Class 09 Mini-Project

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Preparing the Data

Reading in the data

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

Examine the data

```
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
```

Get rid of the "Diagnosis" column because we won't be needing it

```
wisc.data <- wisc.df[,-1]
```

But store "Diagnosis" as a factor to be used later to check our work

```
diagnosis <- as.factor(wisc.df$diagnosis)
```

Q1. How many observations are in this dataset?

```
dim(wisc.data)
```

```
## [1] 569  30
```

569 observations

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

```
table(diagnosis)
```

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

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

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

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

Principal Component Analysis

Checking column means and standard deviation

```
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
```

Perform PCA

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

```
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)?

From row 2 of the summary above, PC1 accounts for 44.27%

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

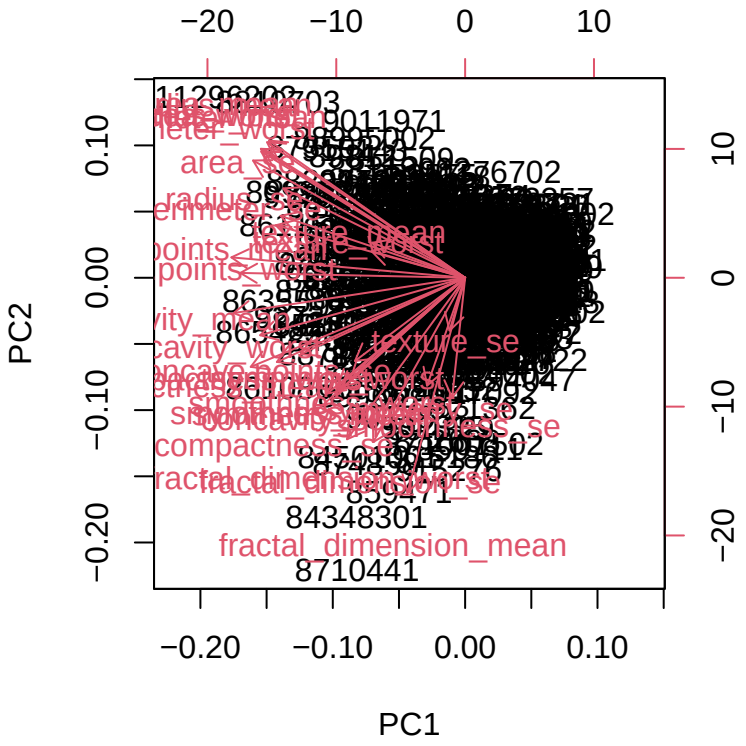
From row 3 of the summary above, 3 PCs are required to describe >70%

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

From row 3 of the summary above, 7 PCs are required to describe >90%

Interpreting PCA Results

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

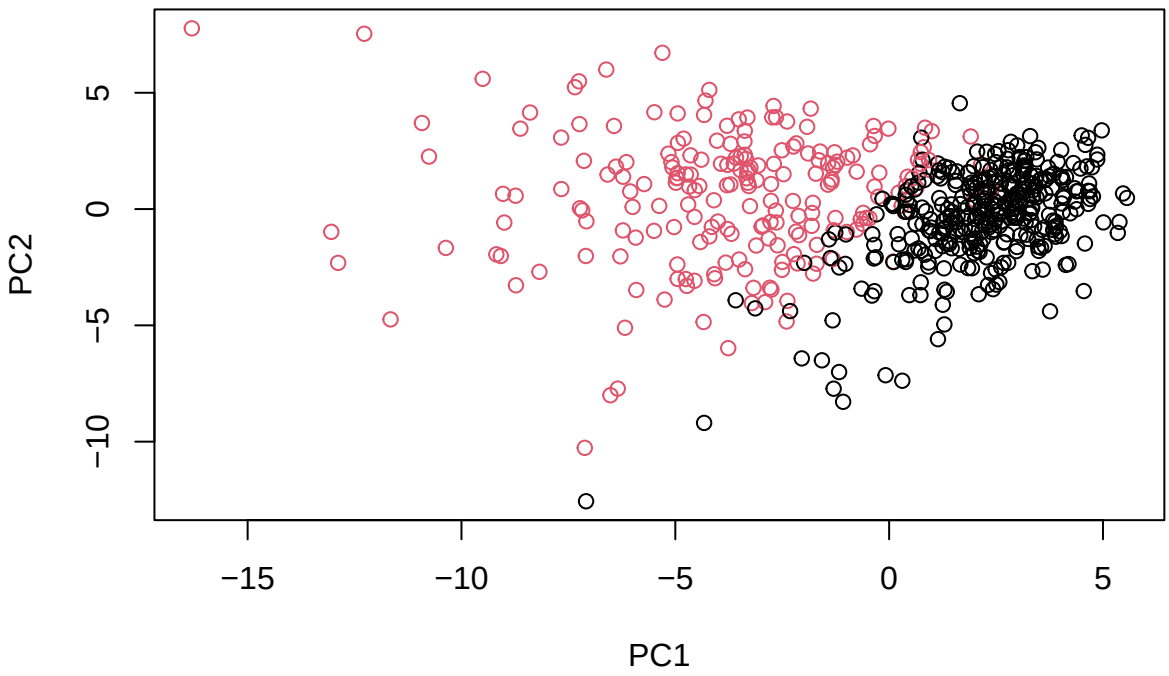


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

There is way too much information on this plot for it to be understood and to be useful.

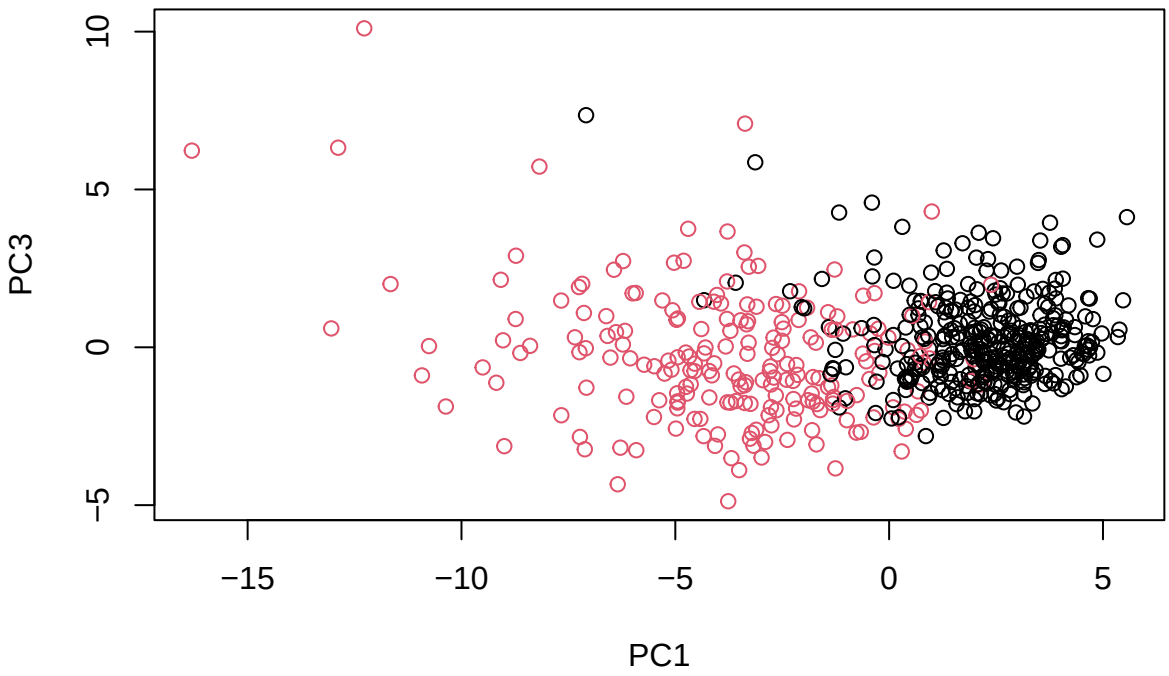
Let's make a better plot

