Lab 9 report (mini-project)

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10/26/2021

#1. Exploratory data analysis

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"

# Input the data and store as wisc.df
wisc.df <- read.csv(fna.data, row.names=1)
```

```
#wisc.df
```

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
```

```
# Create diagnosis vector for later
diagnosis <- factor(wisc.df[,1])
```

```
View(wisc.data)
head(wisc.data)
```

```
##          radius_mean texture_mean perimeter_mean area_mean smoothness_mean
## 842302         17.99        10.38         122.80    1001.0         0.11840
## 842517         20.57        17.77         132.90    1326.0         0.08474
## 84300903       19.69        21.25         130.00    1203.0         0.10960
## 84348301       11.42        20.38          77.58     386.1         0.14250
## 84358402       20.29        14.34         135.10    1297.0         0.10030
## 843786         12.45        15.70          82.57     477.1         0.12780
##          compactness_mean concavity_mean concave.points_mean symmetry_mean
## 842302            0.27760         0.3001             0.14710        0.2419
## 842517            0.07864         0.0869             0.07017        0.1812
## 84300903          0.15990         0.1974             0.12790        0.2069
## 84348301          0.28390         0.2414             0.10520        0.2597
## 84358402          0.13280         0.1980             0.10430        0.1809
## 843786            0.17000         0.1578             0.08089        0.2087
##          fractal_dimension_mean radius_se texture_se perimeter_se area_se
## 842302                  0.07871    1.0950     0.9053        8.589  153.40
## 842517                  0.05667    0.5435     0.7339        3.398   74.08
## 84300903                0.05999    0.7456     0.7869        4.585   94.03
## 84348301                0.09744    0.4956     1.1560        3.445   27.23
## 84358402                0.05883    0.7572     0.7813        5.438   94.44
## 843786                  0.07613    0.3345     0.8902        2.217   27.19
```

```
##          smoothness_se compactness_se concavity_se concave.points_se
## 842302         0.006399        0.04904      0.05373           0.01587
## 842517         0.005225        0.01308      0.01860           0.01340
## 84300903       0.006150        0.04006      0.03832           0.02058
## 84348301       0.009110        0.07458      0.05661           0.01867
## 84358402       0.011490        0.02461      0.05688           0.01885
## 843786         0.007510        0.03345      0.03672           0.01137
##          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
## 843786       0.02165             0.005082        15.47         23.75
##          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
## 843786             103.40      741.6           0.1791            0.5249
##          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
## 843786            0.5355               0.1741         0.3985
##          fractal_dimension_worst
## 842302                   0.11890
## 842517                   0.08902
## 84300903                 0.08758
## 84348301                 0.17300
## 84358402                 0.07678
## 843786                   0.12440
```

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

```
## [1] 569  30
```

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

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

```
length(wisc.data)
```

```
## [1] 30
```

Q1. How many observations are in this dataset?

There are 569 observations in this dataset.

```
table(diagnosis)
```

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

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

There are 212 observations having a malignant diagnosis.

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

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

```
length(grep("_mean", rownames(wisc.data)))
```

```
## [1] 0
```

