Class 09 Unsupervised Learning Mini-Project

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1. Exploratory Data Analysis

Preparing the data

```r
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
```

Let's remove the "diagnosis" column since it gives the answer of whether the cells are malignant or benign.

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]

# Create diagnosis vector for later
diagnosis <- as.numeric(wisc.df$diagnosis == "M")
```

Exploratory Data Analysis

Explore the data you created before (wisc.data and diagnosis) to answer the following questions:

> Q1. How many observations are in this dataset?

```
nrow(wisc.df)
```

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

569 observations in wisc.df

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

```
length(which(diagnosis == 1))
```

```
## [1] 212
```

212 observations

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

```
length(grep(pattern = "_mean", x = colnames(wisc.df)))
```

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

10 variables

2. Principal Component Analysis

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
```

```
# Perform PCA on wisc.data
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)?

44.27%

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

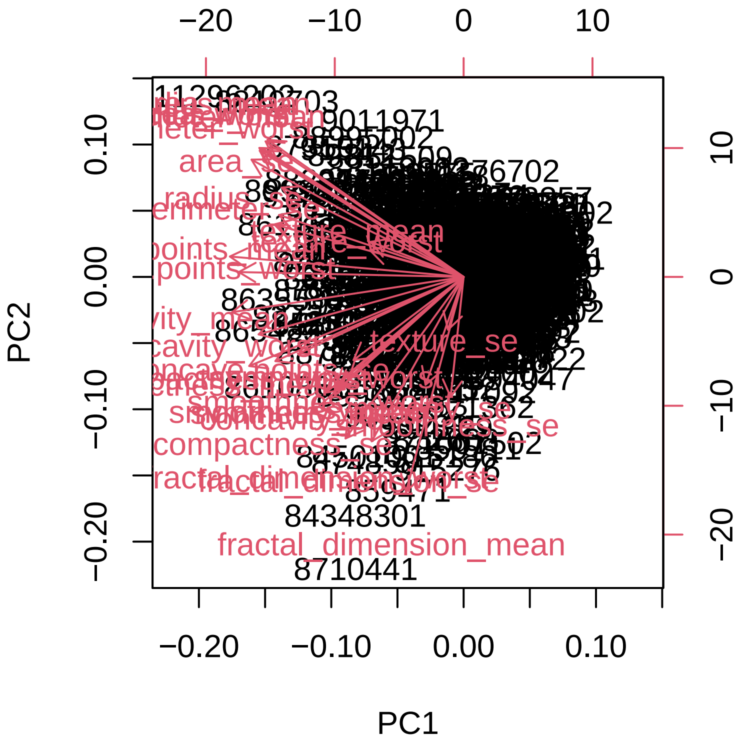
3 (PC1, PC2, and PC3)

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

7 (PC1-7)

Interpreting PCA Results

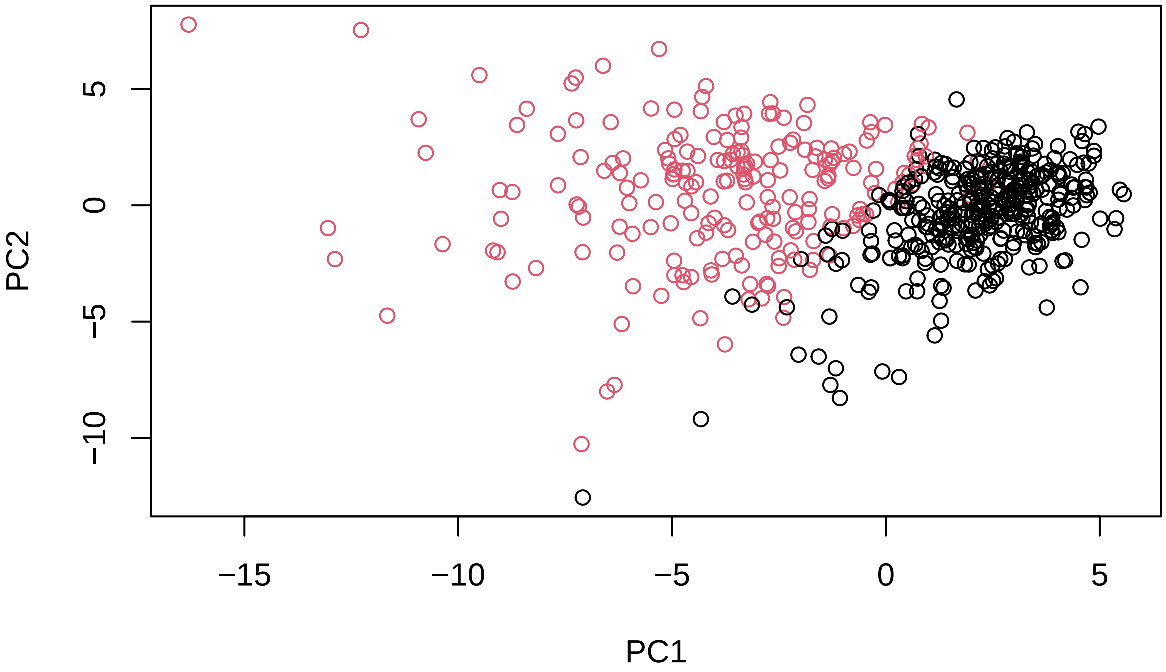
```
# Create a biplot of wisc.pr
biplot(wisc.pr)
```



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

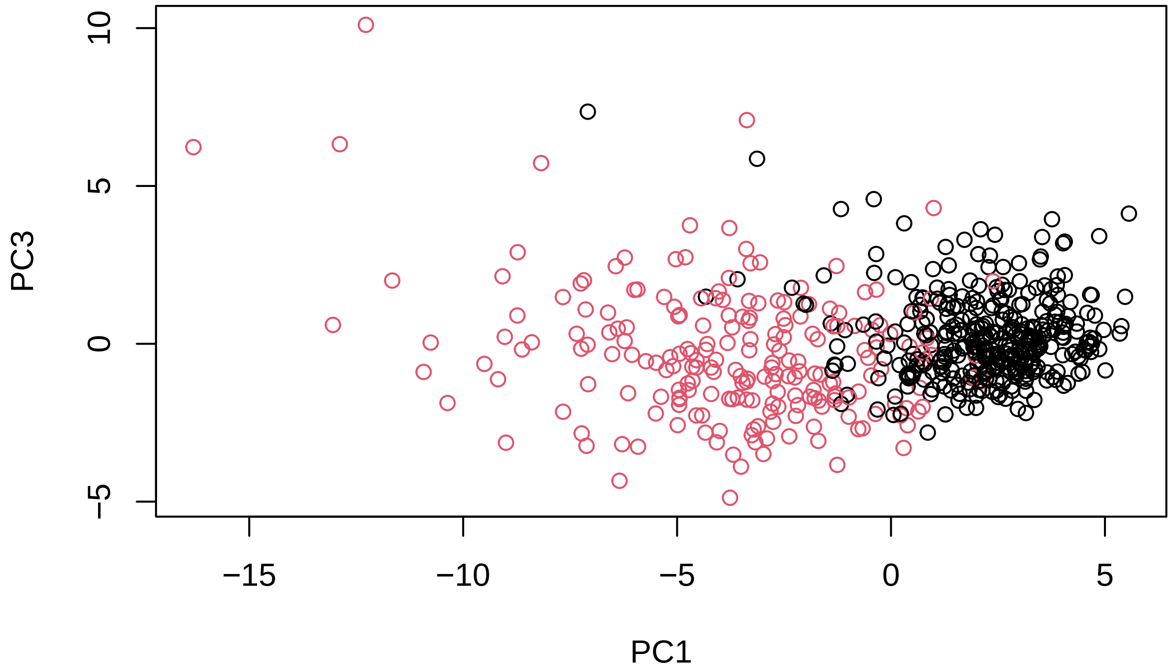
It is very difficult to interpret because everything is clustered together and hard to distinguish from each other.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[, c(1, 2)], col = (diagnosis + 1),
     xlab = "PC1", ylab = "PC2")
```



