Class 8

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Background

In today's class we will apply the methods and techniques clustering and PCA to make sense of a real world breast cancer FNA biopsy data set.

Data Import

We start by importing our data. It is a CSV file so we will use the `read.csv()` function.

```
wisc.report <- read.csv("WisconsinCancer (2).csv")
```

```
wisc.df <- data.frame(wisc.report, row.names=1)
head(wisc.df,4)
```

```
         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
         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
         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
         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
         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
         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
         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
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
```

Make sure to remove the first `diagnosis` column- I don't want to use this for my machine learning models. We will us it later to compare our results to the expert diagnosis.

```r
wisc.data <- wisc.df[,-1]
diagnosis <- wisc.df$diagnosis
```

Exploratory Data Analysis

> Q1. How many observations are in this dataset?

```r
dim(wisc.data)
```

```
[1] 569  30
```

- There are 569 observations in this data set.

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

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

- There are 212 observations that have malignant diagnosis.

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

```r
length(grep("_mean",colnames(wisc.data),TRUE))
```

```
[1] 10
```

- There are 10 variables/features in the data that are suffixed with `_mean`.

Principal Component Analysis

Performing PCA

```r
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 
```

```r
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 
```

- For PCA, the main function is `prcomp()` and we want to make sure we set the optional argument `scale=TRUE`.

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

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                           PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

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

- 44.27% proportion of the original variance is captured by the first principal component (PC1).

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

- 3 PCs are required to describe at least 70% of the original variance in the data since `cumulative proportion` of PC3 is 72.636%.

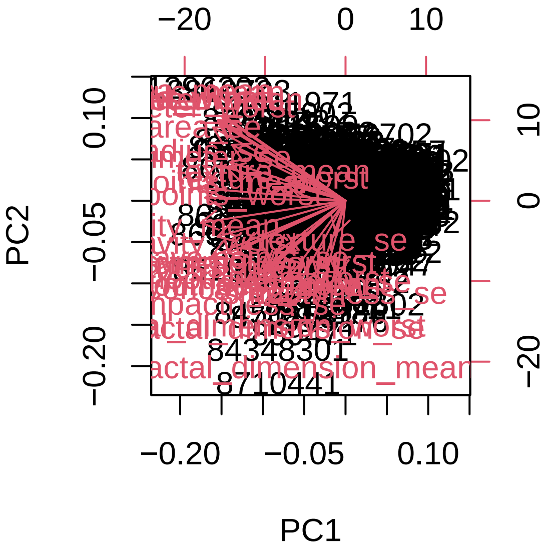
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

- 7 PCs are required to describe at least 90% of the original variance in the data since `cumulative proportion` of PC7 is 91.010%.

Interpreting PCA results

Using so-called bi-plot visualization technique to better understand our PCA model.

