Class 8: Breast Cancer mini project

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Background

Unsupervised learning, supervised learning and reinforcement learning; Focus on unsupervised learning, K-means clustering, Hierarchical clustering, Dimensionality reduction, visualization and analysis, Principal Component Analysis (PCA) Practical considerations and best practices for the analysis of high dimensional datasets.

##Data Import

Our data come from the U. of Wisconsin Medical Center

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

Q1. How many patients /samples are in the dataset?

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

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

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

```
table(wisc.df$diagnosis)
```

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

```
sum(wisc.df$diagnosis== "M")
```

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

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

```
colnames(wisc.df)
```

```
##  [1] "diagnosis"               "radius_mean"
##  [3] "texture_mean"            "perimeter_mean"
##  [5] "area_mean"               "smoothness_mean"
##  [7] "compactness_mean"        "concavity_mean"
##  [9] "concave.points_mean"     "symmetry_mean"
## [11] "fractal_dimension_mean"  "radius_se"
## [13] "texture_se"              "perimeter_se"
## [15] "area_se"                 "smoothness_se"
## [17] "compactness_se"          "concavity_se"
## [19] "concave.points_se"       "symmetry_se"
## [21] "fractal_dimension_se"    "radius_worst"
## [23] "texture_worst"           "perimeter_worst"
## [25] "area_worst"              "smoothness_worst"
## [27] "compactness_worst"       "concavity_worst"
```

```
## [29] "concave.points_worst"    "symmetry_worst"
## [31] "fractal_dimension_worst"
```

```
length( grep("mean", colnames(wisc.df), value = T))
```

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

There is a diagnosis column that is the clinician consense that I want to exclude from any further analysis. We will come back later and compare our results to this diagnosis.

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

```
## [1] M M M M M M
## Levels: B M
```

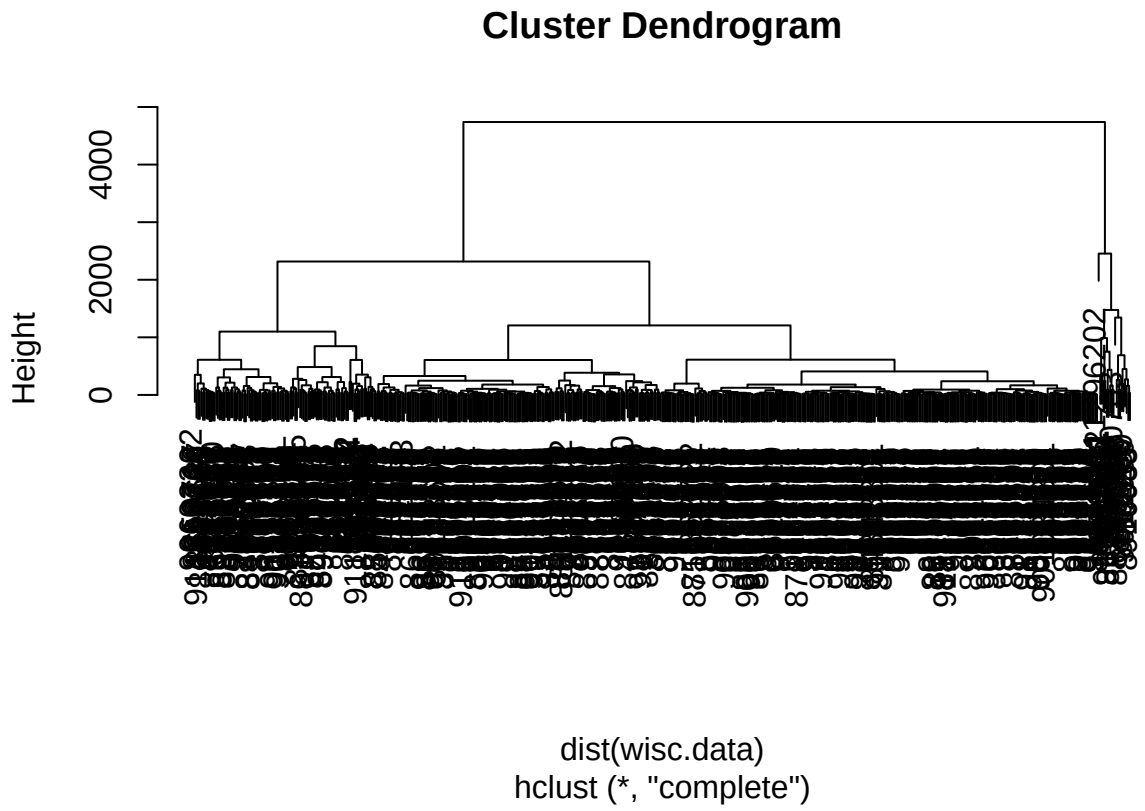
Now we can remove it from the 'wisc.df'

