MiniProject

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Import cancer data

```r
fna.data <- "WisconsinCancer.csv"

#Store as a dataframe and convert sample names to row names
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)
```

```
         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
843786           M       12.45        15.70          82.57     477.1
         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
84358402         0.10030          0.13280         0.1980             0.10430
843786           0.12780          0.17000         0.1578             0.08089
         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
843786          0.2087                0.07613    0.3345     0.8902        2.217
         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
843786     27.19      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
```

```r
dim(wisc.df)
```

```
[1] 569  31
```

Omit the diagnosis column from the data frame

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

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

```
[1] "M" "M" "M" "M" "M" "M"
```

Exploratory data analysis

Q1. How many observations are in this dataset?

```r
# Number of rows and columns in wisc.data
dim(wisc.data)
```

```
[1] 569  30
```

```r
# Number of observations in diagnosis
length(diagnosis)
```

```
[1] 569
```

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

```r
# Returns table of malignant and benign samples
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

```r
grep("_mean", names(wisc.data))
```

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

```r
grep("_mean", diagnosis)
```

```
integer(0)
```

PCA

Check column means and SD; need to scale

```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
```

PCA on wisc.data

```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
```

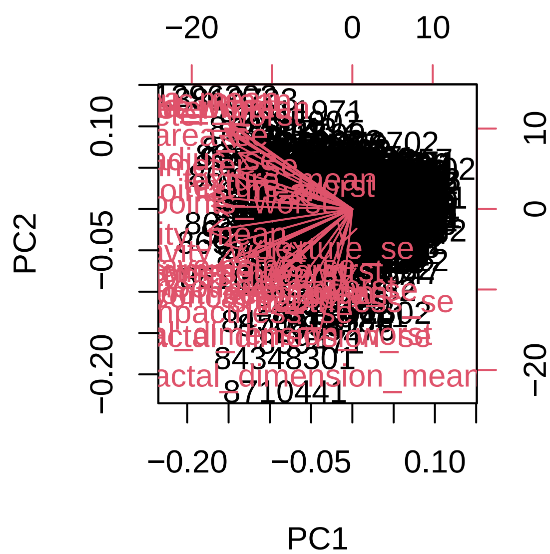
Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)? 44% of the variance is accounted for by PC1. From summary(wisc.pr).

Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? At a minimum, the first 3 PCs are required to desribe 70% of the variance. From summary(wisc.pr).

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. From summary(wisc.pr).

Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? Not easy to understand as there are many data points crowding the plot. There is no discernable pattern to make senseof the PCs.

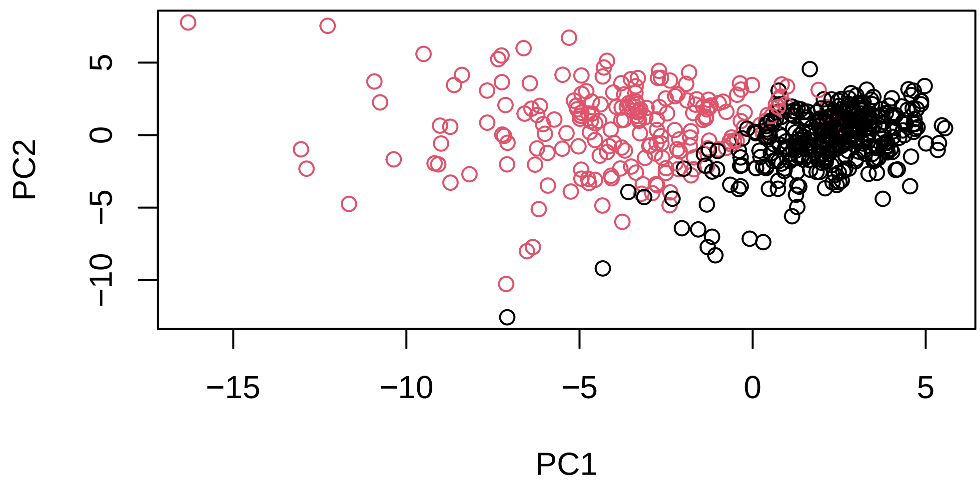
```
biplot(wisc.pr)
```



Scatter plot of PC1 and PC2

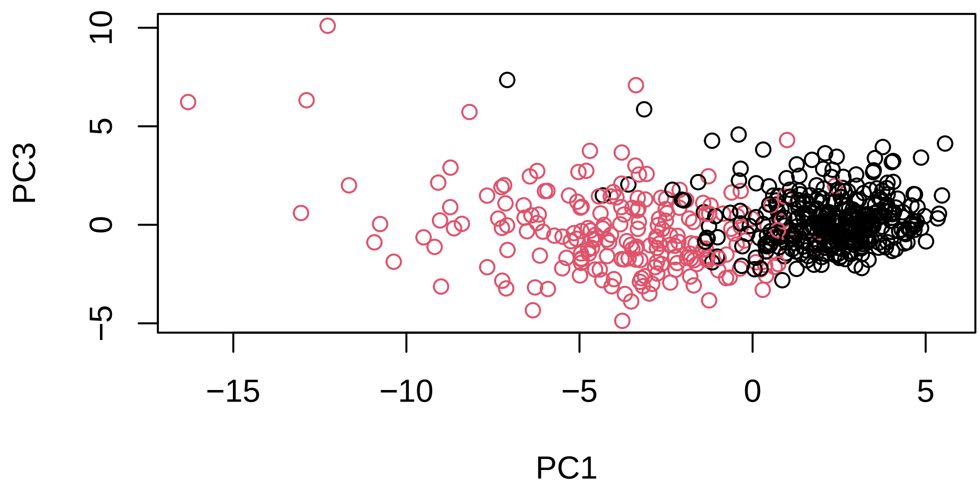
```
# Force R to recognize diagnosis as factor to plot
diagnosis = as.factor(diagnosis)
plot(wisc.pr$x[,1], wisc.pr$x[,2],
```

