Class 08 - Mini Project

Gabriella Tanoto (A18024184)

Table of contents

Background

This mini-project explores unsupervised learning techniques applied to the Wisconsin Breast Cancer Diagnostic Data Set, which contains measurements 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 with different linkage methods. It also includes an optional section on K-means clustering for comparison. The ultimate goal is to combine PCA and 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 comes from the Wisconsin Medical Center. Let's load the saved datasets.

```
wisc.df <- read.csv("WisconsinCancer.csv", row.names=1) #so the ID is just a row name; not a
head(wisc.df, 5)
```

```
         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
         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
         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
         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
         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
         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
         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
         fractal_dimension_worst
```

```
842302                  0.11890
842517                  0.08902
84300903                0.08758
84348301                0.17300
84358402                0.07678
```

Q1. How many observations is in the dataset?

We have *569 patients* in this dataset!

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

```
[1] 569
```

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

There are *212 malignant* diagnosis.

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

```
[1] 212
```

OR:

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

```
  B   M
357 212
```

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

There are *10* column names contains "_mean" in it!

```
grep("_mean", colnames(wisc.df)) #will tell us which column names have the "_mean"
```

```
 [1]  2  3  4  5  6  7  8  9 10 11
```

```
length(grep("_mean", colnames(wisc.df))) #tell us HOW MANY vectors there are that's in my `gr
```

```
[1] 10
```

There is a diagnosis column, that is the clinician's consensus that I wanna exclude from my further analysis. We can come back later and compare our results to this diagnosis!

```
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis) #with the as.factor function, we can see there's level to it.
```

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

Now we can remove it from the `wisc.df`, and save it as a `wisc.data`

```
wisc.data <- wisc.df[,-1]
dim(wisc.data) #now we see we removed the first column -- NO MORE Clinician's DIAGNOSIS!
```

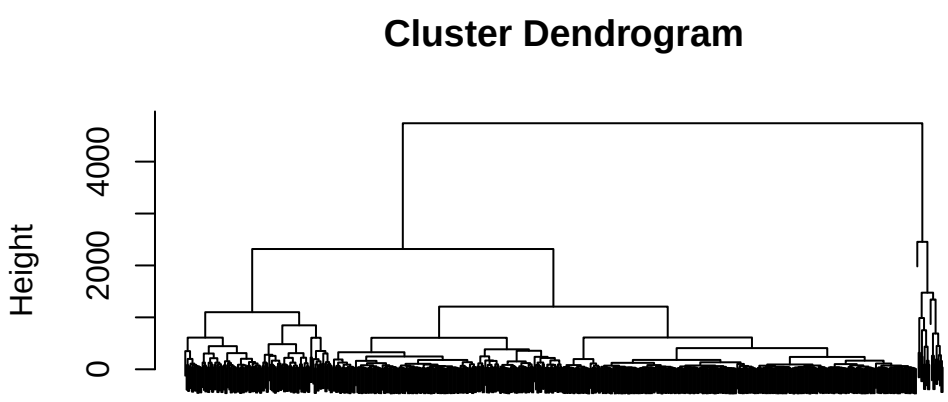
```
[1] 569  30
```

Clustering

We can choose either `kmeans`, `hclust`, or the `pca`.

Let's try the h-clust (Hierarchical clustering)!

```
hc <- hclust(dist(wisc.data))
plot(hc, labels = F)
```



We can extract clusters from the weird dandogram using the `cutree()` function!

```
groups <- cutree(hc, k= 2) #cut the tree into 2 major branches!
table(groups)
```

```
groups
  1   2
549  20
```

Maybe, let's compare it with the diagnosis…

```
table(diagnosis)
```

```
diagnosis
  B   M
357 212
```

To compare the two tables in one, we can do a cross-table that compares our cluster `groups` vectors with our `diagnosis` data:

```
table(diagnosis, groups)
```

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

–> all the weird (most extreme ones the hclust can pick up) is Malignant. But this is bad, cuz it can only pick up the VERY weird ones. We need a better method.

