Suhaas HW 3 ISLR

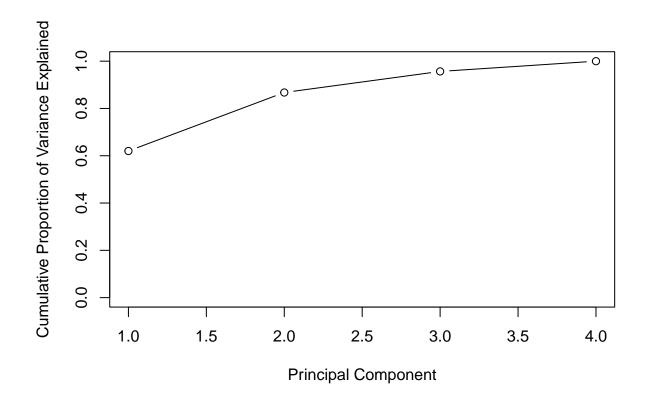
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Homework 3

Question 8

```
library(ISLR) ### a
data(USArrests)
states = row.names(USArrests)
names(USArrests)
## [1] "Murder"
                  "Assault" "UrbanPop" "Rape"
dim(USArrests)
## [1] 50 4
apply(USArrests,2,mean)
##
     Murder Assault UrbanPop
                                  Rape
      7.788 170.760
##
                       65.540
                                21.232
apply(USArrests,2,var)
##
       Murder
                 Assault
                           UrbanPop
                                          Rape
     18.97047 6945.16571 209.51878
pr.out = prcomp(USArrests, scale=TRUE)
pr.var = pr.out$sdev^2
PVE = pr.var/sum(pr.var)
PVE
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
plot(cumsum (PVE ), xlab="Principal Component", ylab = "
Cumulative Proportion of Variance Explained", ylim=c(0,1),
type='b')
```



b

```
pr.loadings = pr.out$rotation
PC1var = var(pr.out$x[,1])
PC2var = var(pr.out$x[,2])
PC3var = var(pr.out$x[,3])
PC4var = var(pr.out$x[,4])

totalVar = (PC1var+PC2var+PC3var+PC4var)

PC1.PVEhand = PC1var/totalVar

PC2.PVEhand = PC2var/totalVar

PC3.PVEhand = PC3var/totalVar

PC4.PVEhand = PC4var/totalVar

PC1.PVEhand = PC4var/totalVar
```

[1] 0.6200604

PC2.PVEhand

[1] 0.2474413

PC3.PVEhand

[1] 0.0891408

PC4.PVEhand

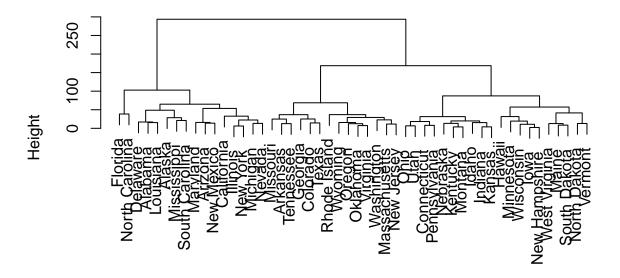
[1] 0.04335752

Question 9

a

```
Arr.complete = hclust(dist(USArrests),method='complete')
plot(Arr.complete,main="Complete Linkage")
```

Complete Linkage

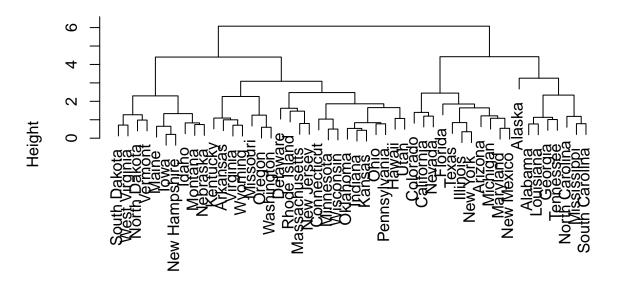


dist(USArrests)
hclust (*, "complete")

