class09

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Getting organized, Preparing the Data

Before we begin our analyses, we'll need to download and import the WisconsinCancer.csv data file using read.csv() and assign the data to an object called "wisc.df".

We can take a look at the data by using head().

```
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)
```

```
##          diagnosis radius_mean texture_mean perimeter_mean area_mean
## 842302           M       17.99        10.38         122.80    1001.0
## 842517           M       20.57        17.77         132.90    1326.0
## 84300903         M       19.69        21.25         130.00    1203.0
## 84348301         M       11.42        20.38          77.58     386.1
## 84358402         M       20.29        14.34         135.10    1297.0
## 843786           M       12.45        15.70          82.57     477.1
##          smoothness_mean compactness_mean concavity_mean concave.points_mean
## 842302           0.11840          0.27760         0.3001             0.14710
## 842517           0.08474          0.07864         0.0869             0.07017
## 84300903         0.10960          0.15990         0.1974             0.12790
## 84348301         0.14250          0.28390         0.2414             0.10520
## 84358402         0.10030          0.13280         0.1980             0.10430
## 843786           0.12780          0.17000         0.1578             0.08089
##          symmetry_mean fractal_dimension_mean radius_se texture_se perimeter_se
## 842302          0.2419                0.07871    1.0950     0.9053        8.589
## 842517          0.1812                0.05667    0.5435     0.7339        3.398
## 84300903        0.2069                0.05999    0.7456     0.7869        4.585
## 84348301        0.2597                0.09744    0.4956     1.1560        3.445
## 84358402        0.1809                0.05883    0.7572     0.7813        5.438
## 843786          0.2087                0.07613    0.3345     0.8902        2.217
##          area_se smoothness_se compactness_se concavity_se concave.points_se
## 842302    153.40      0.006399        0.04904      0.05373           0.01587
## 842517     74.08      0.005225        0.01308      0.01860           0.01340
## 84300903   94.03      0.006150        0.04006      0.03832           0.02058
## 84348301   27.23      0.009110        0.07458      0.05661           0.01867
## 84358402   94.44      0.011490        0.02461      0.05688           0.01885
## 843786     27.19      0.007510        0.03345      0.03672           0.01137
##          symmetry_se fractal_dimension_se radius_worst texture_worst
## 842302       0.03003             0.006193        25.38         17.33
## 842517       0.01389             0.003532        24.99         23.41
```

```
## 84300903     0.02250             0.004571        23.57         25.53
## 84348301     0.05963             0.009208        14.91         26.50
## 84358402     0.01756             0.005115        22.54         16.67
## 843786       0.02165             0.005082        15.47         23.75
##          perimeter_worst area_worst smoothness_worst compactness_worst
## 842302            184.60     2019.0           0.1622            0.6656
## 842517            158.80     1956.0           0.1238            0.1866
## 84300903          152.50     1709.0           0.1444            0.4245
## 84348301           98.87      567.7           0.2098            0.8663
## 84358402          152.20     1575.0           0.1374            0.2050
## 843786            103.40      741.6           0.1791            0.5249
##          concavity_worst concave.points_worst symmetry_worst
## 842302            0.7119               0.2654         0.4601
## 842517            0.2416               0.1860         0.2750
## 84300903          0.4504               0.2430         0.3613
## 84348301          0.6869               0.2575         0.6638
## 84358402          0.4000               0.1625         0.2364
## 843786            0.5355               0.1741         0.3985
##          fractal_dimension_worst
## 842302                   0.11890
## 842517                   0.08902
## 84300903                 0.08758
## 84348301                 0.17300
## 84358402                 0.07678
## 843786                   0.12440
```

The first column in the data frame contains a pathologist-provided diagnosis, which is basically the "answer" to the questions we'll be asking today.

Let's create a data frame that we may work with that omits the column, then save the diagnosis information to a separate vector that we can use to check our results later on.

```
wisc.data <- wisc.df[,-1]
diagnosis <- as.factor(wisc.df[,1])
```

Time to further familiarize ourselves with the data.

The functions dim(), nrow(), table(), length() and grep() may be useful for answering the first 3 questions.

Q1. How many observations are in this dataset?

```
nrow(wisc.data)
```

```
## [1] 569
```

There are 569 observations in the dataset.

Q2. How many of the observations have a malignant diagnosis?

```
table(diagnosis)
```

```
## diagnosis
##   B   M
## 357 212
```

212 of the observations have a malignant diagnosis.

Q3. How many variables/features in the data are suffixed with _mean?

```
length(grep("_mean",colnames(wisc.data)))
```

```
## [1] 10
```

There are 10 variables/features in the data suffixed with "_mean".

Performing PCA

Check column means and standard deviations

```
colMeans(wisc.data)
```

```
##             radius_mean            texture_mean          perimeter_mean
##            1.412729e+01            1.928965e+01            9.196903e+01
##               area_mean         smoothness_mean        compactness_mean
##            6.548891e+02            9.636028e-02            1.043410e-01
##          concavity_mean     concave.points_mean           symmetry_mean
##            8.879932e-02            4.891915e-02            1.811619e-01
##  fractal_dimension_mean               radius_se              texture_se
##            6.279761e-02            4.051721e-01            1.216853e+00
##            perimeter_se                 area_se           smoothness_se
##            2.866059e+00            4.033708e+01            7.040979e-03
##          compactness_se            concavity_se       concave.points_se
##            2.547814e-02            3.189372e-02            1.179614e-02
##             symmetry_se    fractal_dimension_se            radius_worst
##            2.054230e-02            3.794904e-03            1.626919e+01
##           texture_worst         perimeter_worst              area_worst
##            2.567722e+01            1.072612e+02            8.805831e+02
##        smoothness_worst       compactness_worst         concavity_worst
##            1.323686e-01            2.542650e-01            2.721885e-01
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##            1.146062e-01            2.900756e-01            8.394582e-02
```

```
apply(wisc.data,2,sd)
```

```
##             radius_mean            texture_mean          perimeter_mean
##            3.524049e+00            4.301036e+00            2.429898e+01
##               area_mean         smoothness_mean        compactness_mean
##            3.519141e+02            1.406413e-02            5.281276e-02
##          concavity_mean     concave.points_mean           symmetry_mean
##            7.971981e-02            3.880284e-02            2.741428e-02
##  fractal_dimension_mean               radius_se              texture_se
##            7.060363e-03            2.773127e-01            5.516484e-01
##            perimeter_se                 area_se           smoothness_se
##            2.021855e+00            4.549101e+01            3.002518e-03
##          compactness_se            concavity_se       concave.points_se
```

```
##            1.790818e-02            3.018606e-02            6.170285e-03
##             symmetry_se    fractal_dimension_se            radius_worst
##            8.266372e-03            2.646071e-03            4.833242e+00
##           texture_worst         perimeter_worst              area_worst
##            6.146258e+00            3.360254e+01            5.693570e+02
##        smoothness_worst       compactness_worst         concavity_worst
##            2.283243e-02            1.573365e-01            2.086243e-01
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##            6.573234e-02            6.186747e-02            1.806127e-02
```

```
wisc.pr <- prcomp(wisc.data,scale=TRUE)
summary(wisc.pr)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
##                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
## Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
## Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
## Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
##                           PC15    PC16    PC17    PC18    PC19    PC20   PC21
## Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
## Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
## Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
##                           PC22    PC23   PC24    PC25    PC26    PC27    PC28
## Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
## Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
## Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
##                           PC29    PC30
## Standard deviation     0.02736 0.01153
## Proportion of Variance 0.00002 0.00000
## Cumulative Proportion  1.00000 1.00000
```

Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

```
summary(wisc.pr)$importance[2,]
```

```
##     PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8     PC9    PC10
## 0.44272 0.18971 0.09393 0.06602 0.05496 0.04025 0.02251 0.01589 0.01390 0.01169
##    PC11    PC12    PC13    PC14    PC15    PC16    PC17    PC18    PC19    PC20
## 0.00980 0.00871 0.00805 0.00523 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104
##    PC21    PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29    PC30
## 0.00100 0.00091 0.00081 0.00060 0.00052 0.00027 0.00023 0.00005 0.00002 0.00000
```

44.27% of the original variance is captured by the first principal component (PC1).