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

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

#2. Principal Component Analysis Performing PCA

```
# Check column means and standard deviations
colMeans(wisc.data)
```

```
##             radius_mean            texture_mean          perimeter_mean
##            1.412729e+01            1.928965e+01            9.196903e+01
##               area_mean         smoothness_mean        compactness_mean
##            6.548891e+02            9.636028e-02            1.043410e-01
##          concavity_mean     concave.points_mean          symmetry_mean
##            8.879932e-02            4.891915e-02            1.811619e-01
##  fractal_dimension_mean               radius_se              texture_se
##            6.279761e-02            4.051721e-01            1.216853e+00
##            perimeter_se                 area_se          smoothness_se
##            2.866059e+00            4.033708e+01            7.040979e-03
##          compactness_se            concavity_se       concave.points_se
##            2.547814e-02            3.189372e-02            1.179614e-02
##             symmetry_se    fractal_dimension_se            radius_worst
##            2.054230e-02            3.794904e-03            1.626919e+01
##           texture_worst         perimeter_worst              area_worst
##            2.567722e+01            1.072612e+02            8.805831e+02
##        smoothness_worst       compactness_worst         concavity_worst
##            1.323686e-01            2.542650e-01            2.721885e-01
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##            1.146062e-01            2.900756e-01            8.394582e-02
```

```
apply(wisc.data,2,sd)
```

```
##             radius_mean            texture_mean          perimeter_mean
##            3.524049e+00            4.301036e+00            2.429898e+01
##               area_mean         smoothness_mean        compactness_mean
##            3.519141e+02            1.406413e-02            5.281276e-02
##          concavity_mean     concave.points_mean           symmetry_mean
##            7.971981e-02            3.880284e-02            2.741428e-02
##  fractal_dimension_mean               radius_se              texture_se
##            7.060363e-03            2.773127e-01            5.516484e-01
##            perimeter_se                 area_se         smoothness_se
##            2.021855e+00            4.549101e+01            3.002518e-03
##          compactness_se            concavity_se       concave.points_se
##            1.790818e-02            3.018606e-02            6.170285e-03
##             symmetry_se    fractal_dimension_se            radius_worst
##            8.266372e-03            2.646071e-03            4.833242e+00
##           texture_worst         perimeter_worst              area_worst
##            6.146258e+00            3.360254e+01            5.693570e+02
##        smoothness_worst       compactness_worst         concavity_worst
##            2.283243e-02            1.573365e-01            2.086243e-01
##    concave.points_worst          symmetry_worst fractal_dimension_worst
##            6.573234e-02            6.186747e-02            1.806127e-02
```

```
# Perform PCA on wisc.data
wisc.pr <- prcomp(wisc.data, scale = TRUE)
# Look at summary of results
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)?

From my results, 0.4427 (44.27%) of the original variance is caputured by the first principal components (PC1).

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

Based on the Cumulative Proportion, 3 principal components (PCs) are required to describe at least 70% of the original variance in the data (Cumulative Proportion of PC3: 0.72636).

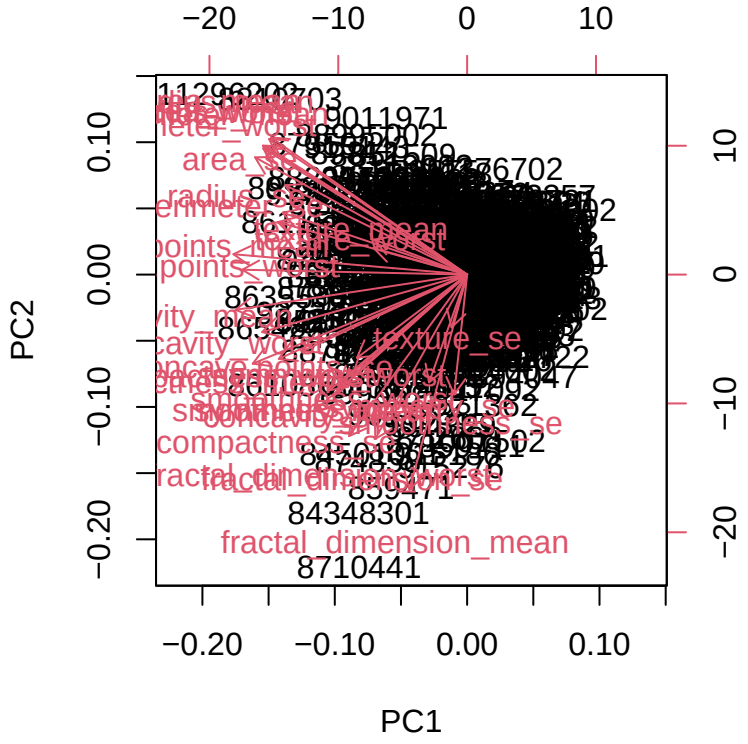
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

Based on the Cumulative Proportion, 7 principal components (PCs) are required to describe at least 90% of the original variance in the data (Cumulative Proportion of PC7: 0.91010).

Interpreting PCA results

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

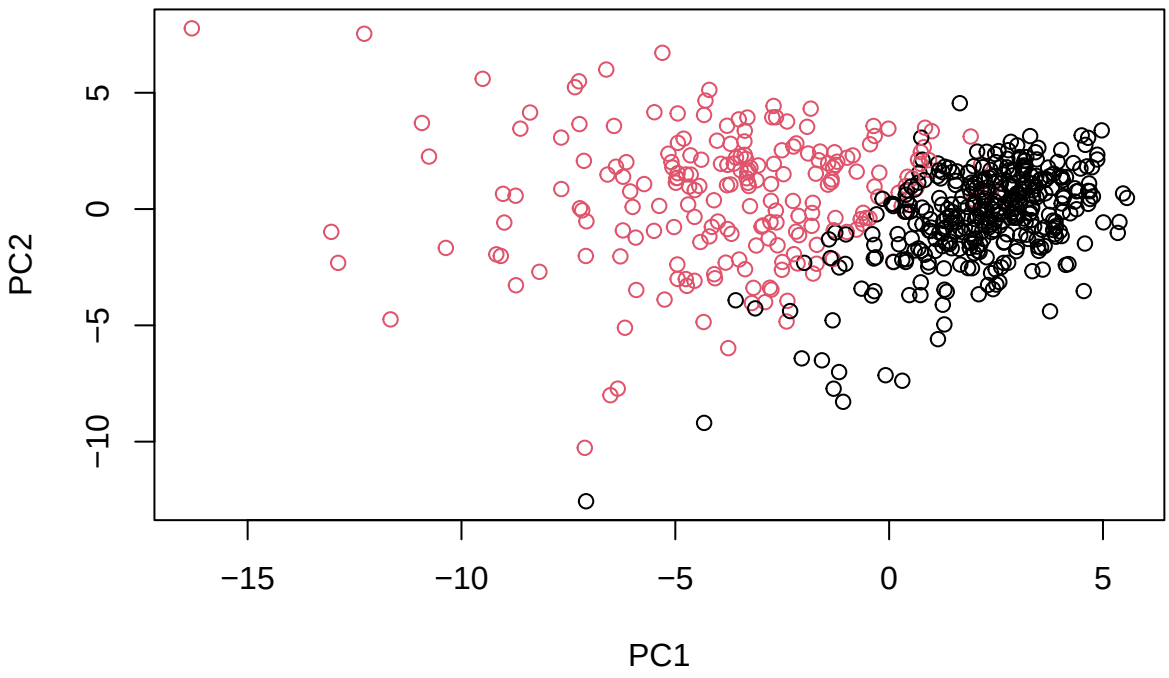
```
biplot(wisc.pr)
```



As this data contains a non-trivial number of observations and variables, this is a hot mess of a plot, which makes it is difficult to understand. We cannot clearly see the distribution pattern of observations and variables in this kind of plot. Thus, we will need to generate our own plots to make sense of this PCA result.

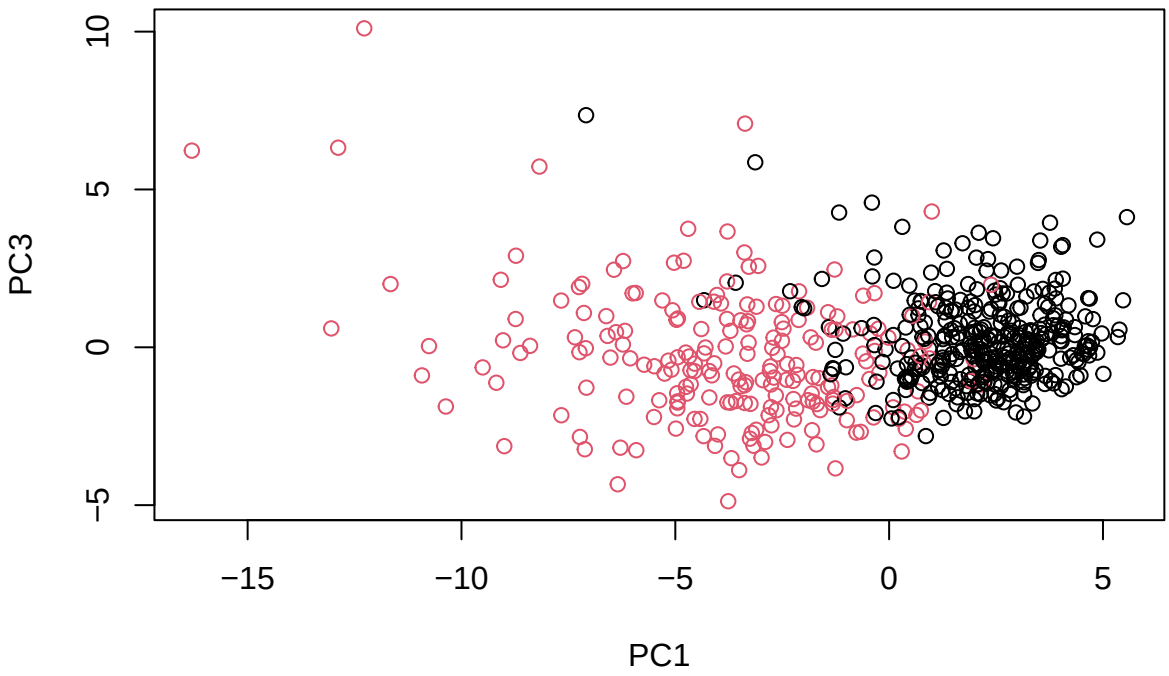
To make this plot ourselves we need access the PCA scores data.