```
plot(wisc.pr$x[,1], wisc.pr$x[,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?

```
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis, xlab = "PC1", ylab = "PC3")
```



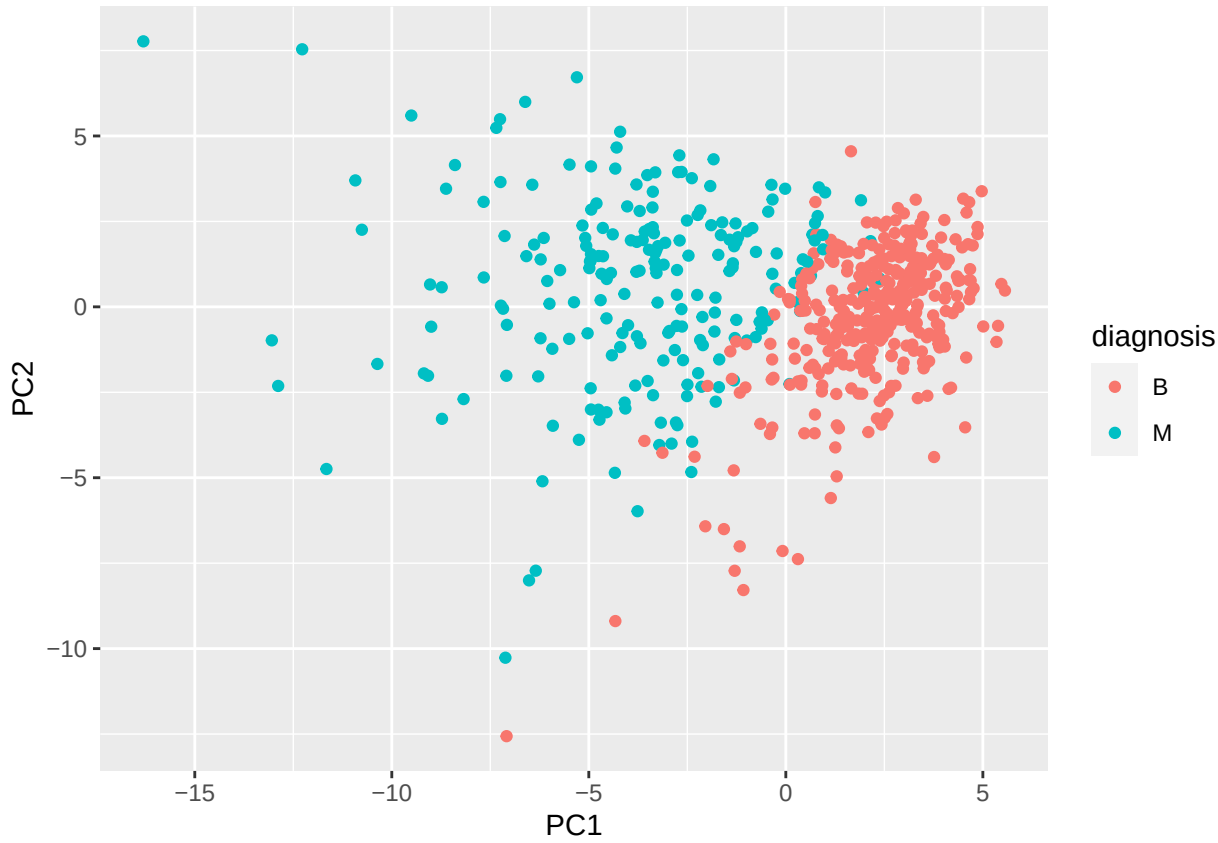
Using ggplot2 to make another plot Turn the PCA into a dataframe, add back diagnosis as a column