PCA

The importance of Scaling

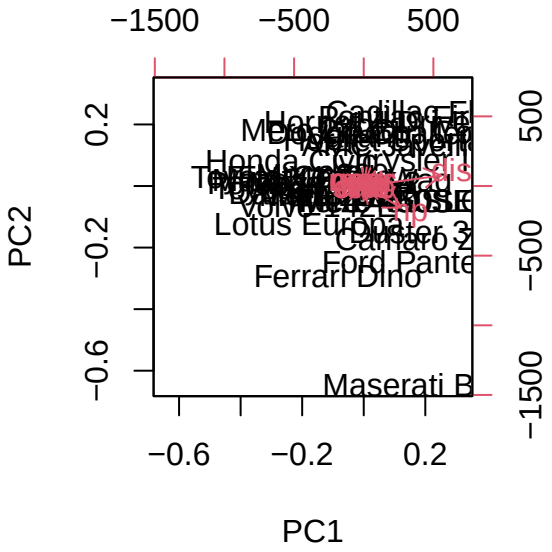
The main function for PCA in base R `prcomp`. It's got a default input parameter of `scale = FALSE`

```
#use the mtcar dataset
head(mtcars,4)
```

```
                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
```

We can do PCA of the data as is, but it could be misleading…

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



Without scaling: the ones that are in the scales of 100-300 (such as the `disp`) are spread out way more than the ones like the `vs` or `am` columns which shows Yes/No values. So, just because the data's got a huge spread, doesn't mean it's more important than the others.

Now let's pay attention to the mean and sd of each columns.

```
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) #2 is code for columns!
```

```
       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 see here that the data is more spread for ones with scales like 100s, because it's got different UNITS. Makes no sense to PCA out of this!

To fix, we can **Scale** the data before PCA, to get a much better representation and analysis of all the columns. Use the function `scale()` to our dataset.

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

Check the means & sd:

```
colMeans(mtscale)
```

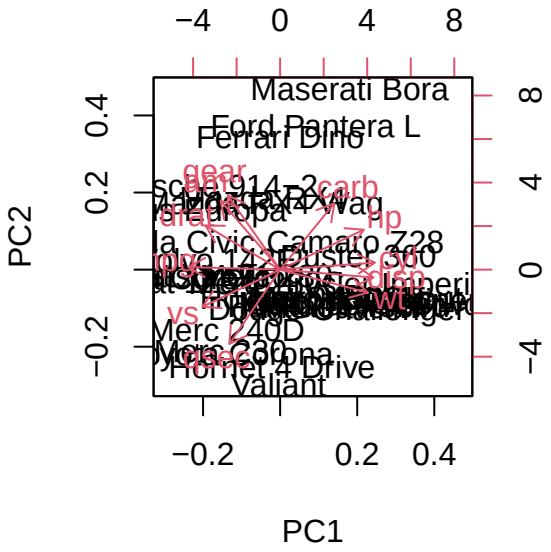
```
          mpg           cyl          disp            hp          drat
 7.112366e-17 -1.474515e-17 -9.085614e-17  1.040834e-17 -2.918672e-16
           wt          qsec            vs            am          gear
 4.682398e-17  5.299580e-16  6.938894e-18  4.510281e-17 -3.469447e-18
         carb
 3.165870e-17
```