```
# Scatter plot observations by components 1 and 2
plot(wisc.pr$x[,1:2], col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



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

```
# Repeat for components 1 and 3
plot(wisc.pr$x[,1], wisc.pr$x[,3], col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```

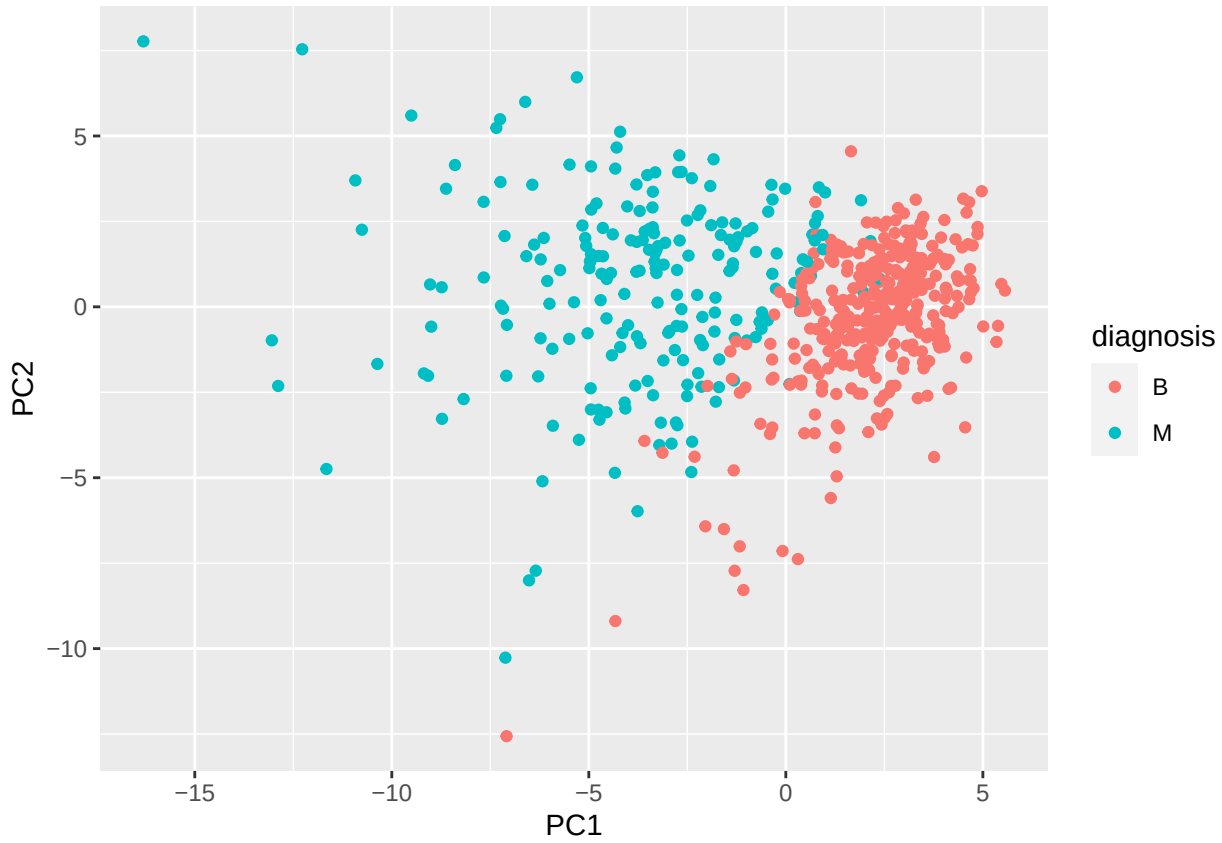


Because principal component 2 explains more variance in the original data than principal component 3, the first plot has a cleaner cut separating the two subgroups. For these plots, they indicate that principal component 1 is capturing a separation of malignant (red) from benign (black) samples. the principal component 2 explains less variance in the original data than principal component 1 but more variance than principal component 3. Thus, the first plot has a cleaner cut separating the two subgroups compared to the second plot (PC1 vs PC3).

