Class 8: Breast Cancer mini project

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Background

This mini project explores unsupervised learning techniques applied to the Wisconsin Breast Cancer Diagnostic Data Set, which contains measuremenst of human breast mass cell nuclei. The project guides the user through exploratory data analysis, performing and interpreting Principal Component Analysis (PCA) to reduce the dimensionality of the data while retaining variance, and applying hierarchical clustering to better separate benign and malignant cell samples, evaluating the results using metrics like sensitivity and specificity, and finally demonstrating how to predict the classification of new samples using the developed PCA model.

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 this 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. 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 consensus 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

```
kmeans(wisc.data, centers = 2)
```

```
K-means clustering with 2 clusters of sizes 438, 131

Cluster means:
  radius_mean texture_mean perimeter_mean area_mean smoothness_mean
1    12.55630     18.57037       81.12347  496.0619       0.0948845
2    19.37992     21.69458      128.23130 1185.9298       0.1012946
  compactness_mean concavity_mean concave.points_mean symmetry_mean
1       0.09109982     0.06243776          0.03343254     0.1780580
2       0.14861298     0.17693947          0.10069878     0.1915397
  fractal_dimension_mean radius_se texture_se perimeter_se  area_se
1             0.06345402 0.3041909   1.215153     2.152881 23.78529
2             0.06060290 0.7428038   1.222538     5.250580 95.67817
  smoothness_se compactness_se concavity_se concave.points_se symmetry_se
1   0.007173263     0.02347469   0.02874551        0.01063632  0.02061358
2   0.006598687     0.03217669   0.04241977        0.01567398  0.02030397
  fractal_dimension_se radius_worst texture_worst perimeter_worst area_worst
1          0.003747503     14.04390      24.70954        91.93751   619.6479
2          0.003953389     23.70947      28.91267       158.49618  1753.0229
  smoothness_worst compactness_worst concavity_worst concave.points_worst
1        0.1299591         0.2233118       0.2192149           0.09132984
```

```
2        0.1404247         0.3577577       0.4493061           0.19243107
  symmetry_worst fractal_dimension_worst
1      0.2835537              0.08328194
2      0.3118817              0.08616550

Clustering vector:
   842302    842517  84300903  84348301  84358402    843786    844359  84458202
        2         2         2         1         2         1         2         1
   844981  84501001    845636  84610002    846226    846381  84667401  84799002
        1         1         1         2         2         1         1         1
   848406  84862001    849014   8510426   8510653   8510824   8511133    851509
        1         2         2         1         1         1         1         2
   852552    852631    852763    852781    852973    853201    853401    853612
        2         2         1         2         2         2         2         1
 85382601    854002    854039    854253    854268    854941    855133    855138
        2         2         2         2         1         1         1         1
   855167    855563    855625    856106  85638502    857010  85713702     85715
        1         1         2         1         1         2         1         1
   857155    857156    857343    857373    857374    857392    857438  85759902
        1         1         1         1         1         2         1         1
   857637    857793    857810    858477    858970    858981    858986    859196
        2         1         1         1         1         1         1         1
 85922302    859283    859464    859465    859471    859487    859575    859711
        1         1         1         1         1         1         2         1
   859717    859983   8610175   8610404   8610629   8610637   8610862   8610908
        2         1         1         2         1         2         2         1
   861103   8611161   8611555   8611792   8612080   8612399  86135501  86135502
        1         1         2         2         1         2         1         2
   861597    861598    861648    861799    861853    862009    862028     86208
        1         1         1         1         1         1         1         2
    86211    862261    862485    862548    862717    862722    862965    862980
        1         1         1         1         1         1         1         1
   862989    863030    863031    863270     86355    864018    864033     86408
        1         1         1         1         2         1         1         1
    86409    864292    864496    864685    864726    864729    864877    865128
        1         1         1         1         1         1         2         2
   865137     86517    865423    865432    865468     86561    866083    866203
        1         2         2         1         1         1         1         2
   866458    866674    866714      8670  86730502    867387    867739    868202
        1         2         1         1         1         1         2         1
   868223    868682    868826    868871    868999    869104    869218    869224
        1         1         1         1         1         2         1         1
   869254    869476    869691  86973701  86973702    869931 871001501 871001502
```