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

```
summary(wisc.pr)$importance[3,]
```

```
##     PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8     PC9    PC10
## 0.44272 0.63243 0.72636 0.79239 0.84734 0.88759 0.91010 0.92598 0.93988 0.95157
##    PC11    PC12    PC13    PC14    PC15    PC16    PC17    PC18    PC19    PC20
## 0.96137 0.97007 0.97812 0.98335 0.98649 0.98915 0.99113 0.99288 0.99453 0.99557
##    PC21    PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29    PC30
## 0.99657 0.99749 0.99830 0.99890 0.99942 0.99969 0.99992 0.99997 1.00000 1.00000
```

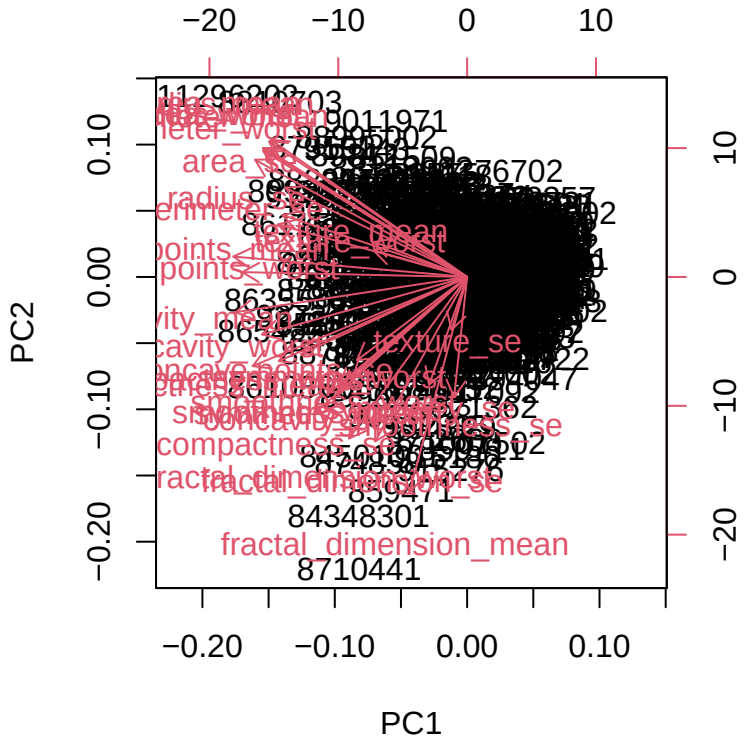
Three PCs are required to describe at least 70% of the original variance in the data (PC1, PC2, and PC3 together describe 72.636% of the original variance).

Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

From above, seven PCs are required to describe at least 90% of the original variance in the data (PC1 through PC7 describe 91.01% of the original variance).

Interpreting PCS results

```
biplot(wisc.pr)
```

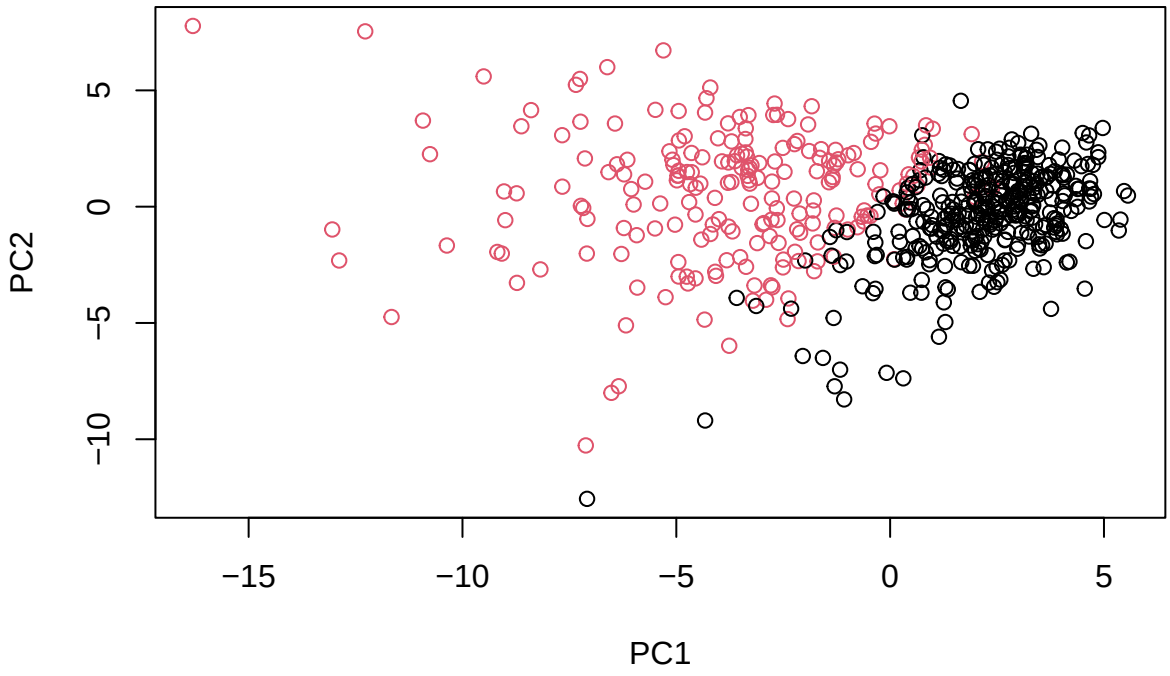


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The plot is not informative because it is extremely crowded. This is not useful for interpreting the PCA results.

Scatter plot observations by components 1 and 2

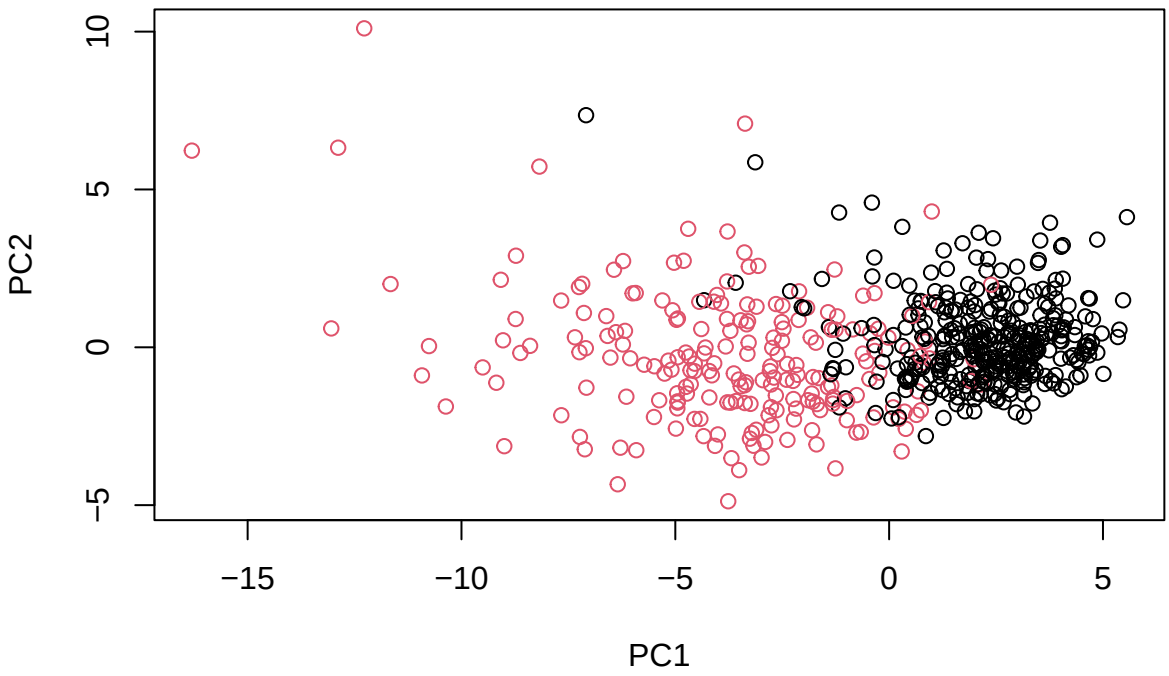
```
plot(wisc.pr$x[,1:2],col=diagnosis,xlab="PC1",ylab="PC2")
```



Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

Scatter plot observations by components 1 and 3

```
plot(wisc.pr$x[,1],wisc.pr$x[,3],col=diagnosis,xlab="PC1",ylab="PC2")
```



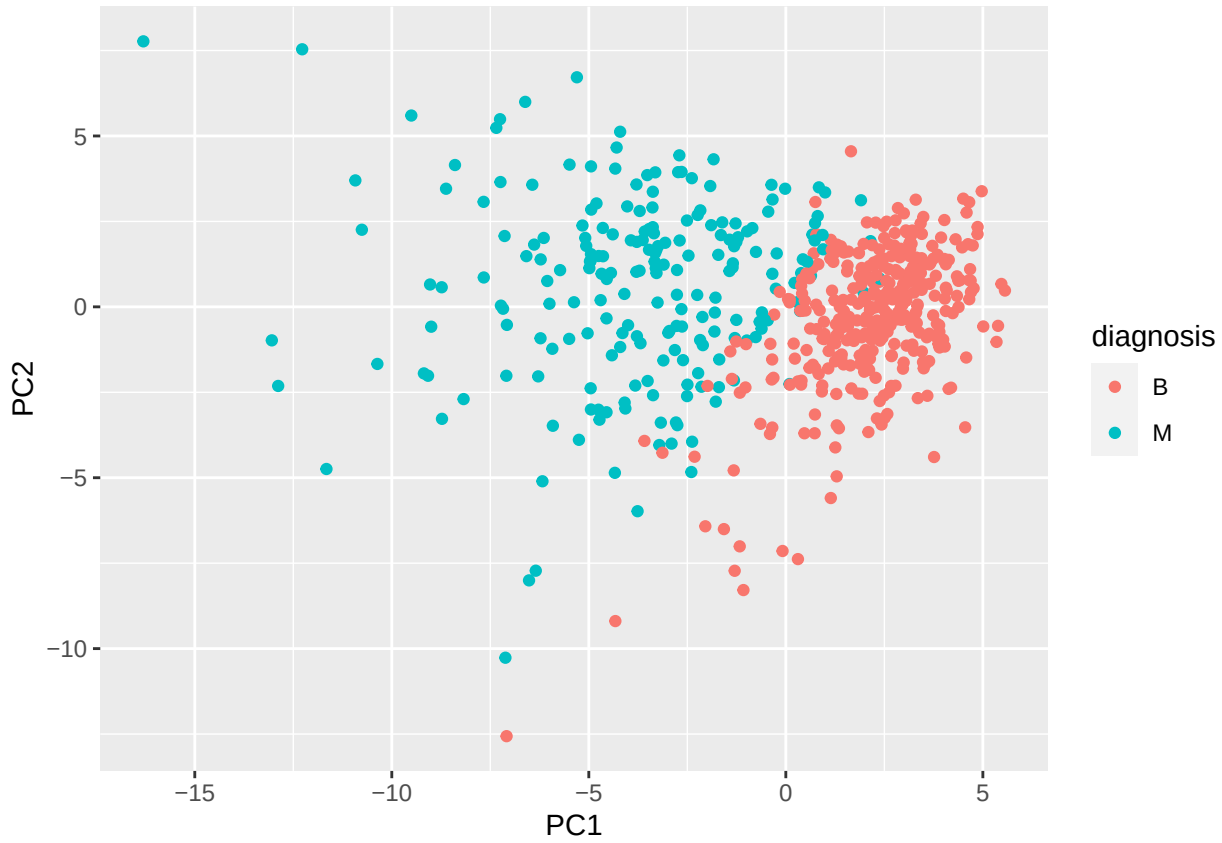
The graphs look somewhat similar; since PC1 accounts for most of the variance in both comparisons, the majority of the distribution of the points is along the x axis. Both plots display that PC1 captures the separation between malignant and benign samples (red v. black). However, PC2 does describe a bit more variance than PC3, so the first plot (PC2 v. PC1) has a bit more spread between the points than the second plot (PC3 v. PC1).

Using ggplot2 for analysis of PCA

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



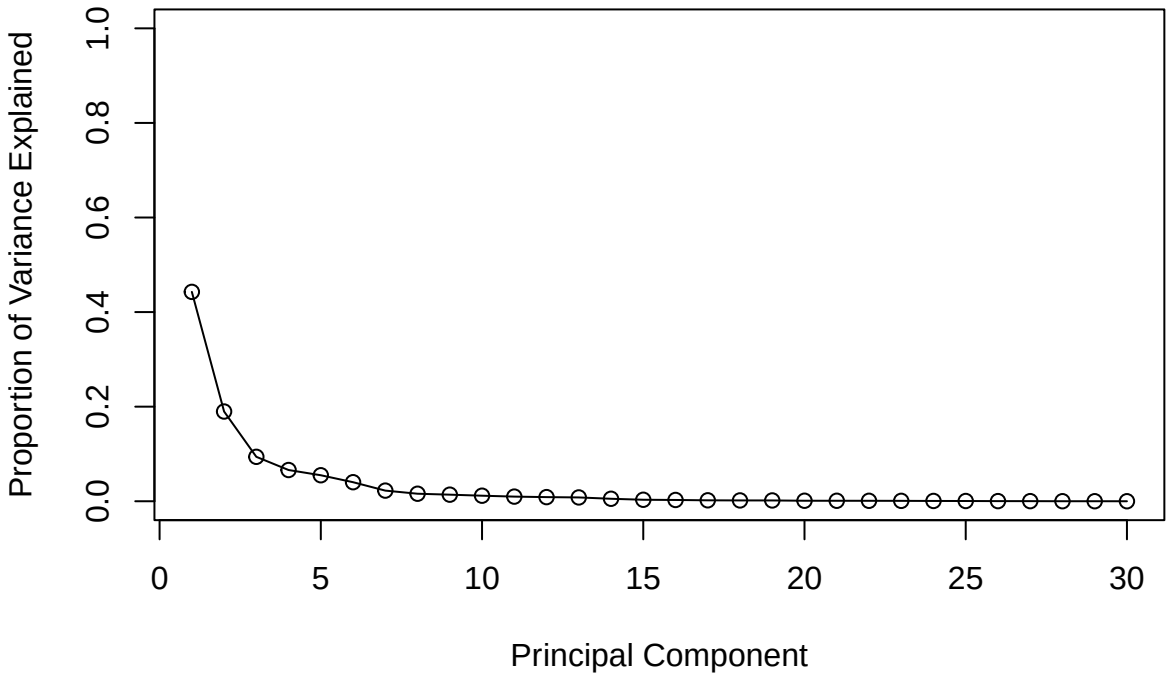
Variance explained (using scree plots)