```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

# Load the ggplot2 package
library(ggplot2)

# Make a scatter plot colored by diagnosis
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



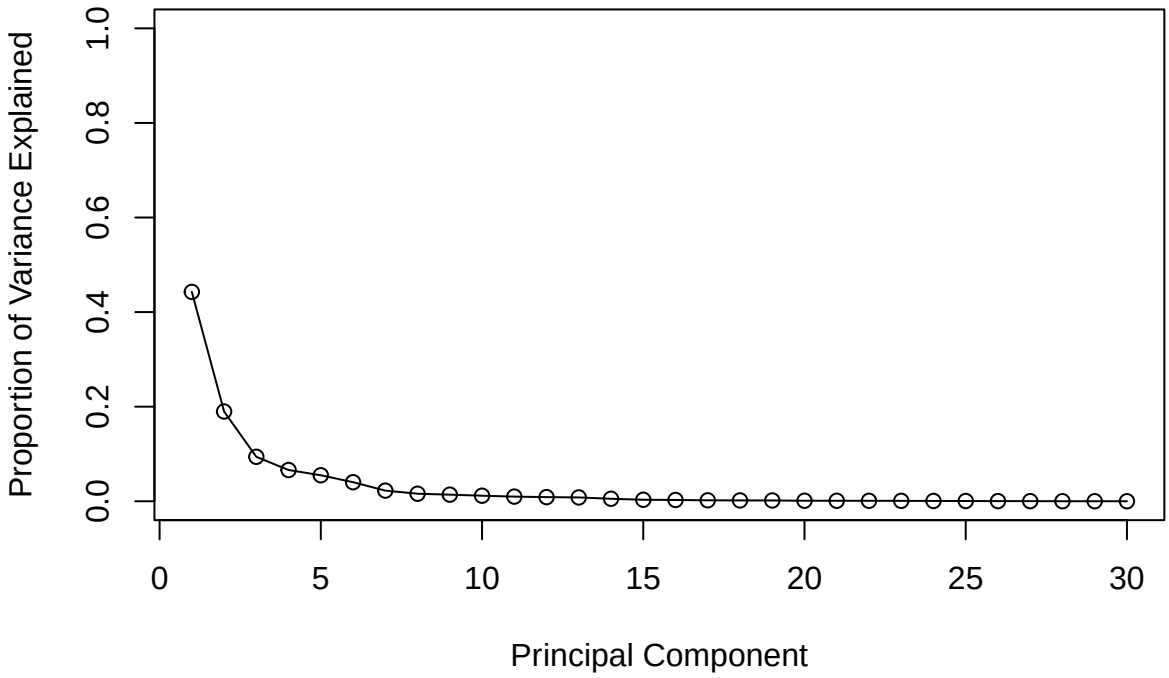
Variance explained

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

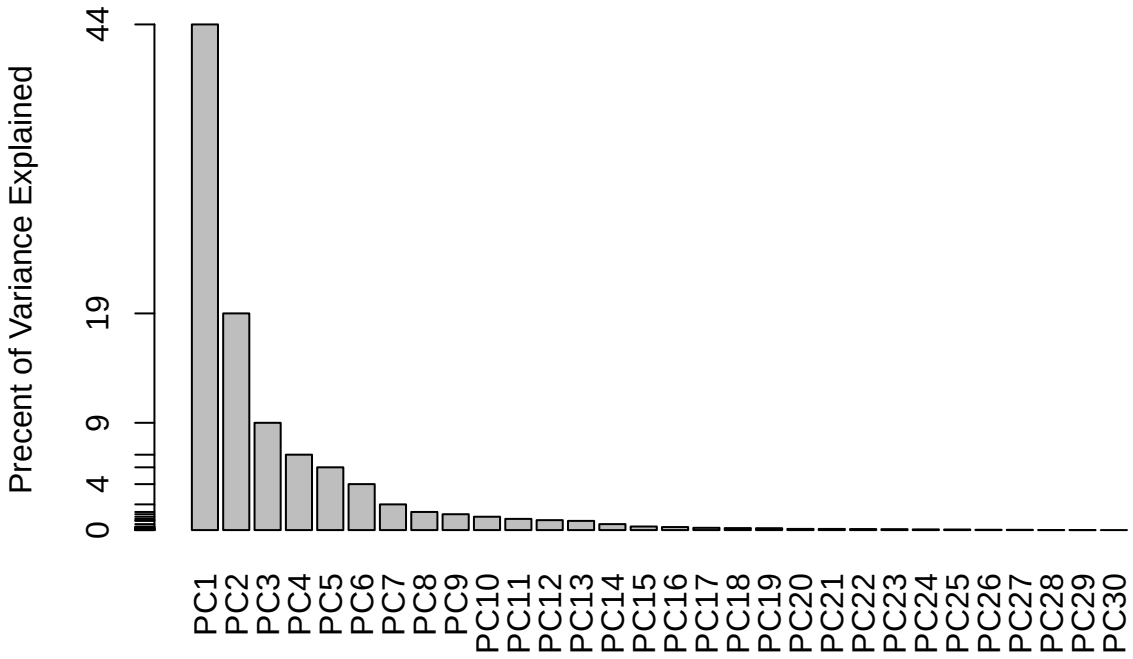
```
## [1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```



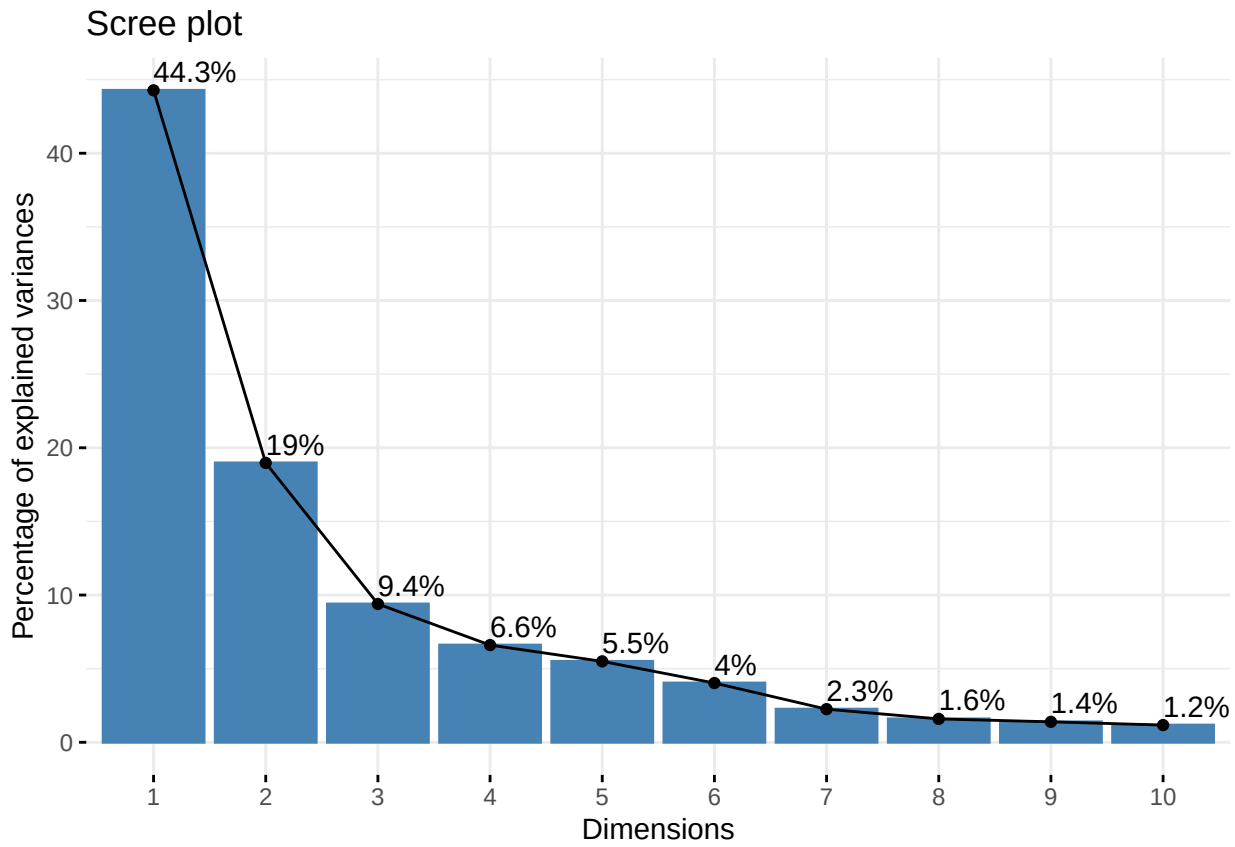

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)
```

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

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



Communicating PCA results ***Q9.*** For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean?

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

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

The component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean is -0.2608538.

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

```
var <- summary(wisc.pr)
var$importance[3,] < 0.8
```

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

```
sum(var$importance[3,] < 0.8)
```

```
## [1] 4
```

```
var
```

```
## 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
```

Based on the Cumulative Proportion, 5 principal components (PCs) are required to describe at least 80% of the original variance in the data (Cumulative Proportion of PC5: 0.84734).

#3. Hierarchical clustering

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

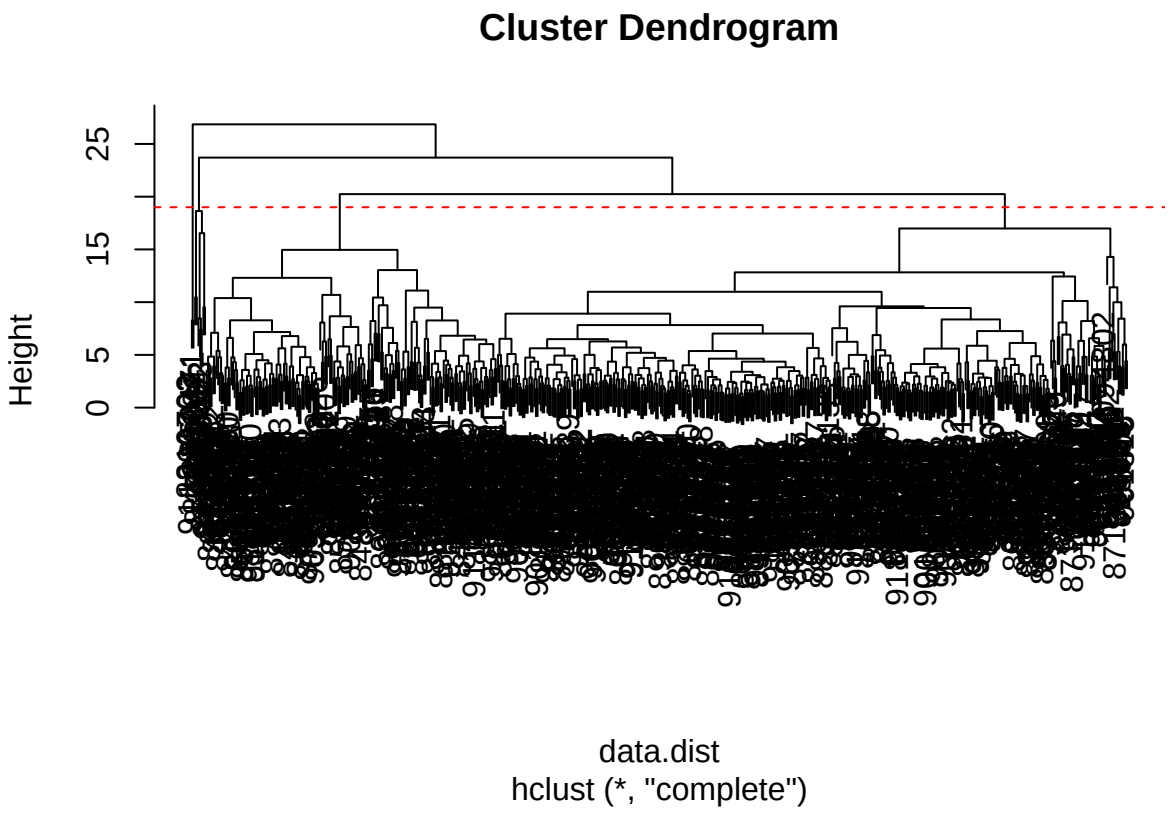
```
#Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset
data.dist <- dist(data.scaled)
```

