Unsupervised Learning Analysis of Human Breast Cancer Cells

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Preparing the data

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

Create a new vector called 'diagnosis' that contains the data from the diagnosis column of the orignal data set and store as a factor

```
diagnosis <- wisc.df$diagnosis
```

Exploratory data analysis

Q1. How many observations are in this dataset?

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

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

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

```
table(diagnosis)
```

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

212 are malignant.

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

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

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

Principle 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 and look at summary of results

```
wisc.pr <- prcomp(x=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)?

0.4427

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

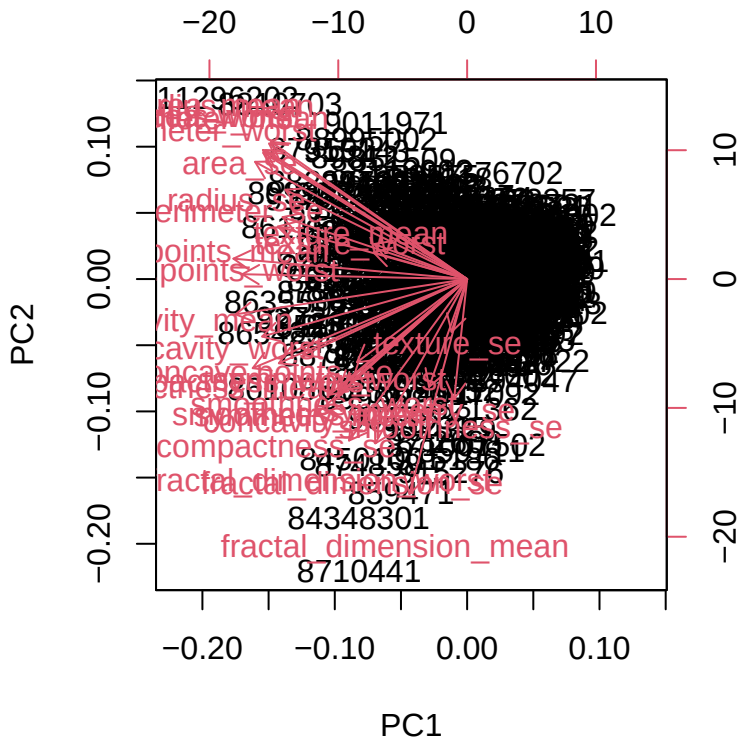
3 PCs

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

7 PCs

Interpreting PCA results

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

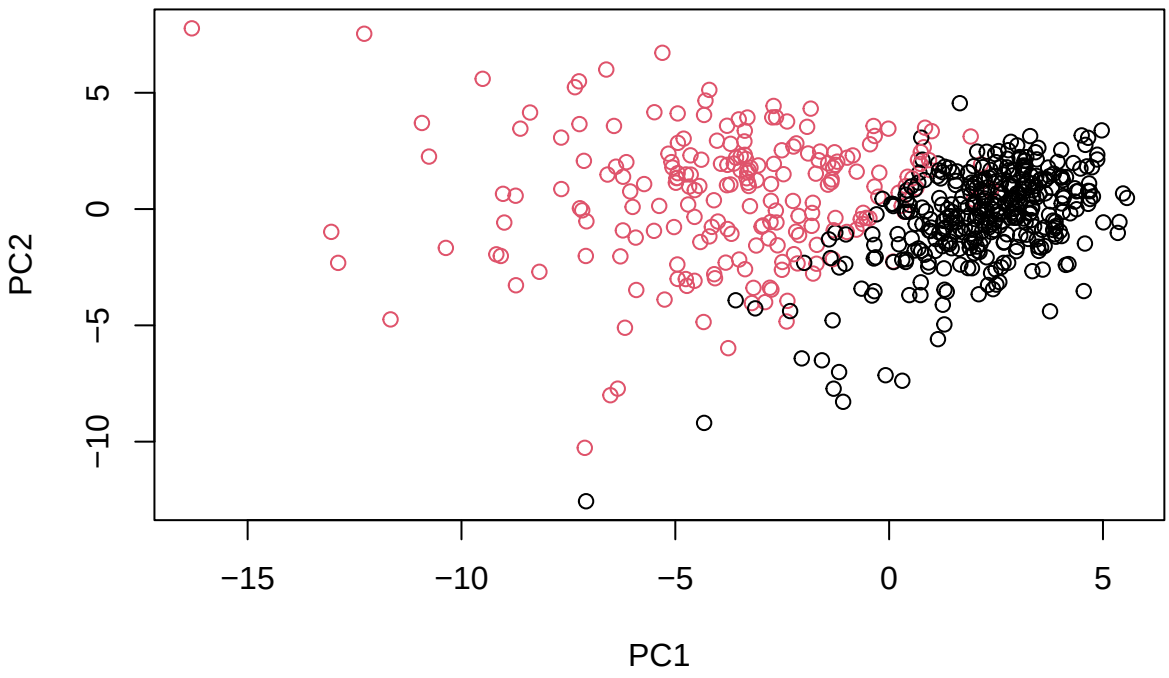


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The graph is very chaotic and messy making it very difficult to read. It's hard to understand because of the rownames being used as the data point characters.

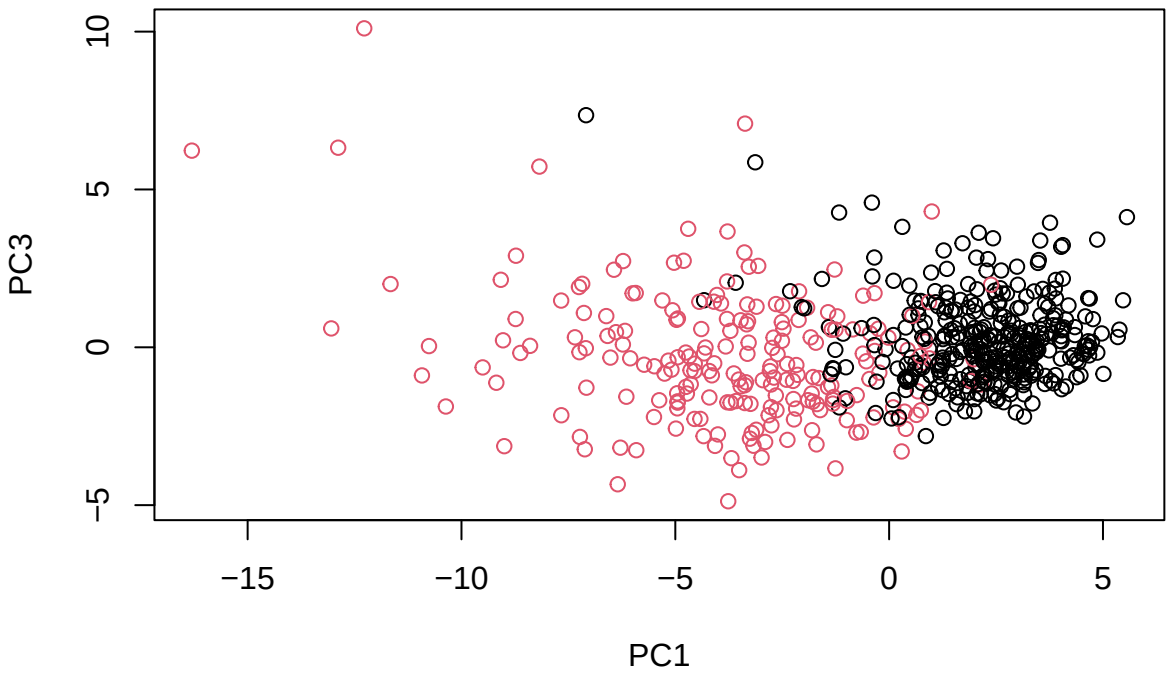
Scatter plot observations by components 1 and 2

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



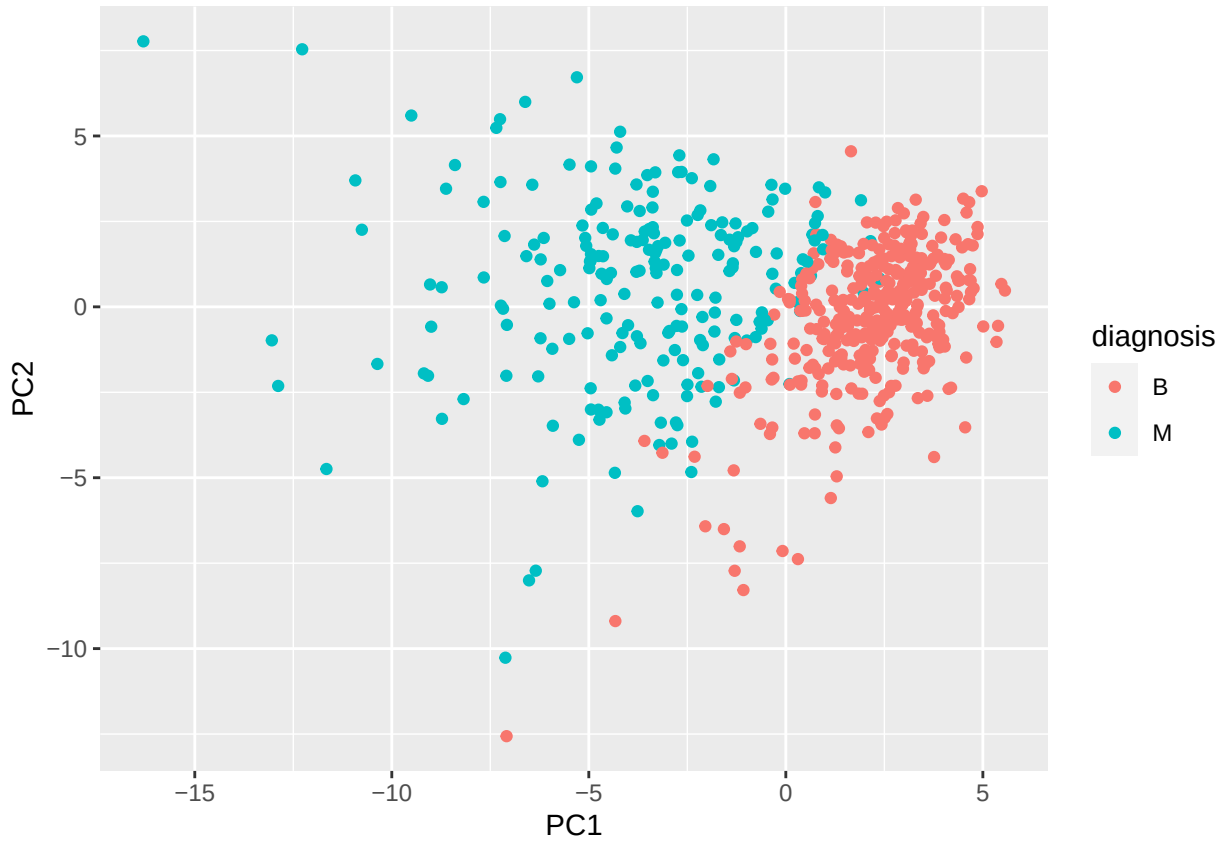
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?

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



It's much easier to visualize the data in these plots as it isn't so crowded and you can actually see the separation between the red(malignant) and black(benign) data points. PC1vsPC2 and PC1vsPC3 only differ in their y-axis.