Calculate variance of each component

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

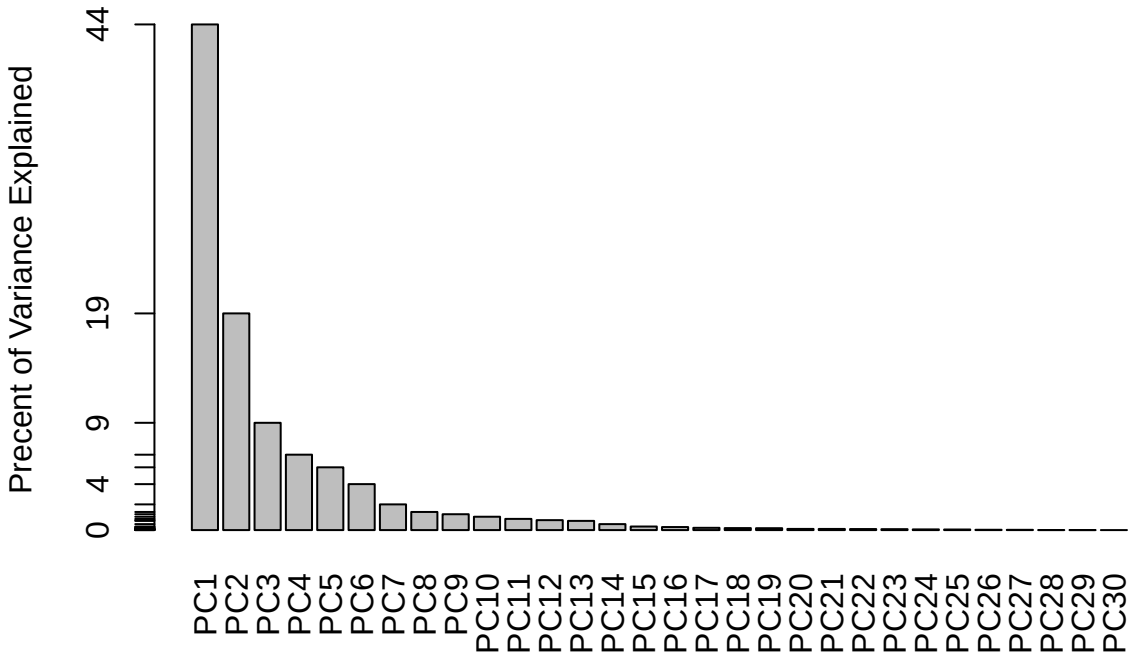
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
pve <- pr.var/sum(pr.var)
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1),type = "o")
```



Alternative scree plot of the same data, note data driven y-axis

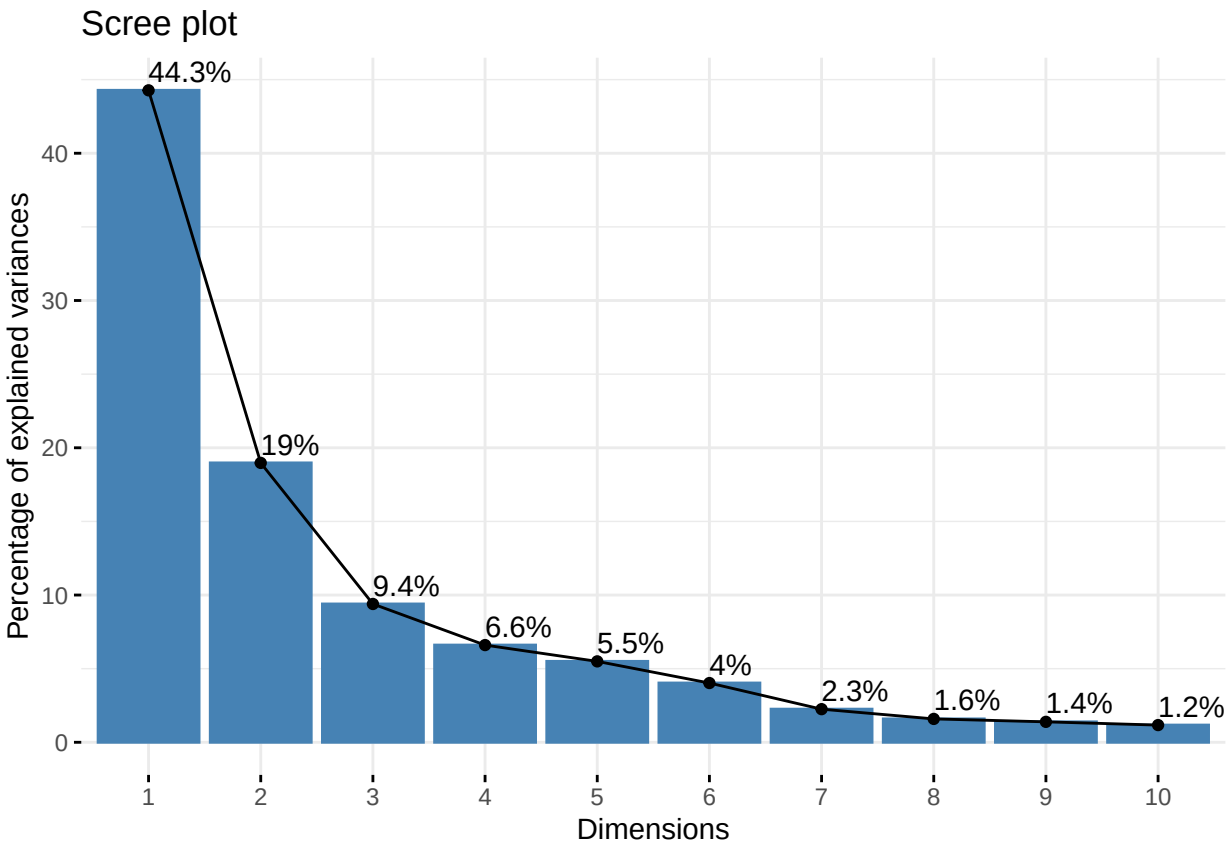
```
barplot(pve,ylab="Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)),las=2,axes=FALSE)
axis(2,at=pve,labels=round(pve,2)*100)
```




```
library(factoextra)
```

```
## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```
fviz_eig(wisc.pr, addlabels = TRUE)
```



Communicating PCA results

Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

```
wisc.pr$rotation[,1]
```

```
##             radius_mean            texture_mean          perimeter_mean
##              -0.21890244              -0.10372458              -0.22753729
##               area_mean         smoothness_mean        compactness_mean
##              -0.22099499              -0.14258969              -0.23928535
##          concavity_mean     concave.points_mean           symmetry_mean
##              -0.25840048              -0.26085376              -0.13816696
##  fractal_dimension_mean                radius_se               texture_se
##              -0.06436335              -0.20597878              -0.01742803
##            perimeter_se                 area_se            smoothness_se
##              -0.21132592              -0.20286964              -0.01453145
##          compactness_se            concavity_se       concave.points_se
##              -0.17039345              -0.15358979              -0.18341740
##             symmetry_se     fractal_dimension_se             radius_worst
##              -0.04249842              -0.10256832              -0.22799663
##           texture_worst         perimeter_worst               area_worst
##              -0.10446933              -0.23663968              -0.22487053
##         smoothness_worst       compactness_worst         concavity_worst
```

```
##             -0.12795256             -0.21009588             -0.22876753
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##             -0.25088597             -0.12290456             -0.13178394
```

The component of the loading vector for concave.points_mean is -0.26085376.

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