b

```
print(sort(cutree(Arr.complete,3),decreasing=TRUE))
##
      Connecticut
                            Hawaii
                                             Idaho
                                                           Indiana
                                                                              Iowa
##
                                                                                 3
                                                                 3
                         Kentucky
##
           Kansas
                                             Maine
                                                        Minnesota
                                                                           Montana
##
                                 3
                                                                 3
##
         Nebraska
                    New Hampshire
                                     North Dakota
                                                              Ohio
                                                                      Pennsylvania
                                                                 3
##
                              Utah
                                                    West Virginia
##
     South Dakota
                                                                         Wisconsin
                                           Vermont
##
                                                 3
                                                                                 3
##
         Arkansas
                          Colorado
                                          Georgia
                                                    Massachusetts
                                                                         Missouri
##
                                                 2
##
                          Oklahoma
                                                     Rhode Island
                                                                        Tennessee
       New Jersey
                                            Oregon
##
                         Virginia
                                                           Wyoming
                                                                           Alabama
##
            Texas
                                       Washington
##
           Alaska
                          Arizona
                                       California
                                                                           Florida
##
                                                          Delaware
##
         Illinois
                        Louisiana
                                         Maryland
                                                         Michigan
                                                                      Mississippi
##
##
##
           Nevada
                       New Mexico
                                         New York North Carolina South Carolina
##
\mathbf{c}
Arrest.scaled = scale(USArrests)
sd(Arrest.scaled[,1])
## [1] 1
sd(Arrest.scaled[,2])
## [1] 1
sd(Arrest.scaled[,3])
## [1] 1
sd(Arrest.scaled[,4])
## [1] 1
Arr.complete.scaled= hclust(dist(Arrest.scaled),method='complete')
plot(Arr.complete.scaled,main="Complete Linkage")
```

Complete Linkage



dist(Arrest.scaled) hclust (*, "complete")

print(sort(cutree(Arr.complete.scaled,3),decreasing=TRUE))

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

 \mathbf{d}

```
threeclust = sum(cutree(Arr.complete,3)==3)
threeclustScale = sum(cutree(Arr.complete.scaled,3)==3)
twoclust = sum(cutree(Arr.complete,3)==2)
twoclustScale = sum(cutree(Arr.complete.scaled,3)==2)
oneclust = sum(cutree(Arr.complete,3)==1)
oneclustScale = sum(cutree(Arr.complete.scaled,3)==1)
print('3 groups raw vs scaled:')
## [1] "3 groups raw vs scaled:"
threeclust
## [1] 20
threeclustScale
## [1] 31
print('2 groups raw vs scaled:')
## [1] "2 groups raw vs scaled:"
twoclust
## [1] 14
twoclustScale
## [1] 11
print('1 group raw vs scaled:')
## [1] "1 group raw vs scaled:"
oneclust
## [1] 16
oneclustScale
## [1] 8
```

We can see using the cutree function, that prior to scaling, the clustering includes less states in larger clusters, and more states in smaller clusters. This likely is a function of the disproportionate variability in the unscaled dataset thus more states are more unique, and thereby more singleton clusters are created. Disproportionate variability in unscaled data can be driven by high values in certain categories, for example urban population in california will be extremely high, and given we are using euclidean distance will be far away from other states if unscaled, this has a disproportionate effect on the state's position wrt arrests, but is not what we are interested in. So yes, I would scale data, IN THIS CASE, in general, the problem is very contextual. For example, if we simply had number of arrests per state, with no other variables included, I perhaps would not need to scale.