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

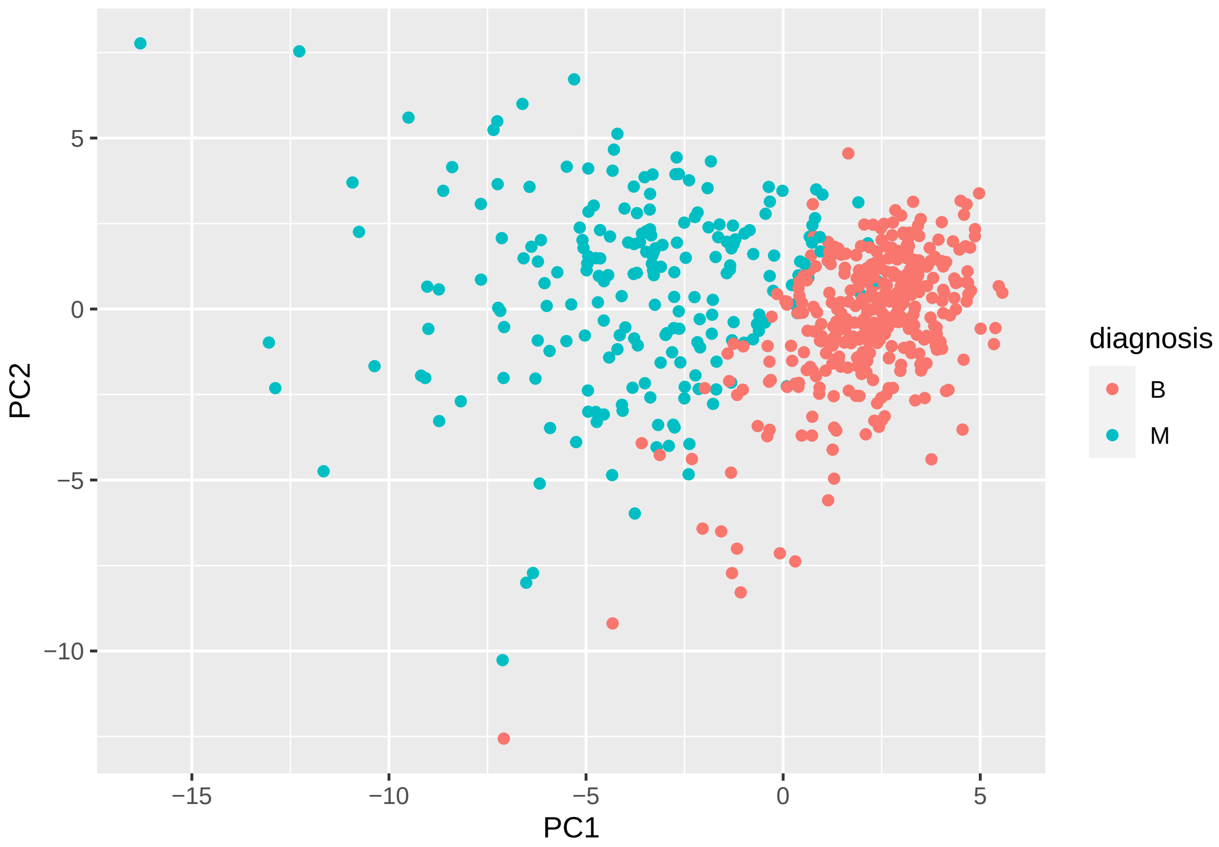
```
# Repeat for components 1 and 3
plot(wisc.pr$x[, c(1, 3)], col = (diagnosis + 1),
     xlab = "PC1", ylab = "PC3")
```



There is clearer separation between the 2 subgroups for the first plot (PC1 vs PC2) compared to the second (PC1 vs PC3). These plots are also much neater than the biplot.