```
summary(wisc.pr)$importance[3,]
```

```
##     PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8     PC9    PC10
## 0.44272 0.63243 0.72636 0.79239 0.84734 0.88759 0.91010 0.92598 0.93988 0.95157
##    PC11    PC12    PC13    PC14    PC15    PC16    PC17    PC18    PC19    PC20
## 0.96137 0.97007 0.97812 0.98335 0.98649 0.98915 0.99113 0.99288 0.99453 0.99557
##    PC21    PC22    PC23    PC24    PC25    PC26    PC27    PC28    PC29    PC30
## 0.99657 0.99749 0.99830 0.99890 0.99942 0.99969 0.99992 0.99997 1.00000 1.00000
```

From above, five PCs are required to describe at least 80% of the original variance in the data (PC1 through PC5 describe 84.734% of the original variance).

Hierarchical clustering

Scale the wisc.data data using the "scale()" function

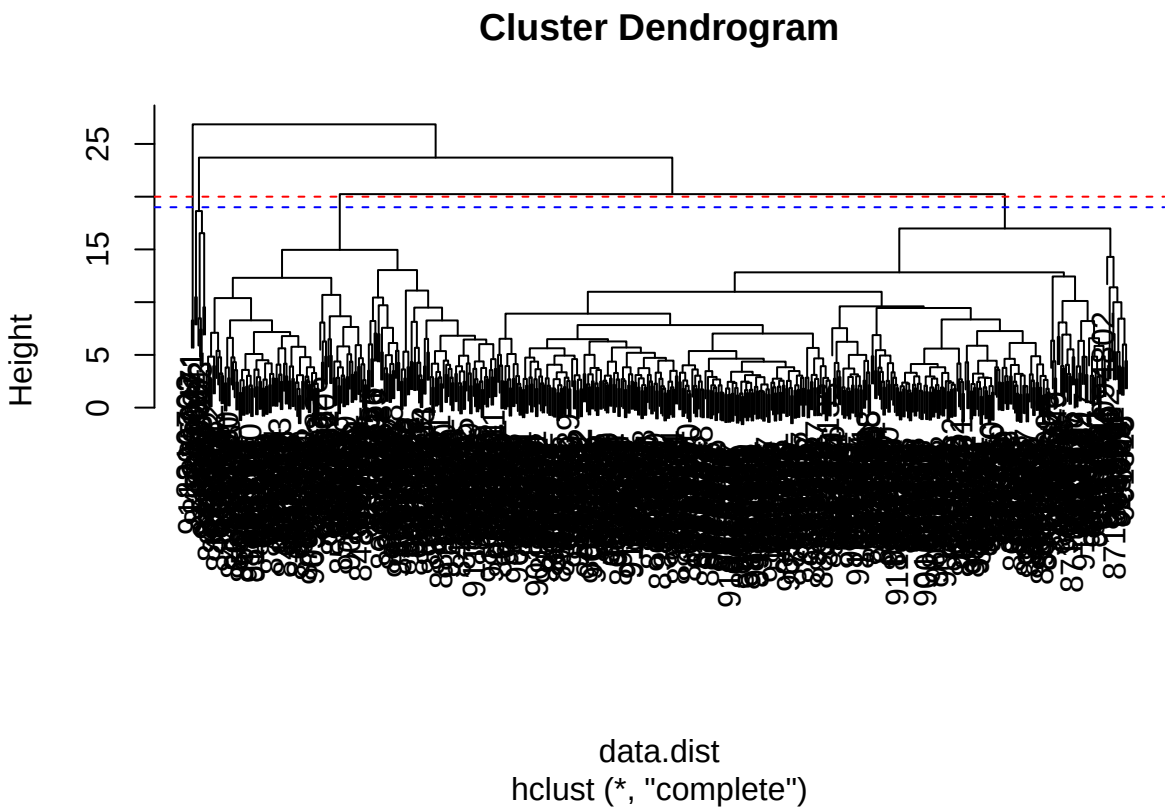
```
data.scaled <- scale(wisc.data)
```

```
data.dist <- dist(data.scaled)
```

```
wisc.hclust <- hclust(data.dist, method="complete")
```

Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

```
plot(wisc.hclust)
abline(h=20, col="red", lty=2)
abline(h=19, col="blue", lty=2)
```



Either h=19 (blue) or h=20 (red) are heights at which the clustering model has 4 clusters.

Selecting number of clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust,h=19)
table(wisc.hclust.clusters,diagnosis)
```

```
##                     diagnosis
## wisc.hclust.clusters   B   M
##                    1  12 165
##                    2   2   5
##                    3 343  40
##                    4   0   2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust.clusters.2 <- cutree(wisc.hclust,h=25)
table(wisc.hclust.clusters.2,diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters.2   B   M
```

```
##                       1 357 210
##                       2   0   2
```

```
wisc.hclust.clusters.3 <- cutree(wisc.hclust,h=22)
table(wisc.hclust.clusters.3,diagnosis)
```

```
##                        diagnosis
## wisc.hclust.clusters.3   B   M
##                       1 355 205
##                       2   2   5
##                       3   0   2
```

```
wisc.hclust.clusters.5 <- cutree(wisc.hclust,h=18)
table(wisc.hclust.clusters.5,diagnosis)
```

```
##                        diagnosis
## wisc.hclust.clusters.5   B   M
##                       1  12 165
##                       2   0   5
##                       3 343  40
##                       4   2   0
##                       5   0   2
```

```
wisc.hclust.clusters.7 <- cutree(wisc.hclust,h=16)
table(wisc.hclust.clusters.7,diagnosis)
```

```
##                        diagnosis
## wisc.hclust.clusters.7   B   M
##                       1  12 165
##                       2   0   3
##                       3 331  39
##                       4   2   0
##                       5  12   1
##                       6   0   2
##                       7   0   2
```

```
wisc.hclust.clusters.9 <- cutree(wisc.hclust,h=13)
table(wisc.hclust.clusters.9,diagnosis)
```

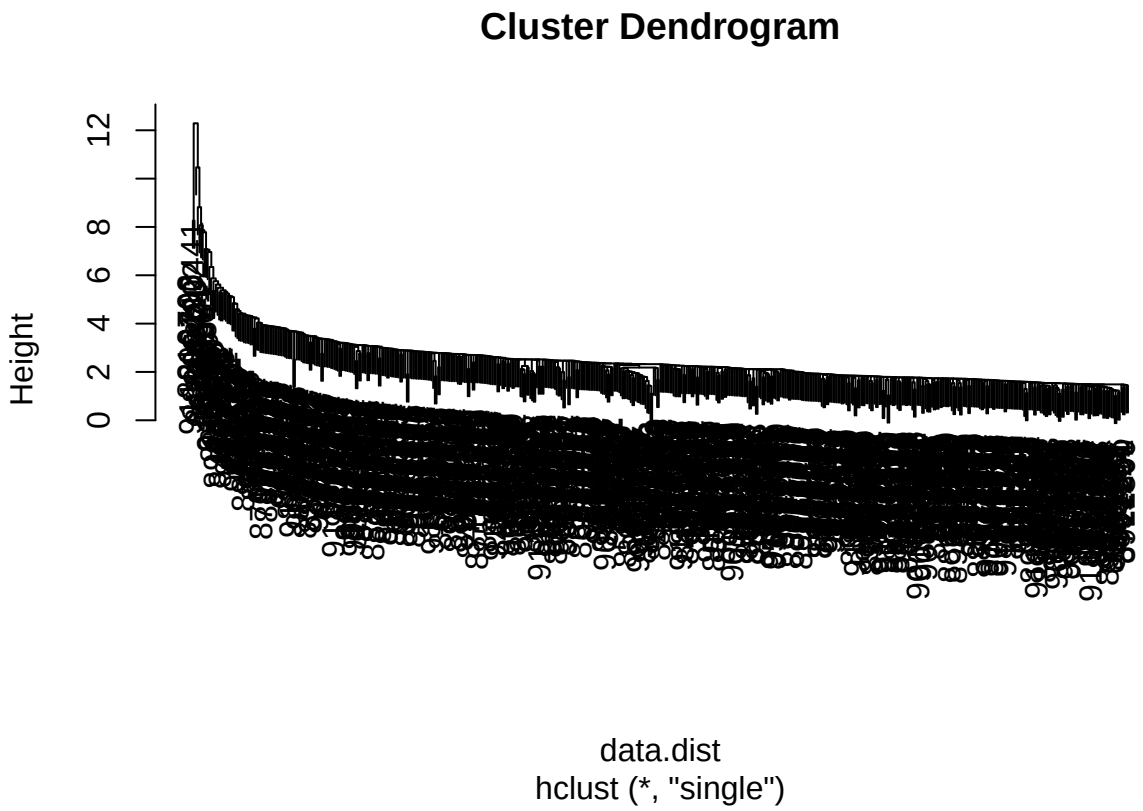
```
##                        diagnosis
## wisc.hclust.clusters.9   B   M
##                      1   12  86
##                      2    0  59
##                      3    0   3
##                      4  331  39
##                      5    0  20
##                      6    2   0
##                      7   12   0
##                      8    0   2
##                      9    0   2
##                      10   0   1
```

Yes; at h=18, using 5 clusters. When using 4 clusters, 1/4 clusters contain only B *or* M, while when using 5 clusters, 3/5 clusters contain only B *or* M.