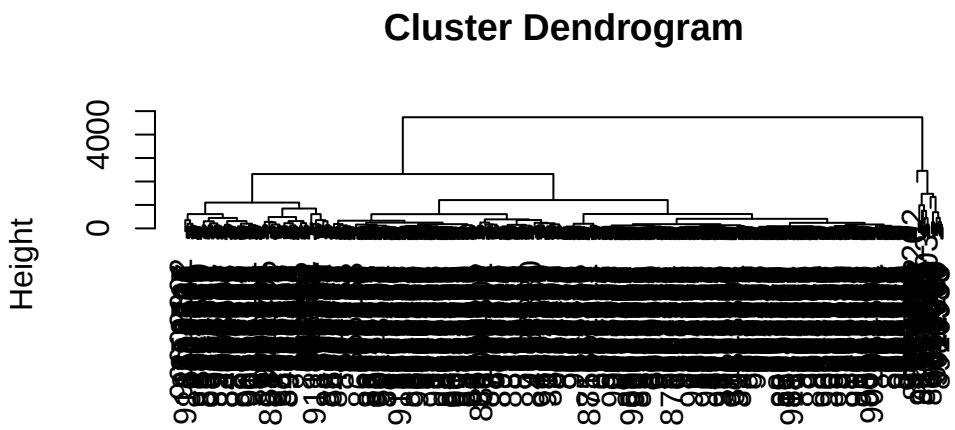
1	1	1	1	1	1	1	1
8710441	87106	8711002	8711003	8711202	8711216	871122	871149
1	1	1	1	2	1	1	1
8711561	8711803	871201	8712064	8712289	8712291	87127	8712729
1	2	2	1	2	1	1	2
8712766	8712853	87139402	87163	87164	871641	871642	872113
2	1	1	1	1	1	1	1
872608	87281702	873357	873586	873592	873593	873701	873843
1	1	1	1	2	2	2	1
873885	874158	874217	874373	874662	874839	874858	875093
1	1	2	1	1	1	1	1
875099	875263	87556202	875878	875938	877159	877486	877500
1	1	1	1	1	2	2	1
877501	877989	878796	87880	87930	879523	879804	879830
1	2	2	1	1	1	1	2
8810158	8810436	881046502	8810528	8810703	881094802	8810955	8810987
1	1	2	1	2	1	1	1
8811523	8811779	8811842	88119002	8812816	8812818	8812844	8812877
1	1	2	2	1	1	1	1
8813129	88143502	88147101	88147102	88147202	881861	881972	88199202
1	1	1	1	1	1	2	1
88203002	88206102	882488	88249602	88299702	883263	883270	88330202
1	2	1	1	2	2	1	2
88350402	883539	883852	88411702	884180	884437	884448	884626
1	1	1	1	2	1	1	1
88466802	884689	884948	88518501	885429	8860702	886226	886452
1	1	2	1	2	2	2	1
88649001	886776	887181	88725602	887549	888264	888570	889403
2	1	2	1	2	2	2	1
889719	88995002	8910251	8910499	8910506	8910720	8910721	8910748
2	2	1	1	1	1	1	1
8910988	8910996	8911163	8911164	8911230	8911670	8911800	8911834
2	1	2	1	1	2	1	1
8912049	8912055	89122	8912280	8912284	8912521	8912909	8913
2	1	2	1	1	1	1	1
8913049	89143601	89143602	8915	891670	891703	891716	891923
1	1	1	1	1	1	1	1
891936	892189	892214	892399	892438	892604	89263202	892657
1	1	1	1	2	1	2	1
89296	893061	89344	89346	893526	893548	893783	89382601
1	1	1	1	1	1	1	1
89382602	893988	894047	894089	894090	894326	894329	894335
1	1	1	1	1	2	1	1