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

Clustering

Lets try a hclust()

```
hc <-hclust(dist(wisc.data))
plot(hc)
```



We can extract clusters from this rather poor dendrogram/tree with the 'cutree()'

```
grps <-cutree(hc, k=2)
```

How many individuals in each cluster?

```
table(grps)
```

```
## grps
##   1   2
## 549  20
```

```
table(diagnosis)
```

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

We can generate a cross-table that compares our cluster 'grps' vector with out 'diagnosis' vectore values

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

```
##          grps
## diagnosis   1   2
##         B 357   0
##         M 192  20
```

Principal Component Analysis

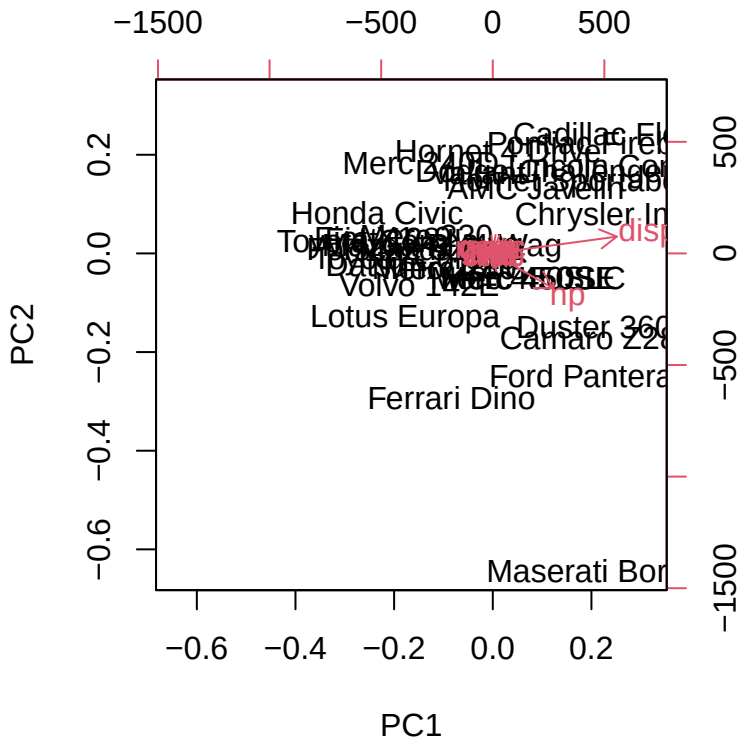
prcomp(x,scale=F,center=F) ### The importance of PCA Data The main function for PCA in base R is 'prcomp()' it has a defualt input parameter of 'scale=FALSE'.

```
#prcomp()
head(mtcars)
```

```
##                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
## Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
## Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
## Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
## Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
## Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
## Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

We could do a PCA of this data as is and it could be mis-leading....

```
pc <- prcomp(mtcars)
biplot(pc)
```



Lets look at the mean values of each column and their standard deviation.

```
colMeans(mtcars)
```

```
##        mpg        cyl       disp         hp       drat         wt       qsec
##  20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750
##         vs         am       gear       carb
##   0.437500   0.406250   3.687500   2.812500
```

```
apply(mtcars, 2, sd)
```

```
##         mpg         cyl        disp          hp        drat          wt
##   6.0269481   1.7859216 123.9386938  68.5628685   0.5346787   0.9784574
##        qsec          vs          am        gear        carb
##   1.7869432   0.5040161   0.4989909   0.7378041   1.6152000
```

We can "scale" this data before PCA to get a much better representation and anlysis of all the columns.