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

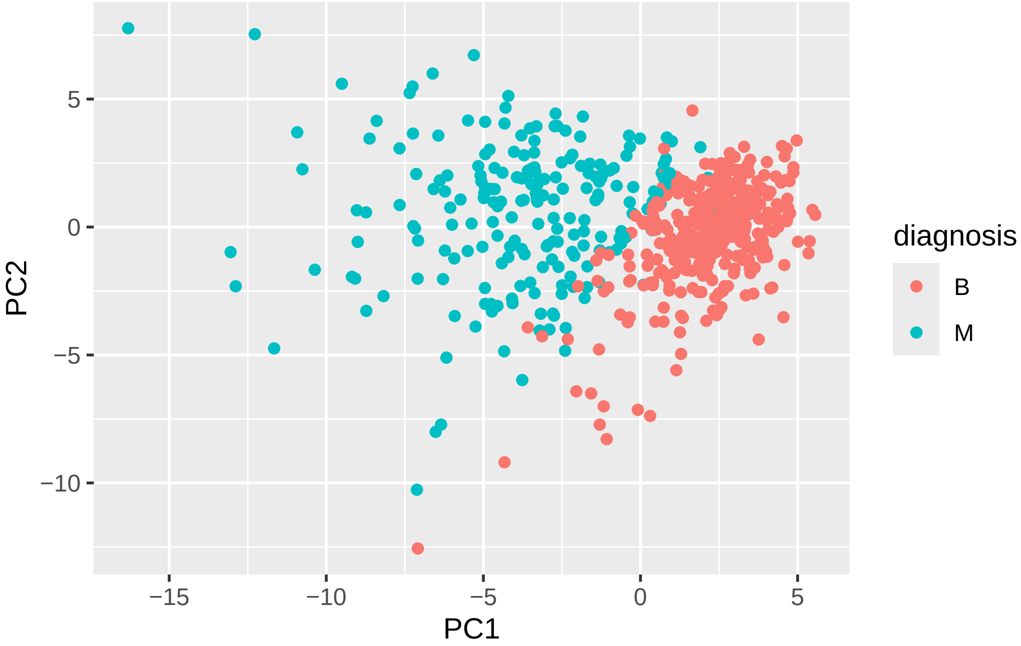


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

- This plot uses row names as the plotting character for every observation in the plot, making trends quite hard to see and the plot looks extremely cluttered. It is quite difficult to read and interpret because there is a lot of overlapping labels on top of each other which makes it hard to see separations or trends, making it harder to understand.

Since the previously made bi-plot was quite difficult to understand, we should make a more standard scatter plot each observation along principal components 1 and 2 (i.e. a plot of PC1 vs PC2 available as the first two columns of wisc.pr$x) and color the points by the diagnosis.

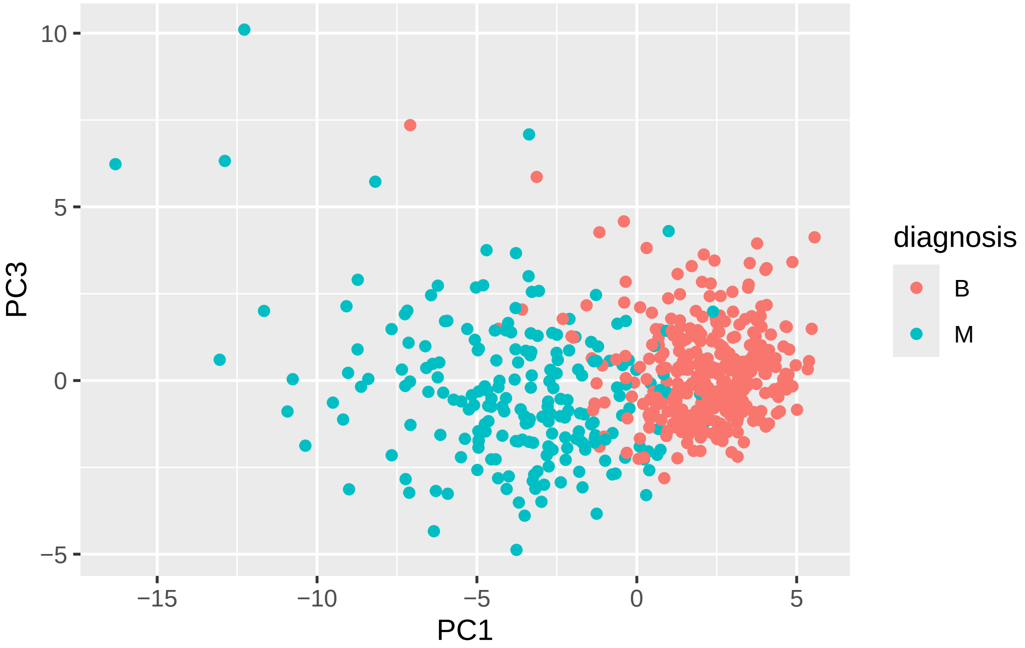
```
library(ggplot2)

ggplot(wisc.pr$x) +
  aes(PC1,PC2, col=diagnosis) +
  geom_point()
```



- The PCA plot shows a separation of Malignant (turquoise) and Benign (red)

  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()
```



- Overall, we can notice from these PCA plots that principal component 1 is capturing most of the separation of Malignant (turquoise) from Benign (red) samples. Principal component 3 does not add much additional separation so the main differences between diagnosis are mainly along principal component 1. This result will be further explored in the upcoming sections.

Variance explained

Calculating the variance of each principal component by squaring the `sdev` component.