894604	894618	894855	895100	89511501	89511502	89524	895299
1	2	1	2	1	1	1	1
8953902	895633	896839	896864	897132	897137	897374	89742801
1	1	1	1	1	1	1	2
897604	897630	897880	89812	89813	898143	89827	898431
1	2	1	2	1	1	1	2
89864002	898677	898678	89869	898690	899147	899187	899667
1	1	1	1	1	1	1	1
899987	9010018	901011	9010258	9010259	901028	9010333	901034301
2	1	1	1	1	1	1	1
901034302	901041	9010598	9010872	9010877	901088	9011494	9011495
1	1	1	1	1	2	2	1
9011971	9012000	9012315	9012568	9012795	901288	9013005	901303
2	2	1	1	2	2	1	1
901315	9013579	9013594	9013838	901549	901836	90250	90251
1	1	1	1	1	1	1	1
902727	90291	902975	902976	903011	90312	90317302	903483
1	1	1	1	1	2	1	1
903507	903516	903554	903811	90401601	90401602	904302	904357
2	2	1	1	1	1	1	1
90439701	904647	904689	9047	904969	904971	905189	905190
2	1	1	1	1	1	1	1
90524101	905501	905502	905520	905539	905557	905680	905686
2	1	1	1	1	1	1	1
905978	90602302	906024	906290	906539	906564	906616	906878
1	2	1	1	1	1	1	1
907145	907367	907409	90745	90769601	90769602	907914	907915
1	1	1	1	1	1	1	1
908194	908445	908469	908489	908916	909220	909231	909410
2	2	1	1	1	1	1	1
909411	909445	90944601	909777	9110127	9110720	9110732	9110944
1	2	1	1	2	1	2	1
911150	911157302	9111596	9111805	9111843	911201	911202	9112085
1	2	1	2	1	1	1	1
9112366	9112367	9112594	9112712	911296201	911296202	9113156	911320501
1	1	1	1	2	2	1	1
911320502	9113239	9113455	9113514	9113538	911366	9113778	9113816
1	1	1	1	2	1	1	1
911384	9113846	911391	911408	911654	911673	911685	911916
1	1	1	1	1	1	1	1
912193	91227	912519	912558	912600	913063	913102	913505
1	1	1	1	1	1	1	2
913512	913535	91376701	91376702	914062	914101	914102	914333

```
       1        1        1        2        2        1        1        1
  914366   914580   914769    91485   914862    91504    91505   915143
       1        1        2        2        1        1        1        2
  915186   915276 91544001 91544002   915452   915460    91550   915664
       1        1        1        1        1        1        1        1
  915691   915940 91594602   916221   916799   916838   917062   917080
       1        1        1        1        2        2        1        1
  917092 91762702    91789   917896   917897    91805 91813701 91813702
       1        2        1        1        1        1        1        1
  918192   918465    91858 91903901 91903902 91930402   919537   919555
       1        1        1        1        1        2        1        2
 91979701   919812   921092   921362   921385   921386   921644   922296
       1        1        1        1        1        1        1        1
  922297   922576   922577   922840   923169   923465   923748   923780
       1        1        1        1        1        1        1        1
  924084   924342   924632   924934   924964   925236   925277   925291
       1        1        1        1        1        1        1        1
  925292   925311   925622   926125   926424   926682   926954   927241
       1        1        1        2        2        2        1        2
   92751
       1

Within cluster sum of squares by cluster:
[1] 28559677 49383423
 (between_SS / total_SS =  69.6 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

let's try `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 our `diagnosis` vector values.

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

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

Principal Component Analysis (PCA)

The Importance of Data Scaling

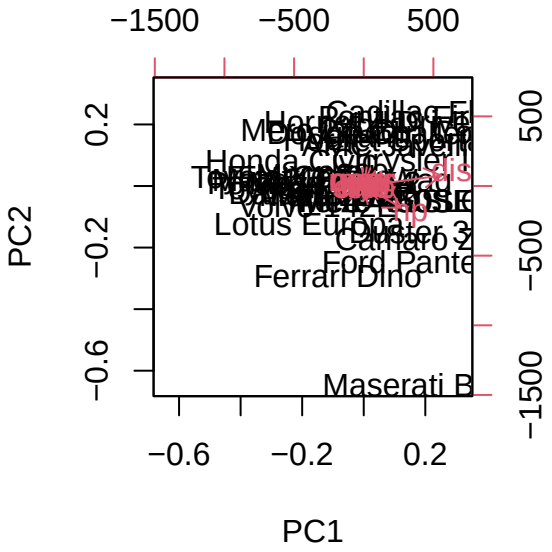
The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale=FALSE`.