```
mtscale <- scale(mtcars)
```

```
round(colMeans(mtscale))
```

```
##  mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
##    0    0    0    0    0    0    0    0    0    0    0
```

```
apply(mtscale,2,sd)
```

```
##  mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
##    1    1    1    1    1    1    1    1    1    1    1
```

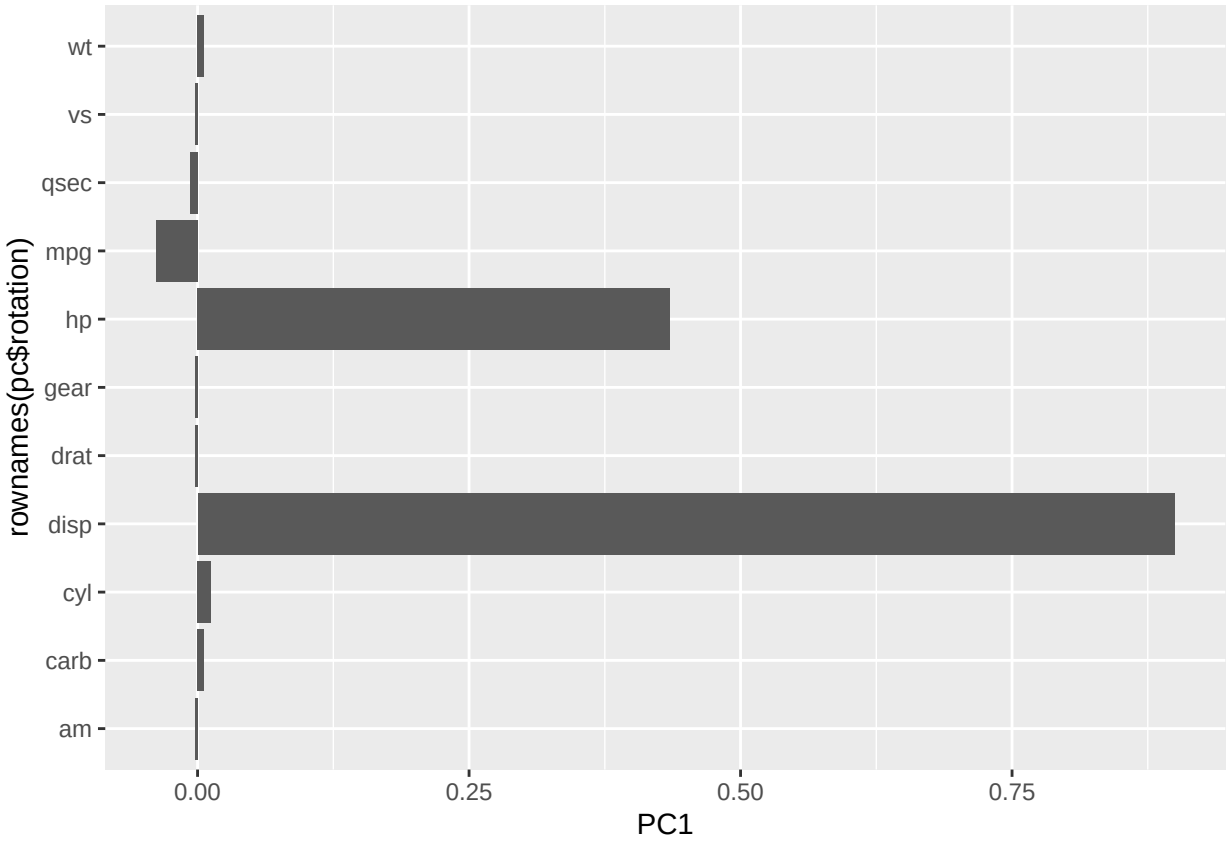
```
pc.scale <-prcomp(mtscale)
```

We can look at the two main results figures from PCA - the 'PCplot" (a.k.a. score plot, orientation plot, or pc1 vs pc2 plot). The "loadings plot" how the original variables contribute to the new PCS.

A loadings plot of the unscalled PCA results

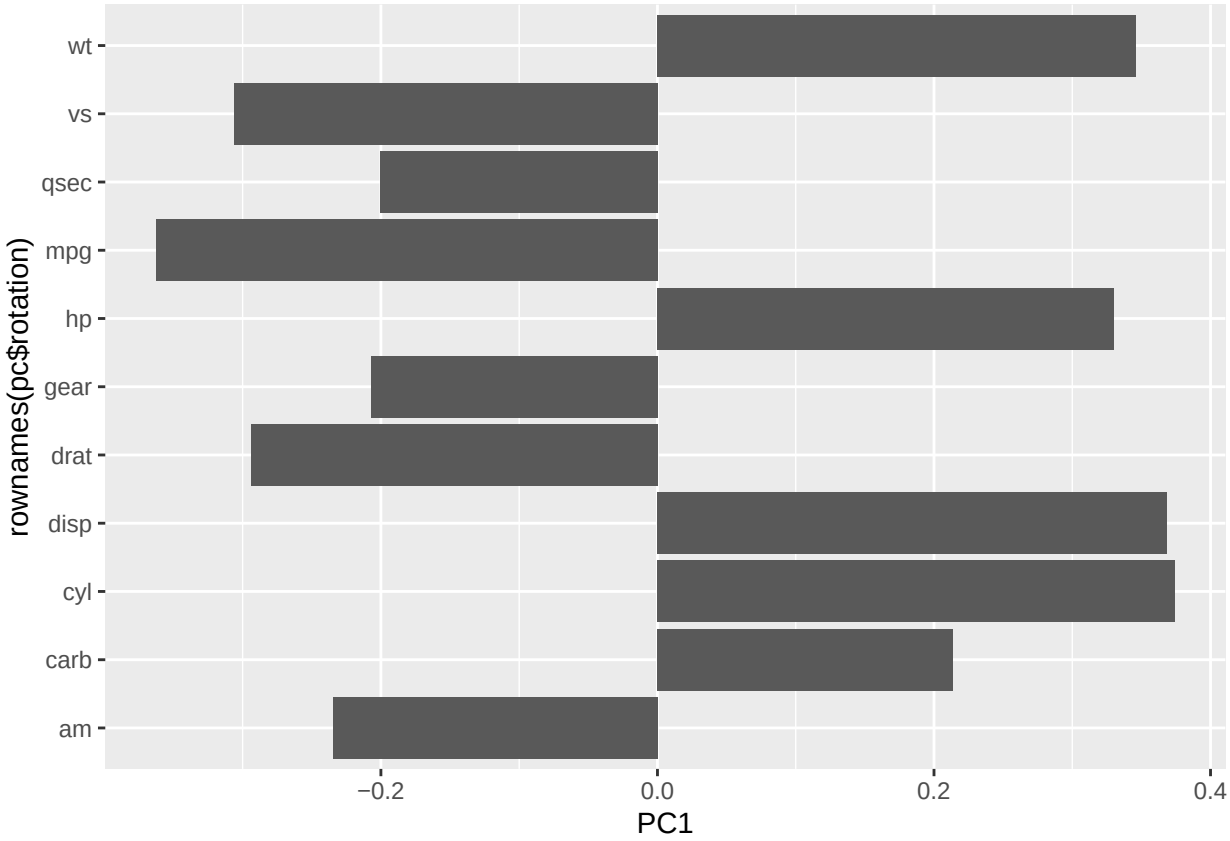
```
library(ggplot2)