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

```
##
## Call:
## hclust(d = data.dist, method = "complete")
##
## Cluster method   : complete
## Distance         : euclidean
## Number of objects: 569
```

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

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



The height at which the clustering model has 4 clusters can be 19.

Selecting number of clusters

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

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

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

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust.clusters2 <- cutree(wisc.hclust, k = 2)
wisc.hclust.clusters3 <- cutree(wisc.hclust, k = 3)
wisc.hclust.clusters4 <- cutree(wisc.hclust, k = 4)
wisc.hclust.clusters5 <- cutree(wisc.hclust, k = 5)
wisc.hclust.clusters6 <- cutree(wisc.hclust, k = 6)
wisc.hclust.clusters7 <- cutree(wisc.hclust, k = 7)
wisc.hclust.clusters8 <- cutree(wisc.hclust, k = 8)
wisc.hclust.clusters9 <- cutree(wisc.hclust, k = 9)
```

```
wisc.hclust.clusters10 <- cutree(wisc.hclust, k = 10)
table(wisc.hclust.clusters2, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters2   B   M
##                     1 357 210
##                     2   0   2
```

```
table(wisc.hclust.clusters3, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters3   B   M
##                     1 355 205
##                     2   2   5
##                     3   0   2
```

```
table(wisc.hclust.clusters4, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters4   B   M
##                     1  12 165
##                     2   2   5
##                     3 343  40
##                     4   0   2
```

```
table(wisc.hclust.clusters5, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters5   B   M
##                     1  12 165
##                     2   0   5
##                     3 343  40
##                     4   2   0
##                     5   0   2
```

```
table(wisc.hclust.clusters6, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters6   B   M
##                     1  12 165
##                     2   0   5
##                     3 331  39
##                     4   2   0
##                     5  12   1
##                     6   0   2
```

```
table(wisc.hclust.clusters7, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters7   B   M
##                     1  12 165
##                     2   0   3
##                     3 331  39
##                     4   2   0
##                     5  12   1
##                     6   0   2
##                     7   0   2
```

```
table(wisc.hclust.clusters8, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters8   B   M
##                     1  12  86
##                     2   0  79
##                     3   0   3
##                     4 331  39
##                     5   2   0
##                     6  12   1
##                     7   0   2
##                     8   0   2
```

```
table(wisc.hclust.clusters9, diagnosis)
```

```
##                       diagnosis
## wisc.hclust.clusters9   B   M
##                     1  12  86
##                     2   0  79
##                     3   0   3
##                     4 331  39
##                     5   2   0
##                     6  12   0
##                     7   0   2
##                     8   0   2
##                     9   0   1
```

```
table(wisc.hclust.clusters10, diagnosis)
```

```
##                        diagnosis
## wisc.hclust.clusters10   B   M
##                      1  12  86
##                      2   0  59
##                      3   0   3
##                      4 331  39
##                      5   0  20
##                      6   2   0
##                      7  12   0
##                      8   0   2
##                      9   0   2
##                      10  0   1
```

As I explore how different numbers of clusters affect the ability of the hierarchical clustering to separate the different diagnoses above, by cutting into a different number of clusters between 2 and 10, I found that as the number of clusters increases, the capacity to separate the different diagnoses is higher. So, I can find a better cluster vs diagnoses match by cutting into a higher number of clusters than 4 (5 clusters can be better for a higher specificity).

Using different methods ***Q13.*** Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

The method "ward.D2" gives my favorite results for the same data.dist dataset. As the method = "ward.D2" creates groups whose variance can be minimized within clusters. So, this has the effect of looking for spherical clusters with the process beginning with all points in individual clusters (bottom up) and then repeatedly merging a pair of clusters such that when merged there is a minimum increase in total within-cluster variance. This process continues until a single group including all points (the top of the tree) is defined, which really makes sense for me so it would be my favorite method.

#4. OPTIONAL: K-means clustering K-means clustering and comparing results

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

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

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

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

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

Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

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

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

Clusters 1, 2, and 4 from the hierarchical clustering model can be interpreted as the cluster 1 equivalent from the k-means algorithm, and cluster 3 can be interpreted as the cluster 2 equivalent.

Based on the table here, k-means separates the two diagnoses well (the first can be interpreted as the group largely corresponding to malignant cells and the second can be seen as the group largely corresponding to benign cells). Compared to my hclust results, k-means seems to separate the two diagnoses better as it has a higher sensitivity (same specificity) than hclust does.

#5. Combining methods

We take the results of our PCA analysis and cluster in this space 'wisc.pr$x'

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

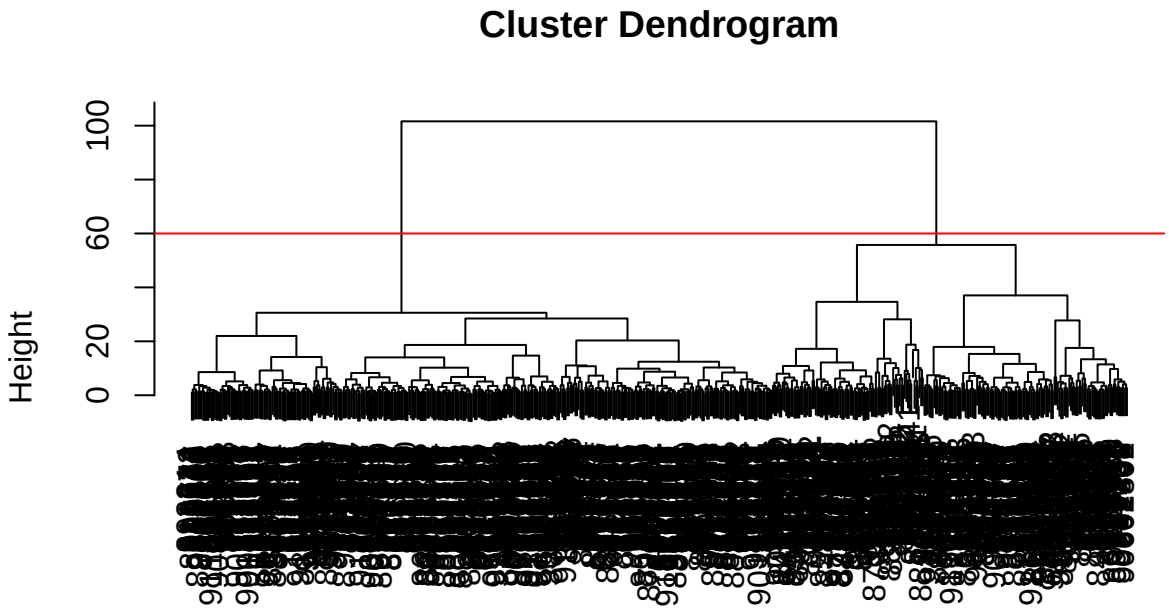
```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion  0.4427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