Variance Explained

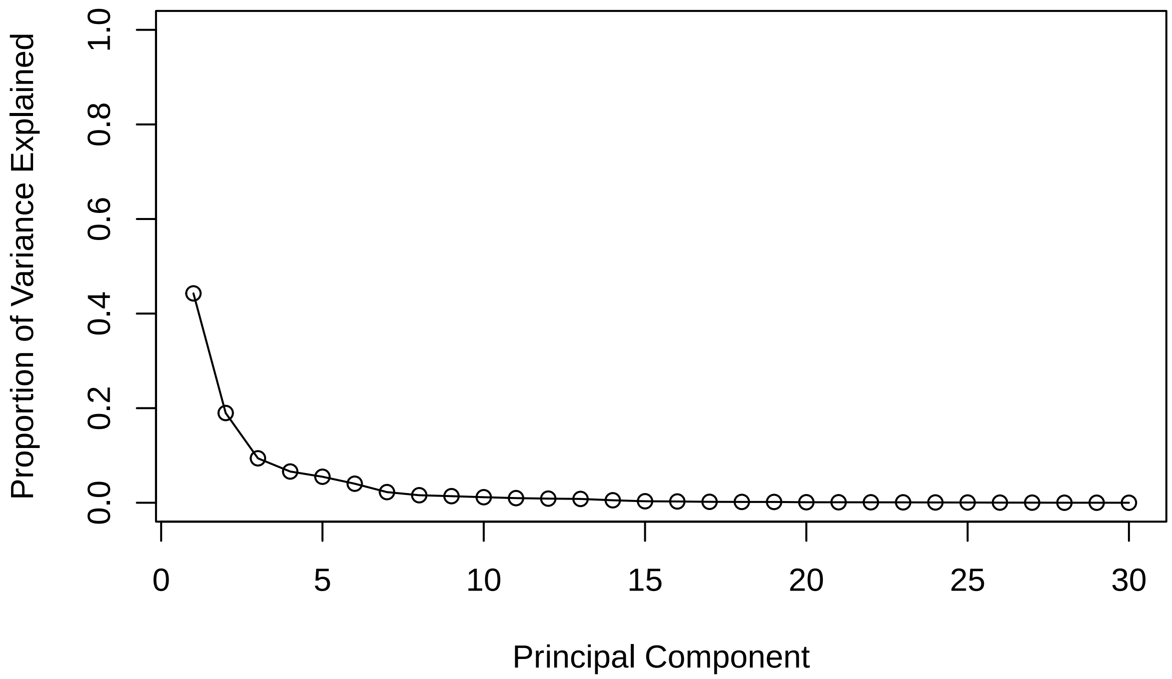
```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- wisc.df$diagnosis

# Load the ggplot2 package
library(ggplot2)

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



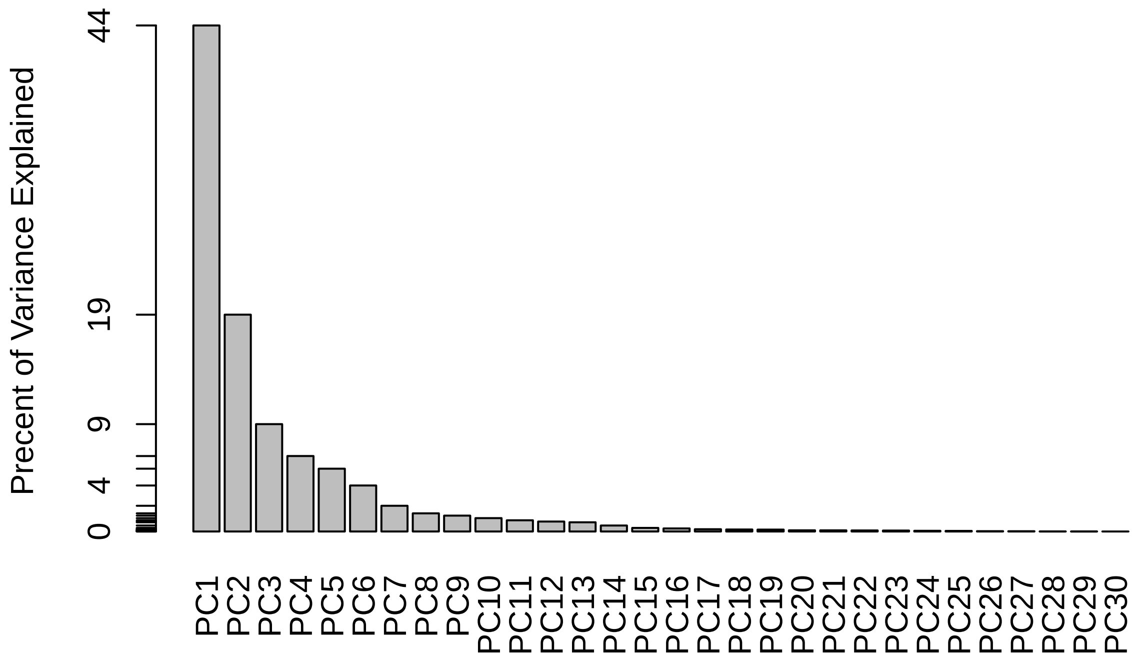
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

```
# Variance explained by each principal component: pve
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 = "o")
```



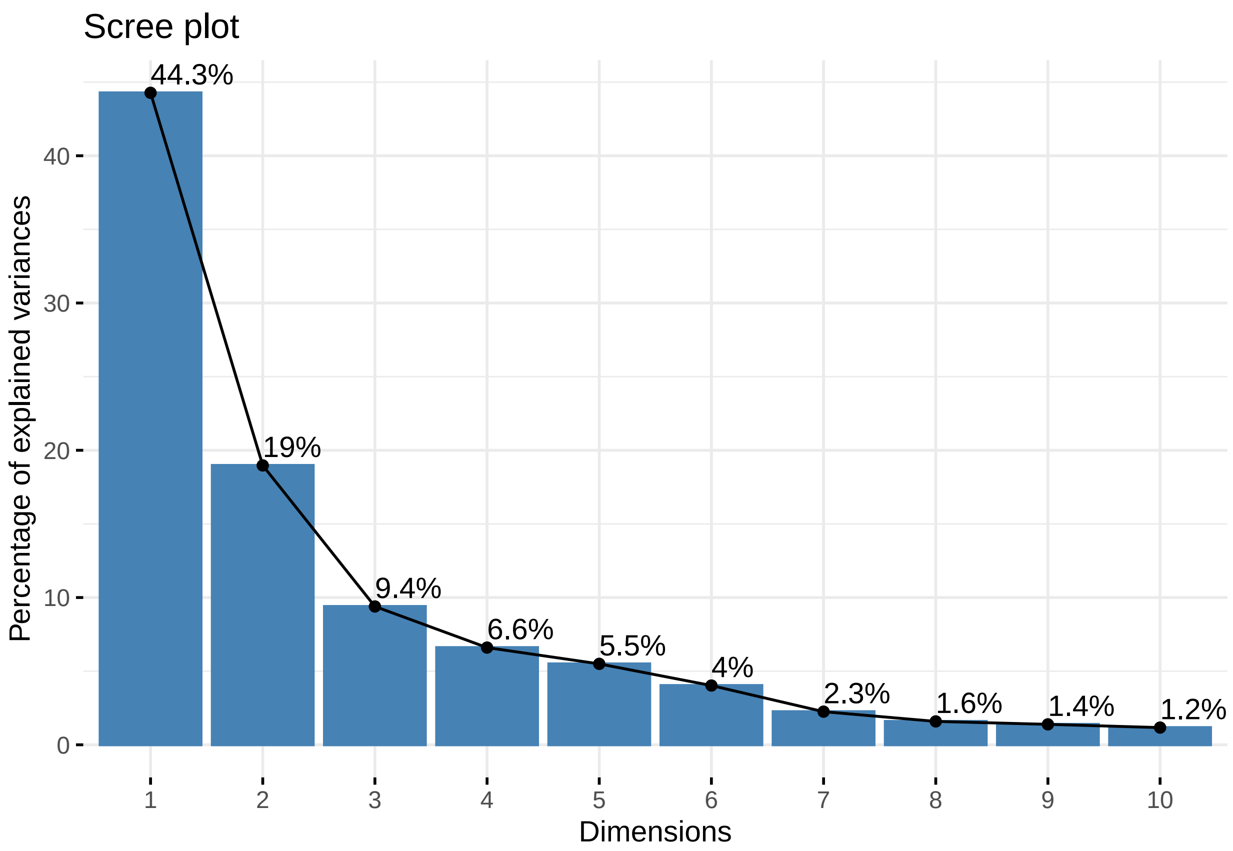
```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg = paste0("PC",1:length(pve)), las = 2, axes = FALSE)
axis(2, at=pve, labels = round(pve, 2)*100 )
```



