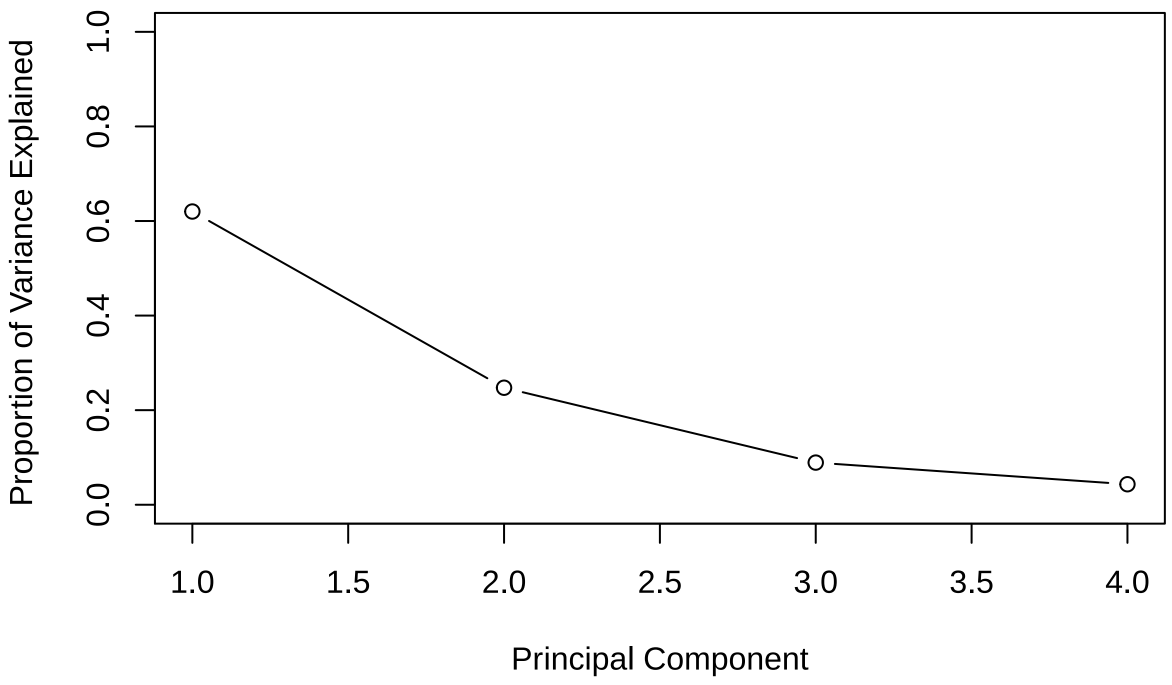
Let's compute the proportional variance as well.

```
pve <- pr.var/sum(pr.var)
pve
```

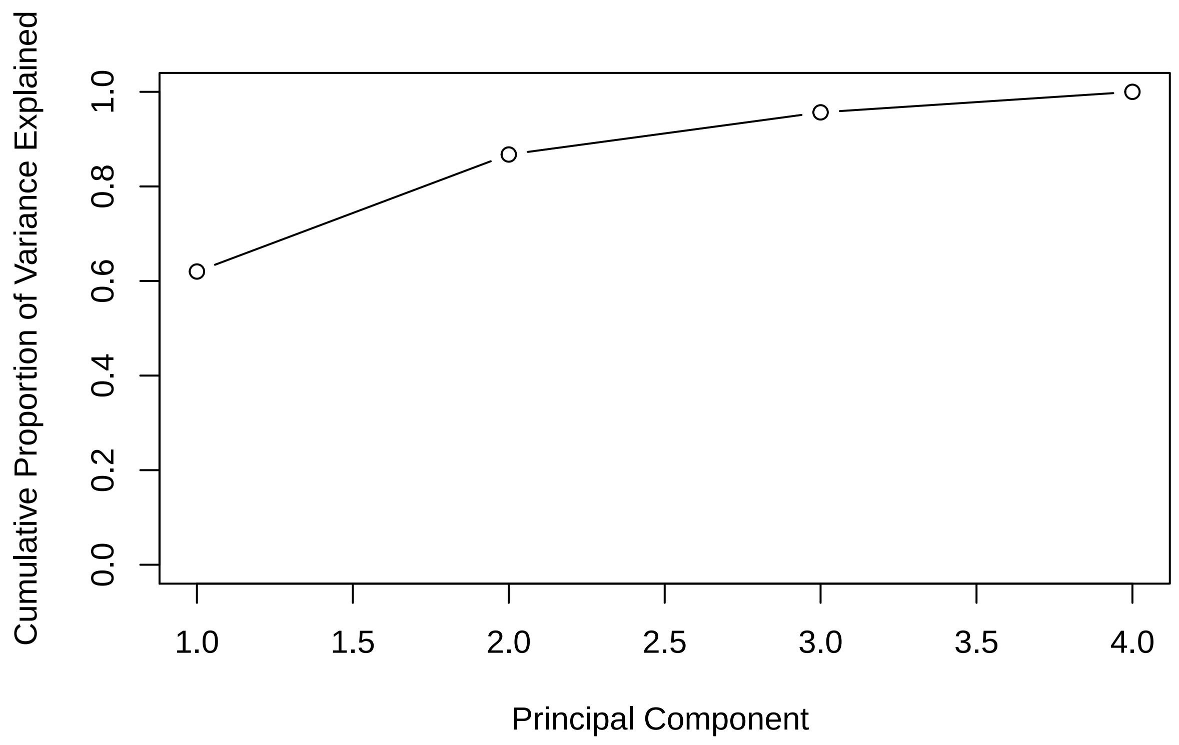
```
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
```

Now we can plot the proportional variance for each principal component.

```
plot(pve, xlab = "Principal Component", ylab = "Proportion of Variance Explained ", ylim = c(0, 1), typ
```



```r
plot(cumsum(pve), xlab = "Principal Component ", ylab = " Cumulative Proportion of Variance Explained "
```



```r
a <- c(1, 2, 8, -3)
cumsum(a)
```

```
## [1]  1  3 11  8
```