```
# 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()
```

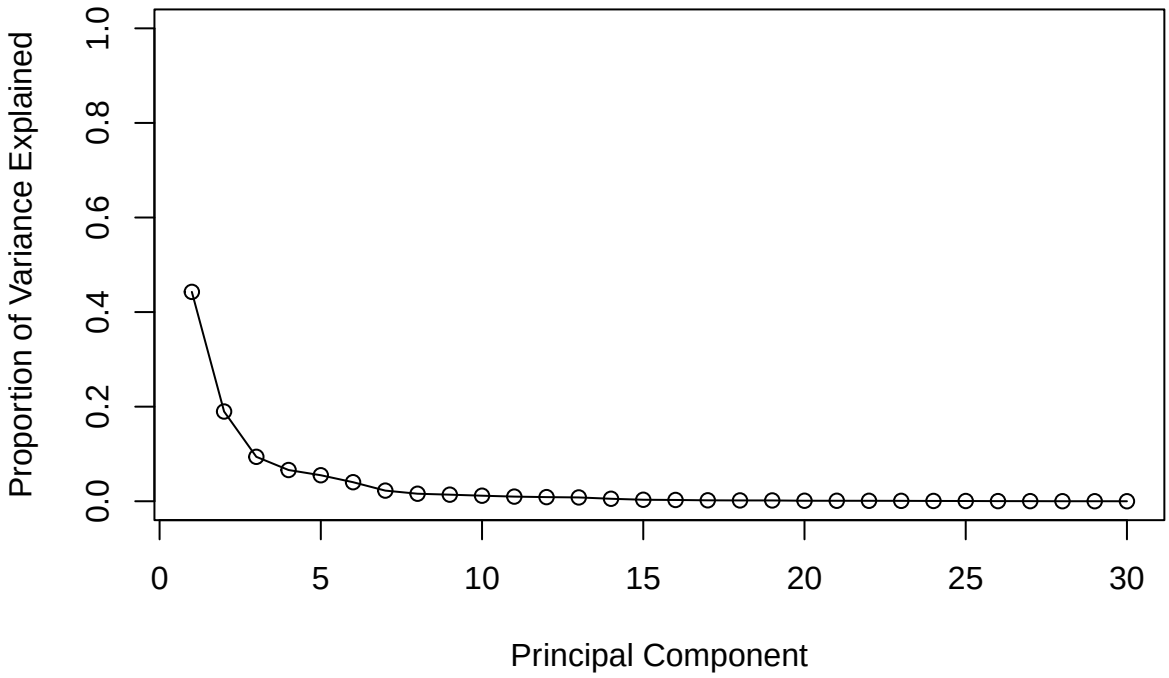


Variance explained

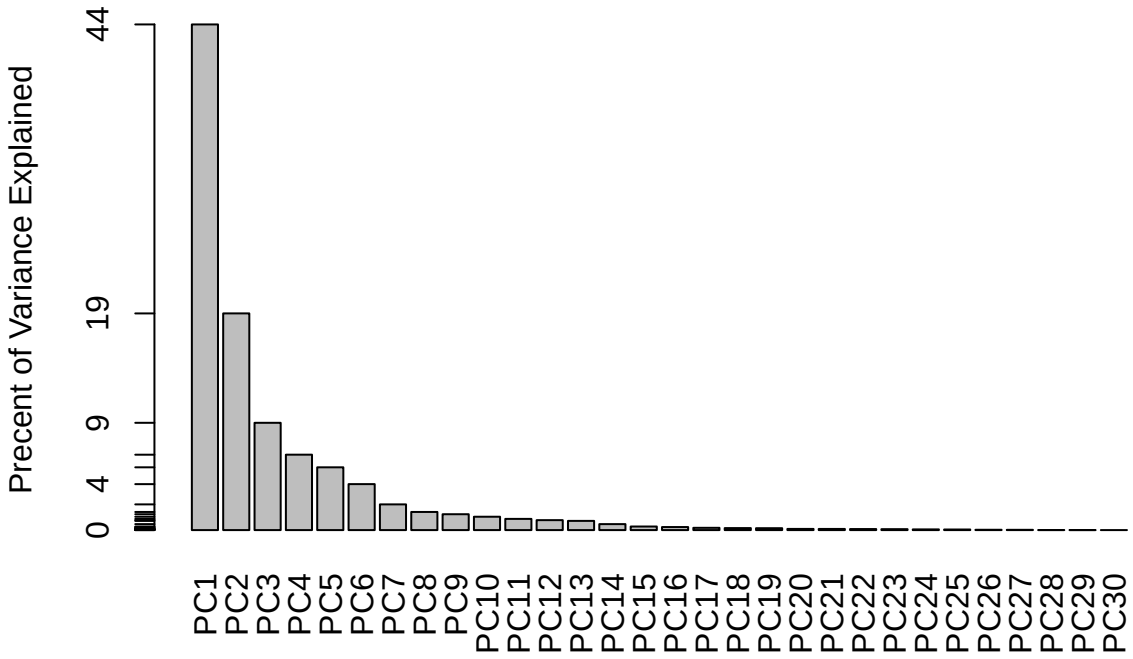
```
# Calculate variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

```
## [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)
# 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?

-0.26085376