```
     xlab = "PC1", ylab = "PC2", col = diagnosis)
```



Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots? Plots are very similar with the exception that PC3 shifts the points downwards and PC1 consistently accounts for the differene between malignant and benign samples.

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

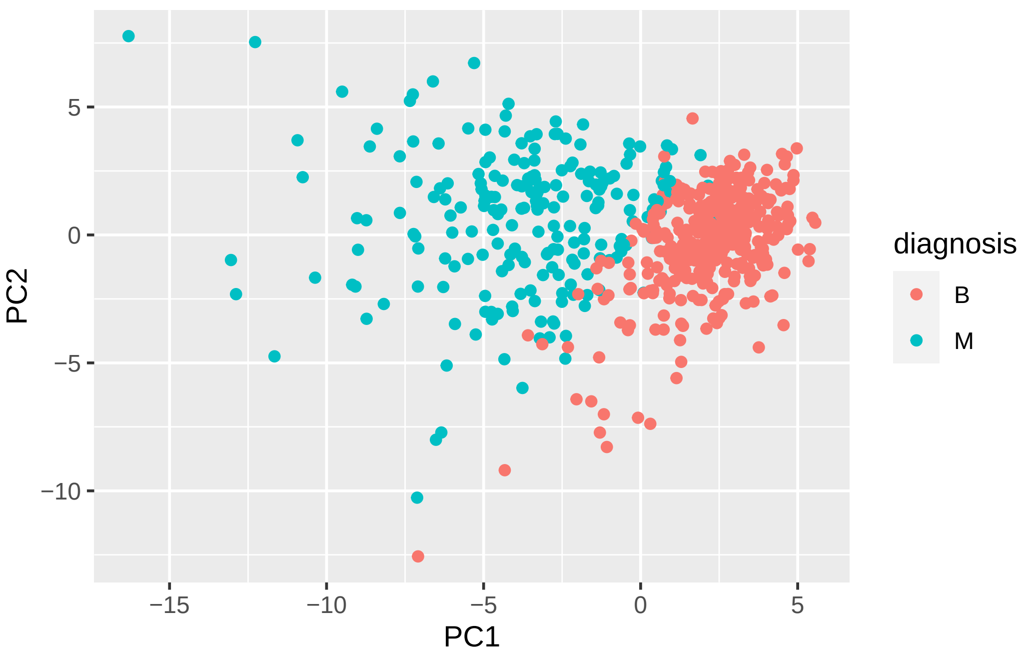


ggplot of PCA

```
#Create dataframe and add diagnosis column
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