##Clustering##

##K-Means Clustering##

In this exercise we use K-Means clustering on randomly generated data using the kmeans() function.

```r
set.seed(2)
x <- matrix(rnorm(50 * 2), ncol = 2)
x[1:25, 1] <- x[1:25, 1] + 3
x[1:25, 2] <- x[1:25, 2] - 4
```

Let's start by clustering the data into two clusters with K = 2.

```r
km.out <- kmeans(x, 2, nstart = 20)
```

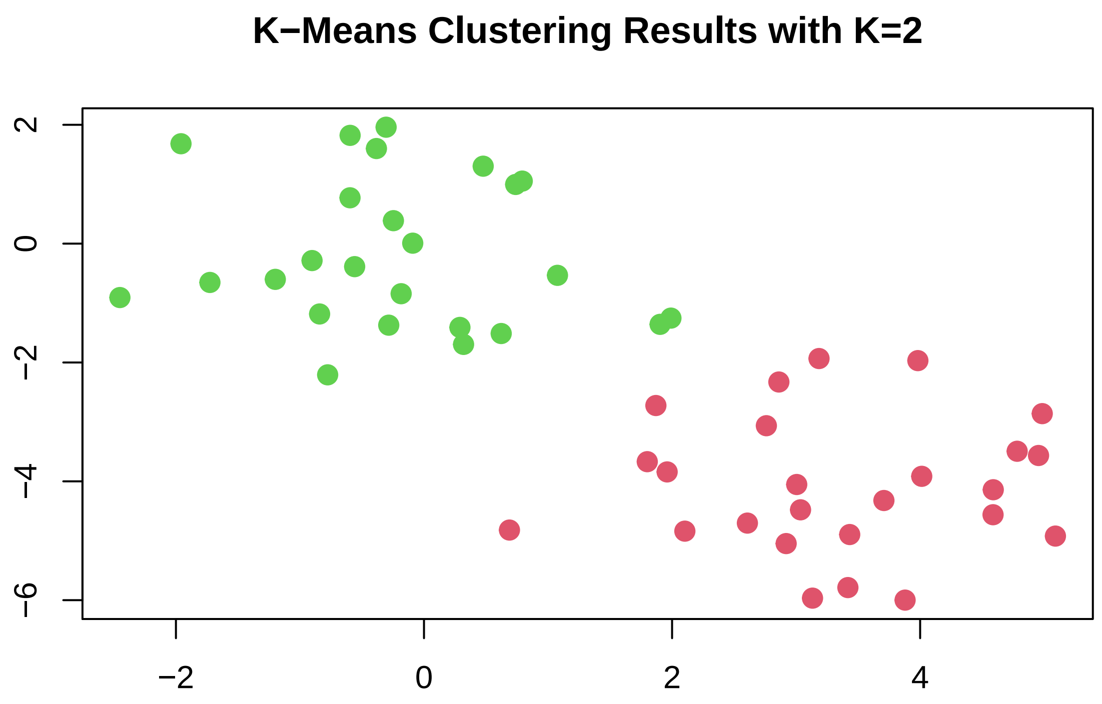
The kmeans() function returns the cluster assignments in the cluster component.

```r
km.out$cluster
```

```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 2 2 2 2 2 2 2
```

Now let's plot the clusters.

```
plot(x, col = (km.out$cluster + 1), main = "K-Means Clustering Results with K=2", xlab = "", ylab = "",
```



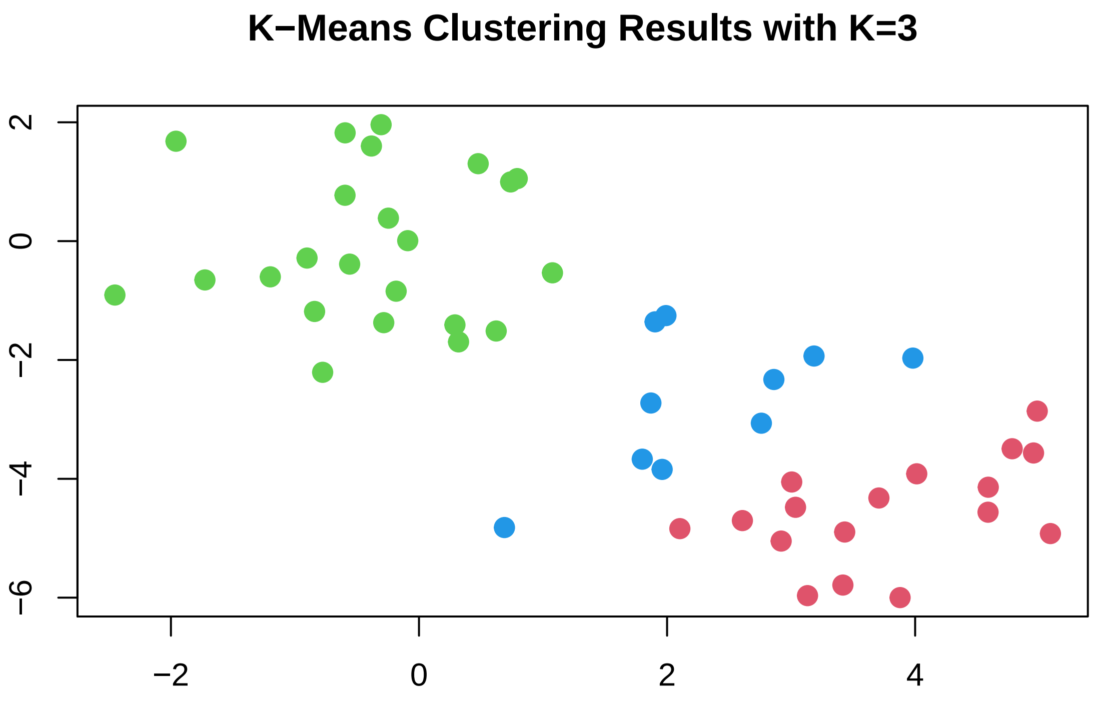
We can run K-means with different values for the number of clusters such as K = 3 and plot the results.

```
set.seed(4)
km.out <- kmeans(x, 3, nstart = 20)
km.out
```

```
## K-means clustering with 3 clusters of sizes 17, 23, 10
##
## Cluster means:
##         [,1]        [,2]
## 1  3.7789567 -4.56200798
## 2 -0.3820397 -0.08740753
## 3  2.3001545 -2.69622023
##
## Clustering vector:
##  [1] 1 3 1 3 1 1 1 3 1 3 1 3 1 3 1 3 1 1 1 1 1 3 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 3 2 3 2 2 2 2
##
## Within cluster sum of squares by cluster:
## [1] 25.74089 52.67700 19.56137
##  (between_SS / total_SS =  79.3 %)
##
```

```
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

```
plot(x, col = (km.out$cluster + 1), main = "K-Means Clustering Results with K=3", xlab = "", ylab = "",
```



We can control the initial cluster assignments with the nstart argument to kmeans().