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

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

Plot my dendrogram

```
plot( wisc.pr.hclust )
abline (h = 60, col = "red")
```



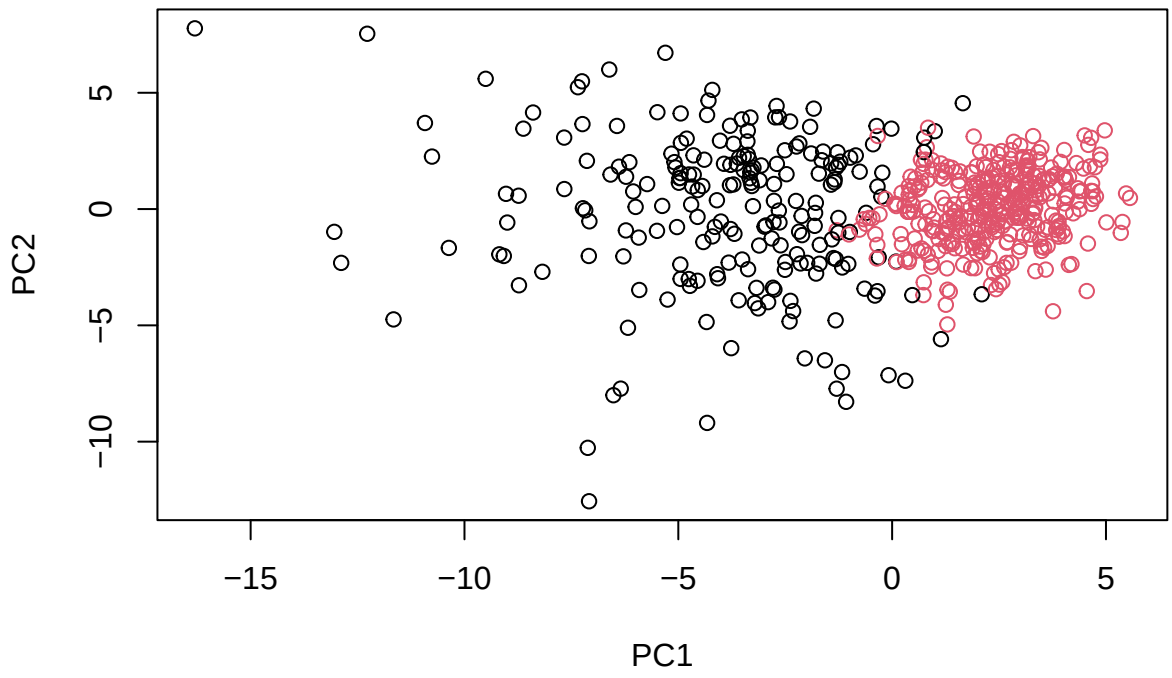

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

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

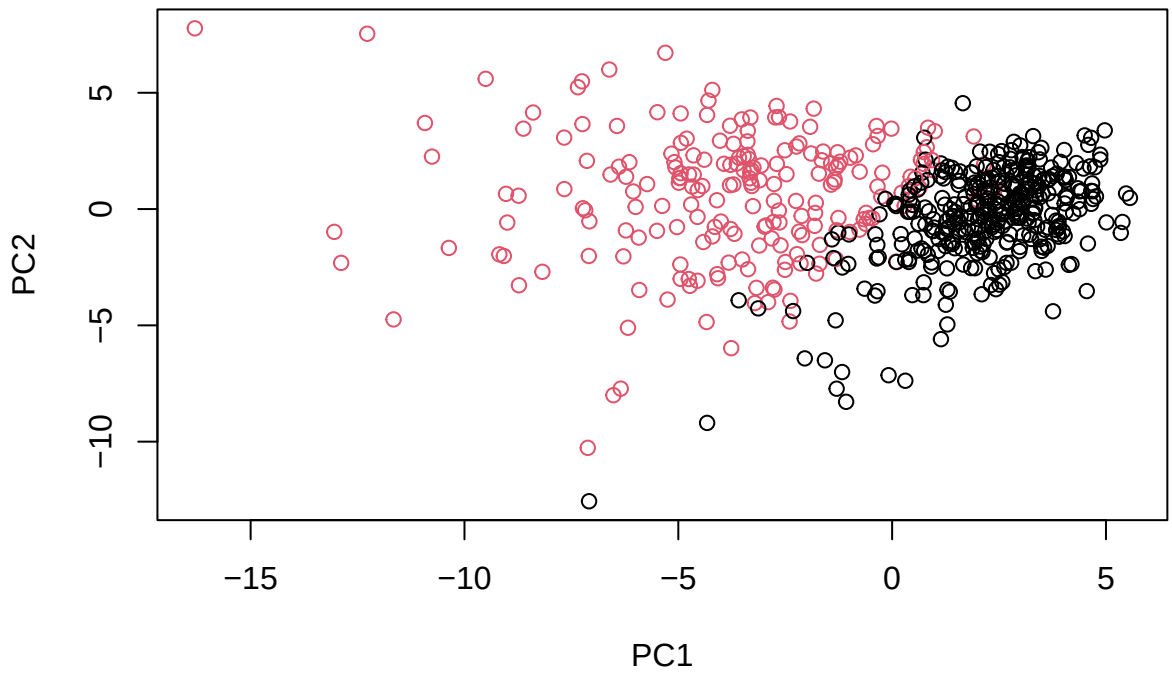
```
table(grps, diagnosis)
```

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

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




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



(practice) Cut the tree into k = 2 groups

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

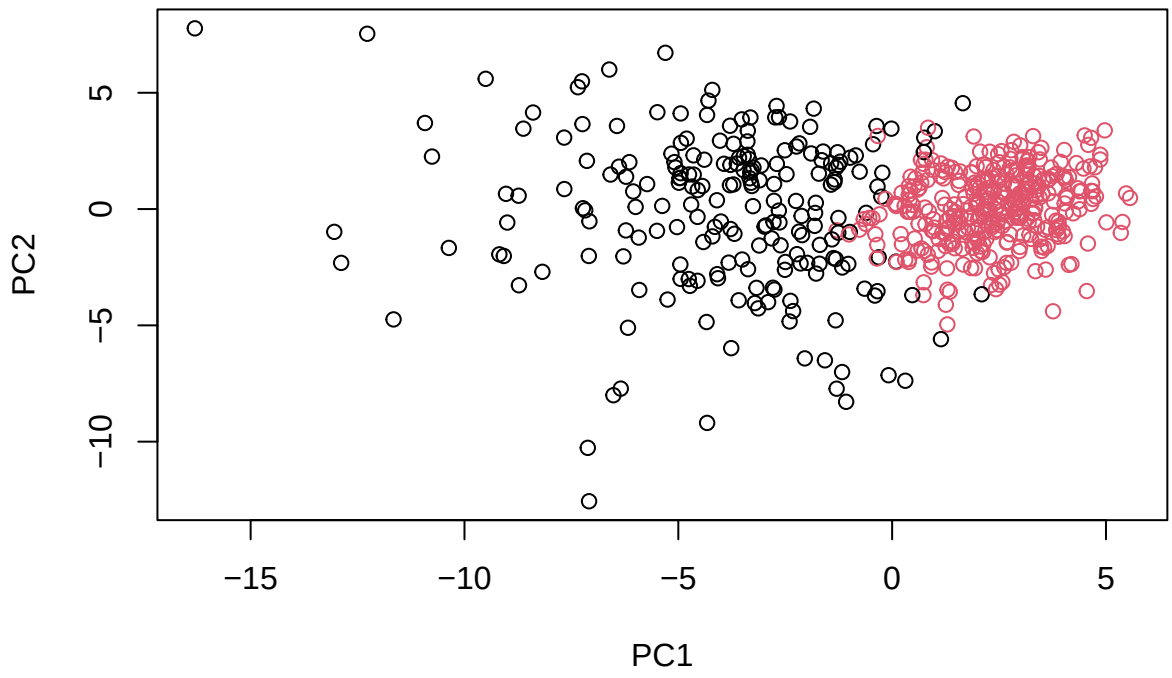
```
## grps
##   1   2
## 216 353
```

Cross table compare of diagnosis and my cluster groups

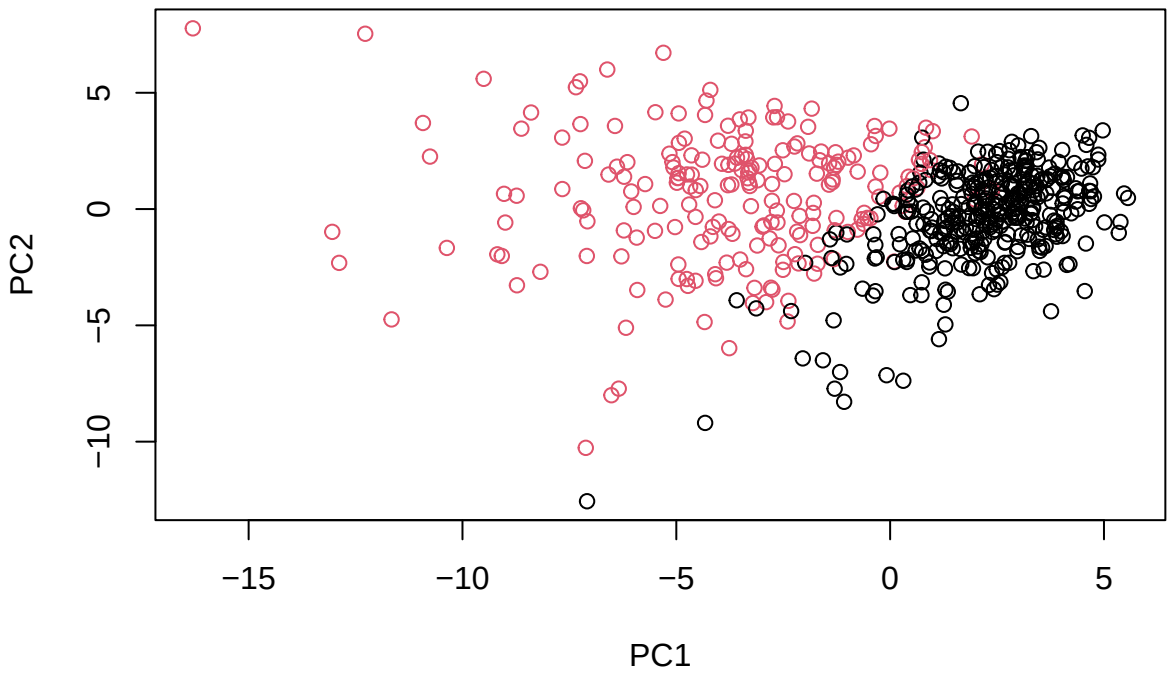
```
table(grps, diagnosis)
```

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