```
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
```

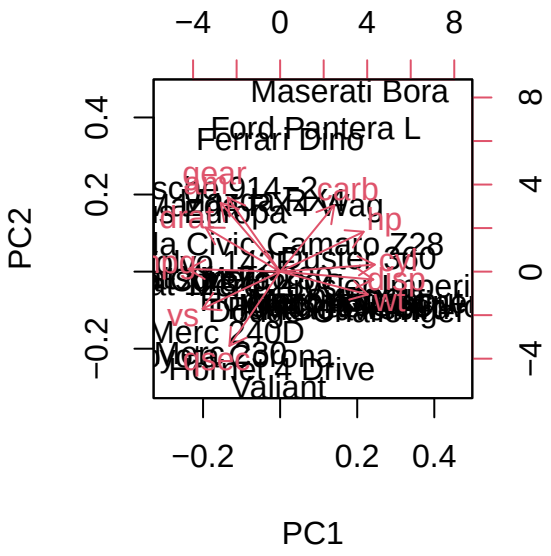
Do prcomp on the scaled data:

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



This 3-step scaling technique can be made as a shortcut into the `prcomp` function by setting `scale=TRUE`:

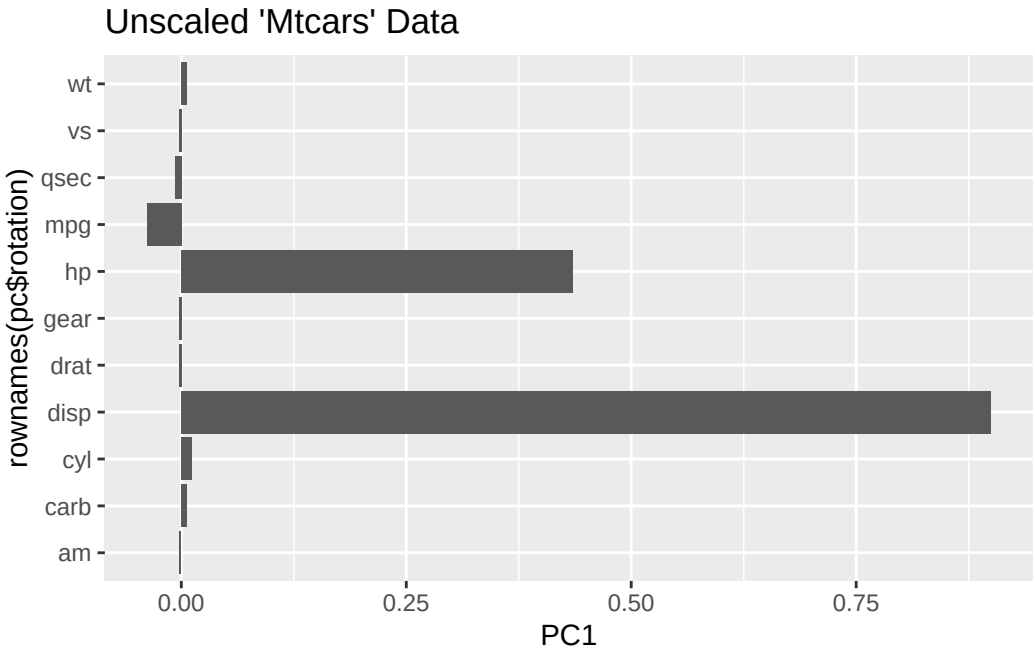
```
pc.scale2 <- prcomp(mtcars, scale.=T)
biplot(pc.scale2)
```



2 figures to represent PCA. Let's do a Loadings Plot od the Unscaled PCA results:

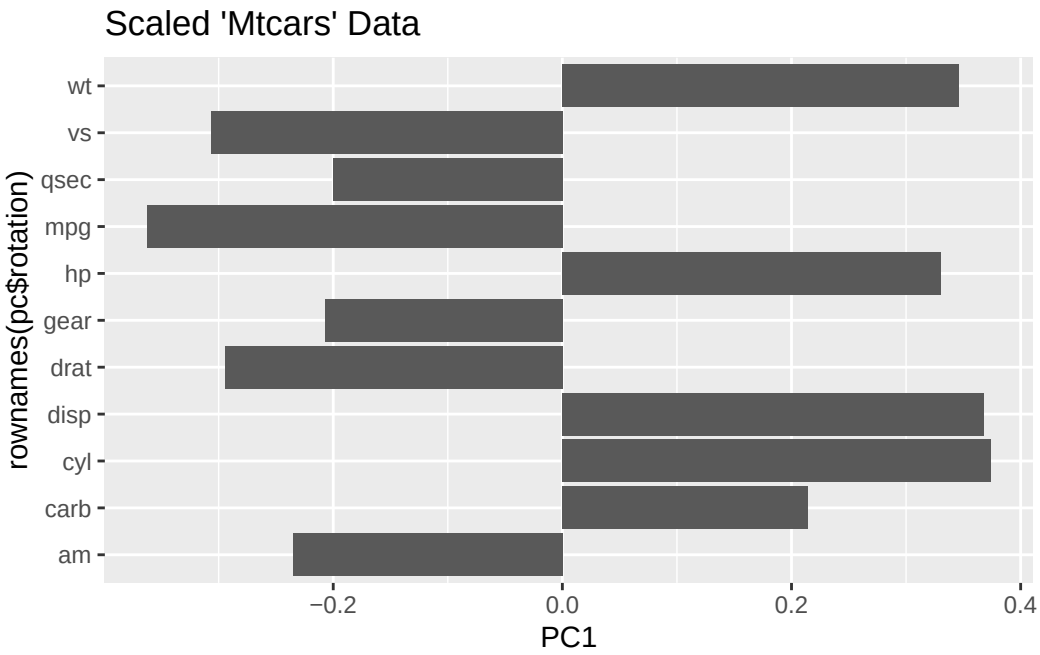
```
library(ggplot2)

ggplot(pc$rotation) +
  aes(PC1, rownames(pc$rotation))+
  geom_col() +
  ggtitle("Unscaled 'Mtcars' Data")
```



Plot of the Scaled PCA:

```
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc$rotation))+
  geom_col()+
  ggtitle("Scaled 'Mtcars' Data")
```



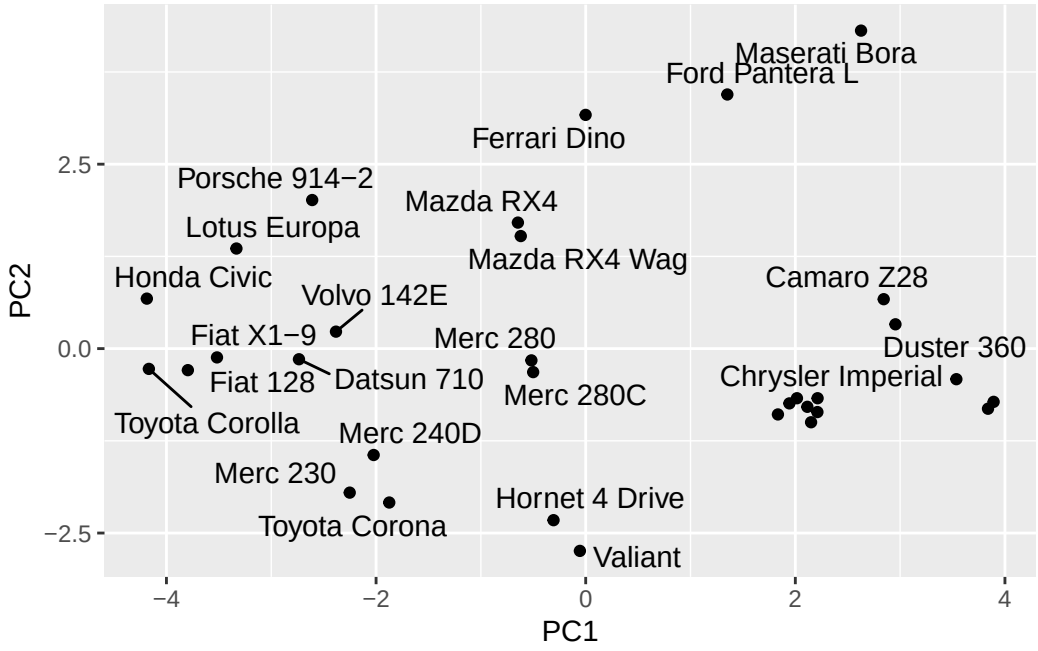
Much better than the unscaled, as we can see that it's not just heavy on the bigger-unit features.

PC plot of Scaled PCA:

```
library(ggrepel)

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

```
Warning: ggrepel: 9 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```



Key Point:
In general, we will set `scale = TRUE` when we do PCA. This isn't the default but it probably should be…

Going back to the Wisc Cancer data:

Now, we can check the SD and the Mean of the `wisc.data` to see if we need to scale it.

```
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
```

We do indeed have to scale it, before making the `prcomp`

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

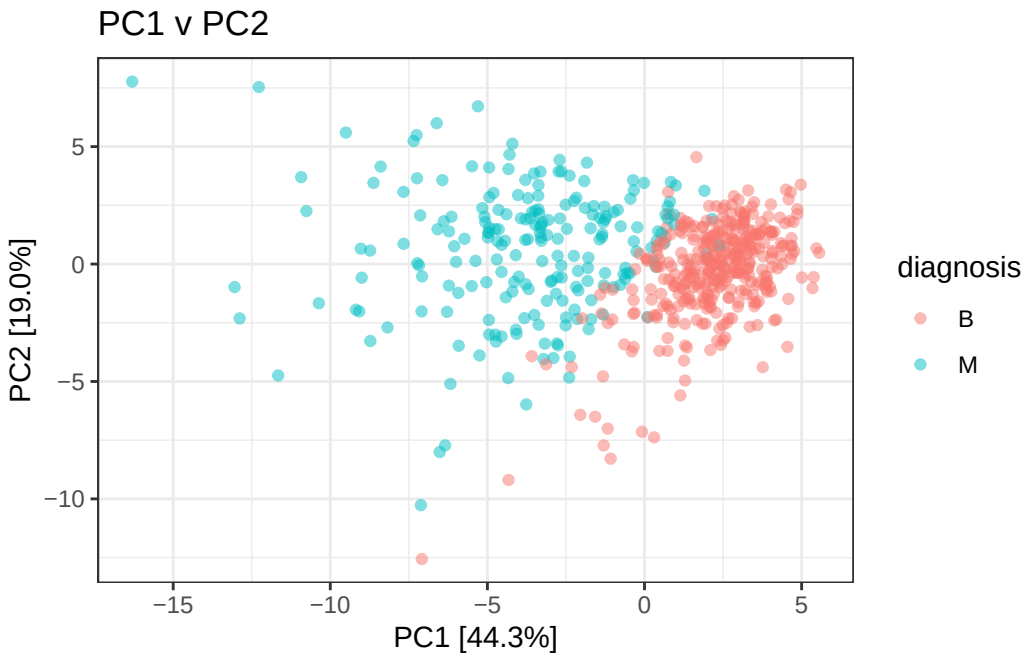
To see how well PCA captures the variance, we can use the `summary` function:

```
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
```

Now, let's make the main PC plot (PC1 v PC2)

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point(alpha=0.5) +
  xlab("PC1 [44.3%]") + ylab("PC2 [19.0%]") +
  ggtitle("PC1 v PC2") +
  theme_bw()
```



This is good, because we can see that it's different enough to determine whether the cell is gonna be 'benign' or 'malignant'. Therefore, we can potentially predict which factor (out of the 30), is the one that's most prominent.
But how, exactly, does PCA do to compress the 30 different factors into 1 dot??

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

We have *44.3% of the variance* captured by PC1.

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

From this info, 70% of the variance is captured in *3 PCs*.

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

90% of the variance is captured in *7 PCs*.

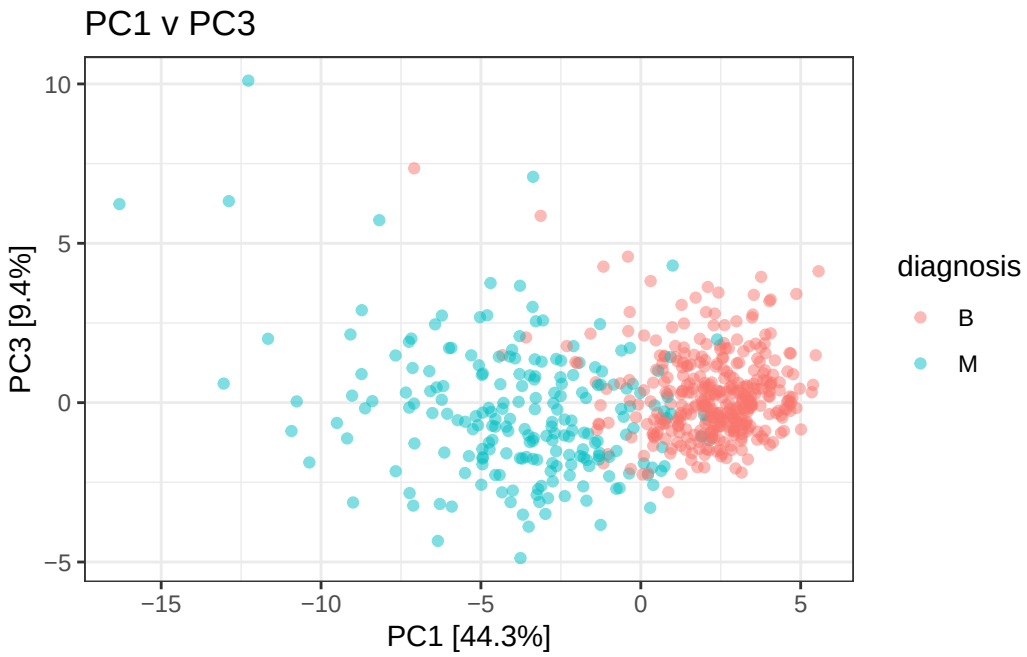
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The PC1 v PC2 plot actually showed that there is a difference between the benign and the malignant cells, as we can see when we color it by the diagnosis.
It is quite easy to undersatnd once I know what PC's are and what it means, because now I know that the

cells vary more along the PC1 (x) axis, and as they are different, they are also different in the diagnosis: more benign cells are in the Right side, and malignant on the Left of the PC1.