```
#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)
```



Let's 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 represenation and analysis 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)
```

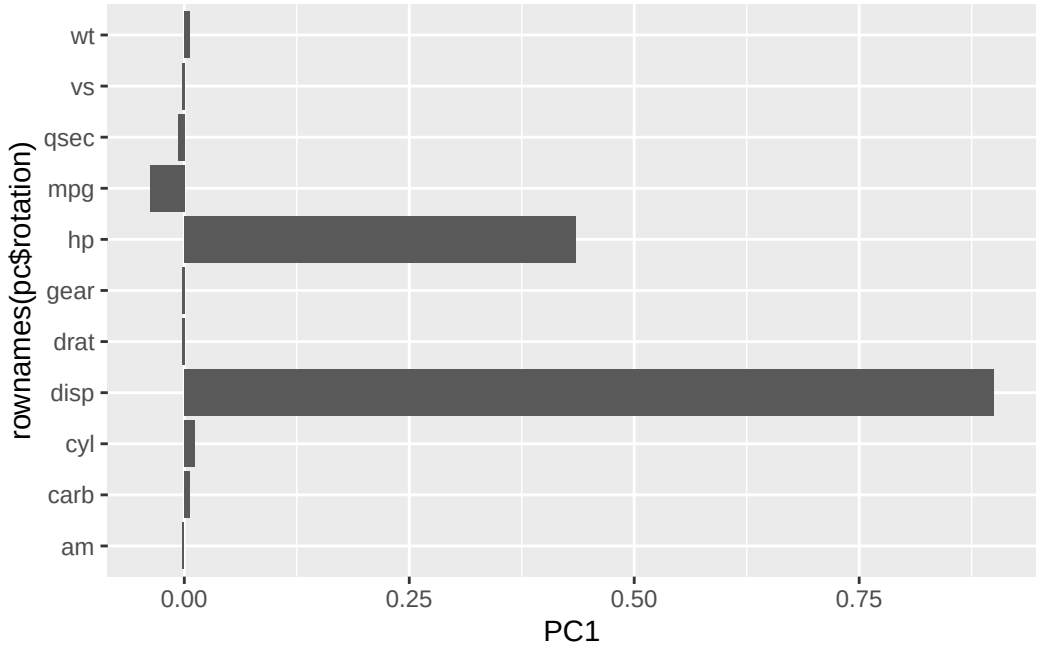
```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb
   1    1    1    1    1    1    1    1    1    1    1
```

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

We can look at the two main results figures from PCA - the "PC plot" (a.k.a. score plot, orientation plot, or PC1 vs PC2 plot). The "loadings plot" says how the original variables contribute to the new PCs.