```
set.seed(3)
km.out <- kmeans(x, 3, nstart = 1)
km.out$tot.withinss
```

```
## [1] 97.97927
```

```
km.out <- kmeans(x, 3, nstart = 20)
km.out$tot.withinss
```

```
## [1] 97.97927
```

##Hierarchical Clustering##

We can use hierarchical clustering on the dataset we generated in the previous exercise using the hclust() function.

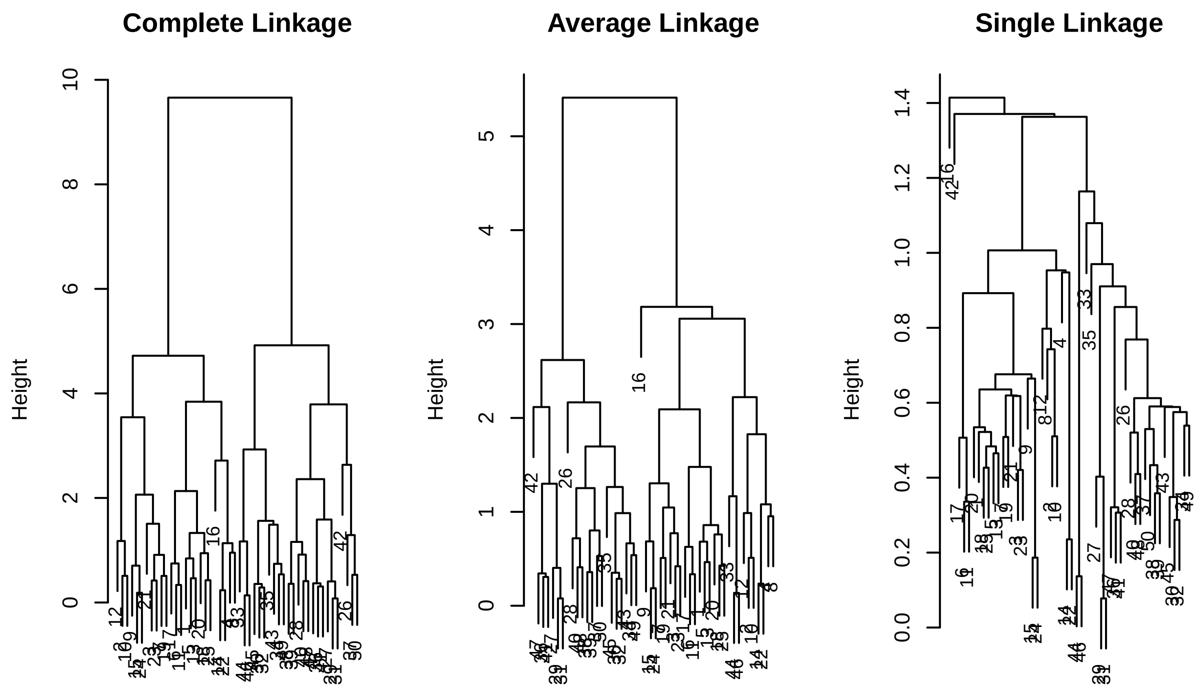
```
hc.complete <- hclust(dist(x), method = "complete")
```

The hclust() function supports various agglomeration methods including “single”, “complete”, and “average” linkages.

```
hc.average <- hclust(dist(x), method = "average")
hc.single <- hclust(dist(x), method = "single")
```

We can compare the different linkages by plotting the results obtained with different methods.

```
par(mfrow = c(1, 3))
plot(hc.complete, main = "Complete Linkage", xlab = "", sub = "", cex = 0.9)
plot(hc.average, main = "Average Linkage", xlab = "", sub = "", cex = 0.9)
plot(hc.single, main = "Single Linkage", xlab = "", sub = "", cex = 0.9)
```



We can cut the tree into different groups using the cutree() function.

```
cutree(hc.complete, 2)
```

```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2
## [39] 2 2 2 2 2 2 2 2 2 2 2 2
```

```
cutree(hc.average, 2)
```

```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 1 2 2 2 2 2
## [39] 2 2 2 2 2 1 2 1 2 2 2 2
```