We can see in unscaled data california is in a singleton cluster, after scaling it is in a 2 state cluster. If we look at the crime values for california and compare to Nevada, whome it was most similarly clustered with, the crime values are highly similar

```
USArrests['California',]
              Murder Assault UrbanPop Rape
## California
                          276
                                     91 40.6
USArrests['Nevada',]
          Murder Assault UrbanPop Rape
## Nevada
            12.2
                      252
                                 81
                                      46
USArrests['Arizona',]
##
           Murder Assault UrbanPop Rape
## Arizona
              8.1
                       294
                                  80
                                       31
```

versus in the unscaled dendrogram, height wise it is similarly singleton to missouri or georgia. Which across all values seem much less similar to values seen in California

```
USArrests['California',]
              Murder Assault UrbanPop Rape
##
## California
                          276
                                     91 40.6
                    9
USArrests['Georgia',]
           Murder Assault UrbanPop Rape
             17.4
                       211
                                 60 25.8
## Georgia
USArrests['Missouri',]
##
            Murder Assault UrbanPop Rape
```

Question 11

Missouri

178

a

70 28.2

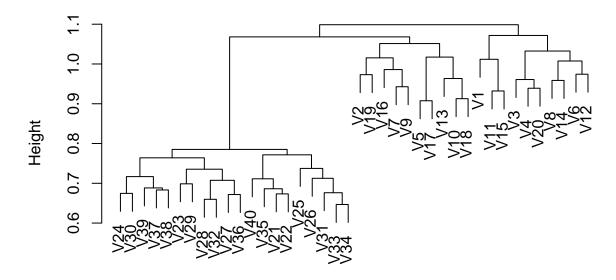
```
getwd()
```

[1] "C:/Users/suhaas.adiraju/Desktop/Statistical ML/StatisticalMLCourse"

 \mathbf{b}

```
sample = names(Ch.Data)
cor.mat.genes= as.dist(1-cor((Ch.Data)))
plot(hclust(cor.mat.genes,method='complete'),main='Correlation-based complete linkage clustering')
```

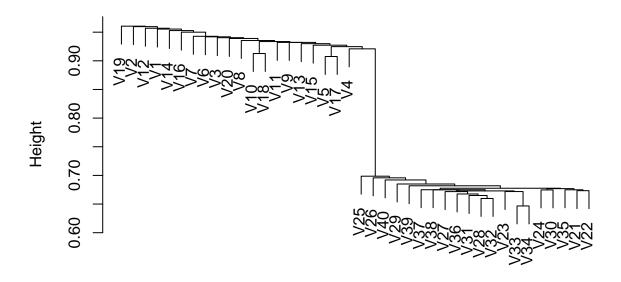
Correlation-based complete linkage clustering



cor.mat.genes hclust (*, "complete")

```
cor.mat.genes= as.dist(1-cor((Ch.Data)))
plot(hclust(cor.mat.genes,method='single'),main='Correlation-based single linkage clustering')
```

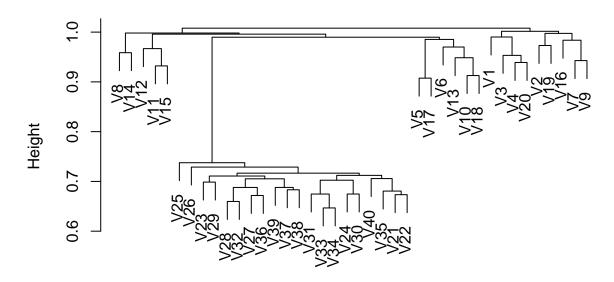
Correlation-based single linkage clustering



cor.mat.genes hclust (*, "single")

cor.mat.genes= as.dist(1-cor((Ch.Data)))
plot(hclust(cor.mat.genes,method='average'),main='Correlation-based average linkage clustering')

Correlation-based average linkage clustering



cor.mat.genes hclust (*, "average")