ggplot(pc$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```



Loadings

```
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```

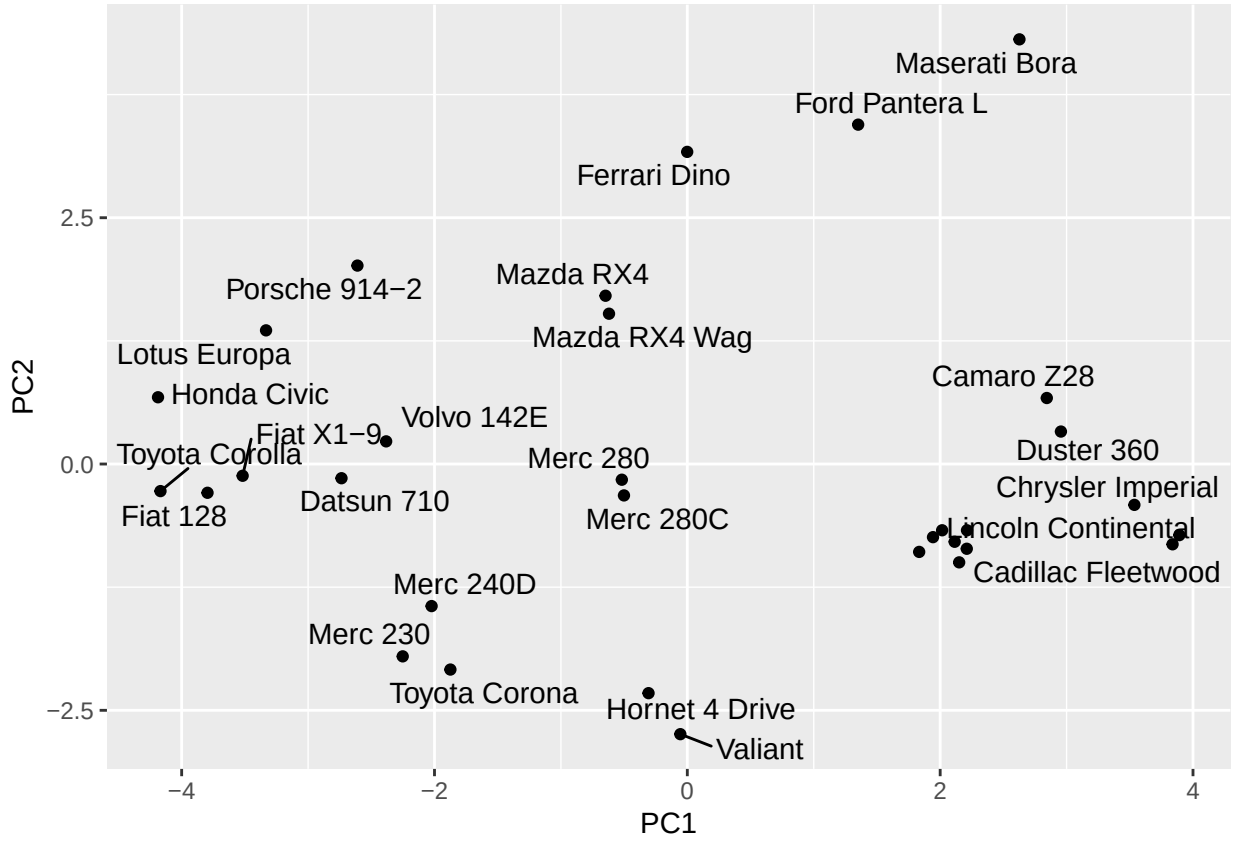


PC plot of scaled PCA results

```
library(ggrepel)

ggplot(pc.scale$x) +
  aes(PC1,PC2, label=rownames(pc.scale$x)) +
  geom_point() +
  geom_text_repel()
```

```
## Warning: ggrepel: 7 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```



Key point: In general we will set 'scale=True' when we do PCA. This is not the defualt but probably should be....

We can check the SD and mean of the different columns in 'wisc.data' to see if we need to sclae - hint; we do!

PCA of wisc.data

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

To see how well PCA is doing here interms capturing the variance (or spread) in the data we can use the 'summary()' function.

```
summary(wisc.pr)
```