```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

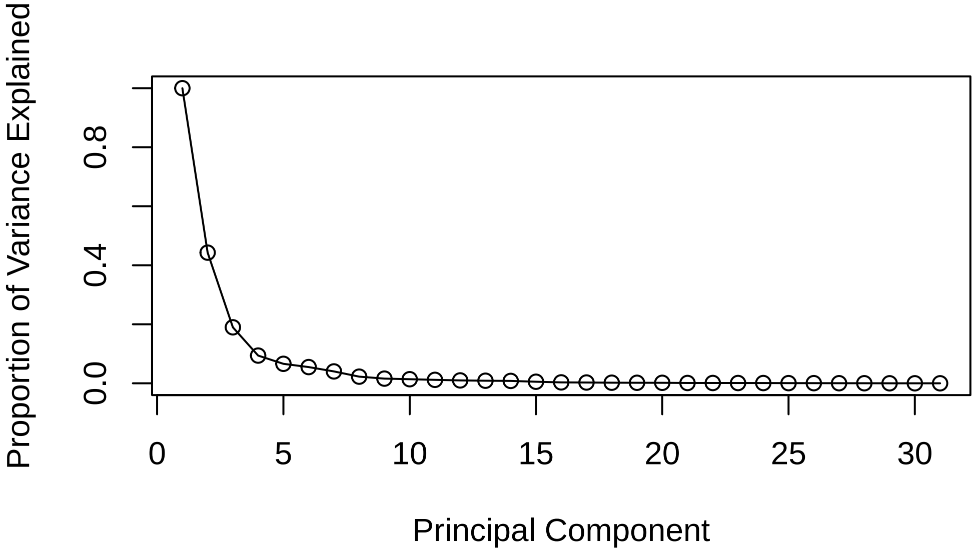
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Calculating the variance explained by each principal component by dividing by the total variance explained of all principal components.

```
pve <- pr.var/ sum(pr.var)
```

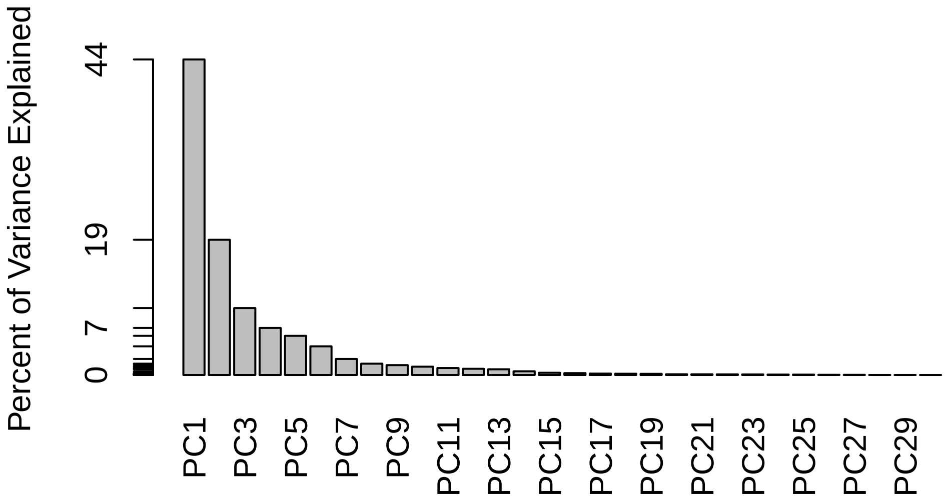
Plot variance explained for each principal component

```
plot(c(1,pve), xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



- Alternative scree plot of the same data (data driven y-axis)

```
barplot(pve, ylab = "Percent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```