#Load ggplot2
library(ggplot2)
```

```
Warning: package 'ggplot2' was built under R version 4.1.3
```

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



Variance of each component

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

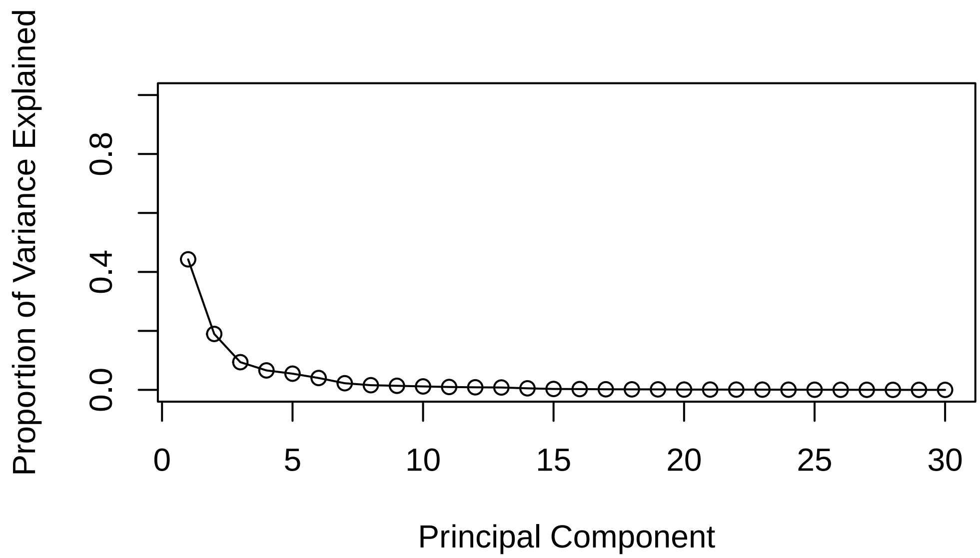
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

Variance explained by each PC

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

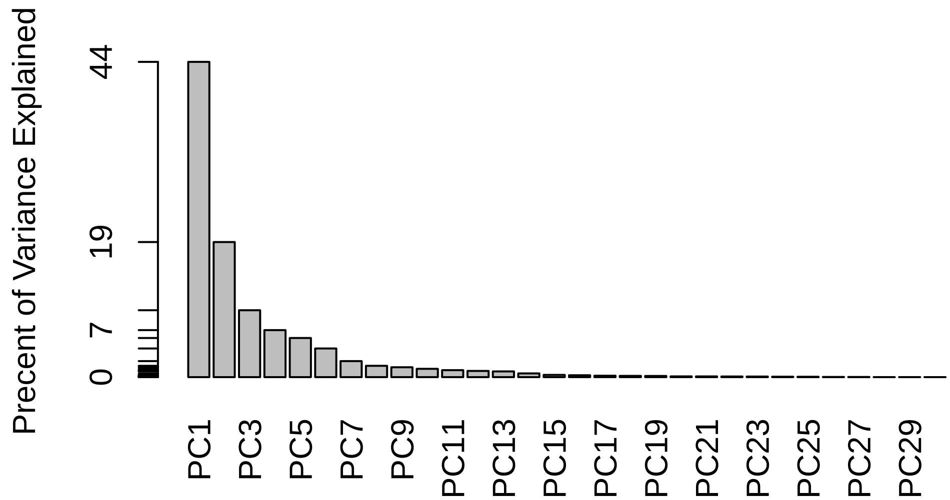
```
 [1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
 [6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

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



Alternative scree plot

```r
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 )
```



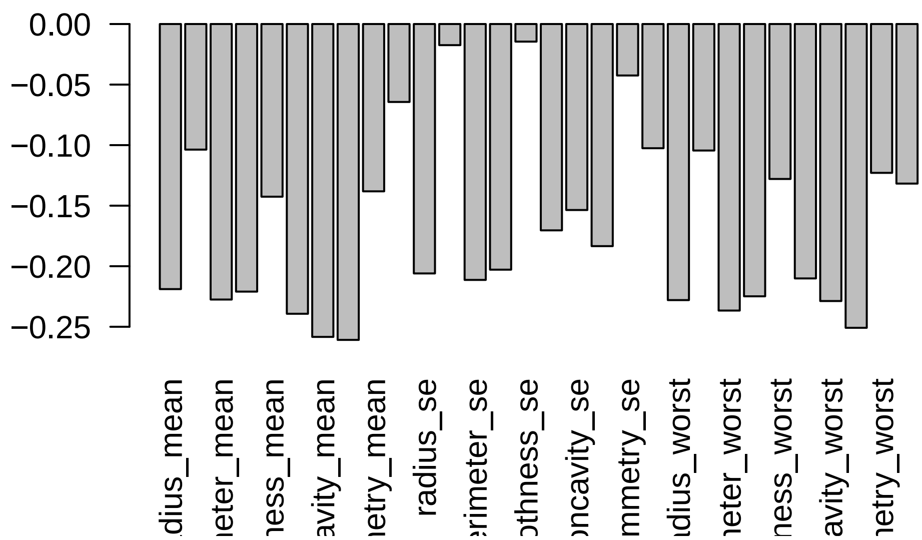
Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean? The loading score for concave.points_mean from PC1 is -0.26.

```
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
```

```r
barplot(wisc.pr$rotation[,1], las=2)
```