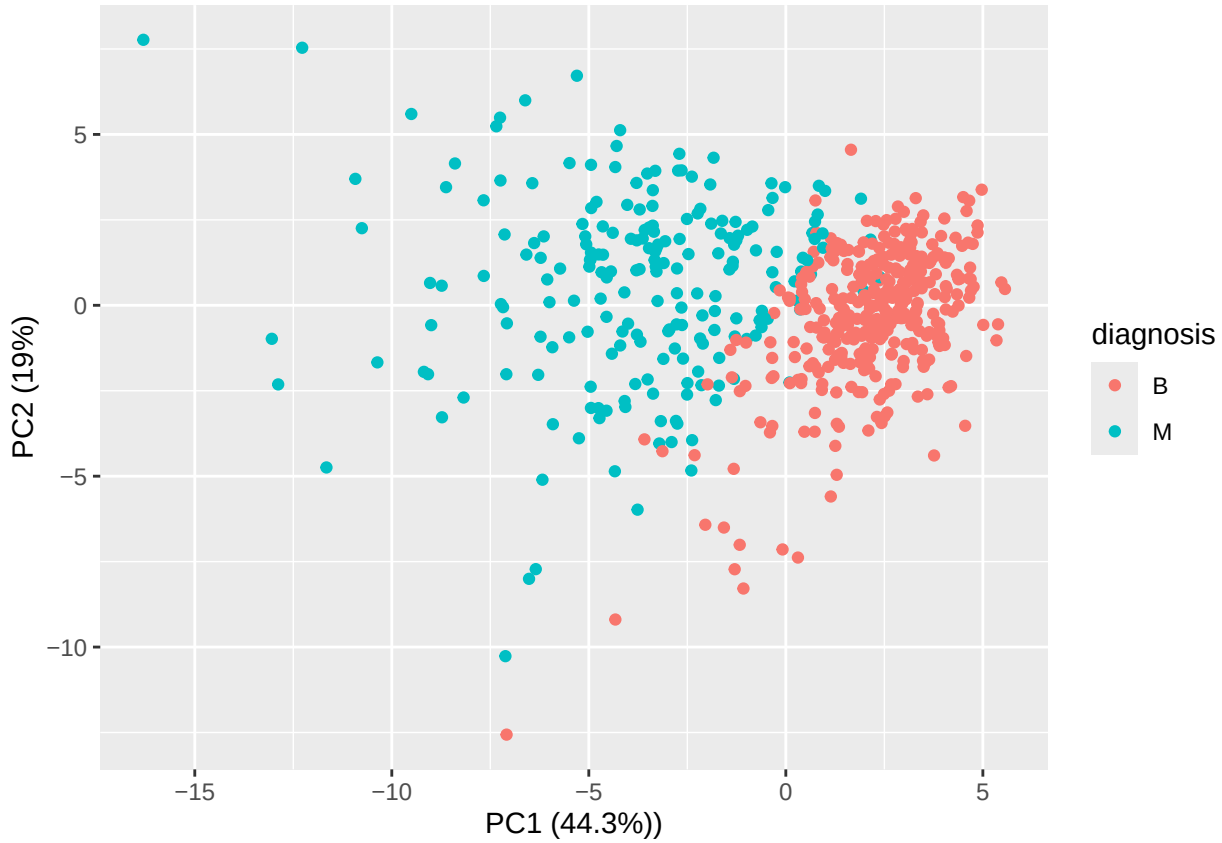
```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion  0.4427 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)?

Lets make the main PC1 VS PC2

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2,col=diagnosis) +
        geom_point() +
  xlab("PC1 (44.3%))") +
  ylab("PC2 (19%)")
```