```
cutree(hc.single, 2)
```

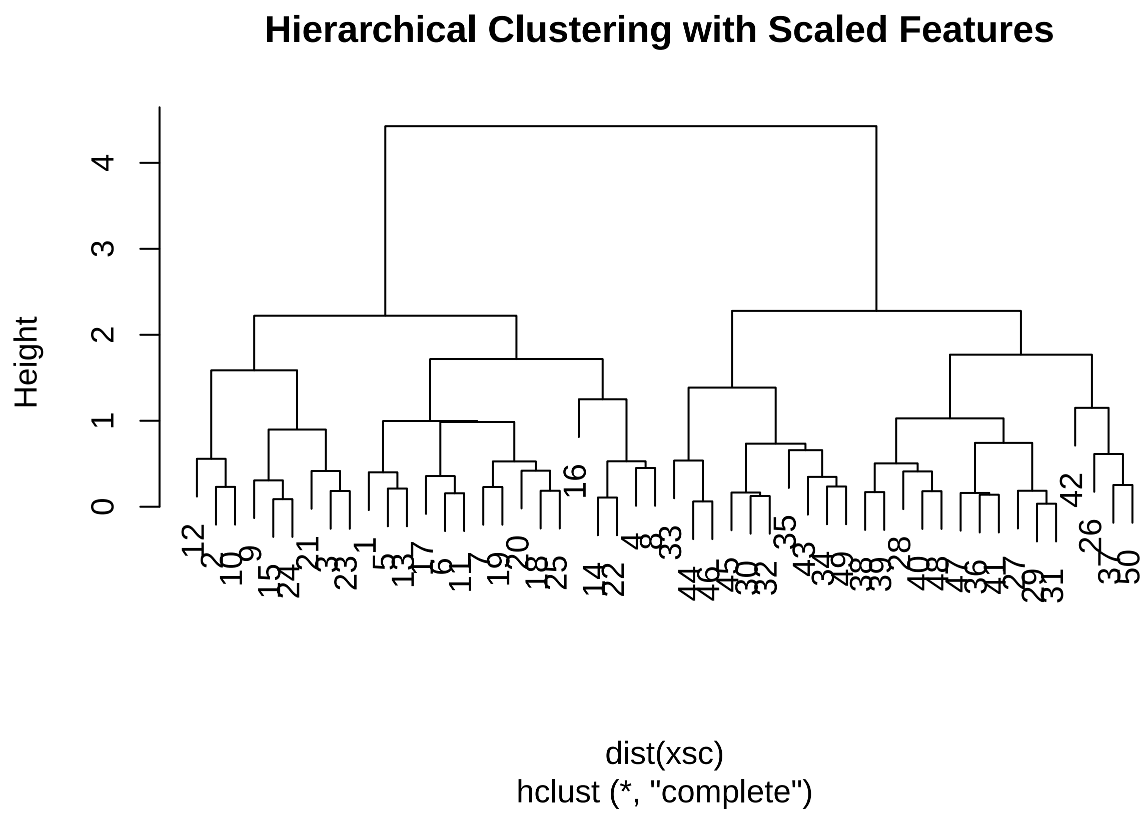
```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [39] 1 1 1 1 1 1 1 1 1 1 1 1
```

```
cutree(hc.single, 4)
```

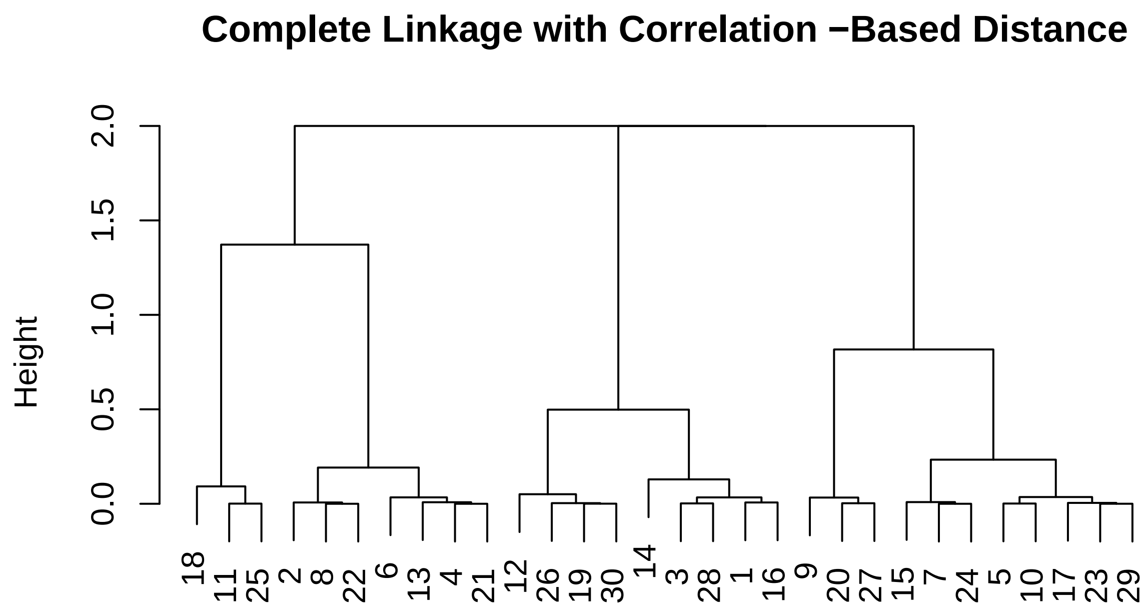
```
##  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 3 3 3 3 3 3 3 3 3 3 3 3 3
## [39] 3 3 3 4 3 3 3 3 3 3 3 3
```

We can scale the dataset before it to the clustering algorithm by first calling scale().

```
xsc <- scale(x)
plot(hclust(dist(xsc), method = "complete"), main = "Hierarchical Clustering with Scaled Features ")
```



```
x <- matrix(rnorm(30 * 3), ncol = 3)
dd <- as.dist(1 - cor(t(x)))
plot(hclust(dd, method = "complete"), main = "Complete Linkage with Correlation -Based Distance", xlab
```



next example

```
library(ISLR)
nci.labs <- NCI60$labs
nci.data <- NCI60$data
```

```
dim(nci.data)
```

```
## [1]   64 6830
```

The table() function can be used to produce crosstabs from the dataset.