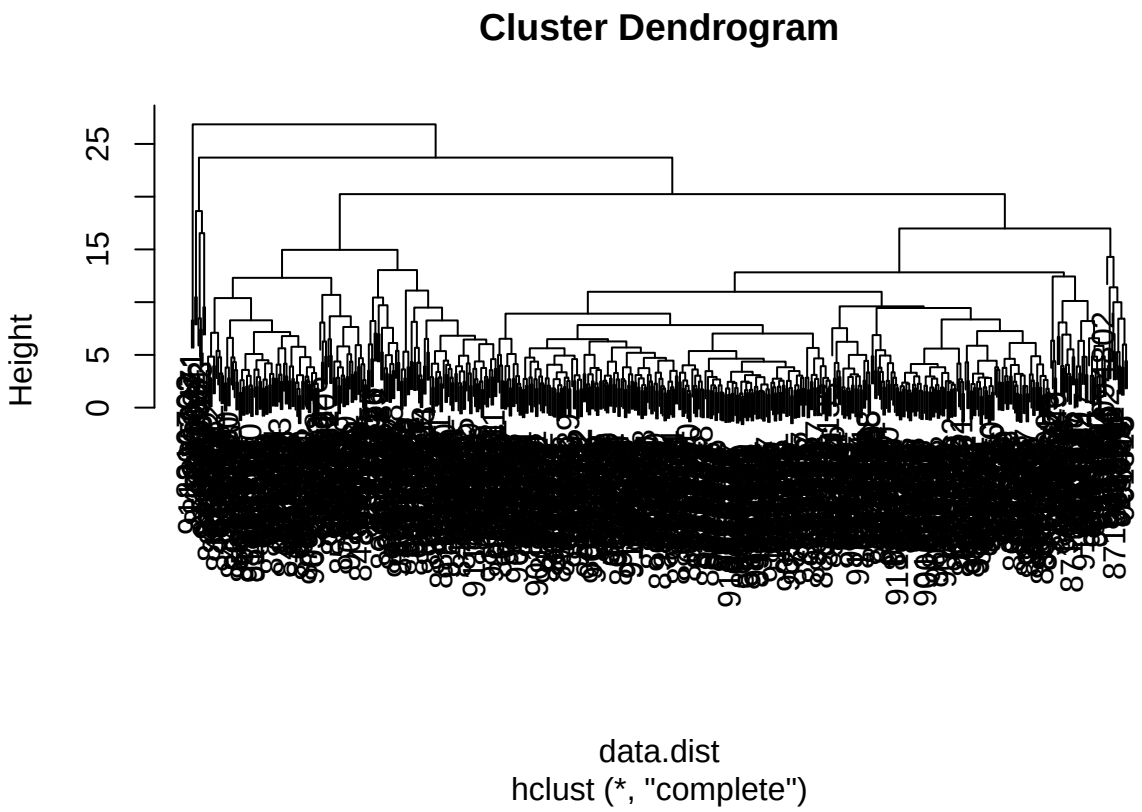
The number of observations in the mixed B *and* M clusters remains approximately the same when using 5 vs. 4 clusters. Adding any more clusters actually introduces additional mixed clusters, and does not improve the separation between B and M observations.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

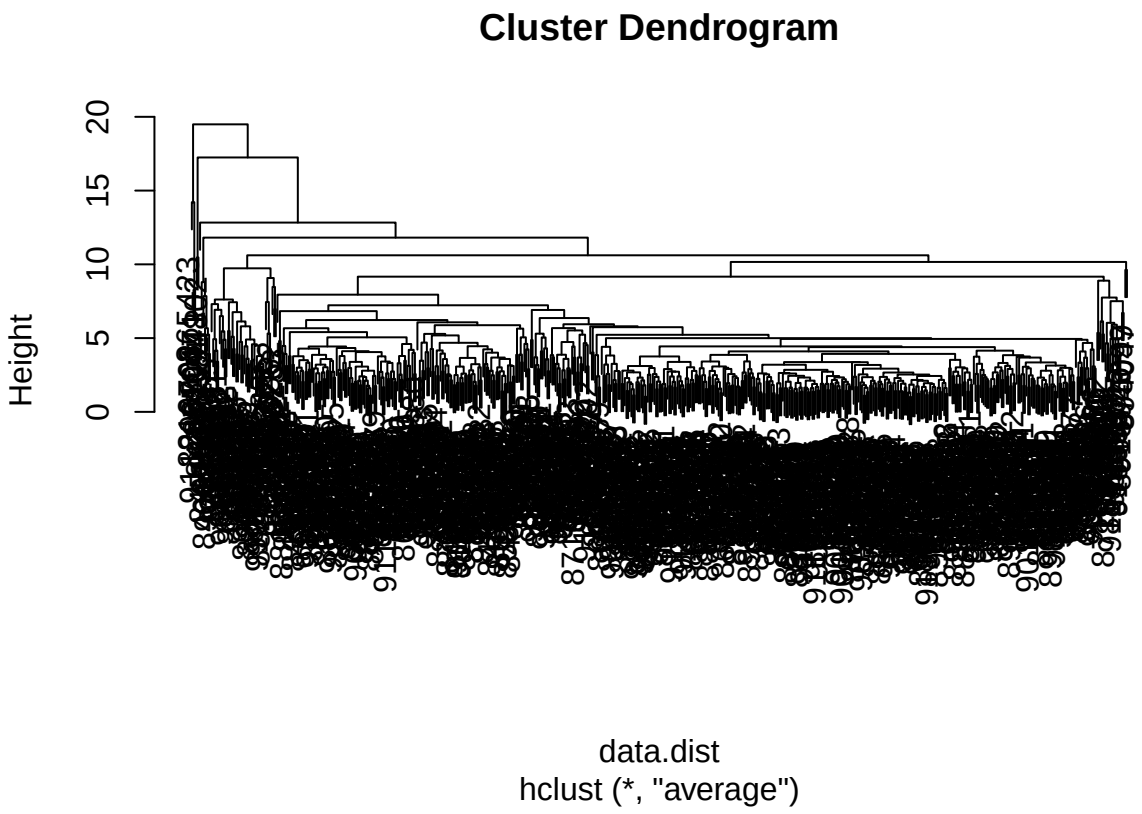
```
plot(hclust(data.dist,method="single"))
```