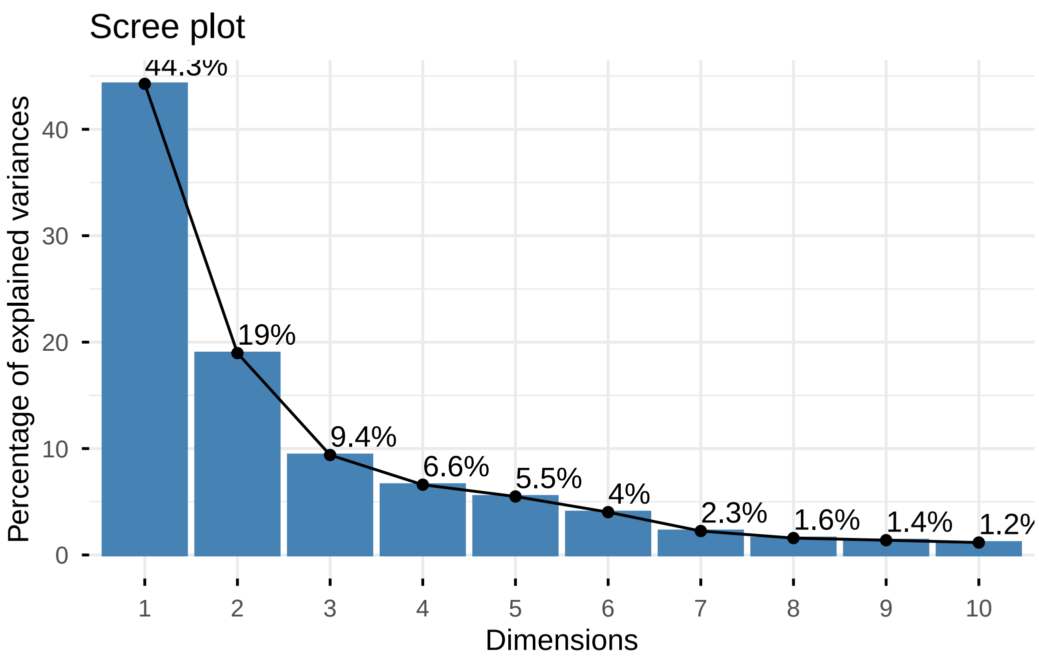
- An optional package useful for exploring PCA is `factoextra` package.

```r
library(factoextra)
```

```
Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```r
fviz_eig(wisc.pr, addlabels = TRUE)
```

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```



Communicating PCA results

```
concave.points_mean1 <- wisc.pr$rotation[,1]
concave.points_mean1
```

```
           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
```

```r
concave.points_mean <- wisc.pr$rotation["concave.points_mean",1]
concave.points_mean
```

```
[1] -0.2608538
```

> 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? This tells us how much this original feature contributes to the first PC. Are there any features with larger contributions than this one?

- The component of the loading vector for the feature concave.points_mean is -0.2608538. There are no features with larger contribution than this one. There are no features with larger contributions than this one but there are a few including concavity_mean (-0.25840048), concave.points_worst (-0.25088597) etc which have similar contributions to the first PC.

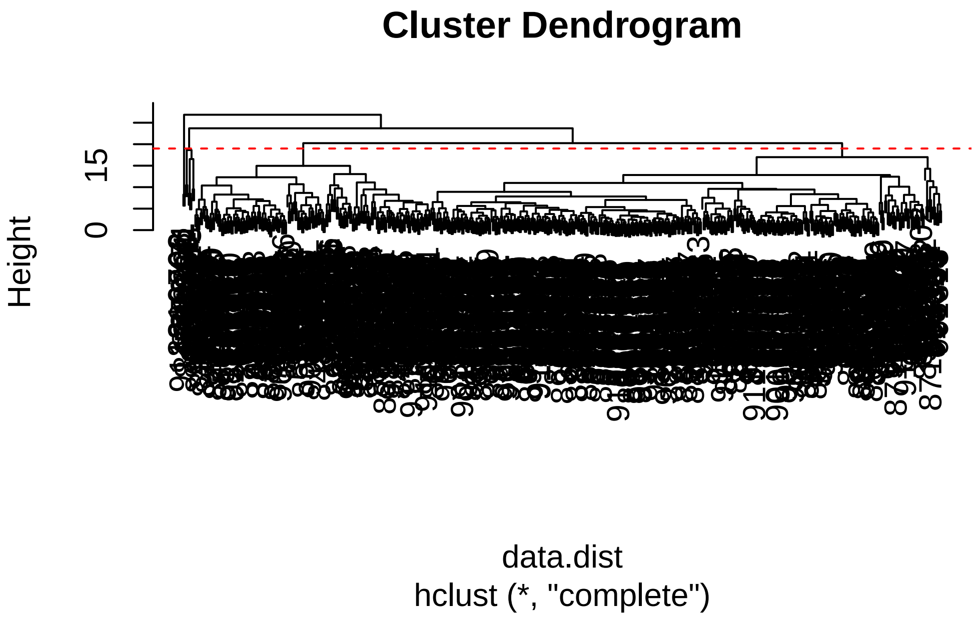
Hierarchical Clustering

- Goal of this section to do hierarchical clustering of the original data to see if there is any obvious grouping into malignant and benign clusters.
- First scale the data with `scale()` function, then calculate a distance matrix (with the `dist()` function). Then cluster with the `hclust()` function and plot.

```r
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "complete")
```