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

```
library(ggplot2)
```

Make a scatter plot colored by diagnosis

```
ggplot(df, aes(PC1, PC2, col = diagnosis)) +
  geom_point()
```



Variance Explained

Calculate variance of each component

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

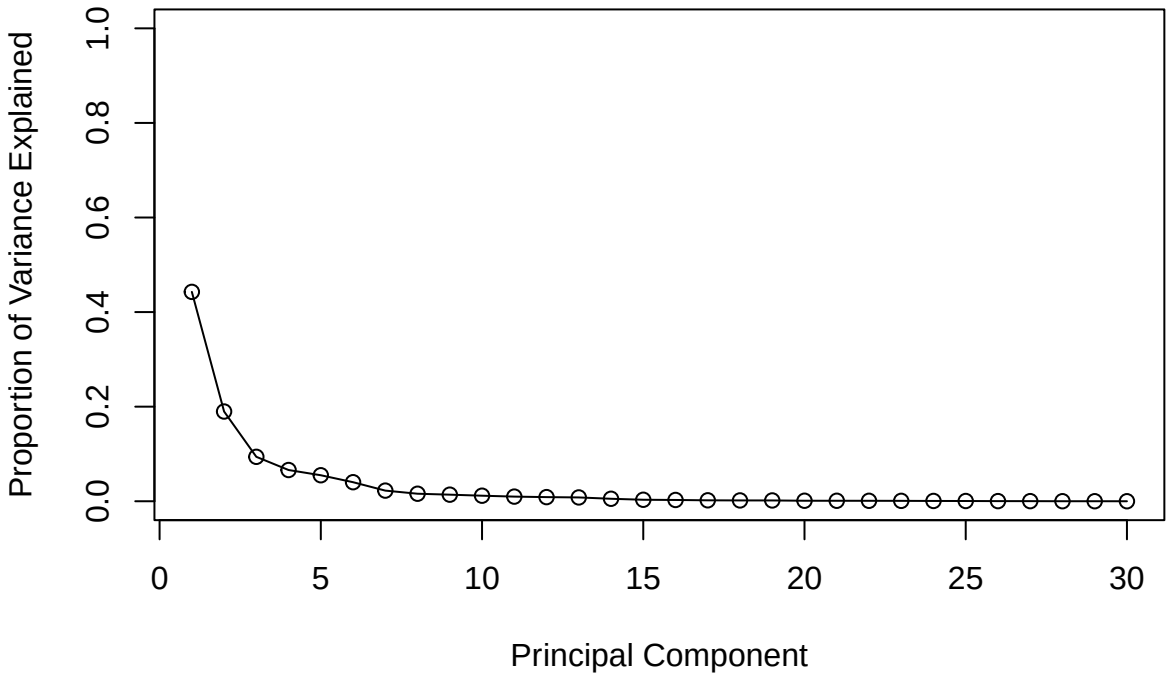
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Calculate the variance explained by each principal component