```
nci.labs[1:4]
```

```
## [1] "CNS"    "CNS"    "CNS"    "RENAL"
```

```
table(nci.labs)
```

```
## nci.labs
##      BREAST         CNS       COLON K562A-repro K562B-repro    LEUKEMIA
##           7           5           7           1           1           6
## MCF7A-repro MCF7D-repro    MELANOMA       NSCLC     OVARIAN    PROSTATE
##            1           1           8           9           6           2
##        RENAL     UNKNOWN
##            9           1
```

PCA on the NCI60 Data

We use prcomp() to run principal component analysis as shown in the PCA exercise above.

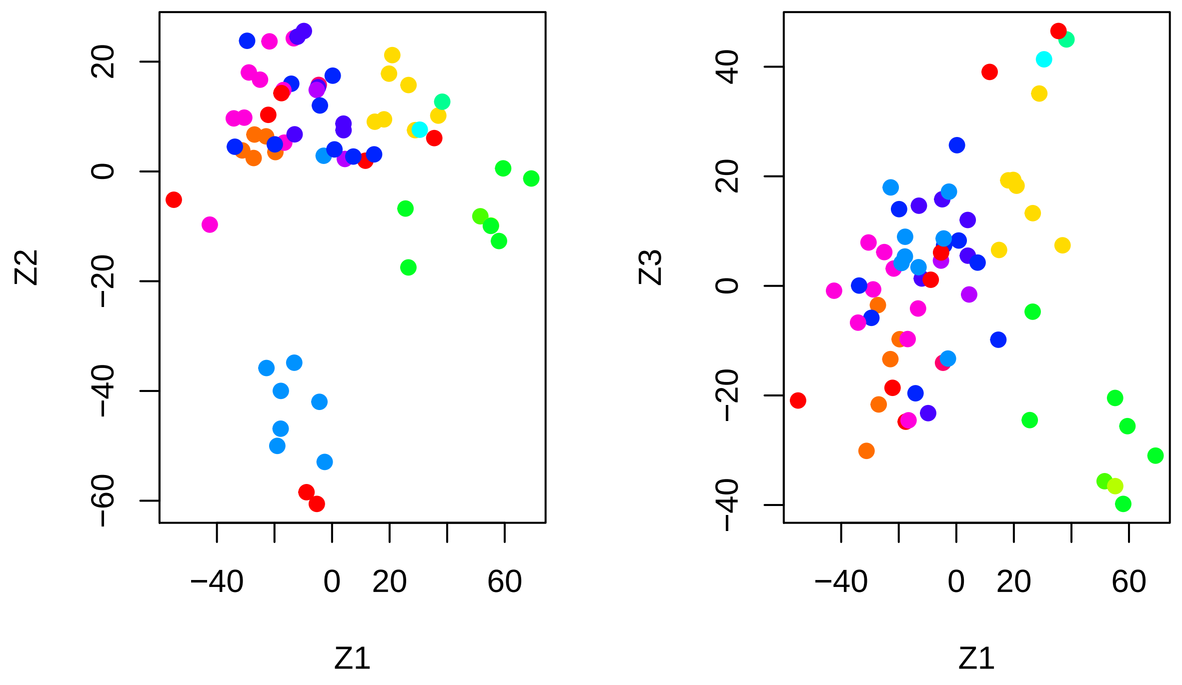
```
pr.out <- prcomp(nci.data, scale = TRUE)
```

We create a function to assign unique colors to each cancer type.

```
Cols <- function(vec) {
    cols <- rainbow(length(unique(vec)))
    return(cols[as.numeric(as.factor(vec))])
}
```

We can now use our Cols() function to plot the PCA results.

```
par(mfrow = c(1, 2))
plot(pr.out$x[, 1:2], col = Cols(nci.labs), pch = 19, xlab = "Z1", ylab = "Z2")
plot(pr.out$x[, c(1, 3)], col = Cols(nci.labs), pch = 19, xlab = "Z1", ylab = "Z3")
```

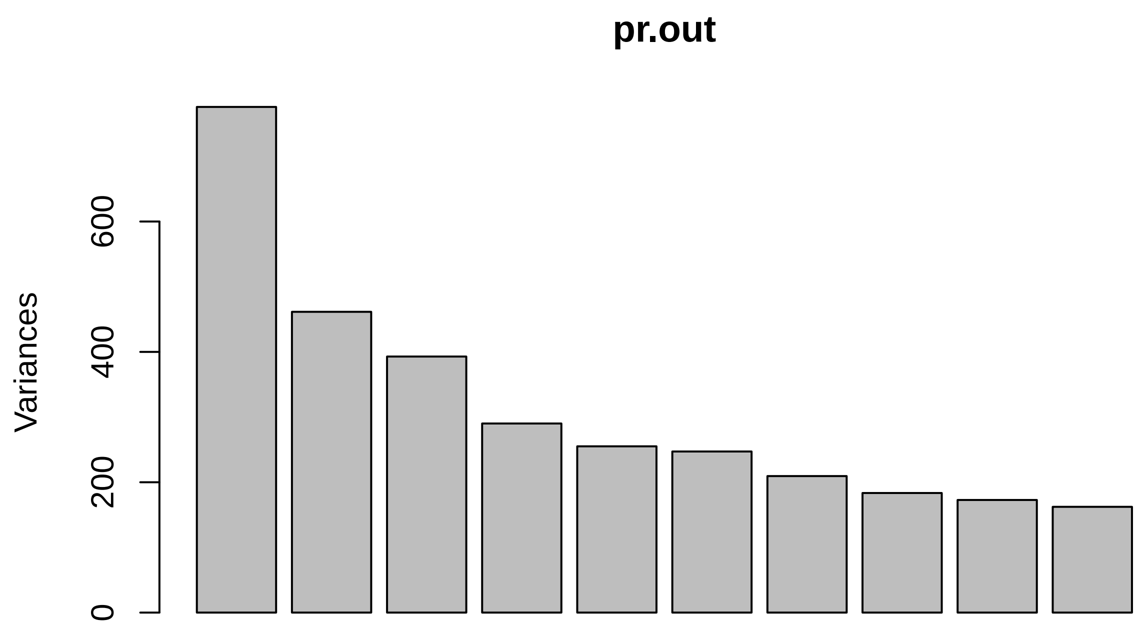


We can get a summary of the proportional variance and plot the variance explained by each principal component.