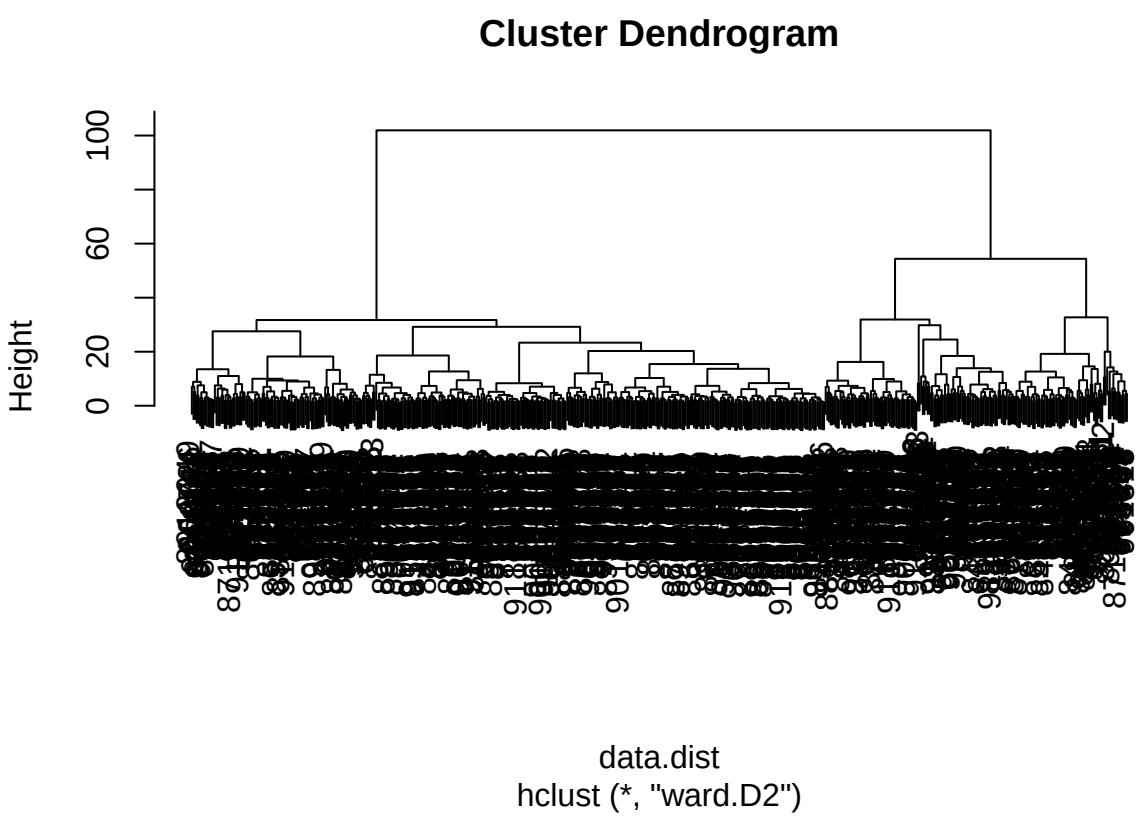

```
plot(hclust(data.dist,method="complete"))
```




```
plot(hclust(data.dist,method="average"))
```




```
plot(hclust(data.dist,method="ward.D2"))
```



I personally prefer the "ward.D2" method, because the terminal nodes of the dendrogram are aligned at the bottom of the graphic (this feels familiar to my prior experience viewing and interpreting dendrograms). The root/early branching of the tree is spread out as well, which would make selecting the cutree() height easier visually speaking.

K-means clustering

```
wisc.km <- kmeans(wisc.data, centers=2, nstart=20)
table(wisc.km$cluster,diagnosis)
```

```
##    diagnosis
##       B   M
##   1   1 130
##   2 356  82
```

```
wisc.hclust.clusters.5 <- cutree(wisc.hclust,h=18)
table(wisc.hclust.clusters.5,diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters.5   B   M
##                      1  12 165
##                      2   0   5
##                      3 343  40
```

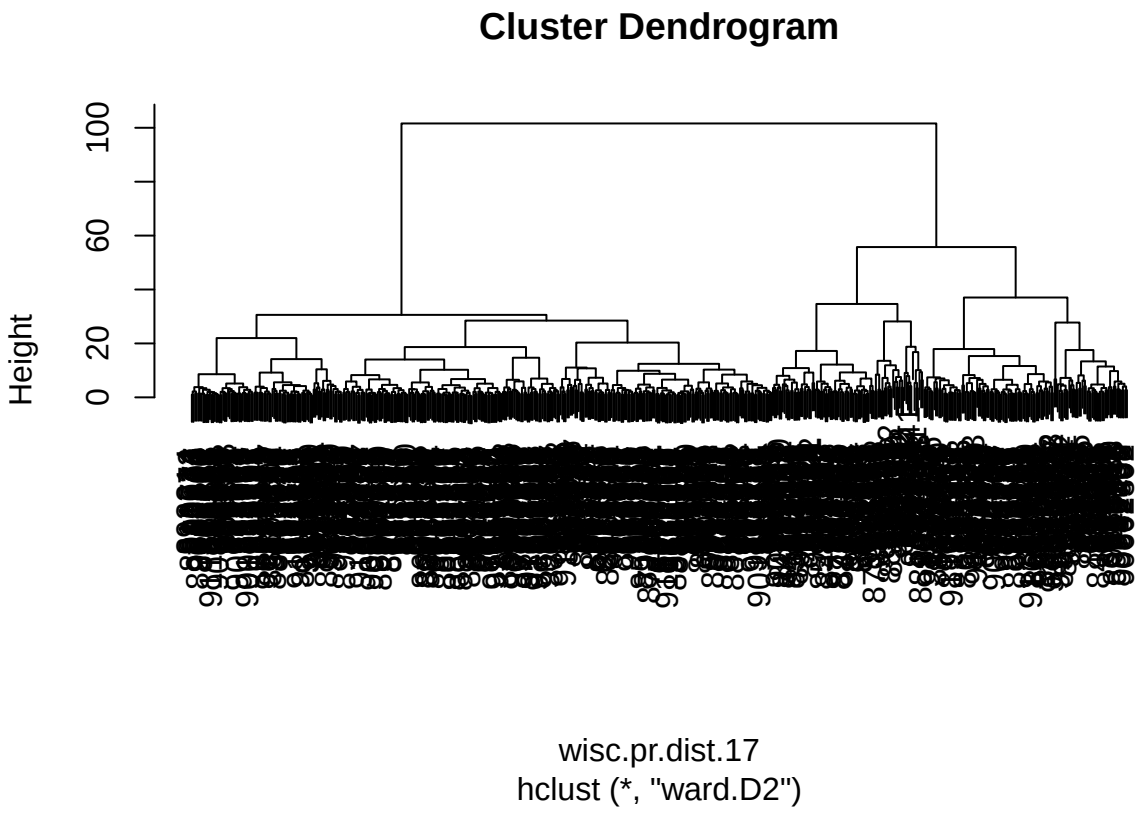
```
##                    4   2   0
##                    5   0   2
```

Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

K-means separates the clusters relatively well; cluster 2 contains mostly M (129/130 obs.), while cluster 1 is slightly less well separated. Compared to hclust, using 5 clusters, the reverse effect is seen. Hclust seems to have better separated out B observations (the predominantly "B" cluster contains half as many "M"s when compared to the K-means method). Overall, niether approach is perfect, but both provide a nice, quick approximation.