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

PC1, PC2 and PC3 is required for at least 70%

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

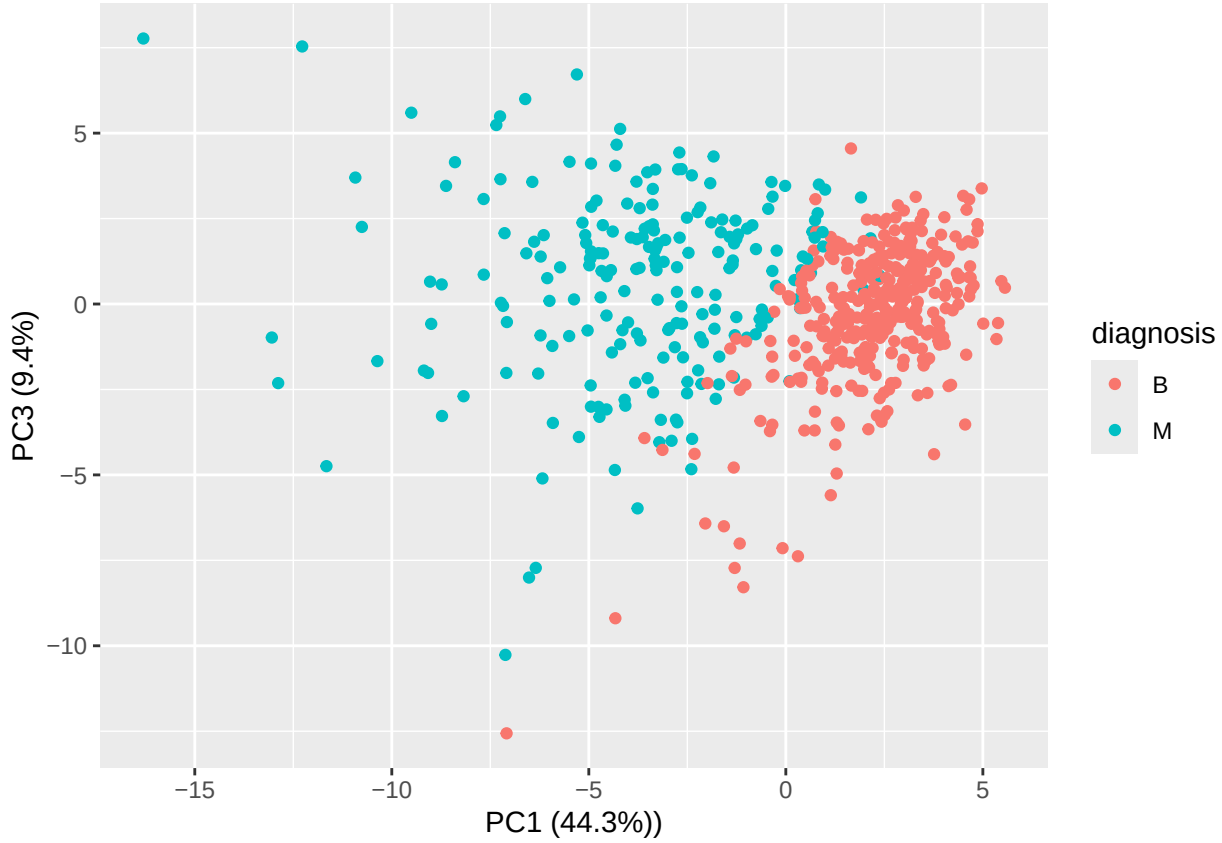
PC1, PC2, PC3, PC4, PC5, PC6, PC7 and PC8.

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

What stands out is that thewre is a clear significance in the causation on the casncer being benign and malignant depending on the data, once creating the PCA axis it will highlight it more to us.

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

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2,col=diagnosis) +
        geom_point() +
  xlab("PC1 (44.3%))") +
  ylab("PC3 (9.4%)")
```



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["concave.points_mean", 1]
```

```
## [1] -0.2608538
```