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

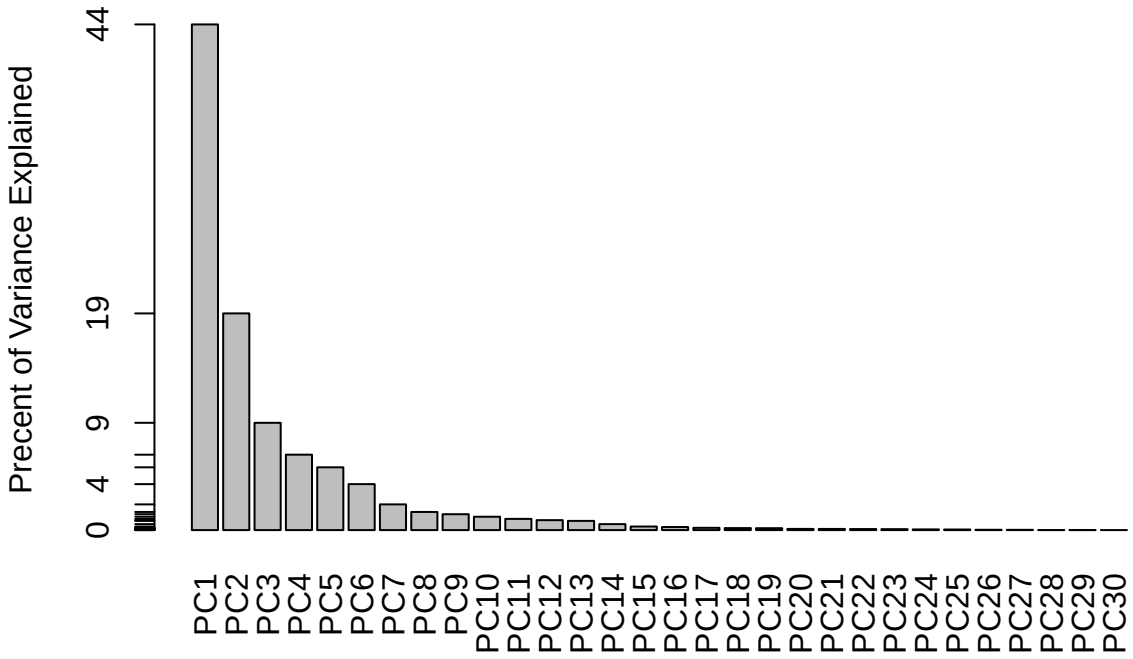
Plot variance explained for each principal component

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



Alternative scree plot of the same data

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

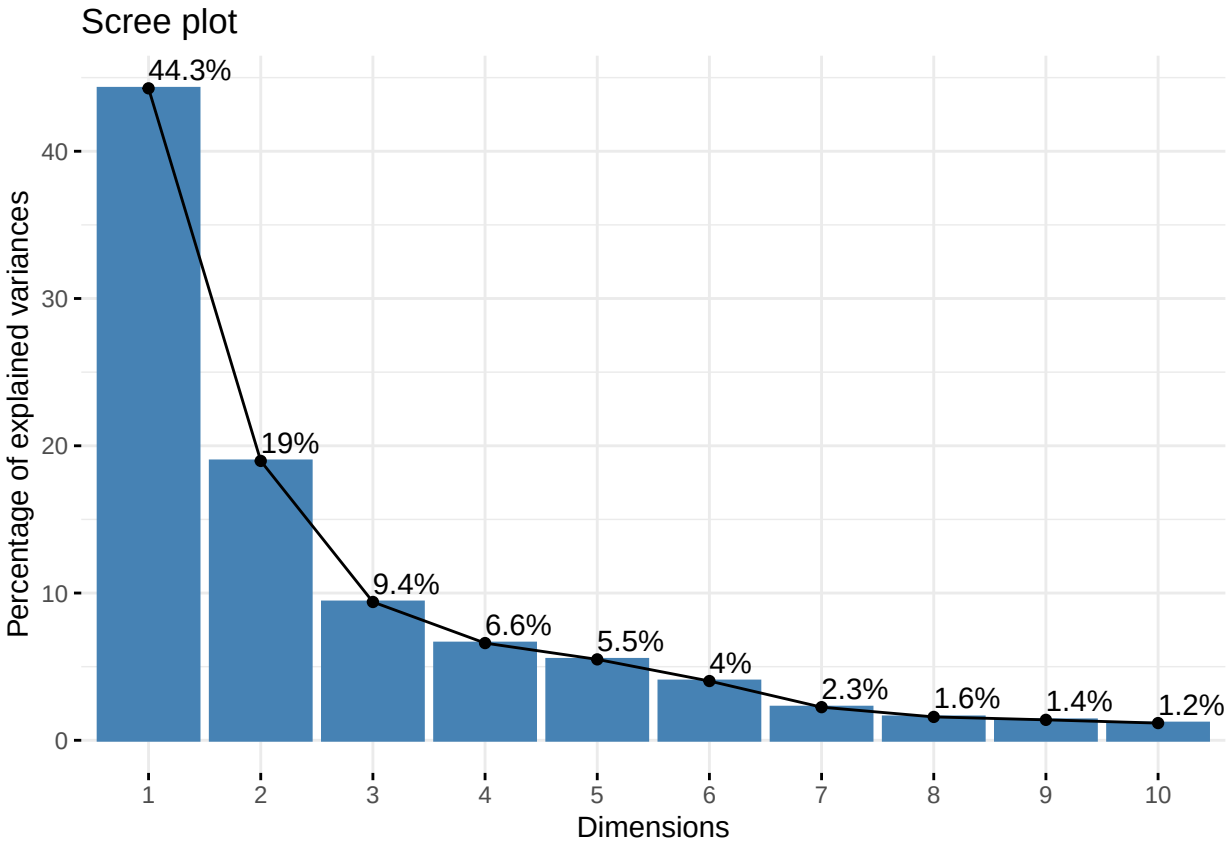


Exploring additional CRAN packages

```
#install.packages("factoextra")
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

Loadings: vectors that explain the mapping from the original features to the PC

> 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 loading vector for concave.points_mean is -0.260

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