```
summary(pr.out)
```

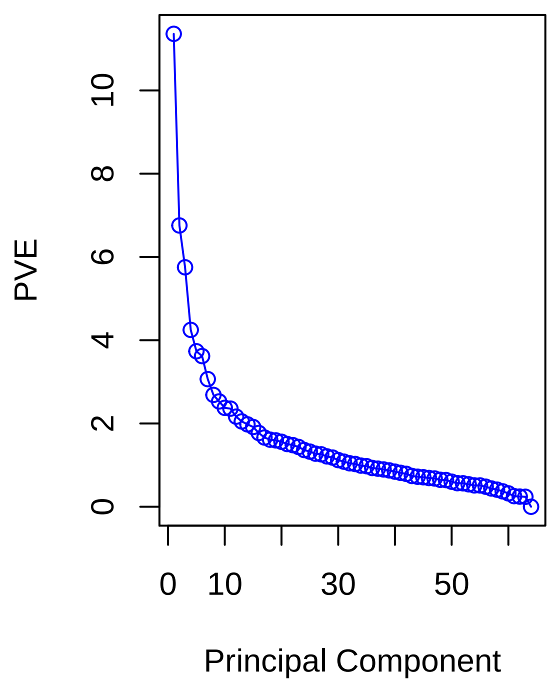
```
## Importance of components:
##                            PC1      PC2      PC3      PC4      PC5      PC6
## Standard deviation     27.8535 21.48136 19.82046 17.03256 15.97181 15.72108
## Proportion of Variance  0.1136  0.06756  0.05752  0.04248  0.03735  0.03619
## Cumulative Proportion   0.1136  0.18115  0.23867  0.28115  0.31850  0.35468
##                             PC7      PC8      PC9     PC10     PC11     PC12
## Standard deviation     14.47145 13.54427 13.14400 12.73860 12.68672 12.15769
## Proportion of Variance  0.03066  0.02686  0.02529  0.02376  0.02357  0.02164
## Cumulative Proportion   0.38534  0.41220  0.43750  0.46126  0.48482  0.50646
##                            PC13     PC14     PC15     PC16     PC17     PC18
## Standard deviation     11.83019 11.62554 11.43779 11.00051 10.65666 10.48880
## Proportion of Variance  0.02049  0.01979  0.01915  0.01772  0.01663  0.01611
## Cumulative Proportion   0.52695  0.54674  0.56590  0.58361  0.60024  0.61635
##                            PC19    PC20     PC21    PC22    PC23    PC24
## Standard deviation     10.43518 10.3219 10.14608 10.0544 9.90265 9.64766
## Proportion of Variance  0.01594  0.0156  0.01507  0.0148 0.01436 0.01363
## Cumulative Proportion   0.63229  0.6479  0.66296  0.6778 0.69212 0.70575
##                           PC25    PC26    PC27   PC28    PC29    PC30    PC31
## Standard deviation     9.50764 9.33253 9.27320 9.0900 8.98117 8.75003 8.59962
## Proportion of Variance 0.01324 0.01275 0.01259 0.0121 0.01181 0.01121 0.01083
## Cumulative Proportion  0.71899 0.73174 0.74433 0.7564 0.76824 0.77945 0.79027
##                           PC32    PC33    PC34    PC35    PC36    PC37    PC38
## Standard deviation     8.44738 8.37305 8.21579 8.15731 7.97465 7.90446 7.82127
## Proportion of Variance 0.01045 0.01026 0.00988 0.00974 0.00931 0.00915 0.00896
## Cumulative Proportion  0.80072 0.81099 0.82087 0.83061 0.83992 0.84907 0.85803
##                           PC39    PC40    PC41   PC42    PC43   PC44    PC45
## Standard deviation     7.72156 7.58603 7.45619 7.3444 7.10449 7.0131 6.95839
## Proportion of Variance 0.00873 0.00843 0.00814 0.0079 0.00739 0.0072 0.00709
## Cumulative Proportion  0.86676 0.87518 0.88332 0.8912 0.89861 0.9058 0.91290
##                          PC46    PC47    PC48    PC49    PC50    PC51    PC52
## Standard deviation     6.8663 6.80744 6.64763 6.61607 6.40793 6.21984 6.20326
## Proportion of Variance 0.0069 0.00678 0.00647 0.00641 0.00601 0.00566 0.00563
## Cumulative Proportion  0.9198 0.92659 0.93306 0.93947 0.94548 0.95114 0.95678
##                           PC53    PC54    PC55    PC56    PC57   PC58    PC59
## Standard deviation     6.06706 5.91805 5.91233 5.73539 5.47261 5.2921 5.02117
## Proportion of Variance 0.00539 0.00513 0.00512 0.00482 0.00438 0.0041 0.00369
## Cumulative Proportion  0.96216 0.96729 0.97241 0.97723 0.98161 0.9857 0.98940
##                           PC60    PC61    PC62    PC63      PC64
## Standard deviation     4.68398 4.17567 4.08212 4.04124 2.148e-14
## Proportion of Variance 0.00321 0.00255 0.00244 0.00239 0.000e+00
## Cumulative Proportion  0.99262 0.99517 0.99761 1.00000 1.000e+00
```

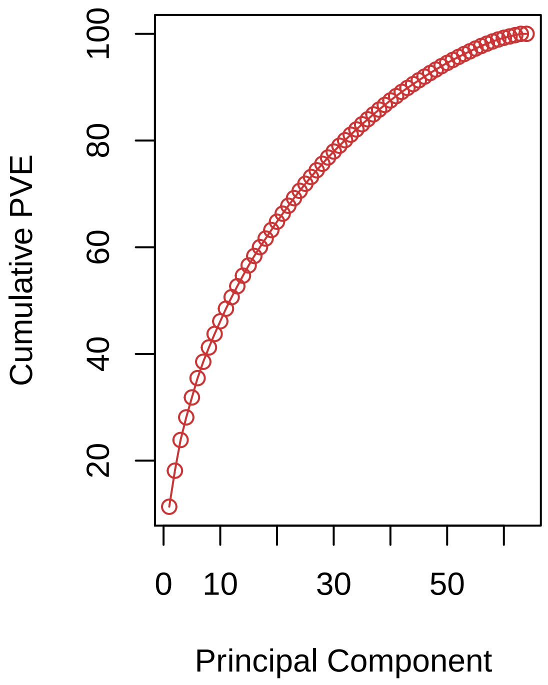
```
plot(pr.out)
```



We can also plot the proportional variance explained (PVE) and the cummulative PVE for each principal component.