> Q10. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

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



- Height = 19

We can also use `cutree()` function with a argument k=4 rather than `h=height`.

```r
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
```

From this result we see that cluster 1 largely corresponds to malignant cells (with diagnosis values of "M") whilst cluster 3 largely corresponds to benign cells (with diagnosis values of "B").

Using different methods

> Q12. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

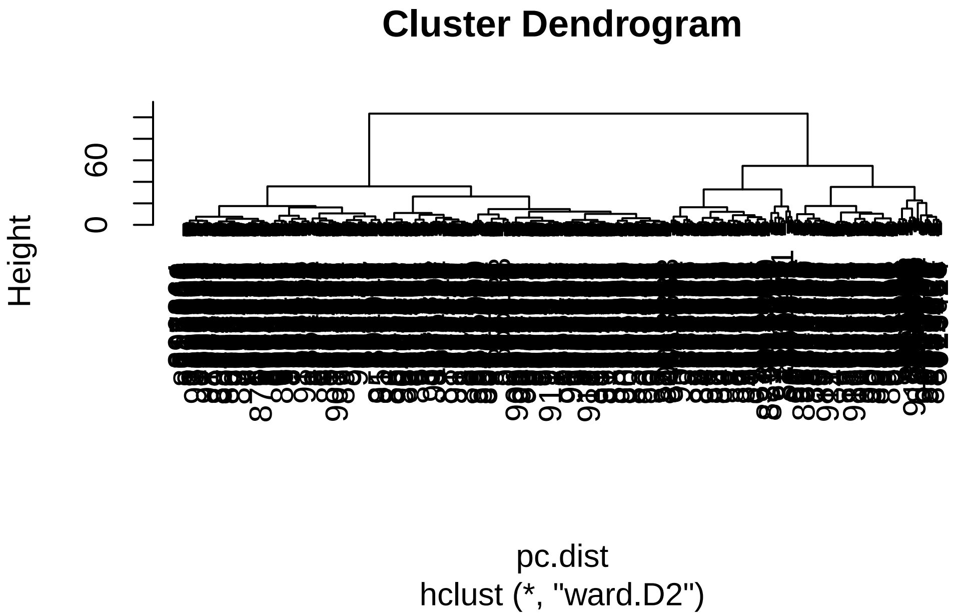
- For the `data.dist` data set, method = "ward.D2" gives my favorite result because it produces clean and more well-separated clusters, minimising the increase in total in-cluster variance.

Combining methods

Clustering on PCA results

Combining PCA and hierarchical clustering: cluster on the PC scores instead of the original 30 features. Here we will essentially take our PCA esults and use those as input for clustering. In other words, our `wisc.pr$x` scores that we plotted above (the main output from PCA- how the data lie on our new principal component axis/variables) and use a subset of these PCs that capture most of the variance as input for `hclust()`.

```
pc.dist <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(pc.dist, method= "ward.D2")
plot(wisc.pr.hclust)
```



- Cut the dendrogram into two main groups/clusters:

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

```
grps
  1   2 
203 366 
```

- I want to know how the clustering in `grps` with values of 1 or 2 correspond the expert `diagnosis`.

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

```
    diagnosis
grps   B   M
   1  24 179
   2 333  33
```

- My clustering **group 1** are mostly "M" diagnosis (179) and my clustering **group 2** are mostly "B" diagnosis (333).