> 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(alpha=0.5) +
  xlab("PC1 [44.3%]") + ylab("PC3 [9.4%]") +
  ggtitle("PC1 v PC3") +
  theme_bw()
```



We can see that the separation still exists, and it's still pretty good. However, the separation between the benign and malignant cells are not as good as plot of 'PC1 and PC2'.

> 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
```

It is *-0.26085376*. There's **NO ONE** factor that makes the cell benign or not, each factor kind of contributes to it.

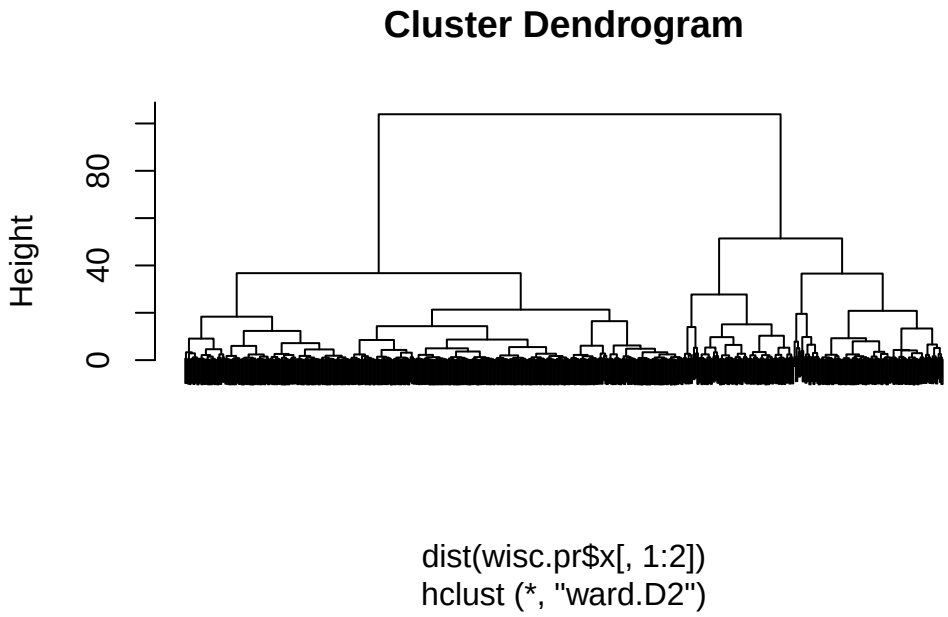
> Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?

5 PCs are required to capture 80% of the variance in the data.

Clustering on PCA results

Now, let's try clustering these cells, based on PC1 and 2, instead of just as is.

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



We can make a `cutree`

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

```
pcgroups
  1   2
195 374
```

Now, crosscheck with the diagnosis table!

```
table(diagnosis, pcgroups)
```

```
         pcgroups
diagnosis   1   2
        B  18 339
        M 177  35
```

^ Most individuals that are benign will fall into Group 2, whereas the ones in Group 1, the vast majority is Malignant. There are still some false positive/ false negatives. We can then estimate the sensitivity.

It's a much better predictor than the last one where we have 18 and 0.

(Q10 gradescope) Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?
WE DIDN'T COVER THIS IN CLASS

(Q12 gradescope) Which method gives your favorite result for the same data.dist dataset?
WE DIDN'T COVER THIS IN CLASS

(Q13 gradescope) How well does the newly created model with four clusters separate out the two diagnoses?
WE DIDN'T COVER THIS IN CLASS

Q15 in class. Which one, using PC 1 and 2 only or using PC1:7 that covers 90% of the variance is better at separating benign vs malignant cells?

```
#using PC 1 through 7, we can capture 90% of the variance in the data.
wisc.pr.hclust90 <- hclust(dist(wisc.pr$x[, 1:7]), method= "ward.D2")
pcgroups90 <- cutree(wisc.pr.hclust90, k= 2)
table(diagnosis, pcgroups90)
```

```
         pcgroups90
diagnosis   1   2
        B  28 329
        M 188  24
```

False negative: When we predict the cell to be benign (B) but it's actually cancerous. False positive: When we predict the cell to be cancerous (M) but it's benign.