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




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



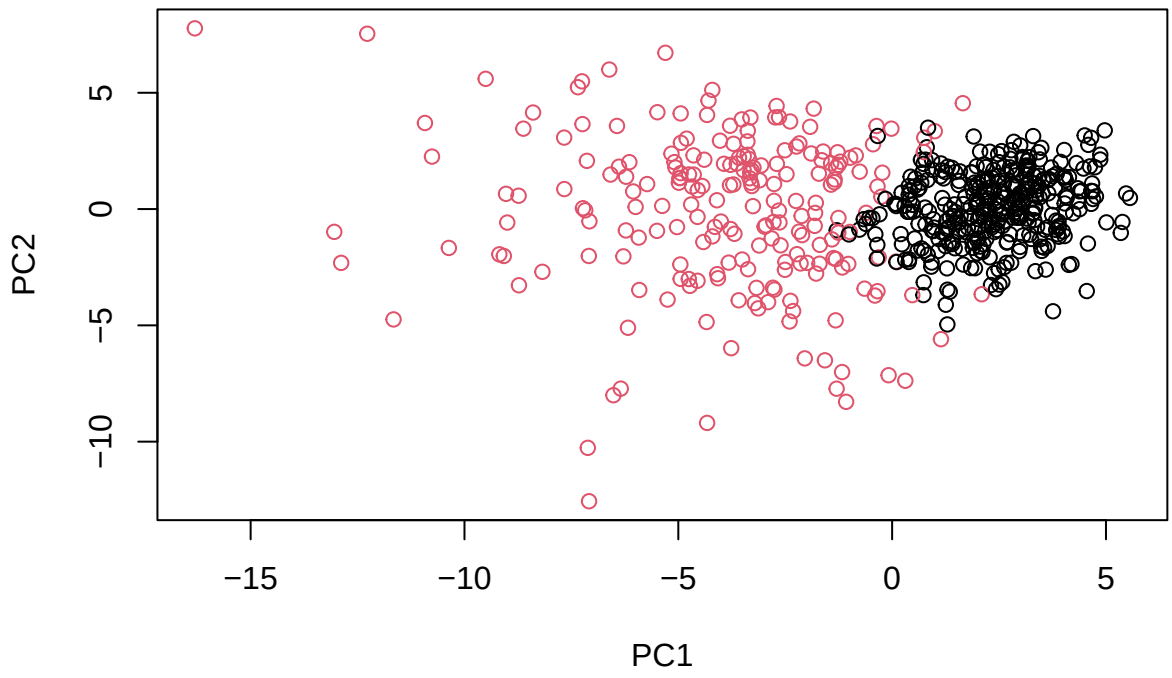

```
g <- as.factor(grps)
levels(g)
```

```
## [1] "1" "2"
```

```
g <- relevel(g,2)
levels(g)
```

```
## [1] "2" "1"
```

```
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)
```




```
library(rgl)
plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s", col=grps)
```

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

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

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

```
# Compare to 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.clusters,diagnosis)
```

```
##                        diagnosis
```

```
## wisc.pr.hclust.clusters   B   M
##                       1  28 188
##                       2 329  24
```

The newly created model with four clusters separates out the two diagnoses really well.

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.