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
```

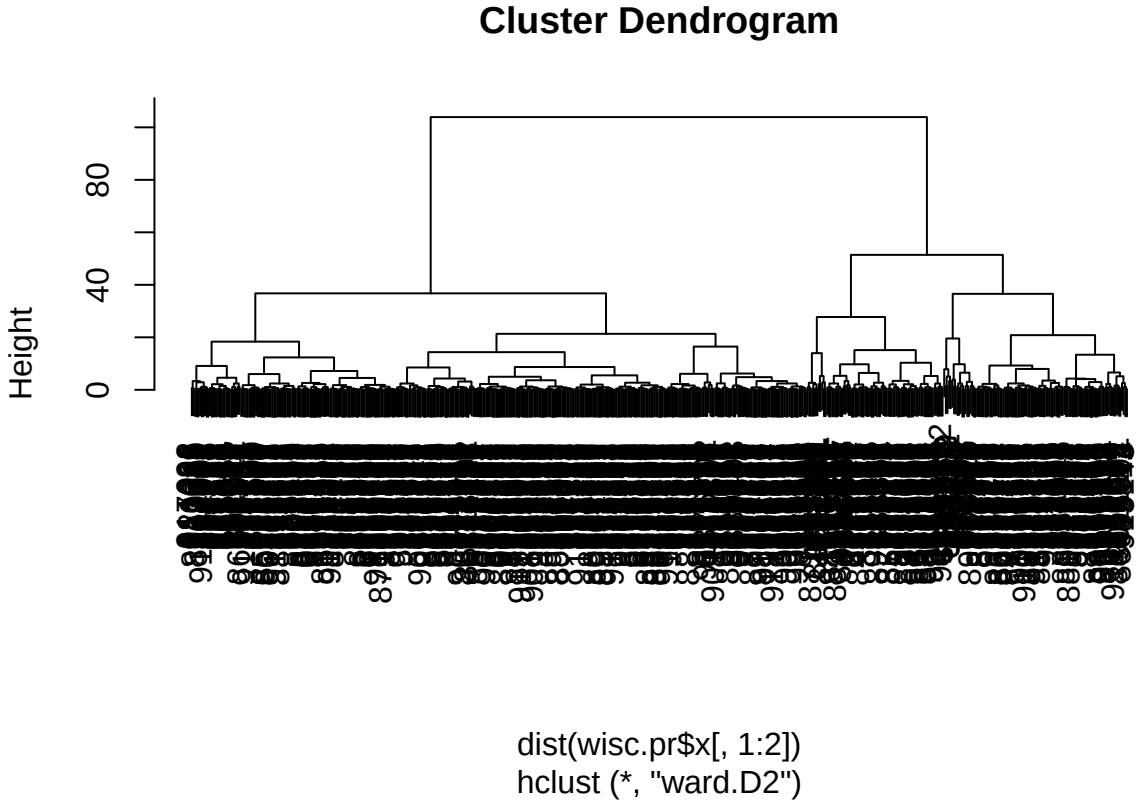
```
## Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
##                            PC8    PC9    PC10   PC11    PC12    PC13    PC14
## Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
## Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 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
```

It would include PC30-PC9 which includes rest of 20%

5. Combining methods

Clustering on PCA results

```
wisc.pr.hclust <- hclust( dist(wisc.pr$x[,1:2]), method="ward.D2")
plot(wisc.pr.hclust)
```



We can "cut" this tree to yield out cluster (groups):

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

```
## pc.grps
##   1   2
## 195 374
```

How do my cluster grps compare to the expert diagnosis

```
table(diagnosis,pc.grps)
```

```
##          pc.grps
## diagnosis   1   2
##         B  18 339
##         M 177  35
```

```
table(diagnosis)
```

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

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

```
# Run k-means with 4 clusters on PCA-reduced data
set.seed(123)  # For reproducibility
wisc.km.4 <- kmeans(wisc.pr$x[, 1:3], centers = 4)

# Compare clusters to actual diagnoses
table(wisc.km.4$cluster, diagnosis)
```

```
##    diagnosis
##       B   M
##   1   0  96
##   2  48  73
##   3 284   6
##   4  25  37
```

It did it really well, had a shown a great differences in our patients diagnosis through the family tree and if needed we could further make the groups even more specific.

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.

They did really badly. We do much better after PCA - the new PCA variables (what we call a basis set) give us much better separation of M and B

##7. Prediction

We can use out PCA model for the analysis of new "unseen" data. In this case from U. Mich.

```
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
```

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

```
head((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
```

```
prioritize <- npc[, "PC1"] < -5
# adjust threshold based on earlier plots

npc[prioritize, ]
```

```
##      PC1 PC2 PC3 PC4 PC5 PC6 PC7 PC8 PC9 PC10 PC11 PC12 PC13 PC14 PC15 PC16
##      PC17 PC18 PC19 PC20 PC21 PC22 PC23 PC24 PC25 PC26 PC27 PC28 PC29 PC30
```

Patients with strongly negative PC1 scores — for example, those with PC1 < -5 — should be prioritized for follow-up. These patients are projected close to where malignant cases cluster in the PCA analysis and may have a higher risk of malignancy.