Using the PC method, we can group each cells to either cluster 1 (where they are predicted to be Malignant/cancerous), or cluster 2. When we use this clustering to predict, people who is in group 1 is gonna be considered (+) for Malignant. When looking at group 1, there's **MORE false positive** (12.96%) using the 91% clustering, compared to the previous one that covers 63% of the variance (9.23% false positives).

If you are in group 2, you're more likely to be benign. There is **LESS** chance that you get a *false negative* (cancer but predicted to be OK) compared to when the PC just covers 63% of the variance.

I think the better one would be the 90%, because we can catch more potentially malignant patients; although we might accidentally cause panic (false positives).

Q16 (Q14 gradescope). 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.

We didn't do the K-means, but we did group the using the hierarchical cluster (before doing any PCA analysis). Below is the code for the comparison between h-clustering groups:

```
table(groups, diagnosis)
```

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

As we can see, it is of very low quality, we cannot use the grouping result of h-clustering to predict if one were to be a malignant or benign tumor cell.

If we just force ourselves to see the pattern, we'll see that the Group 2 tend to be malignant, but 35% of group 1 is also malignant. There would be way too many false negatives with this data.

However, once we used PCA to take into account the whole thing, we can see that the data actually gets clustered pretty well.

Prediction

We can use the PCA data to analyse new "unseen" data. In this case, we use data from U of Michigan.

```
new <- read.csv("new_samples.csv")
npc <- predict(wisc.pr, newdata=new)
npc
```

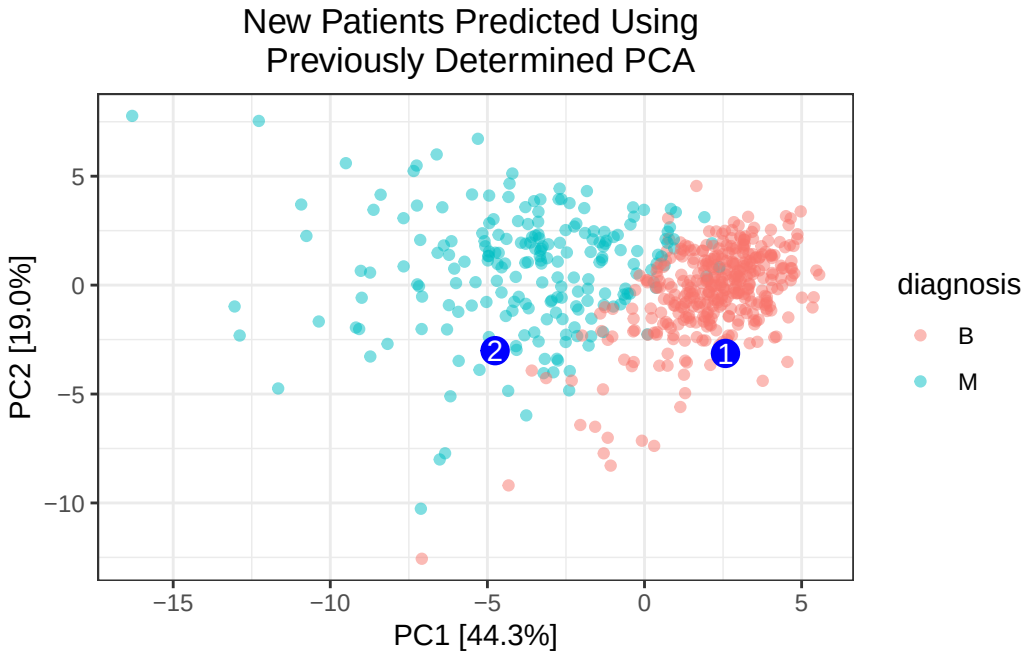
```
           PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
           PC8       PC9       PC10      PC11      PC12      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?

```
library(ggeasy)

plotpc <- ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point(alpha=0.5) +
  xlab("PC1 [44.3%]") + ylab("PC2 [19.0%]") +
  ggtitle("New Patients Predicted Using \n Previously Determined PCA")+
  theme_bw() + ggeasy::easy_center_title()

#Add the new patients we wanna predict as blue dots; and adding the labels.
plotpc + annotate("point", npc[,1], npc[,2], color="blue", size = 4.5) +
  annotate("text", npc[,1], npc[,2], color="white", label= c("1", "2"))
```



From this newly generated plot, we can see that patient #1 is likely to be benign, and patient #2 is likely to have a malignant cell. Therefore, we should prioritize the patient 2, as they are more likely to suffer from cancer.