```r
pve <- 100 * pr.out$sdev^2/sum(pr.out$sdev^2)
par(mfrow = c(1, 2))
plot(pve, type = "o", ylab = "PVE", xlab = "Principal Component", col = " blue ")
plot(cumsum(pve), type = "o", ylab = "Cumulative PVE", xlab = "Principal Component ", col = " brown3 ")
```





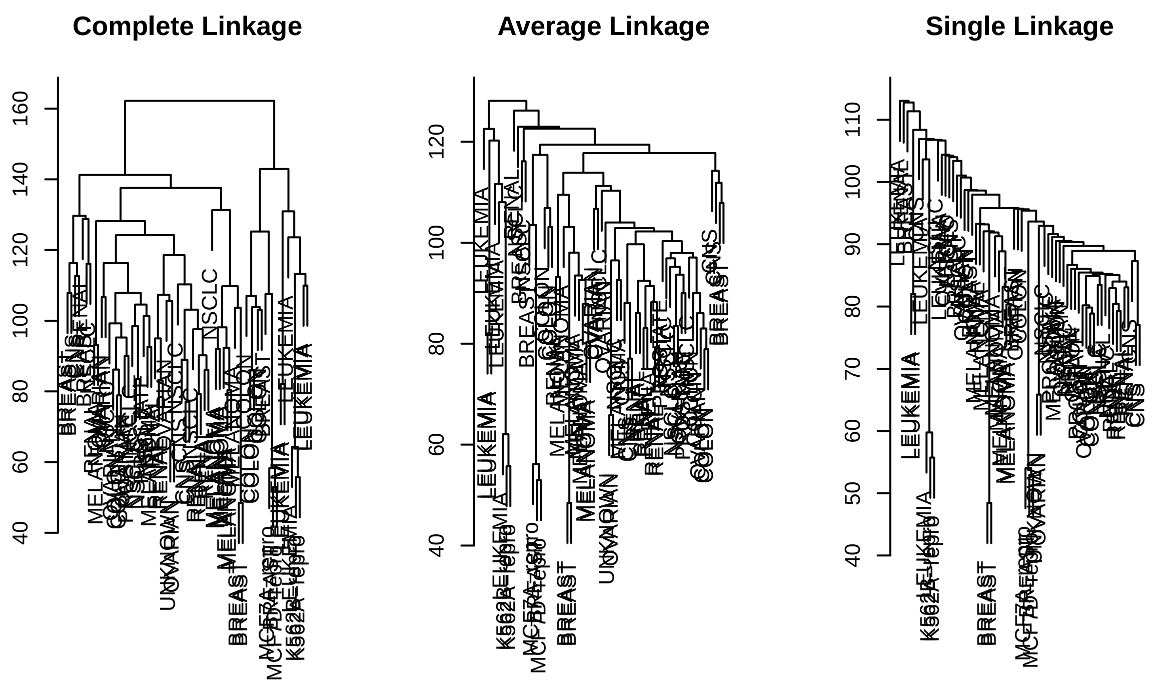
Clustering the Observations of the NCI60 Data

In this final exercise we use heirchical and K-means clustering on the NC160 dataset. We first scale the data to have a zero mean and standard deviation of one.

```
sd.data <- scale(nci.data)
```

We run heirchical clustering with different linakges and plot the results.

```
par(mfrow = c(1, 3))
data.dist <- dist(sd.data)
plot(hclust(data.dist), labels = nci.labs, main = "Complete Linkage", xlab = "", sub = "", ylab = "")
plot(hclust(data.dist, method = "average"), labels = nci.labs, main = "Average Linkage", xlab = "", sub
plot(hclust(data.dist, method = "single"), labels = nci.labs, main = "Single Linkage", xlab = "", sub =
```



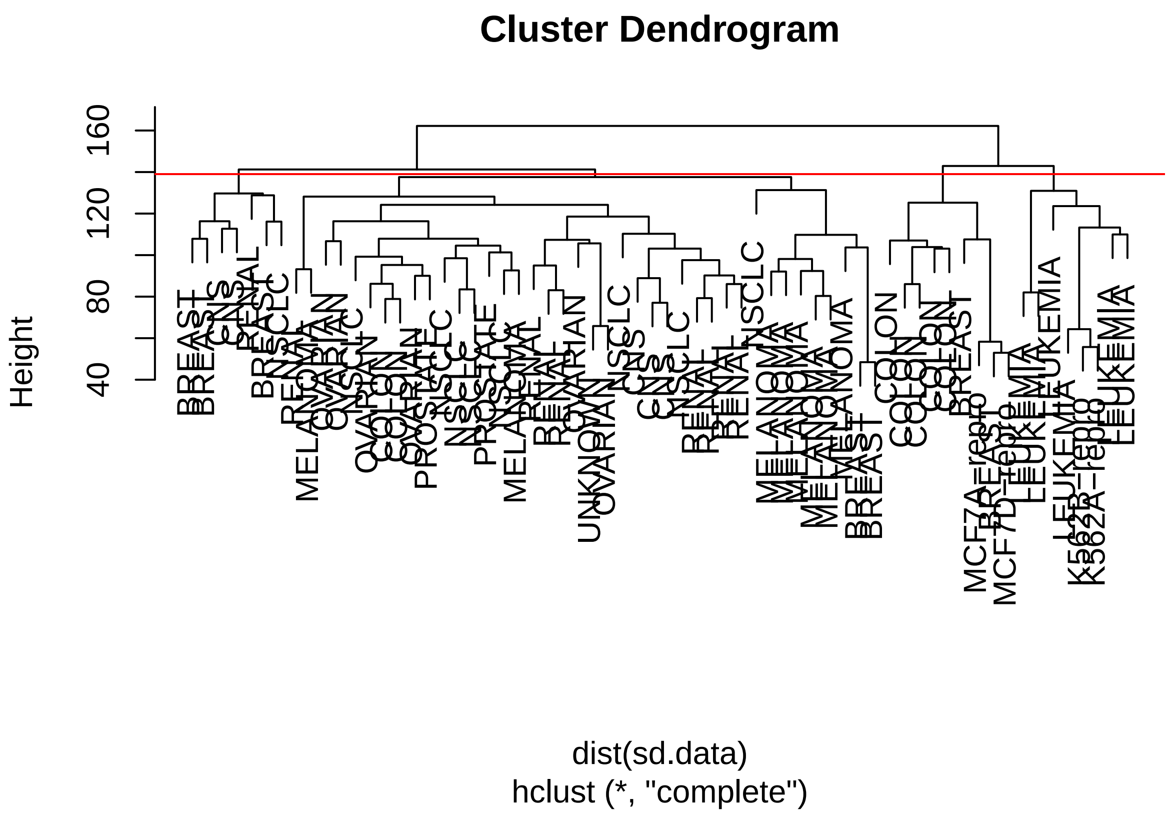
We cut the tree to give us four clusters using cutree().