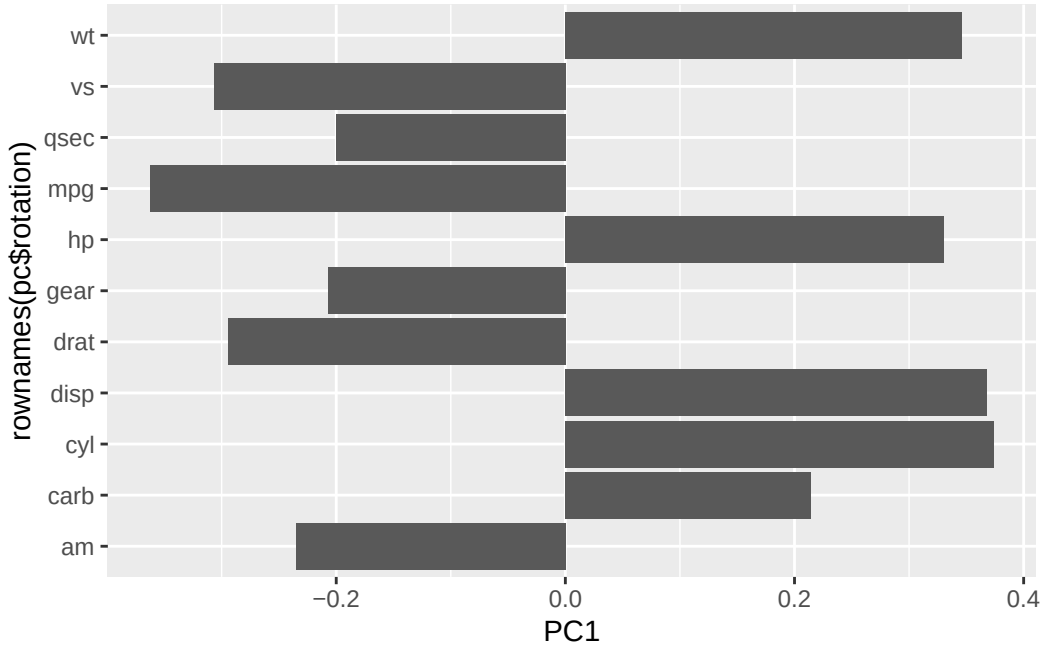
A loadings plot of the unscaled PCA results

```
library(ggplot2)

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



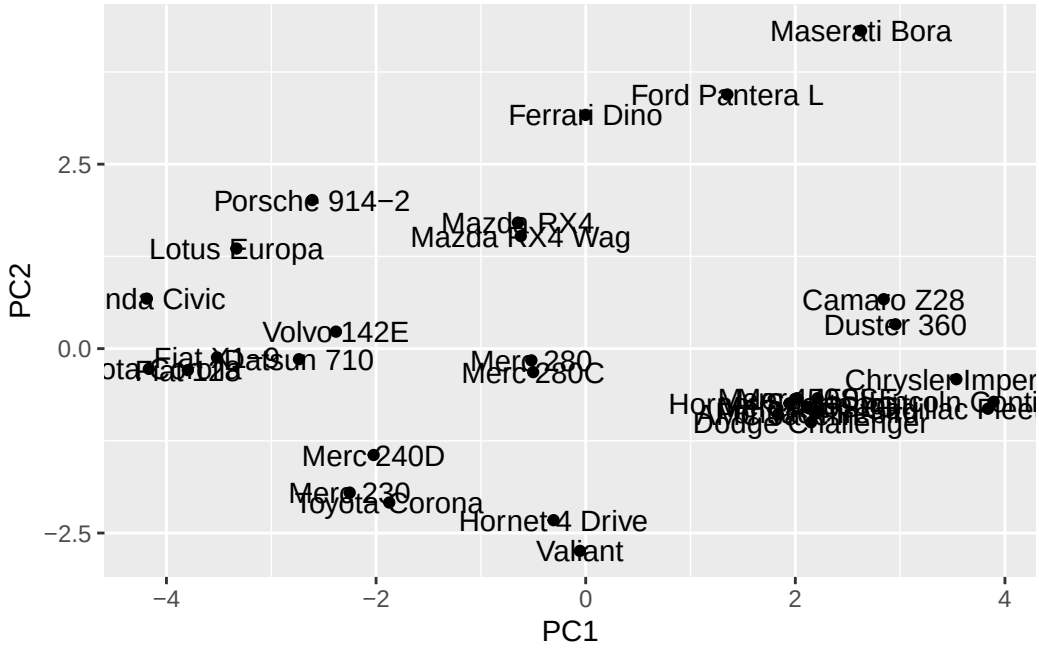
Loadings plot of the scaled data.