```
# ggplot based graph
#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

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
```

-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 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
```

5 (PC1-5)

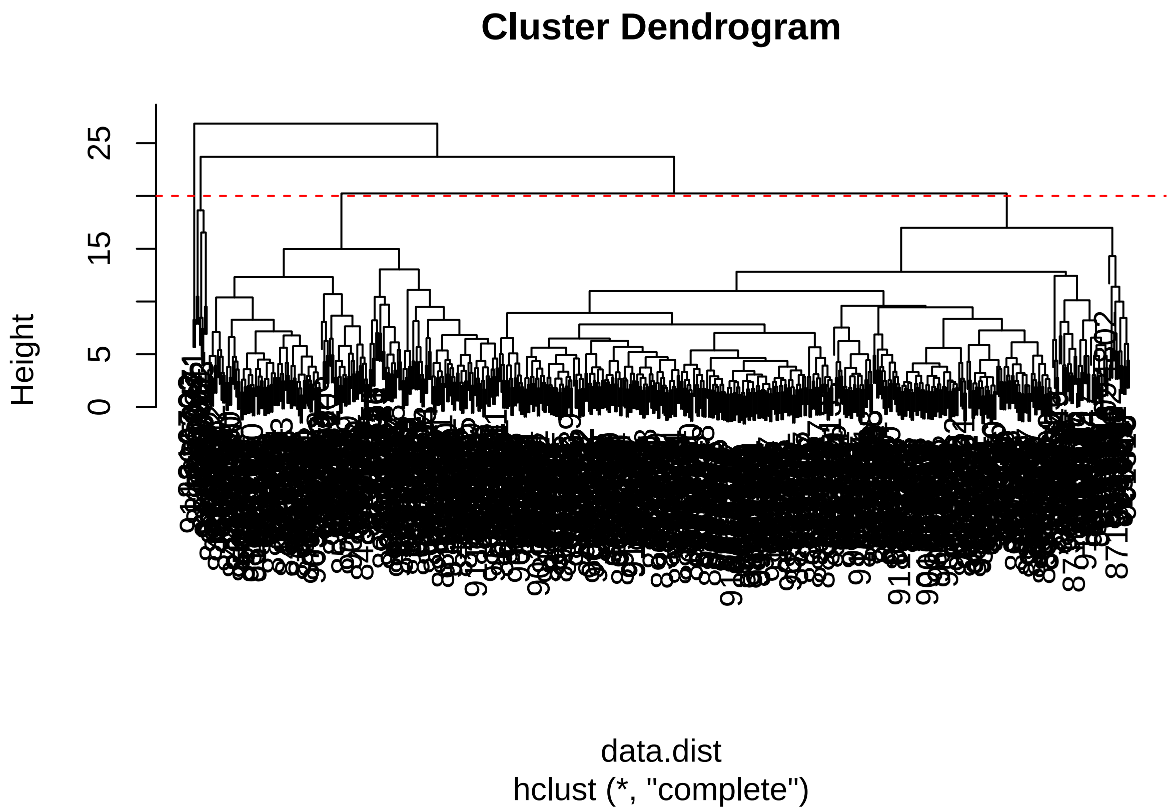
3. Hierarchical Clustering

```
# 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")
```

Results of Hierarchical Clustering

> 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)
```



20

Selecting Number of Clusters

```
# Cut tree so that it has 4 clusters: wisc.hclust.clusters
wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)

# Compare cluster membership to actual diagnoses
table(wisc.hclust.clusters, diagnosis)
```

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

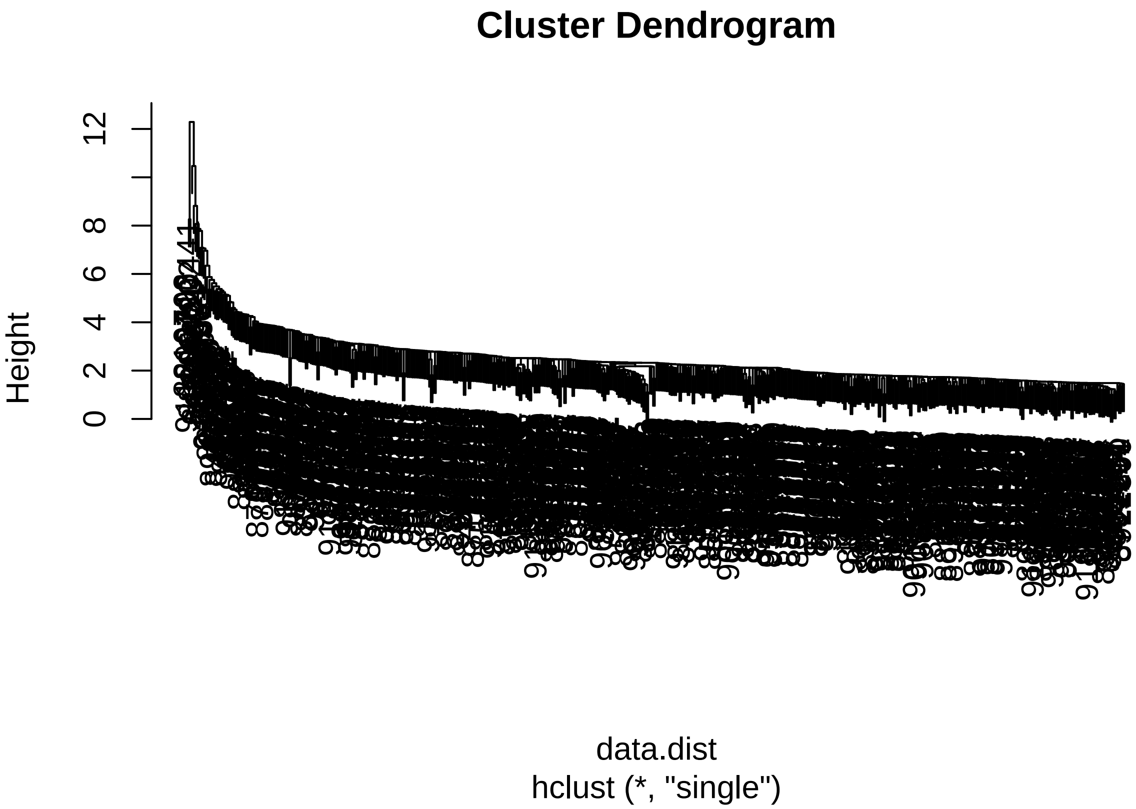
Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
# Cut tree so that it has 3 clusters: wisc.hclust.clusters
wisc.hclust.clusters0 <- cutree(wisc.hclust, k = 3)

# Compare cluster membership to actual diagnoses
table(wisc.hclust.clusters0, diagnosis)
```