```
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
```

You need 5 principal components to explain >80% of the variance

Hierarchical Clustering

First scale the data

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

Calculate the distances between all pairs of observations

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

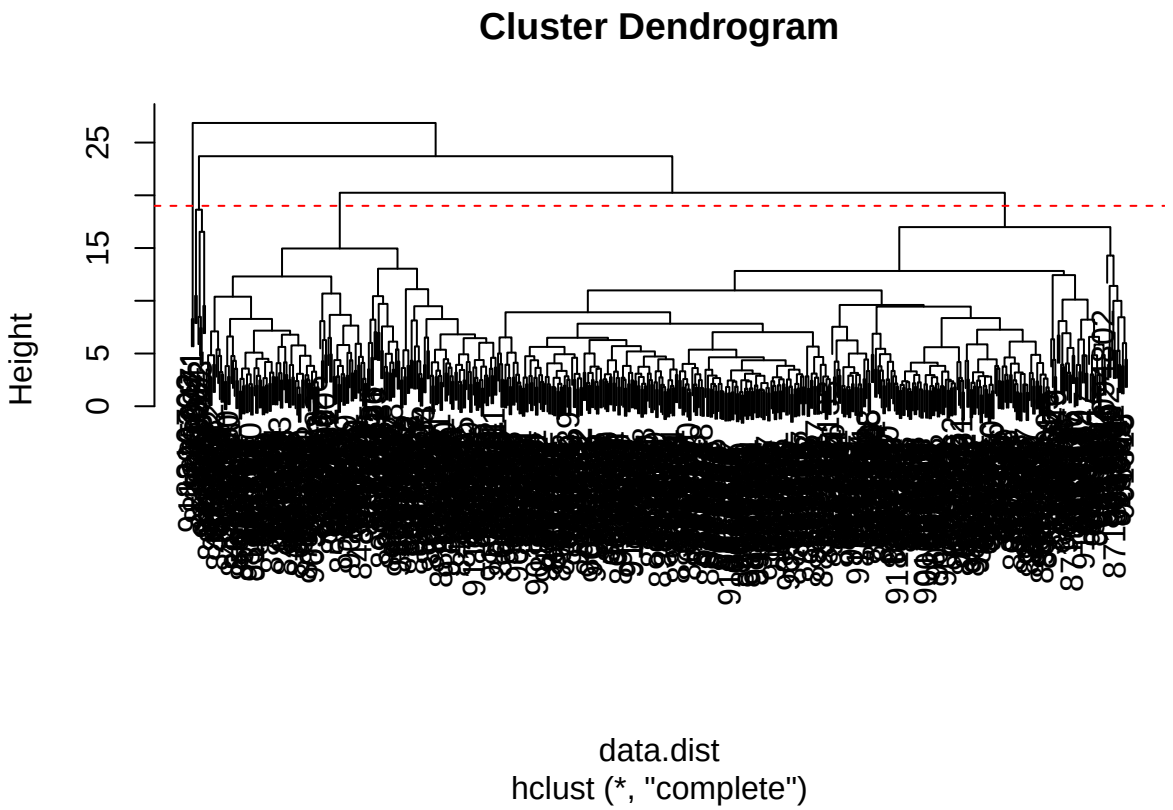
Create hierarchical clustering model

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

Results of HClustering

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

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



There are four clusters at about height 19

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

```
##               diagnosis
## wisc.xclusters   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
```

```
wisc.xclusters <- cutree(wisc.hclust, h = 15)
table(wisc.xclusters, diagnosis)
```

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

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

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

```
wisc.xclusters <- cutree(wisc.hclust, h = 20)
table(wisc.xclusters, diagnosis)
```

```
##               diagnosis
## wisc.xclusters   B   M
```

```
##              1  12 165
##              2   2   5
##              3 343  40
##              4   0   2
```

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

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

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