```
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
```

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

5 PCs

Hierarchial clustering

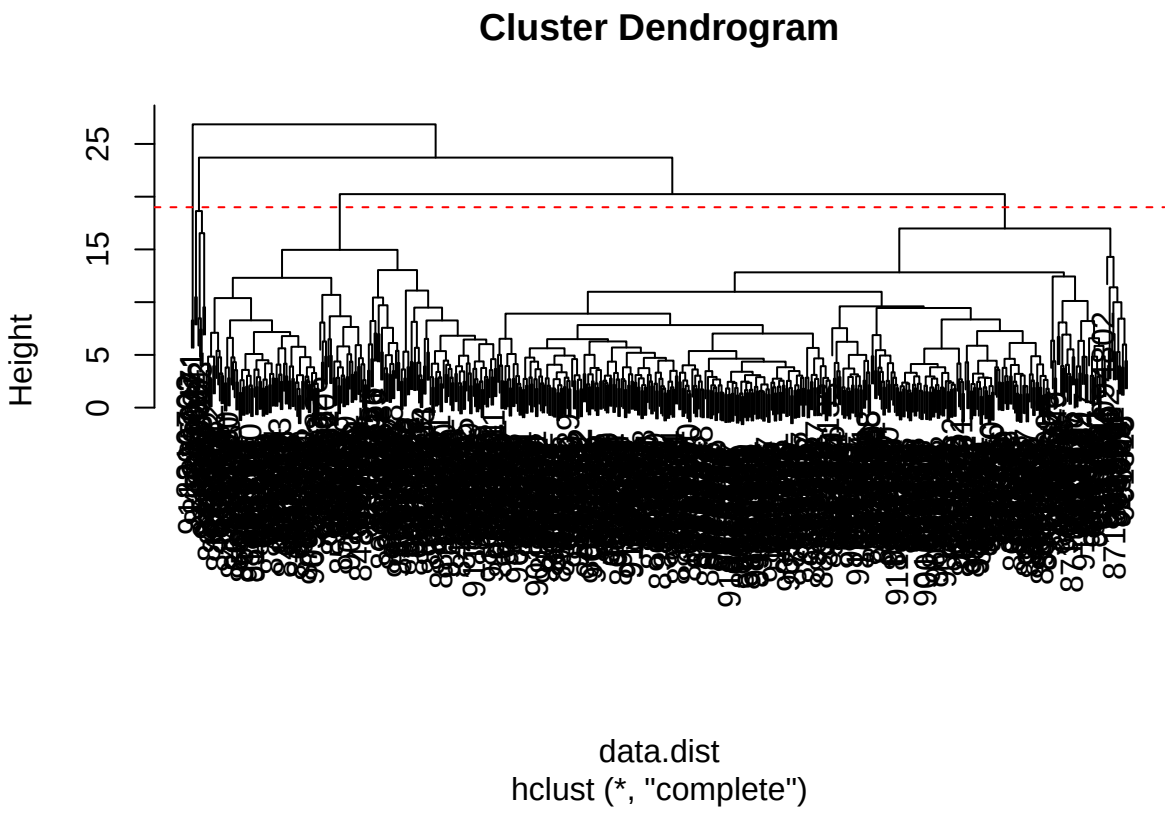
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)

# Calculate the Euclidean distances between all pairs of observations
data.dist <- dist(data.scaled)

# Create a hierarchical clustering model using complete linkage
wisc.hclust <- hclust(data.dist, method = "complete")
```