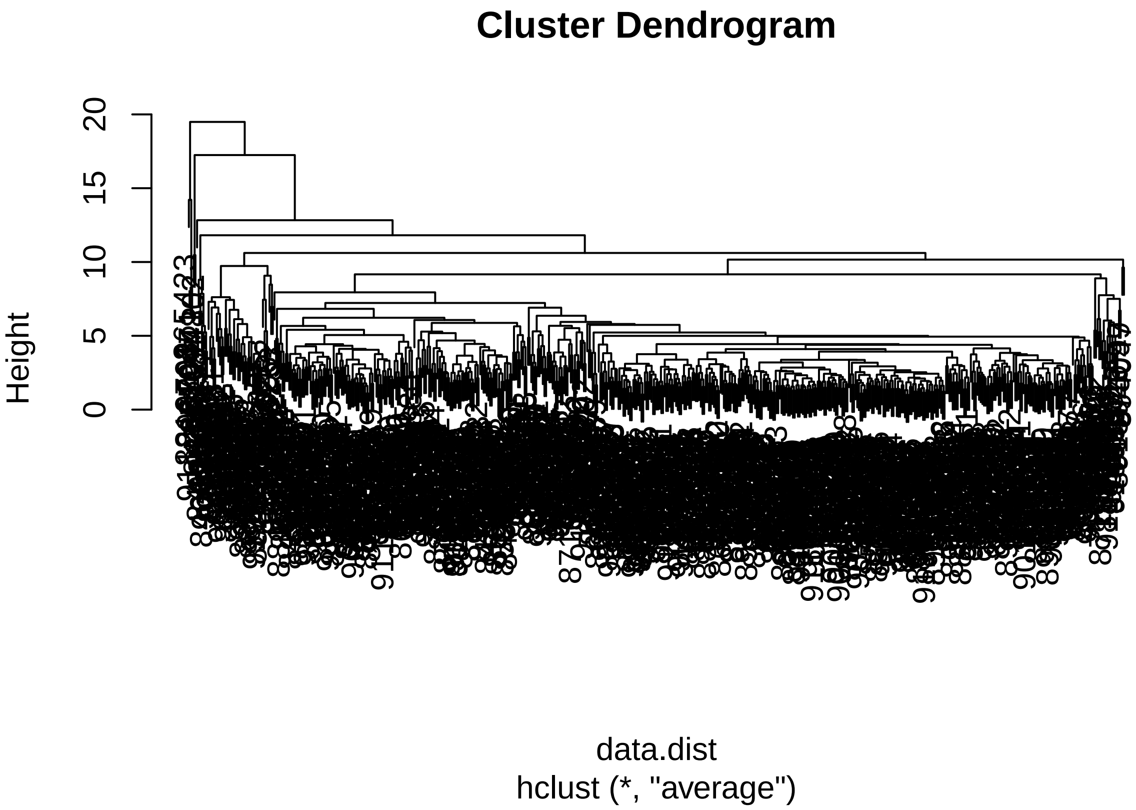
```
##                       diagnosis
## wisc.hclust.clusters0   0   1
##                     1 355 205
##                     2   2   5
##                     3   0   2
```

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

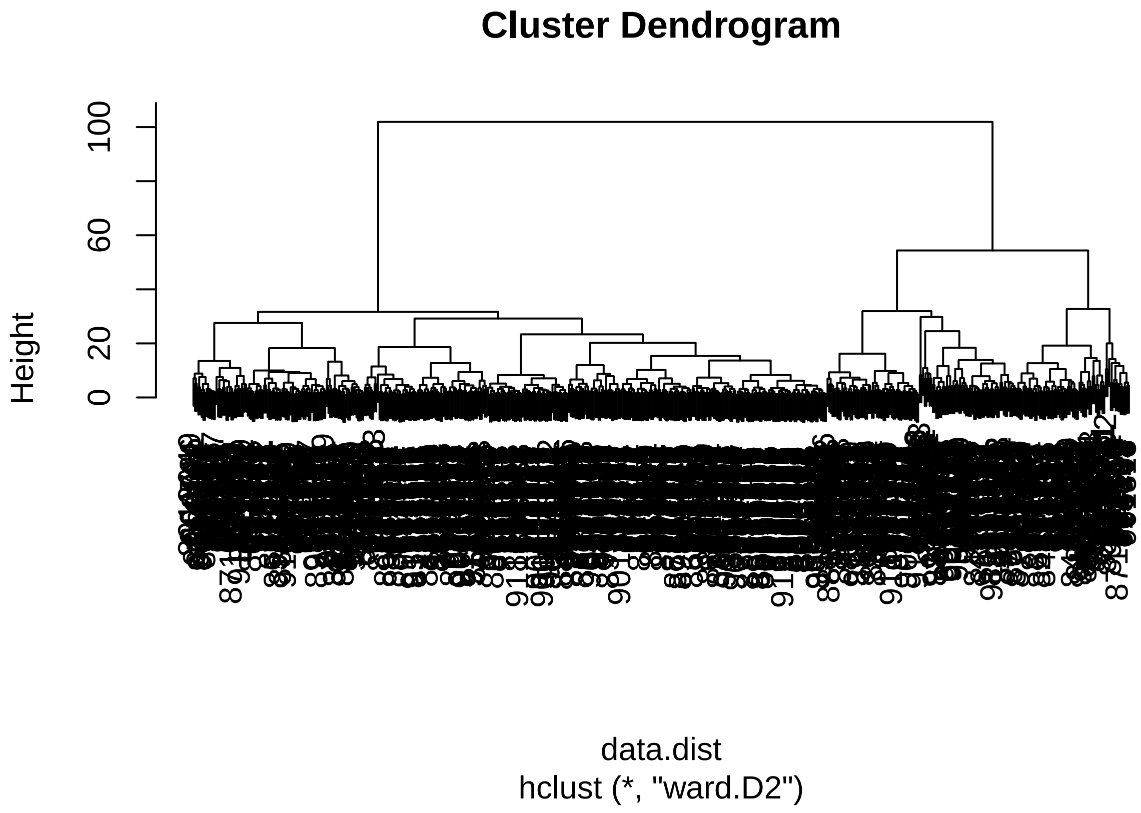
```
wisc.hclust1 <- hclust(data.dist, method = "single")
plot(wisc.hclust1)
```



```
wisc.hclust2 <- hclust(data.dist, method = "average")
plot(wisc.hclust2)
```



```
wisc.hclust3 <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust3)
```