```
##               diagnosis
## wisc.xclusters   B   M
##              1 357 210
##              2   0   2
```

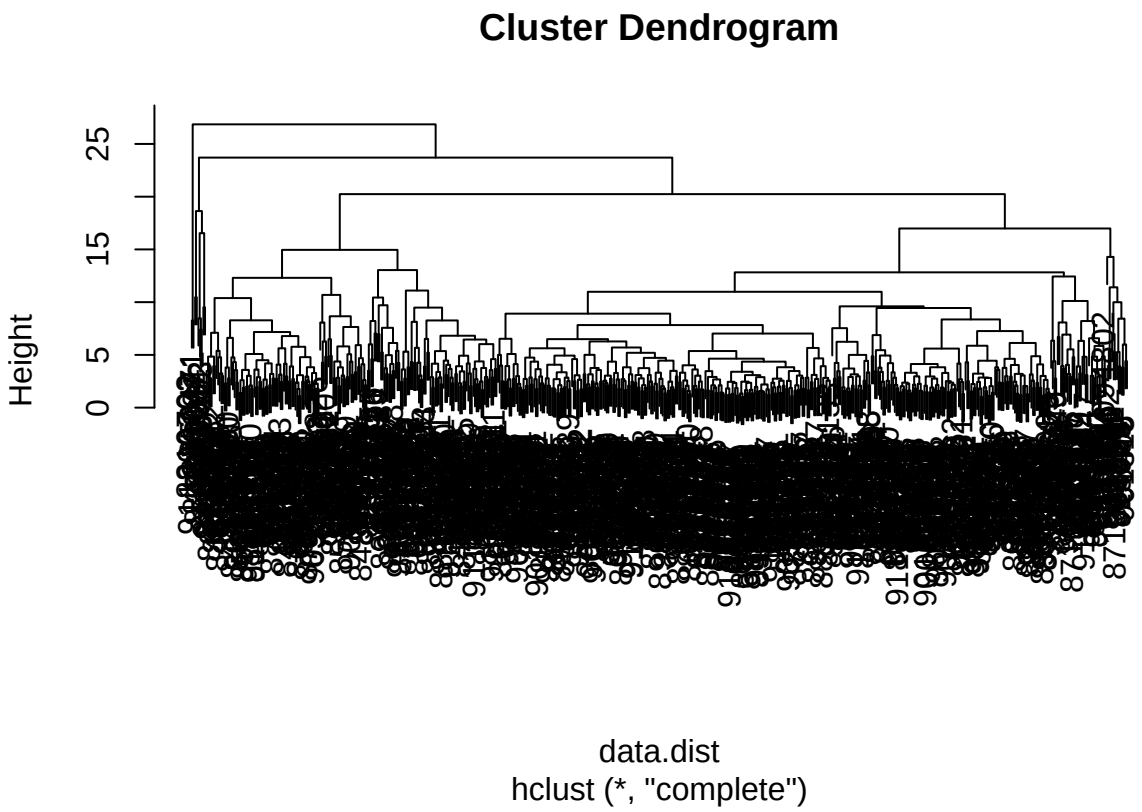
4 cluster provided some of the best results but using 5 clusters, at h = 18, could be a better decision. The two main benign and malignant groups retain the same values as in the original 4 cluster model but now, the additional three clusters are at least 100% benign or 100% malignant. In the 4 cluster model, one of the additional clusters was a mix of benign (29%) and malignant (71%).

Using Different Methods

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

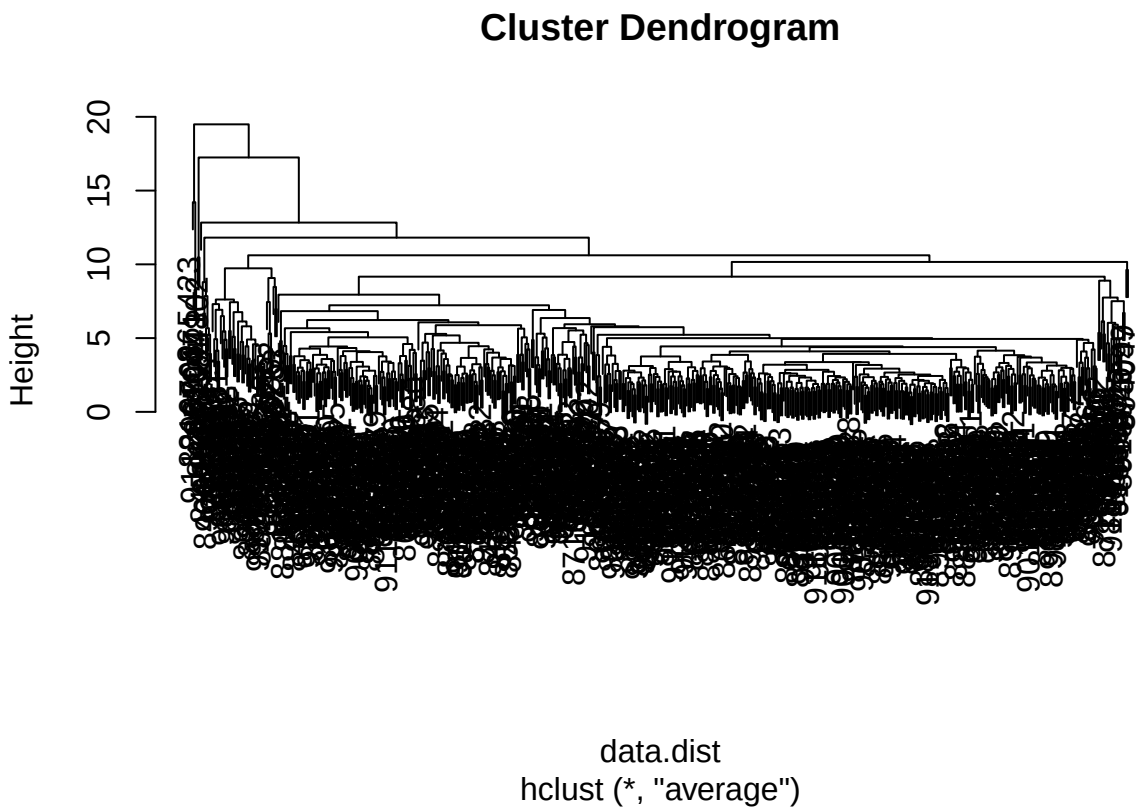
"complete" for reference