24 FP, 179 TP, 33 TN, 33 FN.

- Sensitivity TP/(TP+FN)

```
179/(179+33)
```

```
[1] 0.8443396
```

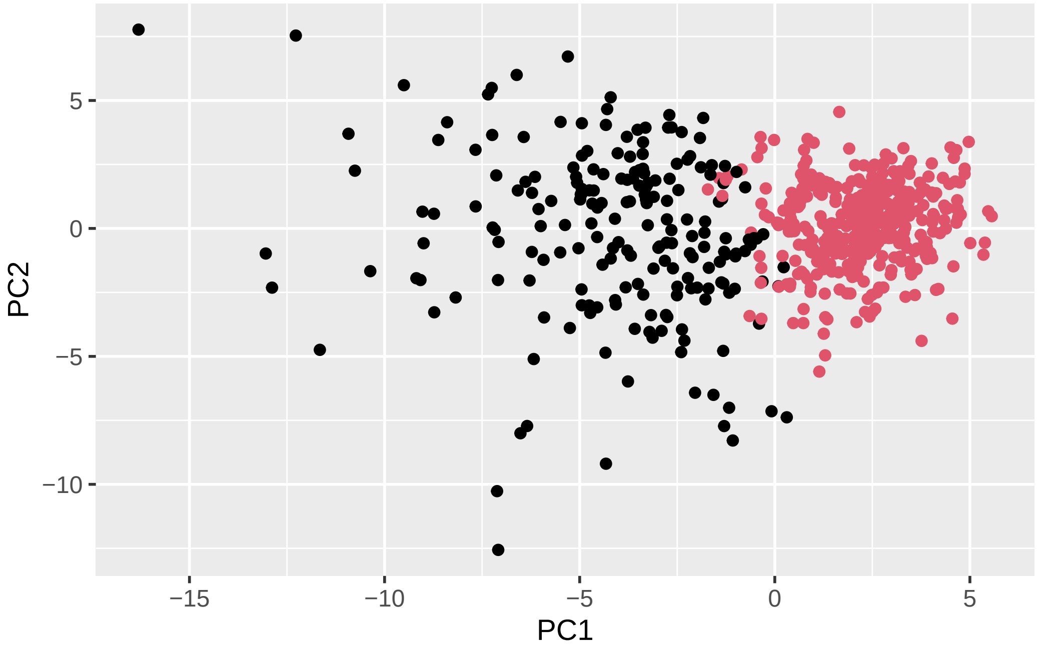
- Specificity TN/(TN+FP)

```
333/(333+24)
```

```
[1] 0.9327731
```

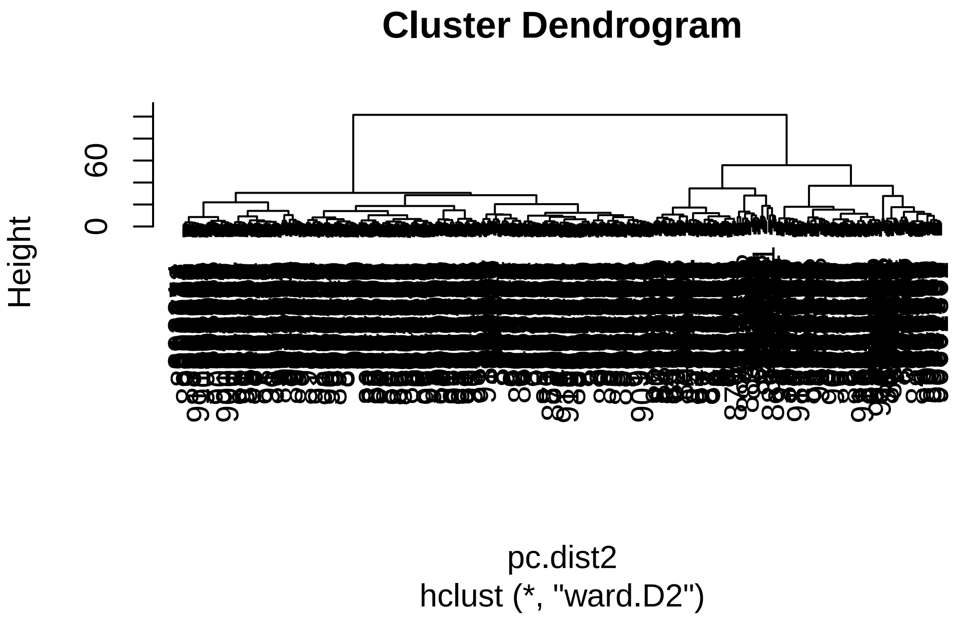
- ggplot

```
ggplot(wisc.pr$x) +
  aes(PC1, PC2) +
  geom_point(col=grps)
```