I like the ward.D2 method because it separated the results into 2 clear groups.

4. OPTIONAL: K-means Clustering

K-means Clustering and Comparing Results

```
# Create a k-means model on wisc.data: wisc.km
wisc.km<-kmeans(scale(wisc.data), centers = 2, nstart = 20)

# Compare k-means to actual diagnoses
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##       0   1
##   1  14 175
##   2 343  37
```

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

Clusters 1, 2, and 4 in the hierarchical clustering model seem to be like cluster 1 from the k-means method. Cluster 3 from the hierarchical clustering model seems to be like cluster 2 from the k-means method.

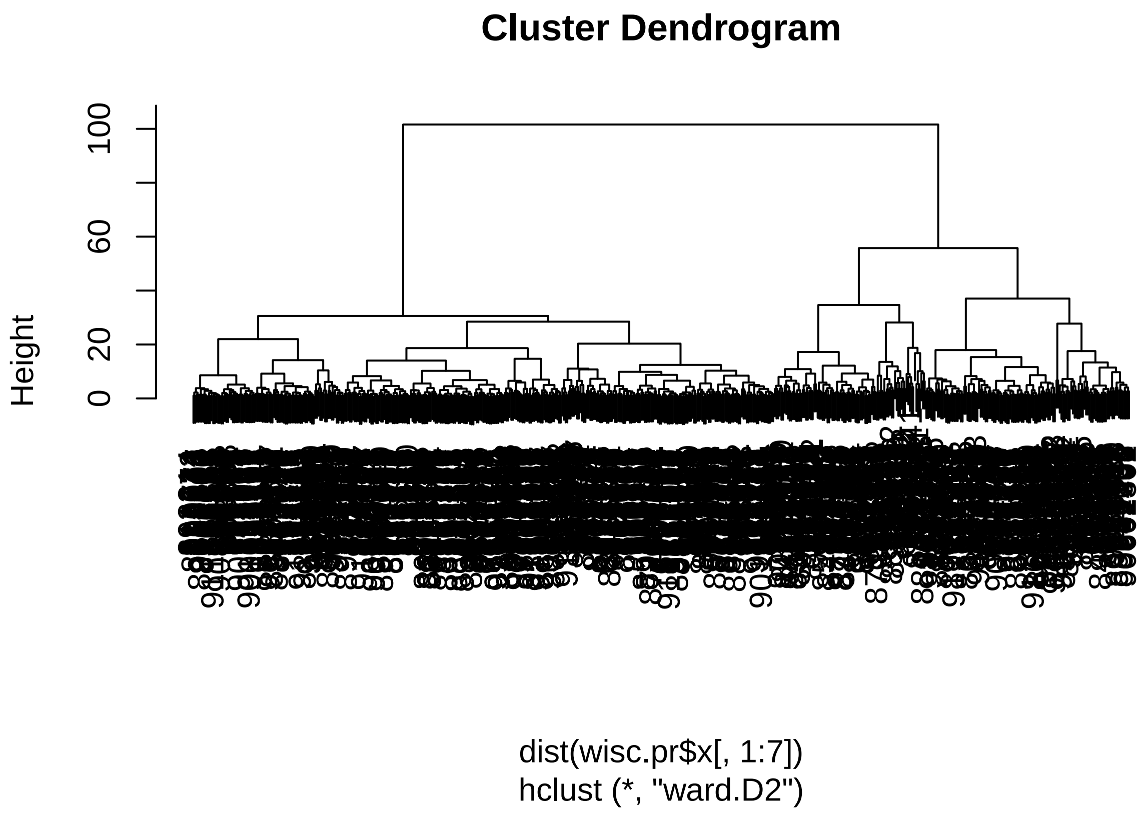
```
table(wisc.hclust.clusters, wisc.km$cluster)
```

```
##
## wisc.hclust.clusters   1   2
##                    1 160  17
##                    2   7   0
##                    3  20 363
##                    4   2   0
```