```
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()
```



Key point: In general, we will set `scale=TRUE` when we do PCA. This is not the default but probably should be...

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

PCA of this wisc.data

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

To see how well this PCA data is doing in terms of capturing the variance (or spread) in the data, we can use the `summary()` function.

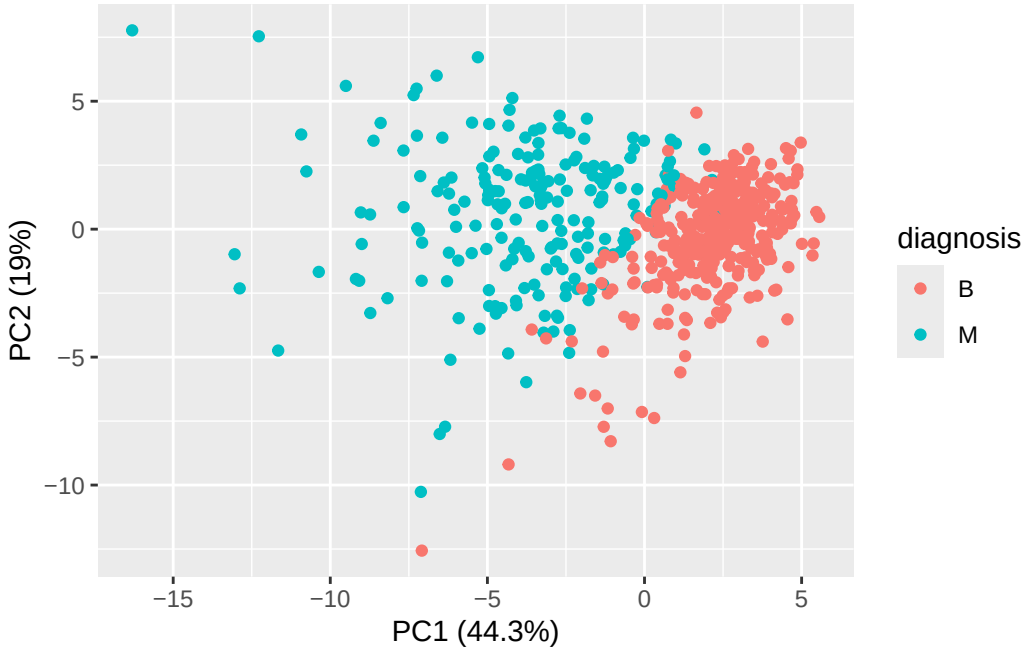
```
summary(wisc.pr)
```