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

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

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

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

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

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

Before PCA, the k-means and hierarchical clustering models separate the diagnoses well. In the k-means model, group 1 can be interpreted as the group largely corresponding to benign cells, and group 2 can be seen as the group largely corresponding to malignant cells. In the hierarchical clustering model, group 1 can be seen as the group largely corresponding to malignant cells, and group 3 can be interpreted as the group largely corresponding to benign cells. Compared to my hclust results, k-means seems to separate the two diagnoses better as it has a higher sensitivity (same specificity) than hclust does.

#6. Sensitivity/Specificity **Accuracy** What proportion did we get correct if we call cluster 1 M and cluster 2 B

```
(329 + 188)/nrow(wisc.data)
```

```
## [1] 0.9086116
```

Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

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

```
## [1] 0.8867925
```

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

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

```
## [1] 0.9215686
```

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

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

```
##     diagnosis
## grps   B   M
##    1  28 188
##    2 329  24
```

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

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

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

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

```
#specificity
PCA_hierarchical_clustering_spe <- 329/(329+28)
kmeans_clustering_spe <- 343/(343+14)
hierarchical_clustering_spe <- 343/(343+12+2)
PCA_hierarchical_clustering_spe
```

```
## [1] 0.9215686
```

```
kmeans_clustering_spe
```

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

```
hierarchical_clustering_spe
```

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

```
#sensitivity
PCA_hierarchical_clustering_sen <- 188/(188+24)
kmeans_clustering_sen <- 175/(175+37)
hierarchical_clustering_sen <- 172/(165+5+2+40)
PCA_hierarchical_clustering_sen
```

```
## [1] 0.8867925
```

```
kmeans_clustering_sen
```

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

```
hierarchical_clustering_sen
```

```
## [1] 0.8113208
```

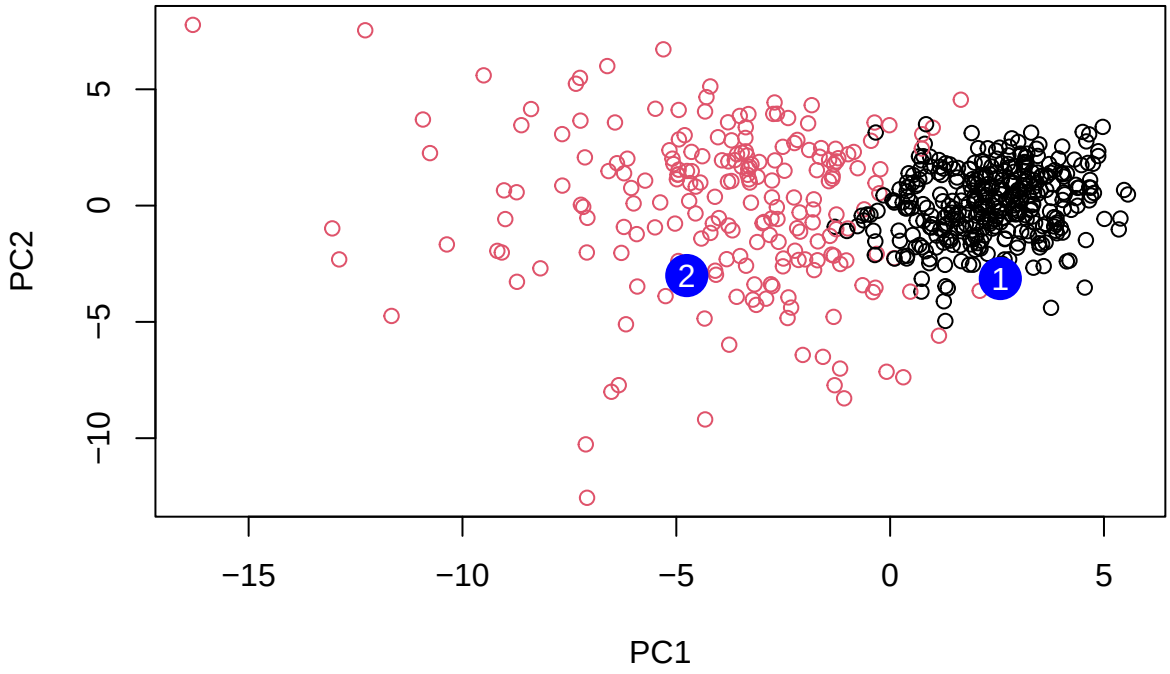
The k-means and hierarchical clustering resulted in a clustering model with the best specificity, and the PCA hierarchical clustering resulted in a clustering model with the best sensitivity.

#7. Prediction

```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
##            PC1       PC2        PC3        PC4       PC5        PC6        PC7
## [1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
## [2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
##             PC8       PC9       PC10      PC11      PC12      PC13     PC14
## [1,] -0.2307350 0.1029569 -0.9272861 0.3411457  0.375921 0.1610764 1.187882
## [2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
##           PC15       PC16        PC17        PC18        PC19       PC20
## [1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
## [2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
##            PC21       PC22       PC23       PC24        PC25         PC26
## [1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121  0.078884581
## [2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
##              PC27        PC28         PC29         PC30
## [1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
## [2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

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



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

New patients in 2 (Patients 2). Based on my results, since patients in 2 are in the cluster identified as predominantly malignant (cancerous), we should prioritize these new patients for follow up.

#About this document

```
sessionInfo()
```

```
## R version 4.1.1 (2021-08-10)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Big Sur 11.6
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.1-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1-arm64/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
```

```
##
## other attached packages:
## [1] rgl_0.107.14     factoextra_1.0.7 ggplot2_3.3.5
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_1.1.1  xfun_0.26         purrr_0.3.4       haven_2.4.3
##  [5] carData_3.0-4     colorspace_2.0-2  vctrs_0.3.8       generics_0.1.1
##  [9] htmltools_0.5.2   yaml_2.2.1        utf8_1.2.2        rlang_0.4.11
## [13] pillar_1.6.3      ggpubr_0.4.0      foreign_0.8-81    glue_1.4.2
## [17] withr_2.4.2       DBI_1.1.1         readxl_1.3.1      lifecycle_1.0.1
## [21] stringr_1.4.0     cellranger_1.1.0  munsell_0.5.0     ggsignif_0.6.3
## [25] gtable_0.3.0      zip_2.2.0         htmlwidgets_1.5.4 evaluate_0.14
## [29] forcats_0.5.1     labeling_0.4.2    knitr_1.36        rio_0.5.27
## [33] fastmap_1.1.0     curl_4.3.2        fansi_0.5.0       highr_0.9
## [37] broom_0.7.9       Rcpp_1.0.7        scales_1.1.1      backports_1.2.1
## [41] jsonlite_1.7.2    abind_1.4-5       farver_2.1.0      hms_1.1.1
## [45] digest_0.6.28     openxlsx_4.2.4    stringi_1.7.5     rstatix_0.7.0
## [49] dplyr_1.0.7       ggrepel_0.9.1     grid_4.1.1        tools_4.1.1
## [53] magrittr_2.0.1    tibble_3.1.5      crayon_1.4.1      tidyr_1.1.4
## [57] car_3.0-11        pkgconfig_2.0.3   ellipsis_0.3.2    data.table_1.14.2
## [61] assertthat_0.2.1  rmarkdown_2.11    R6_2.5.1          compiler_4.1.1
```