5. Combining Methods

Clustering on PCA Results

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method = "ward.D2")
plot(wisc.pr.hclust)
```



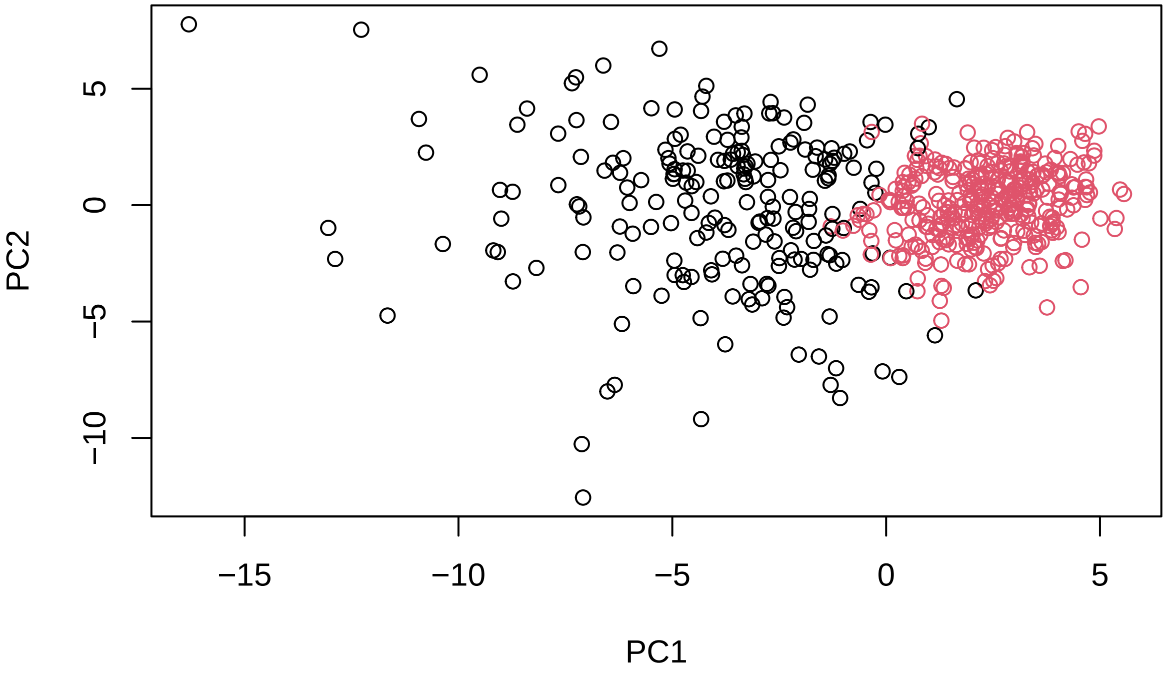
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

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

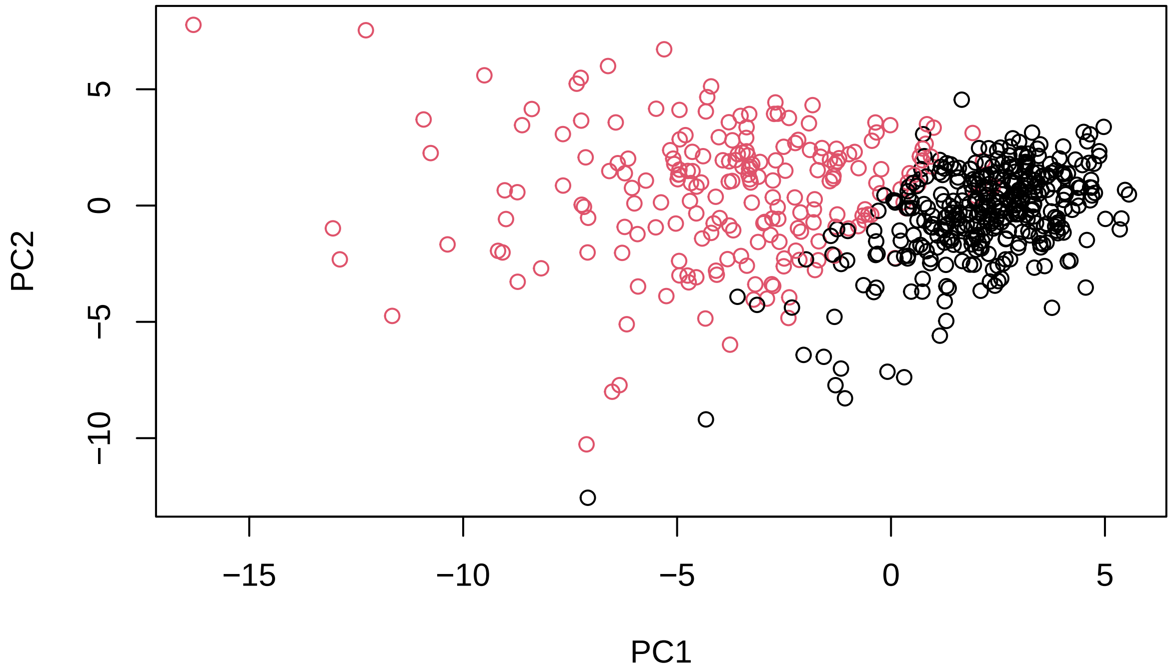
```
table(grps, diagnosis)
```

```
##     diagnosis
## grps   0   1
##    1  28 188
##    2 329  24
```

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



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



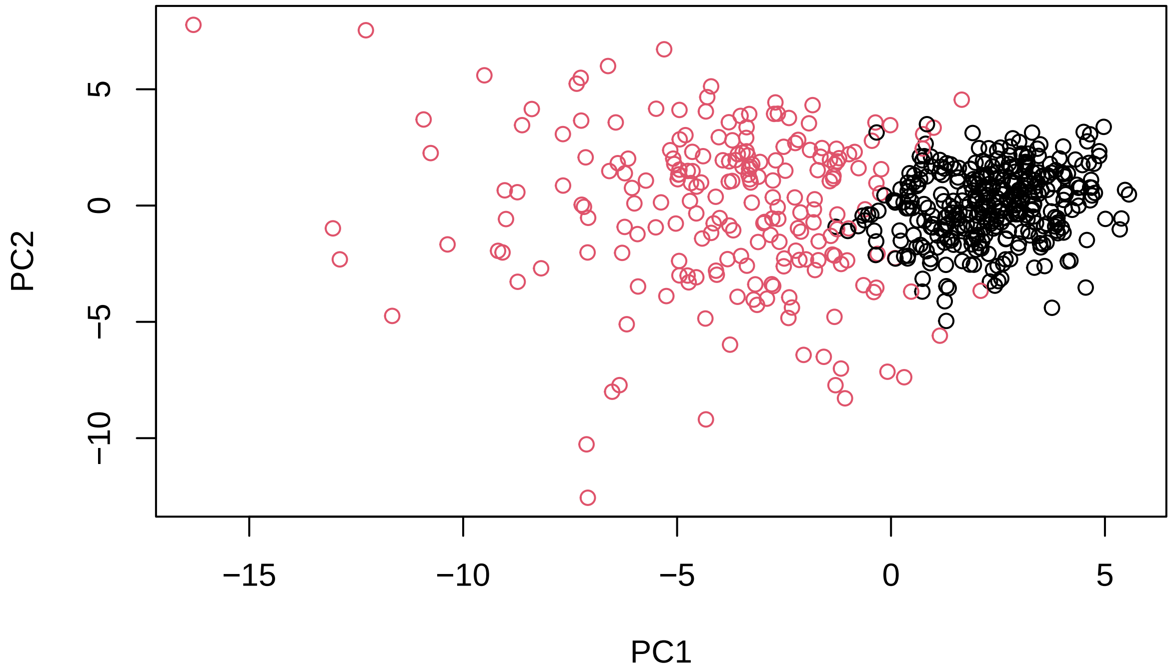
```
g <- as.factor(grps)
levels(g)
```

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

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

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

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col = g)
```



```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")

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

Q15. How well does the newly created model with four clusters separate out the two diagnoses?