Results of hierarchial clustering

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

At height 19, the model has 4 clusters.

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



Selecting number of clusters

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4)
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?

After experimenting with clusters between 2 and 10, cutting by into clusters of 2 presents the most simplified results.

Using different methods

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

"ward.D2" gives my favorite results because the data is easiest to read due to the limited variance within clusters.

OPTIONAL: K-means clustering

K-means clustering and comparing results

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

```
##    diagnosis
##       B   M
##   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 from hclust is equivalent to cluster 1 from kmeans while cluster 3 is the kmeans cluster 2.

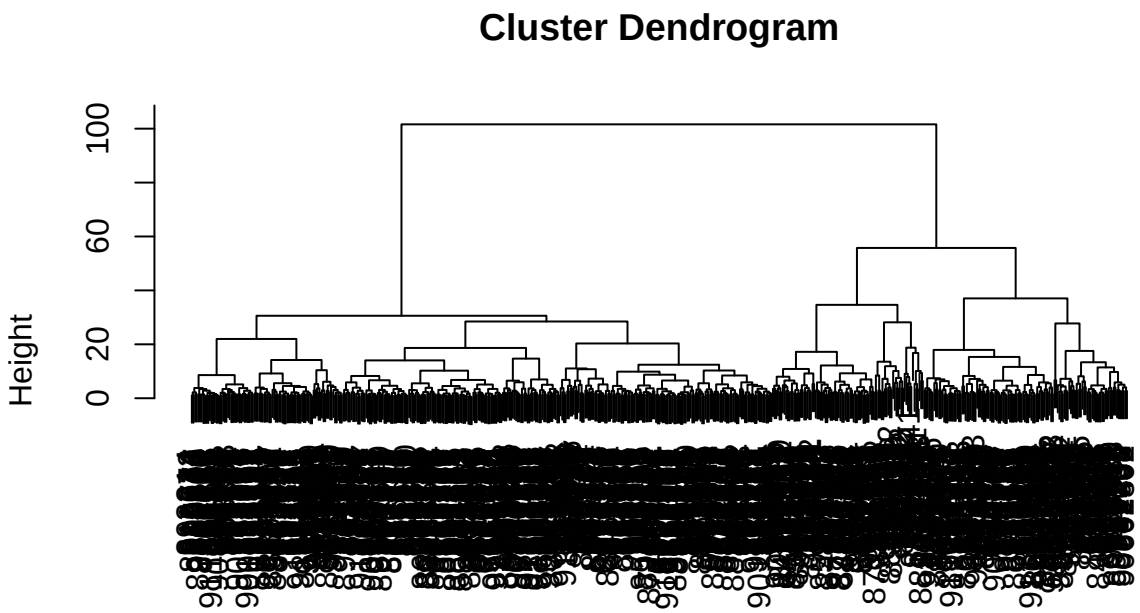
```
table(wisc.hclust.clusters, wisc.km$cluster)
```

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

Combining methods

Clustering on PCA results

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



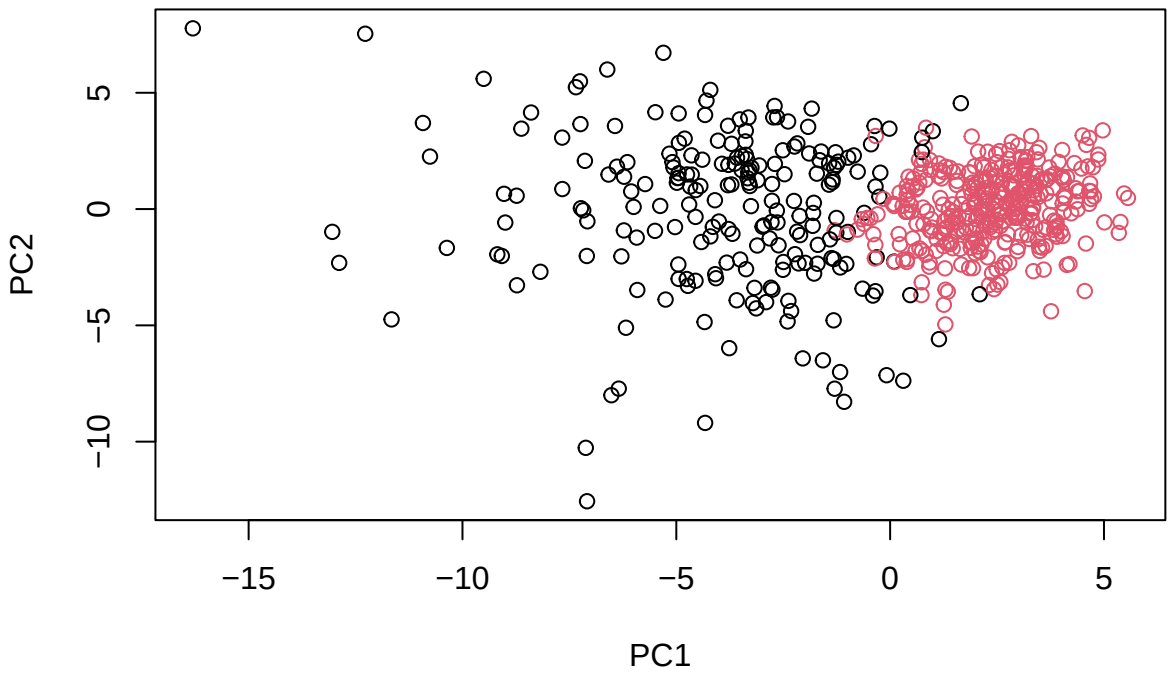

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

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

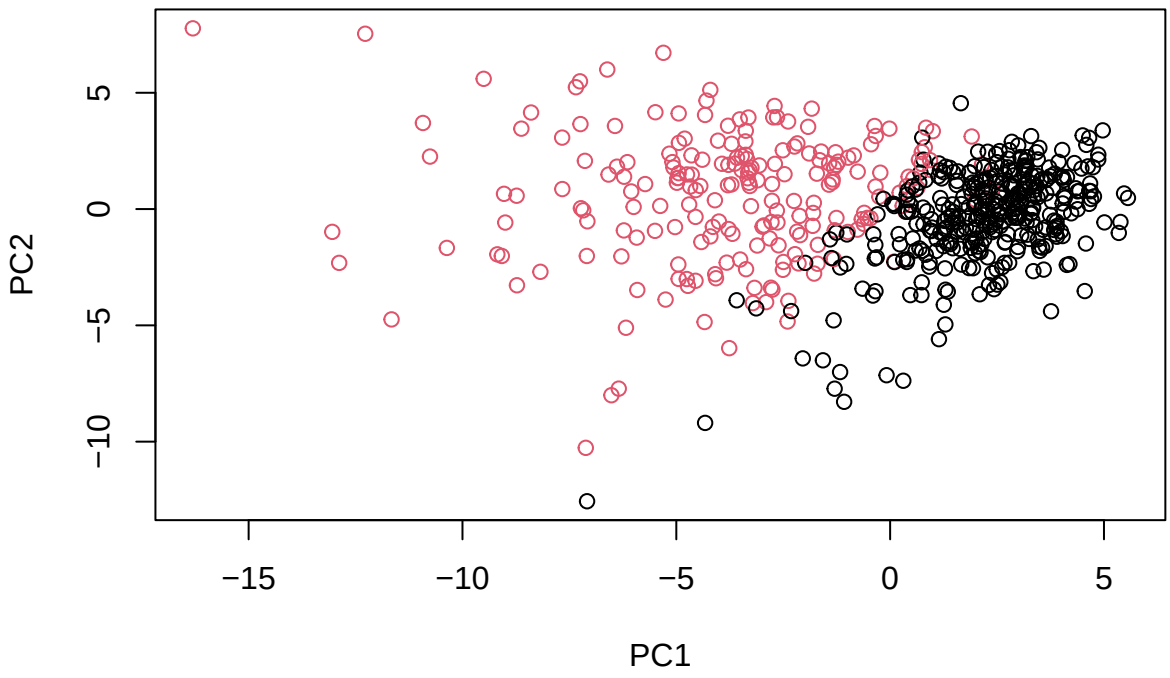
```
table(grps, diagnosis)
```