- Now, Use the distance along the first 7 PCs for clustering

```
pc.dist2 <- dist(wisc.pr$x[,1:7])
wisc.pr.hclust2 <- hclust(pc.dist2, method= "ward.D2")
plot(wisc.pr.hclust2)
```



```
wisc.pr.hclust.clusters2 <- cutree(wisc.pr.hclust2, k=2)
```

Q13. How well does the newly created hclust model with two clusters separate out the two "M" and "B" diagnoses?

```
table(wisc.pr.hclust.clusters2,diagnosis)
```

```
                        diagnosis
wisc.pr.hclust.clusters2   B   M
                       1  28 188
                       2 329  24
```

- The newly created hclust model separates diagnosis fairly well but not perfectly as it shows that clustering **group 1** are mostly "M" diagnosis (188) and my clustering **group 2** are mostly "B" diagnosis (329). Therefore, it can be said that it correctly identifies most of the beningn vs malignant cases. However, it does give us some false positives in group 1 (28) and some false negative in group 2 (24).

28 FP, 188 TP, 329 TN, 24 FN.

- Sensitivity TP/(TP+FN)

```
188/ (188+24)
```

```
[1] 0.8867925
```

- Specificity TN/(TN+FP)

```
329/(329+28)
```

```
[1] 0.9215686
```

> Q14. How well do the hierarchical clustering models you created in the previous sections (i.e. without first doing PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.hclust.clusters and wisc.pr.hclust.clusters) with the vector containing the actual diagnoses.

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

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

```
table(wisc.pr.hclust.clusters2, diagnosis)
```

```
                        diagnosis
wisc.pr.hclust.clusters2   B   M
                       1  28 188
                       2 329  24
```

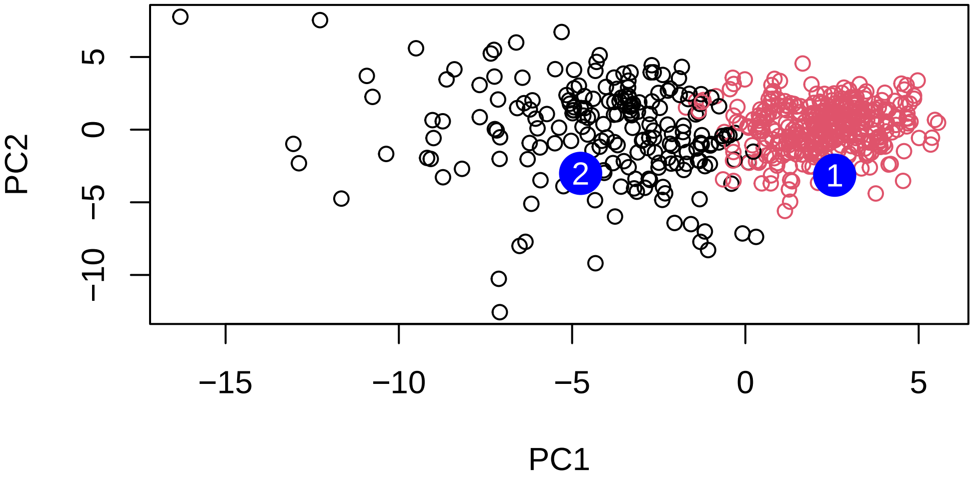
- PCA based hierarchial clustering does a better job separating the diagnosis since it clearly shows that cluster 1 has majorly malignant diagnosis (with 28 FP) while cluster 2 has majorly benign diagnosis (24 FN). This separation is fairly clean. On the other hand, hierarchial clustering without PCA does only a poorer job separating the diagnosis- cluster 1 is mostly malignant but has 12 FP, cluster 3 is mostly benign but has considerable 40 FN while cluster 2 and 4 are quite small and contain a mix, highlighting the fact that PCA based hierarchial clustering does a comparitively better job separating the diagnosis.

Prediction

```r
#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
```

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



Q16. Which of these new patients should we prioritize for follow up based on your results?

- Based on these results, we should prioritize patients from cluster/group 2 for follow up because their results match the results/fall in the region of the malignant diagnosis thereby indicating that they are at a higher risk.