```
plot(wisc.hclust)
```



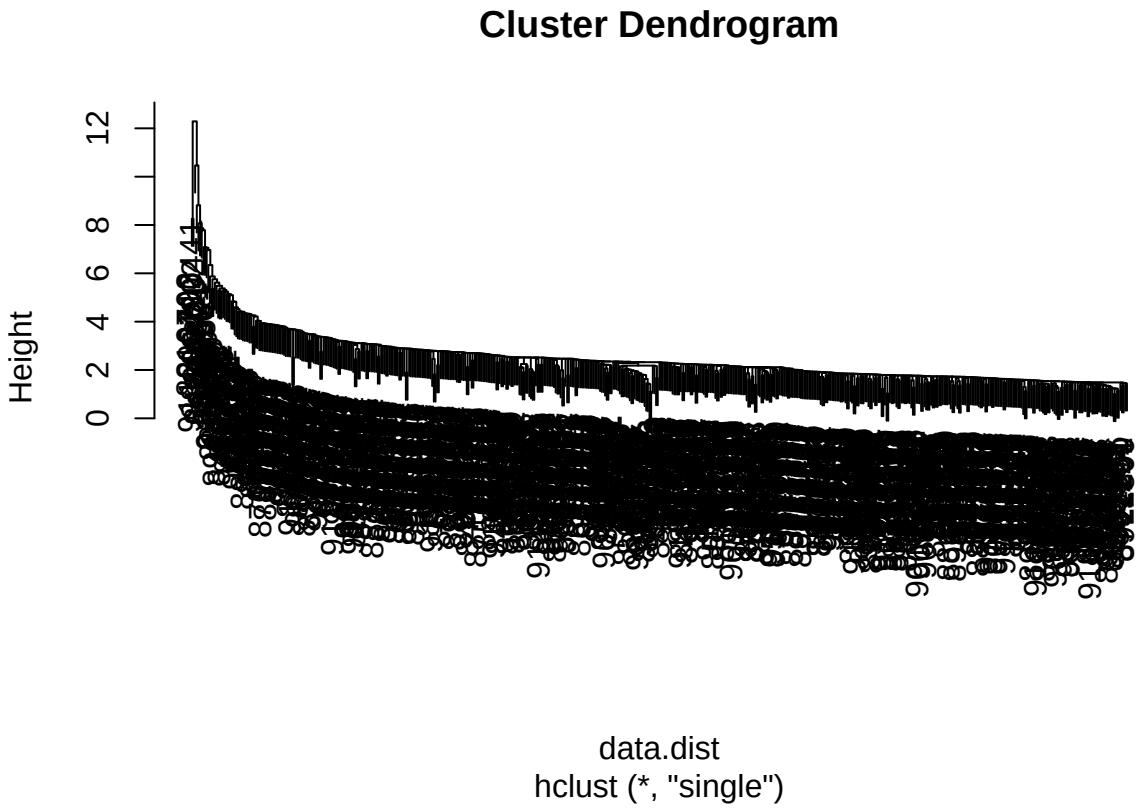
“average”

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



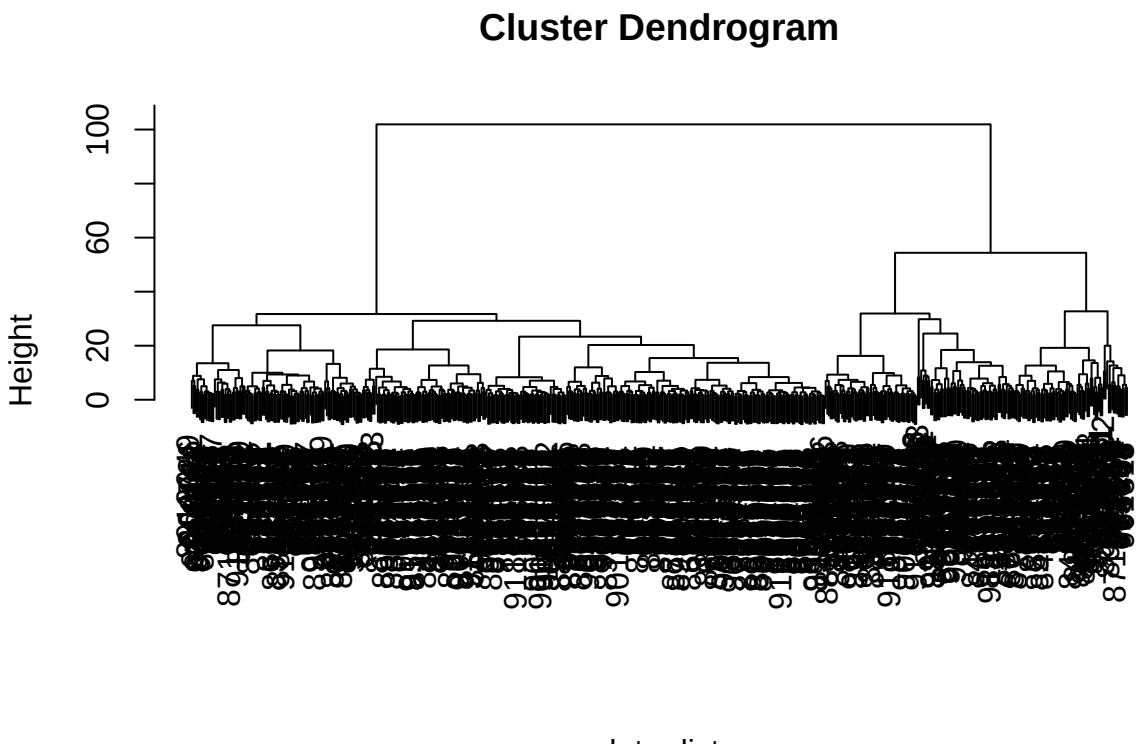
"single"

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



“ward.D2”

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

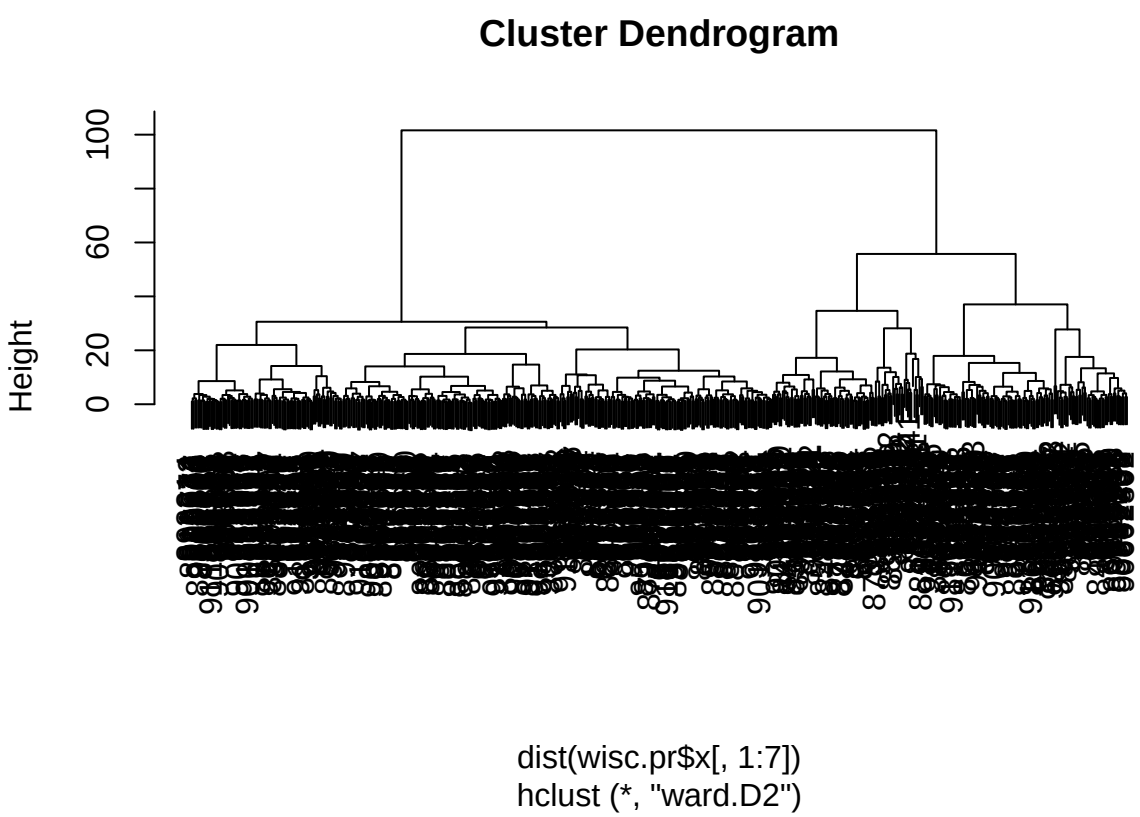


My favorite method was ward.D2 because it was the easiest to read. The symmetry of the plot made the larger clusters much easier to see. Additionally, all branches ended in the same place on a horizontal line which makes more conceptual sense to me.

Combining Methods

Does PCA improve or degrade the performance of hierarchical clustering?

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



Are these two main branches representative of malignant and benign tumors?

TO BE CONT.