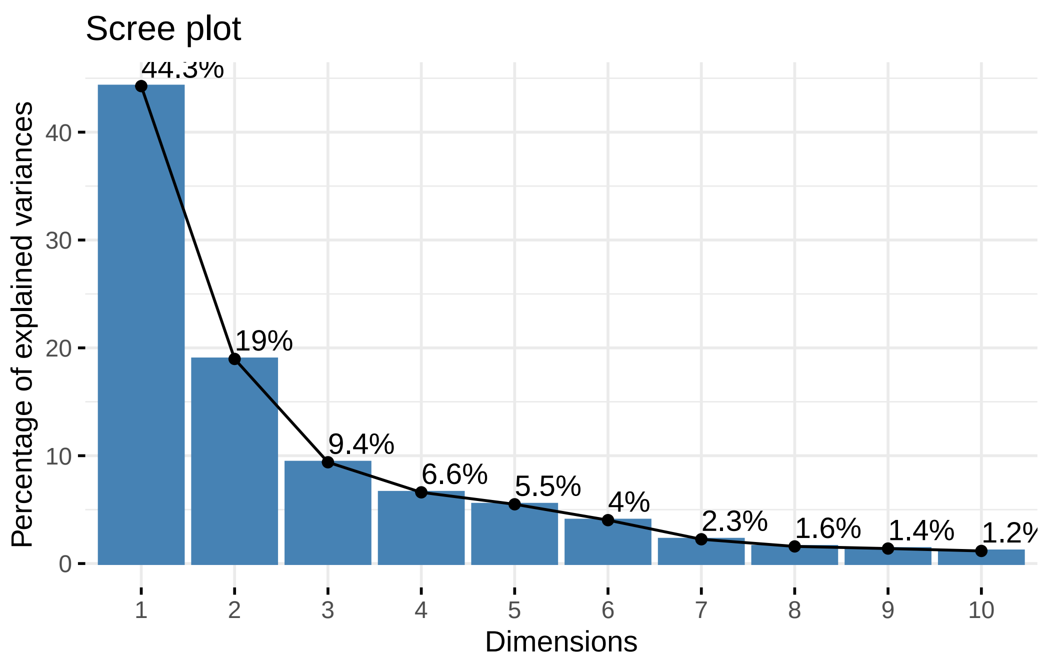
Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? 5 PCs are the minimum number of principal components needed to explain 80% of the variance.

```r
library(factoextra)
```

```
Warning: package 'factoextra' was built under R version 4.1.3
```

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

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




```
var <- round((wisc.pr$sdev^2)/sum(wisc.pr$sdev^2) * 100)
var
```

```
 [1] 44 19  9  7  5  4  2  2  1  1  1  1  1  1  0  0  0  0  0  0  0  0  0  0  0
[26]  0  0  0  0  0
```