```
##     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=as.factor(diagnosis))
```



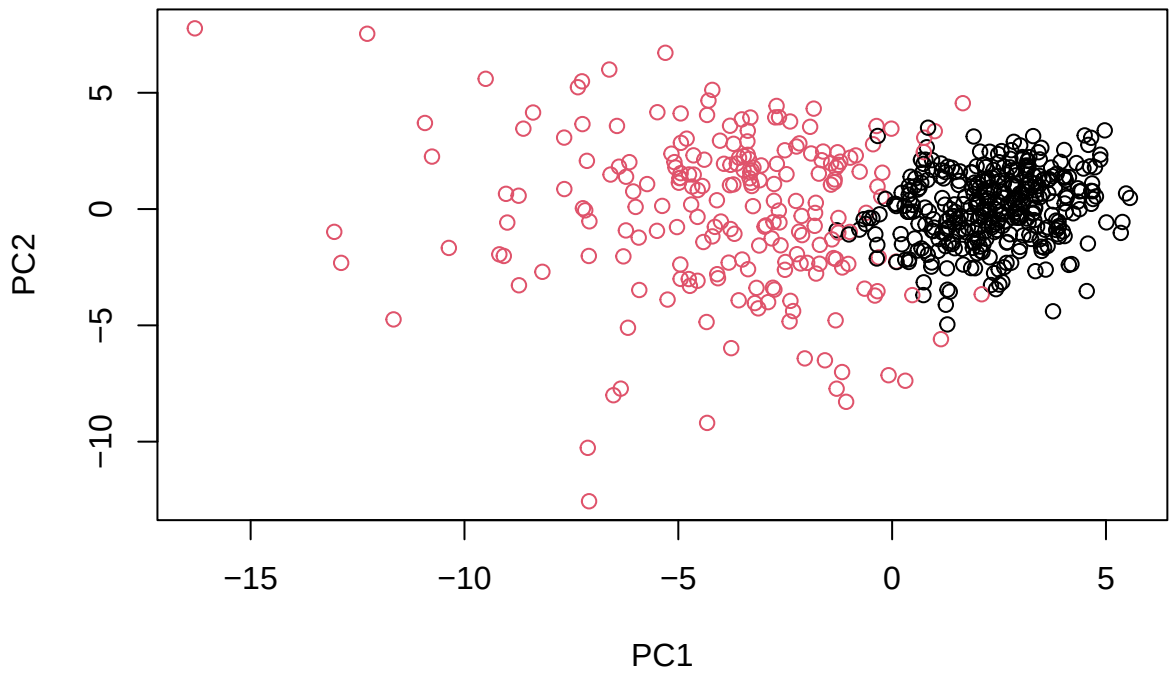

```
g <- as.factor(grps)
levels(g)
```

```
## [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)
```




```
# 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)
```

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
data.dist <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust <- hclust(data.dist, method="ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)
```

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

The newly created model separates the two diagnoses pretty well. There is a clear distinction between the malignant and benign tumors shown by the color. However the slight overlap between the black and red makes it a little unclear.

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

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

K-means and hclust do alright with separating the diagnoses as you can tell there are 2 main clusters in each, but the PCA model does it best.

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

```
##    diagnosis
##       B   M
##   1  14 175
##   2 343  37
```

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

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

Sensitivity/Specificity

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

Both kmeans and hclust have the best specificity, while kmeans has the best sensitivity.