```
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
```

Let's make the main PC1 vs PC2

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



Q10. Please answer up to this Q10… ;

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

[44.3%]

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

3 principal components are required to describe at least 70% of the original variance in the data.

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

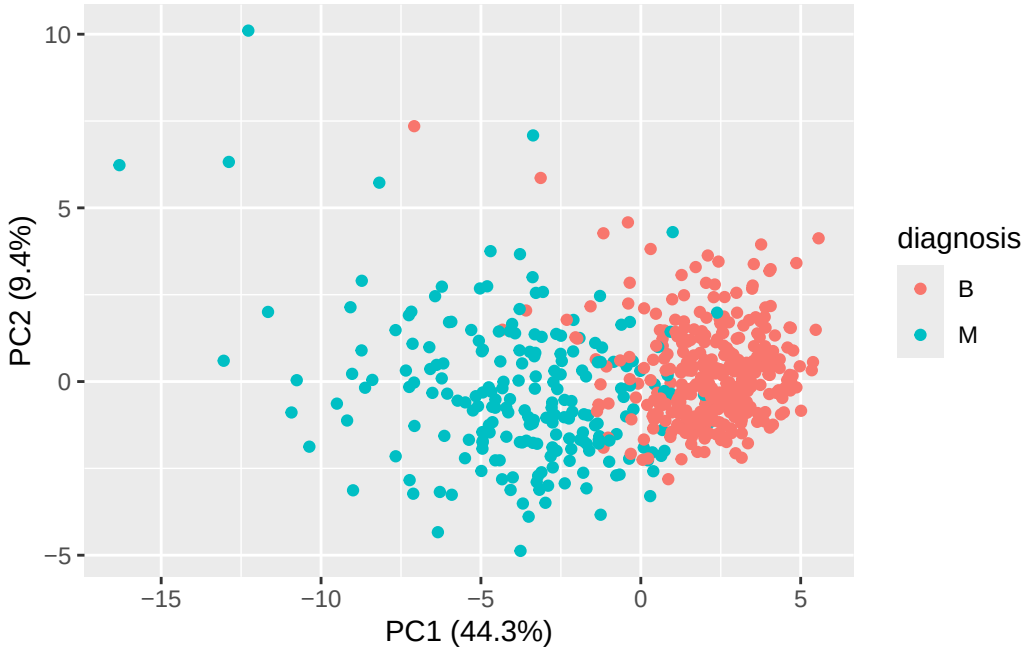
7 principal components are required to describe at least 70% of the original variance in the data.

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

The difference diagnosises are grouped very visibly by color and their distinct groupings stand out to me. It is easy to understand and see, due to being able to see where they fall on the scatter plot.

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

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



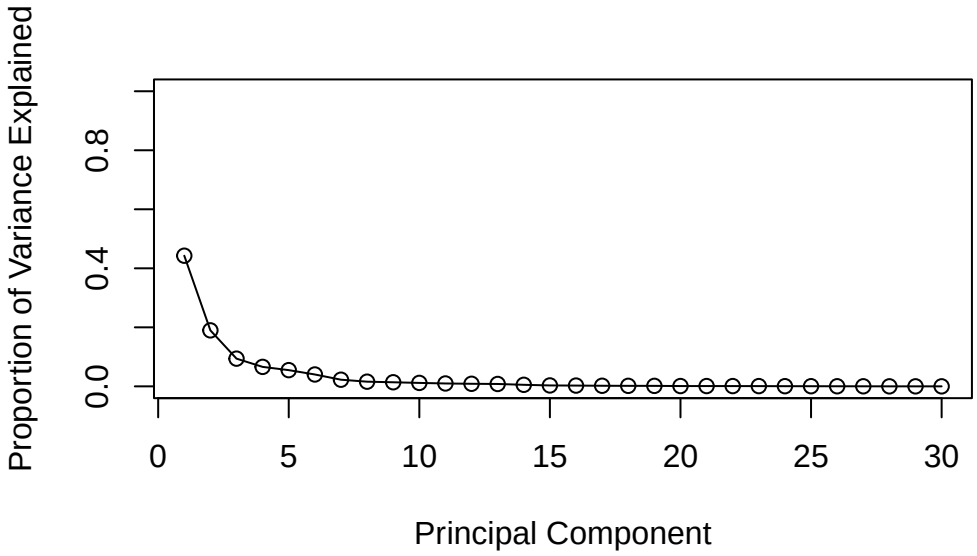
After generating a similar plot, I notice that the diagnosises of benign or malignant are still grouped together, but are at a lower percentage on the y-axis. This is because the PC3 proportion of variance is lower, and so the shift is to be expected. I also notice slightly more overlap between the two diagnosises, in comparison to the PC1 and PC2 plot from before.

> 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?