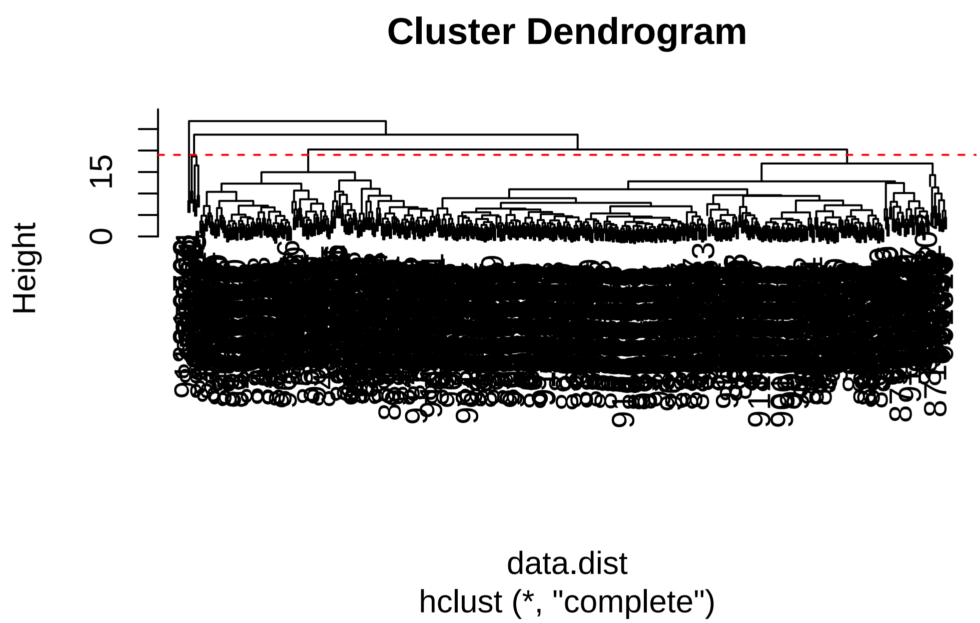
Hierarchical clustering

Scale the wisc.data

```
data.scaled <- scale(wisc.data)

#Eucladian distance
data.dist <- dist(data.scaled)

#Hierachical clustering assignment
wisc.hclust <- hclust(data.dist, method = "complete")
```

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)
```



Number of clusters

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

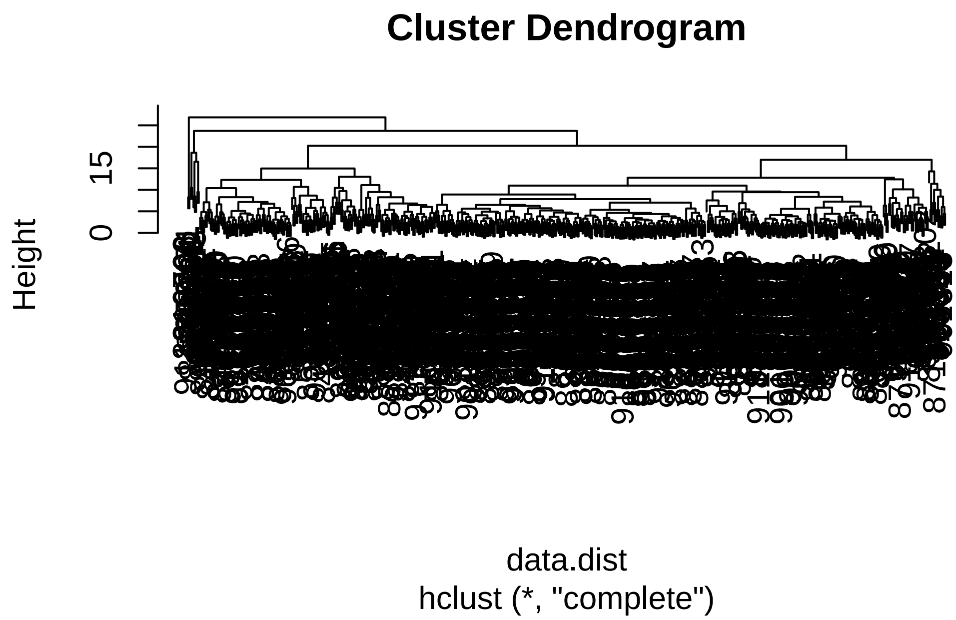
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? Cluster 4 is the best cluster as additional clusters do not add greater separation.

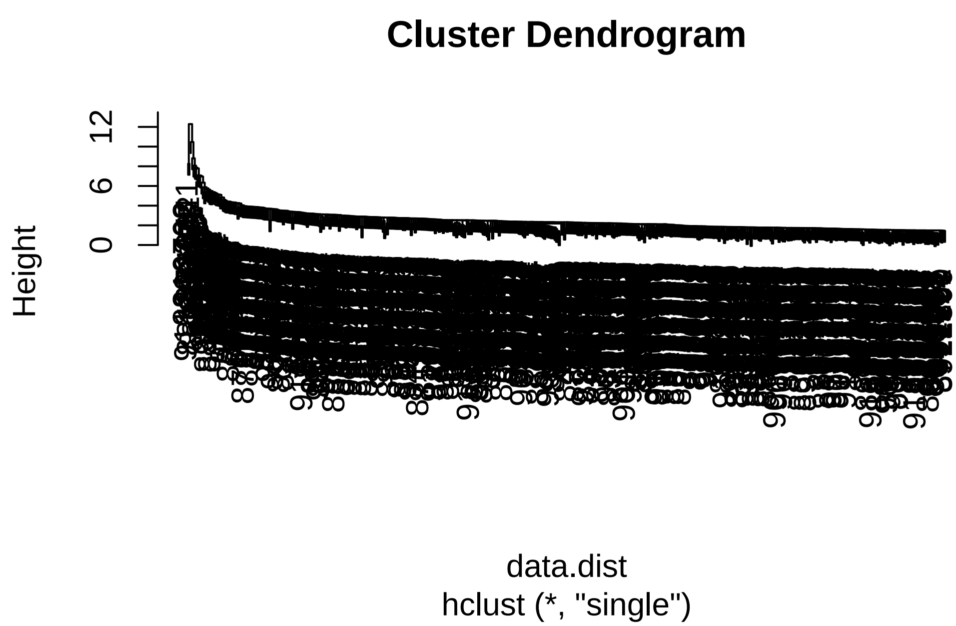
```
# k = 2
#wisc.hclust.clusters <- cutree(wisc.hclust, k=2)
#table(wisc.hclust.clusters, diagnosis)