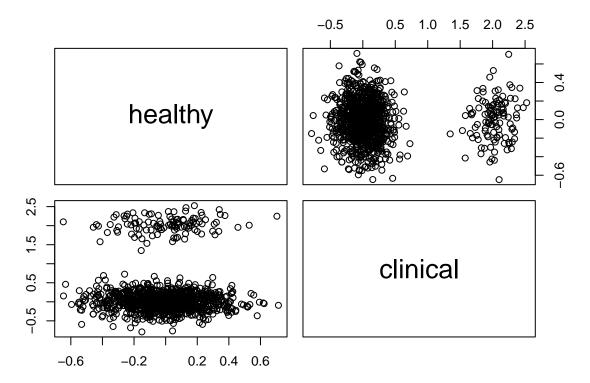
The separation of genes in to simply two groups is not trivial/automatic, but depends on the clustering used. none of the dendrograms only form two clusters, but using average and complete distances certainly provide a better 2 cluster estimation compared to single. Another way to show this result

```
sort(cutree(hclust(cor.mat.genes,method='average'),2))
                         V9 V16 V19 V20
                                         ۷5
                                              ۷6
                                                  V8 V10 V11 V12 V13 V14 V15
                                                   2
                                                                2
                                                                    2
##
                                               2
   V21 V22 V23 V24 V25 V26 V27
                                V28
                                    V29
                                        V30
                                            V31 V32 V33 V34 V35 V36
                                                                     V37 V38
                                                                              V39 V40
                          2
                              2
                                  2
                                      2
                                                                2
sort(cutree(hclust(cor.mat.genes,method='complete'),2))
                                                  ۷5
                                                          V9 V10 V13 V16 V17
##
                    V8 V11 V12 V14 V15 V20
                                              V2
                                                   2
                                                       2
                                                                2
                                                                    2
           V23
                   V25
                        V26
                                V28
                                    V29
                                        V30
                                             V31 V32 V33 V34
                                                             V35
                                                                 V36
                                                                      V37
                                                                          V38
                                                                              V39
                                                                                  V40
sort(cutree(hclust(cor.mat.genes,method='single'),2))
                                     V9 V10 V11 V12 V13 V14 V15 V16 V17 V18
                                                                              V20 V21
                   V26
                            V28
                                V29
                                    V30
                                        V31 V32 V33 V34 V35
                                                             V36
                                                                 V37 V38 V39
```

We can see single linkage clustered every sample except for V19 in cluster 1, this is clearly not useful.

There are several ways we can explore this question, I would start with very basic exploratory analysis and plotting. We know our two groups already, this is an advantage, we can average each gene(row) across samples, within each respective group of healthy versus diseased. Then use the pairs function to see if there are major differences plotting healthy versus diseased gene average values:

```
healthy = apply(Ch.Data[,1:20],1,mean)
clinical = apply(Ch.Data[,21:40],1,mean)
gene.frame = data.frame(healthy,clinical)
pairs(gene.frame)
```

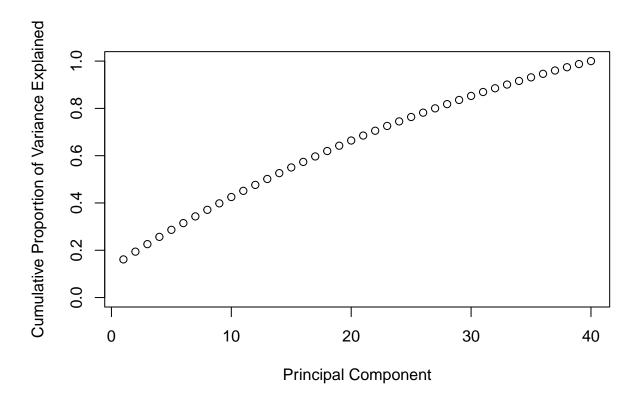


Look at that! it seems that indeed there is a subgroup of genes that express much higher mean values in the clinical group. We could pull out the identity of these genes by setting a threshold and indexing the data frame

```
clinical.hit.genes= which((gene.frame$clinical>1.0),useNames = TRUE)
clinical.hit.genes
##
                                      18
                                          19
                                              20 501 502 503 504 505 506 507 508
          11
              12
                  13
                      14
                          15
                              16
                                  17
    [19] 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526
##
    [37] 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544
    [55] 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562
    [73] 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580
    [91] 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598
  [109] 599 600
```