```
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
##                        diagnosis
## wisc.pr.hclust.clusters   0   1
##                       1  28 188
##                       2 329  24
```

Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

```
table(wisc.km$cluster, diagnosis)
```

```
##    diagnosis
##        0   1
##   1   14 175
##   2  343  37
```

```
table(wisc.hclust.clusters, diagnosis)
```

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

6. Sensitivity/Specificity

> Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

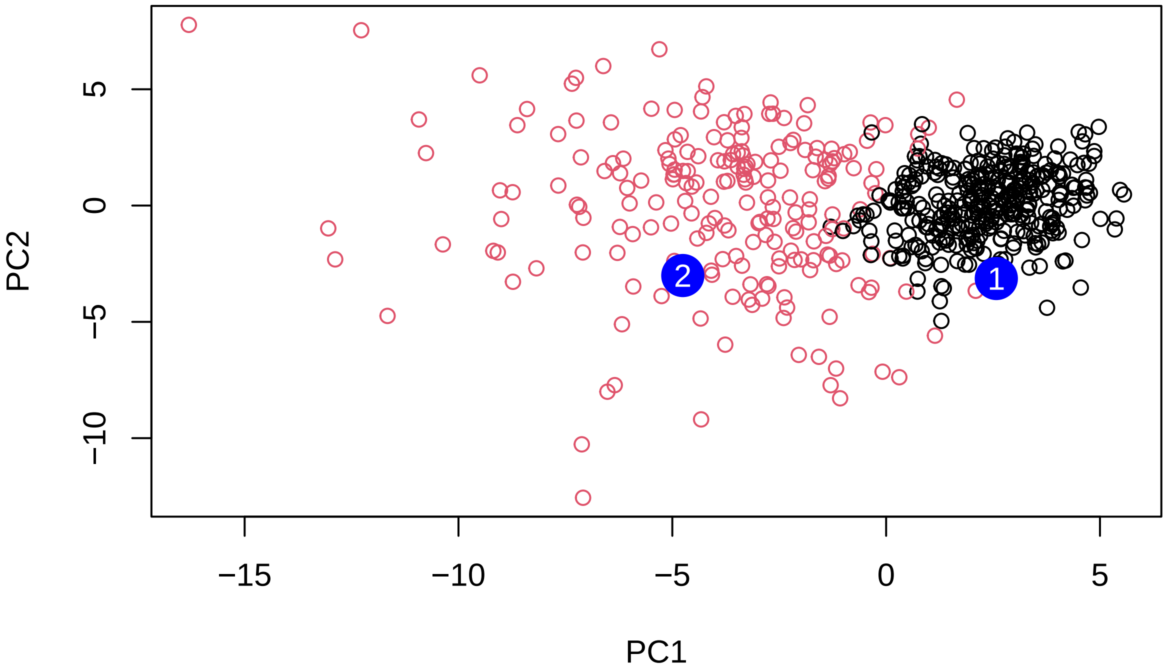
Kmeans resulted in the best specificity and sensitivity.

7. Prediction

```
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
##            PC1       PC2        PC3        PC4       PC5        PC6        PC7
## [1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
## [2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
##             PC8       PC9       PC10      PC11      PC12      PC13     PC14
## [1,] -0.2307350 0.1029569 -0.9272861 0.3411457  0.375921 0.1610764 1.187882
## [2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
##           PC15       PC16        PC17        PC18        PC19       PC20
## [1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
## [2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
##            PC21       PC22       PC23       PC24        PC25         PC26
## [1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121  0.078884581
## [2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
##              PC27        PC28         PC29         PC30
## [1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
## [2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

```
plot(wisc.pr$x[,1:2], col = g)
points(npc[,1], npc[,2], col = "blue", pch = 16, cex = 3)
text(npc[,1], npc[,2], c(1,2), col = "white")
```



Q18. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize following up with those patients represented by the black circles overlapping with the red circles because their cells are similar to cells of malignant tumors.

About This Document

```
sessionInfo()
```

```
## R version 4.1.2 (2021-11-01)
## Platform: x86_64-w64-mingw32/x64 (64-bit)
## Running under: Windows 10 x64 (build 19043)
##
## Matrix products: default
##
## locale:
## [1] LC_COLLATE=English_United States.1252
## [2] LC_CTYPE=English_United States.1252
## [3] LC_MONETARY=English_United States.1252
## [4] LC_NUMERIC=C
## [5] LC_TIME=English_United States.1252
##
```

```
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
## [1] factoextra_1.0.7 ggplot2_3.3.5
##
## loaded via a namespace (and not attached):
##  [1] Rcpp_1.0.8        ggpubr_0.4.0      pillar_1.6.4      compiler_4.1.2
##  [5] highr_0.9         tools_4.1.2       digest_0.6.27     evaluate_0.14
##  [9] lifecycle_1.0.1   tibble_3.1.6      gtable_0.3.0      pkgconfig_2.0.3
## [13] rlang_0.4.11      DBI_1.1.2         ggrepel_0.9.1     yaml_2.2.1
## [17] xfun_0.29         withr_2.4.3       stringr_1.4.0     dplyr_1.0.7
## [21] knitr_1.37        generics_0.1.1    vctrs_0.3.8       grid_4.1.2
## [25] tidyselect_1.1.1  glue_1.6.0        R6_2.5.1          rstatix_0.7.0
## [29] fansi_0.5.0       rmarkdown_2.11    carData_3.0-5     car_3.0-12
## [33] tidyr_1.1.4       purrr_0.3.4       farver_2.1.0      magrittr_2.0.1
## [37] backports_1.4.1   scales_1.1.1      ellipsis_0.3.2    htmltools_0.5.1.1
## [41] abind_1.4-5       assertthat_0.2.1  colorspace_2.0-2  ggsignif_0.6.3
## [45] labeling_0.4.2    utf8_1.2.2        stringi_1.7.6     munsell_0.5.0
## [49] broom_0.7.11      crayon_1.4.2
```