# k =3
#wisc.hclust.clusters <- cutree(wisc.hclust, k=3)
#table(wisc.hclust.clusters, diagnosis)

# k = 5
#wisc.hclust.clusters <- cutree(wisc.hclust, k=5)
#table(wisc.hclust.clusters, diagnosis)

# k = 6
#wisc.hclust.clusters <- cutree(wisc.hclust, k=6)
#table(wisc.hclust.clusters, diagnosis)

# k = 7
#wisc.hclust.clusters <- cutree(wisc.hclust, k=7)
#table(wisc.hclust.clusters, diagnosis)

# k = 8
#wisc.hclust.clusters <- cutree(wisc.hclust, k=8)
#table(wisc.hclust.clusters, diagnosis)

# k = 9
#wisc.hclust.clusters <- cutree(wisc.hclust, k=9)
#table(wisc.hclust.clusters, diagnosis)

# k = 10
#wisc.hclust.clusters <- cutree(wisc.hclust, k=10)
#table(wisc.hclust.clusters, diagnosis)
```

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning. Ward.D2 is my favorite as it is the most aesthetically pleasing and easiest to interpret.

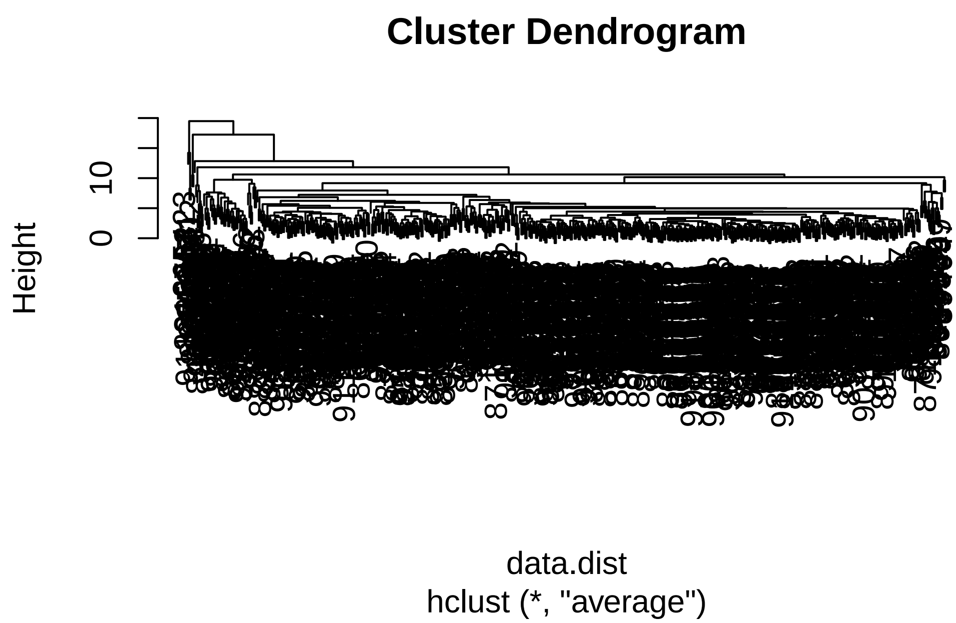
```
wisc.hclust_complete <- hclust(data.dist, method = "complete")
plot(wisc.hclust_complete)
```



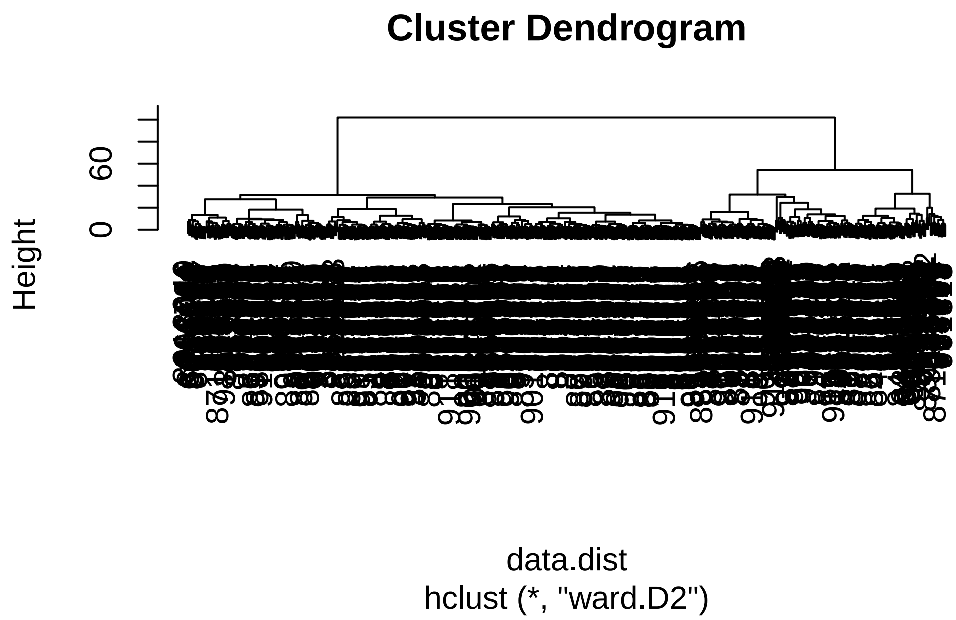

```r
wisc.hclust_single <- hclust(data.dist, method = "single")
plot(wisc.hclust_single)
```



```
wisc.hclust_average <- hclust(data.dist, method = "average")
plot(wisc.hclust_average)
```




```
wisc.hclust_ward.D2 <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust_ward.D2)
```



K means clustering

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

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

Q14. Optional

Combining results

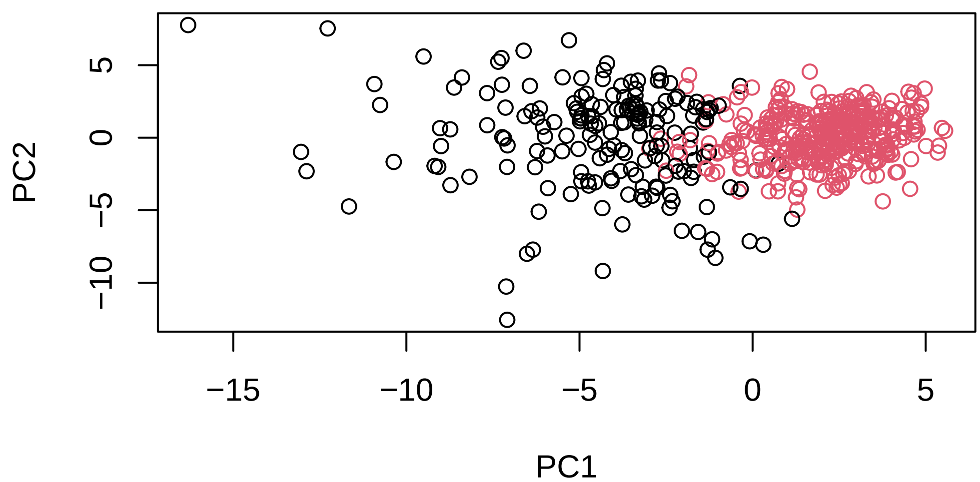
```
wisc.pr.hclust <- hclust(data.dist, method = "ward.D2")

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

```
grps
  1   2 
184 385 
```