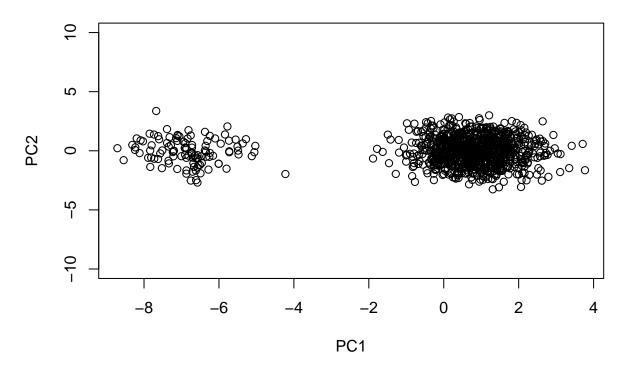
although this is useful information, when we average across samples in each group, we are assuming a lot of stability across samples or rather overlooking the within group variability, as well as other nuances. To take a more fine-grained approach of preserving individual sample contributions lets use PCA

```
pr.out.gene = prcomp((Ch.Data), scale=TRUE)
pr.var.gene = pr.out.gene$sdev^2
PVE.gene = pr.var.gene/sum(pr.var.gene)
PVE.gene
    [1] 0.16130137 0.03280179 0.03176830 0.03075558 0.02972109 0.02847757
##
##
    [7] 0.02833663 0.02783324 0.02736489 0.02674424 0.02610345 0.02519941
  [13] 0.02499759 0.02484029 0.02396715 0.02339585 0.02313948 0.02299186
  [19] 0.02250569 0.02193219 0.02091515 0.02041673 0.02023852 0.01921437
  [25] 0.01863679 0.01836530 0.01819977 0.01786939 0.01757227 0.01708818
  [31] 0.01658588 0.01587270 0.01569743 0.01524706 0.01516708 0.01485582
## [37] 0.01409545 0.01388385 0.01331786 0.01258275
plot(cumsum (PVE.gene ), xlab="Principal Component", ylab =
Cumulative Proportion of Variance Explained", ylim=c(0,1)
)
```



We see from our cumulative plot and the proportion of variance explained values that our first component captures the highest proportion of variance, and all following components add about the same small amount of information. lets plot our data mapped in the first 2 components.

Gene data projected on to first 2 PCs



We can see in this plot the data varies a lot on PC1, and a little on PC2, and via the PC1 variance, there is a distinct data cloud with large negative score values, these could be positive too, as PCA weights are identical up to sign changes. Basically, these genes differ alot among the samples. We should index them, and sort them, to see which genes they are and which are the most variable along PC1

```
gene.hits.pca.idx = which(pr.out.gene$x[,'PC1'] <= -4,useNames = TRUE)
top.genes = data.frame(gene.hits.pca.idx, -(pr.out.gene$x[gene.hits.pca.idx
,'PC1']))
sorted.top.genes = order(top.genes$X..pr.out.gene.x.gene.hits.pca.idx...PC1...,decreasing=TRUE)
top.genes[sorted.top.genes,1]
##
     [1] 551 589 508 548 509 511 566 565 540 534 561 502 584 586
                                                                  12 558 593 568
##
    [19] 582 578 503
                     13 549 572 538 505 554 587 545 550 521
                                                              11 522 526 560 555
##
    [37] 570 597 559 541 516 590 571 576 517
                                              14 546 600 520 529 515 514 506 535
    [55] 537 596 542 523 595 594 512 599 562 591 536 556 544 527 575
                                                                      20 533 564
    [73] 530 539 579 18 513 543 567 524 501 569 583 563 588 531
                                                                 16 585 592 581
              15 574 553 580 598 17 519 507 547 552 504 557 510 577 573 528 525
##
    [91]
         19
## [109] 532 518
```