```
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")
```



The component of the loading vector `wisc.pr$rotation[,1]` for the feature of `concave.points_mean` is -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?

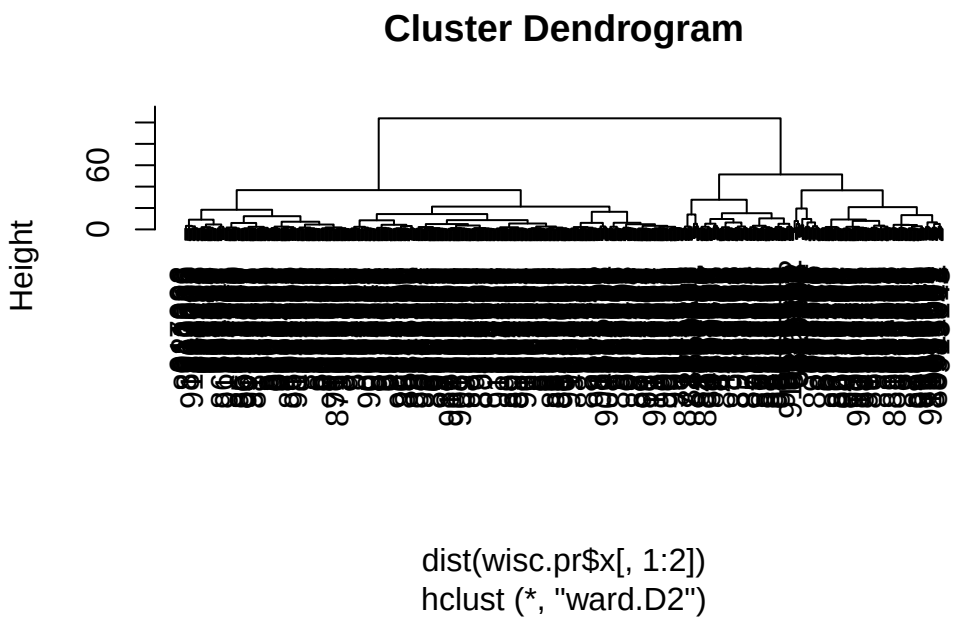
The minimum number of principal components required to explain 80% of the variance of the data is 5 components combined.

5. Combining Methods

We can take our PCA results and use them as a basis set for other analysis such as clustering.

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 our clusters (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 from

```
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?

The newly created model with four clusters separates the two diagnoses in a cleaner way, but has the potential to be hard to read; whereas a model that separates via two clusters could be more distinct and helpful in visualization.

> 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) gives us much better separation of M and B.

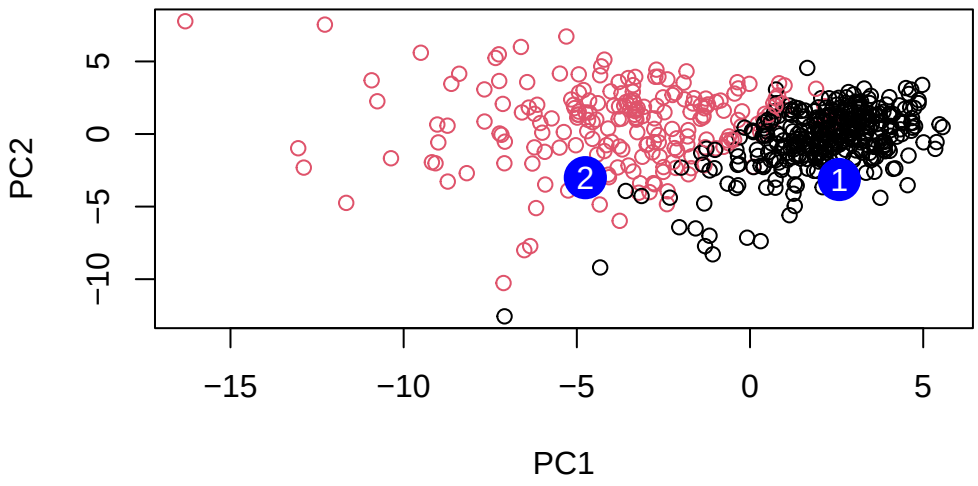
7. Prediction

We can use our PCA model for 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
```

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

Patient 2 for sure.

answer questions 1-10, 15, 16, 18 for homework.