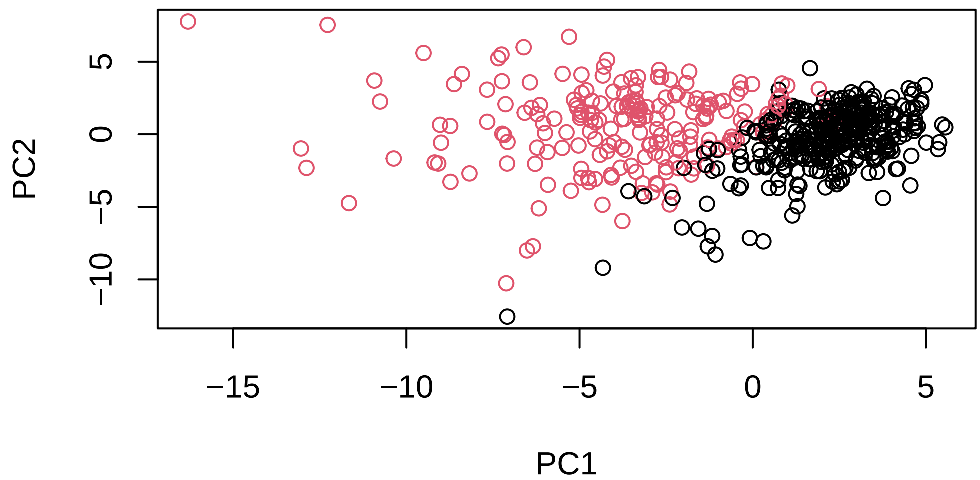
```
table(grps, diagnosis)
```

```
    diagnosis
grps   B   M
   1  20 164
   2 337  48
```

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




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



First 7 PCs

```
# 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")

# 2 clusters
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? This model separates the four clusters well and minimizes the clusters into 2.

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

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

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. The k means model approximates this new model much more closely while maintaining clear clustering. The hierarchical clustering model isn't the best approximation of this new model as it contains 2 additional clusters.

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

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

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

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

Sensitivity/Specificity

Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity? The k means method provides the highest sensitivity, while the hierarchical clustering method has the highest specificity.

```
#Combined method sensitivity
188/(188+24)
```

```
[1] 0.8867925
```

```
#Combined method specificity
329/(329+28)
```

```
[1] 0.9215686
```

```
#K means method sensitivity
175/(175+14)
```

```
[1] 0.9259259
```

```
#K means method specificity
343/(343+37)
```

```
[1] 0.9026316
```

```
#hc method sensitivity
165/(165+5+40+2)
```

```
[1] 0.7783019
```

```
#hc method specificity
343/(12+2+343)
```

```
[1] 0.9607843
```

Prediction

Load in new sample data

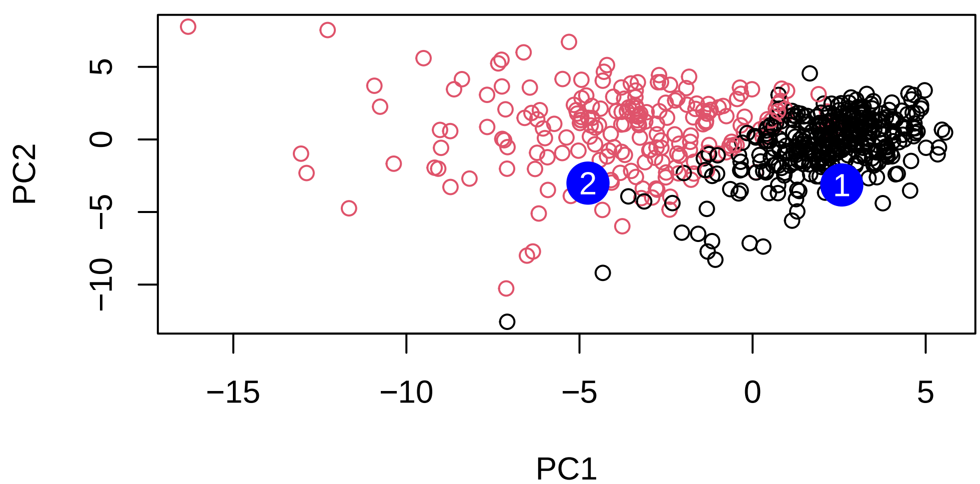
```
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
npc <- predict(wisc.pr, newdata=new)
npc
```

```
           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 predicted data

```r
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 is localized to PC2 which comprises the majority of the malignant samples.