```
hc.out <- hclust(dist(sd.data))
hc.clusters <- cutree(hc.out, 4)
table(hc.clusters, nci.labs)
```

```
##            nci.labs
## hc.clusters BREAST CNS COLON K562A-repro K562B-repro LEUKEMIA MCF7A-repro
##           1      2   3     2           0           0        0           0
##           2      3   2     0           0           0        0           0
##           3      0   0     0           1           1        6           0
##           4      2   0     5           0           0        0           1
##            nci.labs
## hc.clusters MCF7D-repro MELANOMA NSCLC OVARIAN PROSTATE RENAL UNKNOWN
##           1           0        8     8       6        2     8       1
##           2           0        0     1       0        0     1       0
##           3           0        0     0       0        0     0       0
##           4           1        0     0       0        0     0       0
```

And plot the results with four clusters.

```
par(mfrow = c(1, 1))
plot(hc.out, labels = nci.labs)
abline(h = 139, col = "red")
```



We can get a summary of the result from the return value of hclust().

```
hc.out
```

```
##
## Call:
## hclust(d = dist(sd.data))
##
## Cluster method   : complete
## Distance         : euclidean
## Number of objects: 64
```

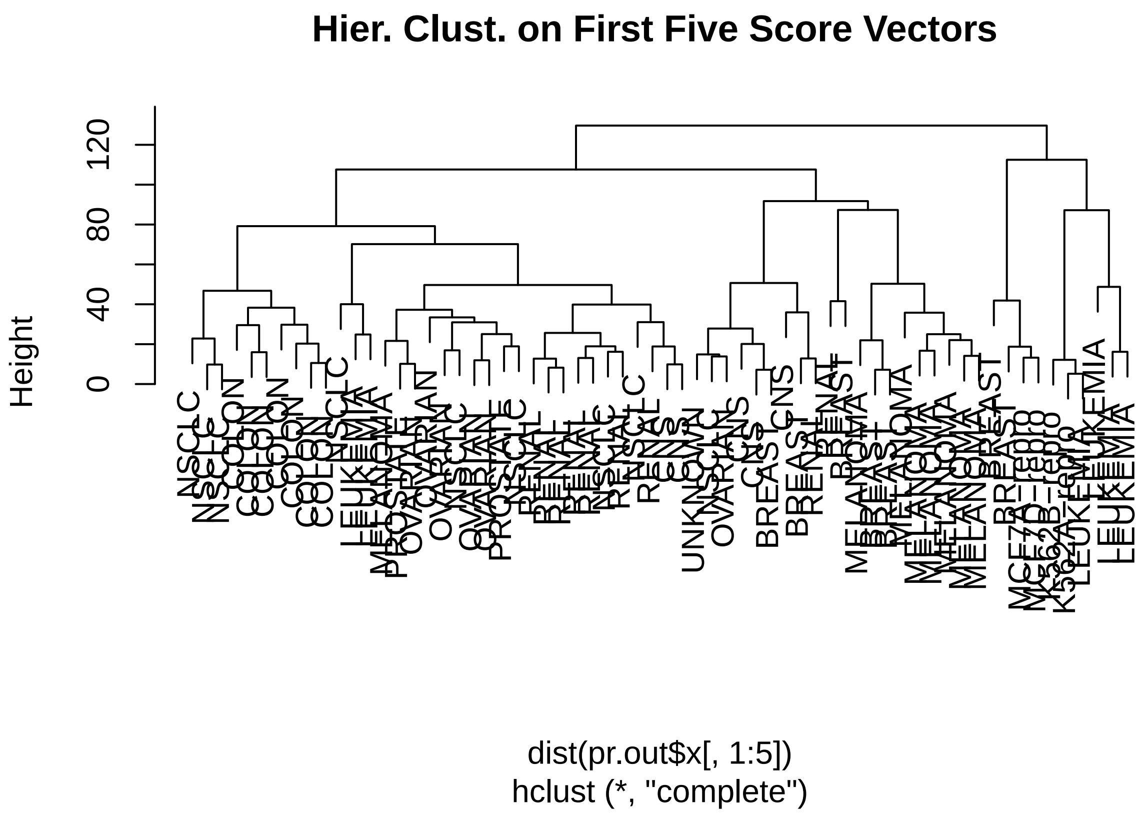
For clustering the cancer types in four groups with K-means, we simply run kmeans() with K = 4.

```
set.seed(2)
km.out <- kmeans(sd.data, 4, nstart = 20)
km.clusters <- km.out$cluster
table(km.clusters, hc.clusters)
```

```
##            hc.clusters
## km.clusters  1  2  3  4
##           1 11  0  0  9
##           2 20  7  0  0
##           3  9  0  0  0
##           4  0  0  8  0
```

We can also combine the different algorithms by first running principal component analysis and then performing heirchical clustering on the first few principal components.

```r
hc.out <- hclust(dist(pr.out$x[, 1:5]))
plot(hc.out, labels = nci.labs, main = "Hier. Clust. on First Five Score Vectors ")
```



```r
table(cutree(hc.out, 4), nci.labs)
```

```
##    nci.labs
##     BREAST CNS COLON K562A-repro K562B-repro LEUKEMIA MCF7A-repro MCF7D-repro
##   1      0   2     7           0           0        2           0           0
##   2      5   3     0           0           0        0           0           0
##   3      0   0     0           1           1        4           0           0
##   4      2   0     0           0           0        0           1           1
##    nci.labs
##     MELANOMA NSCLC OVARIAN PROSTATE RENAL UNKNOWN
##   1        1     8       5        2     7       0
##   2        7     1       1        0     2       1
##   3        0     0       0        0     0       0
##   4        0     0       0        0     0       0
```