Combining methods, clustering on PCA results

```
wisc.pr.dist.17 <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(wisc.pr.dist.17,method="ward.D2")
plot(wisc.pr.hclust)
```



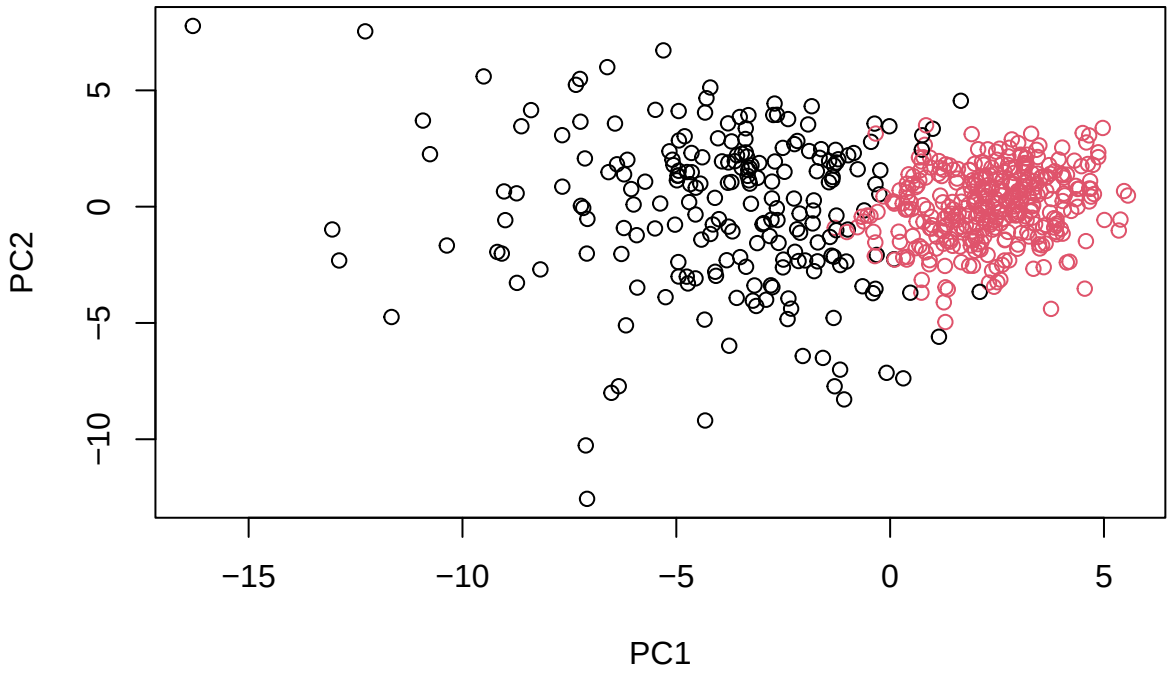

```
grps <- cutree(wisc.pr.hclust,k=2)
table(grps)
```

```
## grps
##   1   2
## 216 353
```

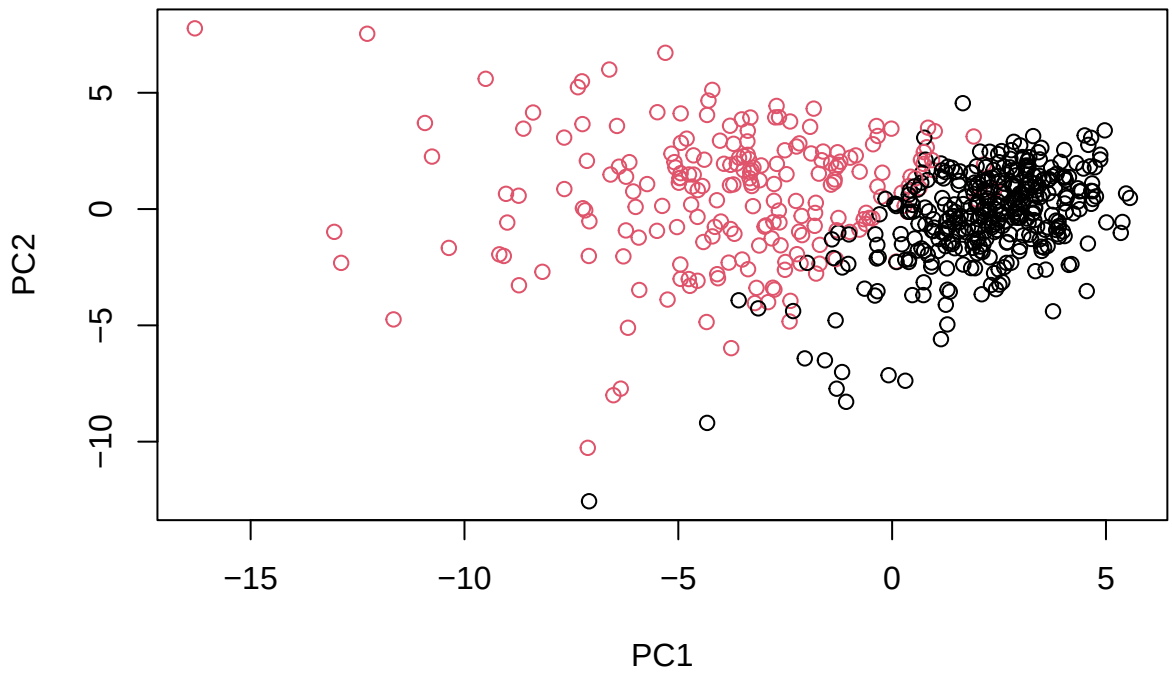
```
table(grps,diagnosis)
```

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

```
plot(wisc.pr$x[,1:2],col=grps)
```




```
plot(wisc.pr$x[,1:2],col=diagnosis)
```



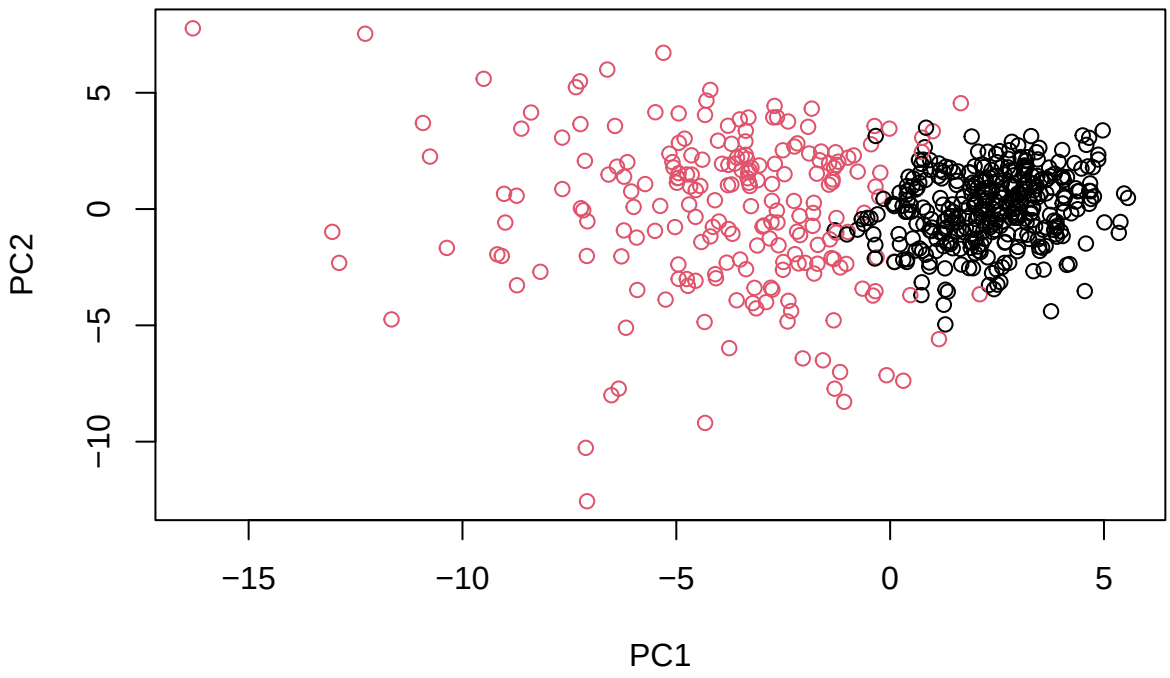

```
g <- as.factor(grps)
levels(g)
```

```
## [1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
## [1] "2" "1"
```

```
plot(wisc.pr$x[,1:2], col=g)
```




```
#library(rgl)
#plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s", col=grps)
#rglwidget(width = 400, height = 400)
```