Specificity = TP/(TP+FN)

```
# for hclust
343/(343+12+2)
```

```
## [1] 0.9607843
```

```
# for kmeans
343/(343+14)
```

```
## [1] 0.9607843
```

Sensitivity = TN/(TN+FN)

```
# for hclust
165/(165+5+40+2)
```

```
## [1] 0.7783019
```

```
# for kmeans
175/(175+37)
```

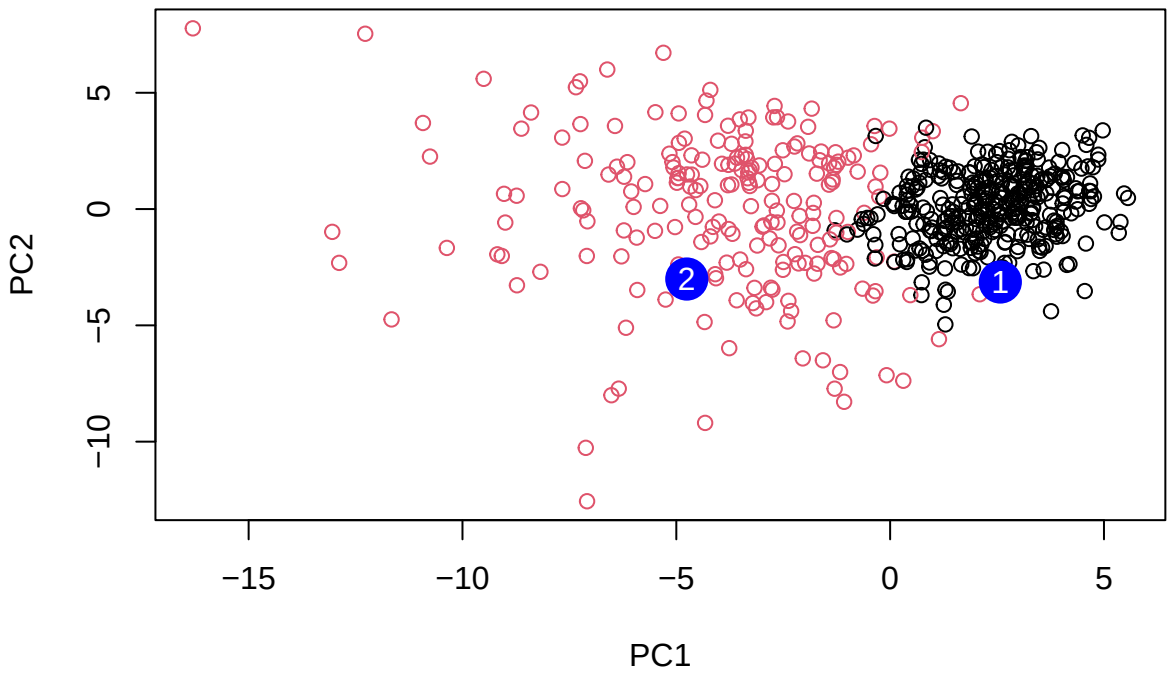
```
## [1] 0.8254717
```

Prediction

```
#url <- "new_samples.csv"
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 patient 2 for follow up due to the location in the red cluster, which signifies malignant cells.

```
sessionInfo()
```

```
## R version 4.1.2 (2021-11-01)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Big Sur 10.16
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
## [1] ggplot2_3.3.5
##
## loaded via a namespace (and not attached):
```

```
##  [1] pillar_1.7.0     compiler_4.1.2   highr_0.9        tools_4.1.2
##  [5] digest_0.6.29    evaluate_0.14    lifecycle_1.0.1  tibble_3.1.6
##  [9] gtable_0.3.0     pkgconfig_2.0.3  rlang_1.0.0      cli_3.1.1
## [13] rstudioapi_0.13  yaml_2.2.2       xfun_0.29        fastmap_1.1.0
## [17] withr_2.4.3      stringr_1.4.0    dplyr_1.0.8      knitr_1.37
## [21] generics_0.1.2   vctrs_0.3.8      grid_4.1.2       tidyselect_1.1.1
## [25] glue_1.6.1       R6_2.5.1         fansi_1.0.2      rmarkdown_2.11
## [29] farver_2.1.0     purrr_0.3.4      magrittr_2.0.2   scales_1.1.1
## [33] ellipsis_0.3.2   htmltools_0.5.2  colorspace_2.0-2 labeling_0.4.2
## [37] utf8_1.2.2       stringi_1.7.6    munsell_0.5.0    crayon_1.4.2
```