Class 8 Mini Project: Unsupervised Learning Analysis of Human Breast Cancer Cells

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Data import

We first have to download and import our data correctly into our R session. We can use the `read.csv()` function to read the CSV (comma-separated values) file containing the data (avaliable from our class website).

```
# Save your input data file into your Project directory
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names = 1)
```

Examine your input data to ensure column names are set correctly.

```
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
```

We need to take out the first column `wisc.df$diagnosis` because it has the "answer". We

don't want to include this in our analysis. We need to create a new data.frame that omits this first column.

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

Setup a new separate vector called `diagnosis` that contains the data from the diagnosis column of the original dataset. We will store this as a *factor* (useful for plotting) and use this later to check our results.

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

Exploratory data analysis

Q1. How many observations are in this dataset?

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

```
[1] 569
```

There are 569 observations in this dataset.

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

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

```
  B   M
357 212
```

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

First find the column names.

```
colnames(wisc.data)
```

```
 [1] "radius_mean"             "texture_mean"
 [3] "perimeter_mean"          "area_mean"
 [5] "smoothness_mean"         "compactness_mean"
 [7] "concavity_mean"          "concave.points_mean"
 [9] "symmetry_mean"           "fractal_dimension_mean"
[11] "radius_se"               "texture_se"
[13] "perimeter_se"            "area_se"
[15] "smoothness_se"           "compactness_se"
[17] "concavity_se"            "concave.points_se"
[19] "symmetry_se"             "fractal_dimension_se"
[21] "radius_worst"            "texture_worst"
[23] "perimeter_worst"         "area_worst"
[25] "smoothness_worst"        "compactness_worst"
[27] "concavity_worst"         "concave.points_worst"
[29] "symmetry_worst"          "fractal_dimension_worst"
```

Next I need to search within the column names for "_mean" pattern. The `grep()` function might help us.

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

```
[1] 10
```

Q. How many dimensions are in this dataset?

```
ncol(wisc.data)
```

```
[1] 30
```

Principal Component Analysis

Performing PCA

It's important to check if the data needs to be scaled before performing PCA, because the input variables might use different units of measurement or have significantly different variances.

```
# Check column means and standard devations
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

```
round(apply(wisc.data, 2, sd), 3)
```

radius_mean	texture_mean	perimeter_mean
3.524	4.301	24.299
area_mean	smoothness_mean	compactness_mean
351.914	0.014	0.053
concavity_mean	concave.points_mean	symmetry_mean
0.080	0.039	0.027
fractal_dimension_mean	radius_se	texture_se
0.007	0.277	0.552
perimeter_se	area_se	smoothness_se
2.022	45.491	0.003
compactness_se	concavity_se	concave.points_se
0.018	0.030	0.006
symmetry_se	fractal_dimension_se	radius_worst
0.008	0.003	4.833
texture_worst	perimeter_worst	area_worst
6.146	33.603	569.357
smoothness_worst	compactness_worst	concavity_worst
0.023	0.157	0.209

```
   concave.points_worst          symmetry_worst fractal_dimension_worst
                  0.066                   0.062                   0.018
```

Execute PCA with the `prcomp()` function on the `wisc.data`, scaling if appropriate, and assign the output model to `wisc.pr`. It also looks like we need to scale the 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 captures by the first principal components (PC1)?

44.27%

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

3 PCs capture about 72%.

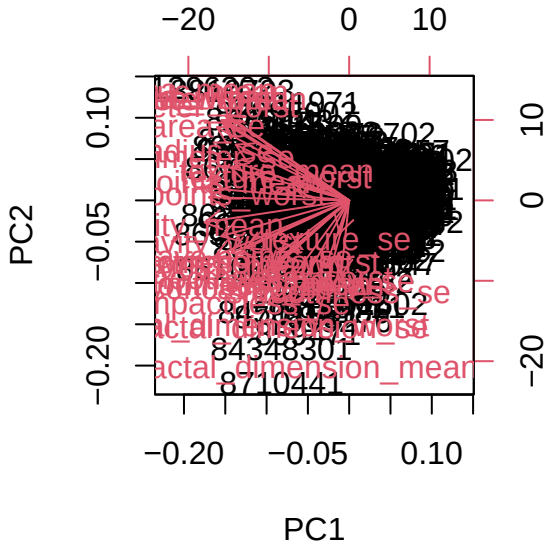
Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs capture about 91%.

##Interpreting PCA results

Create a biplot of the `wisc.pr` using the `biplot()` function.

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

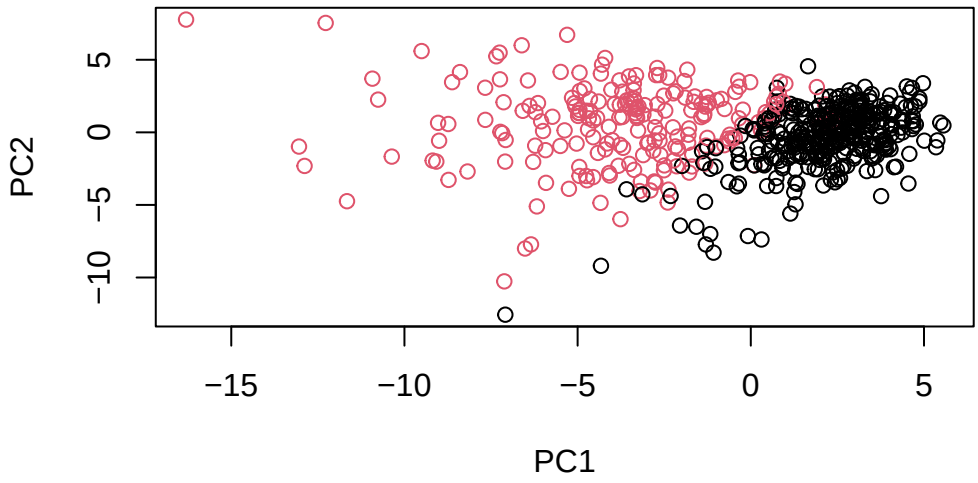


Q7. What stands out to you about this plot? Is it easy or difficult to understand?

All the points seem to originate from one common place. It's difficult to understand, because it's hard to make out the values. Everything is clustered together.

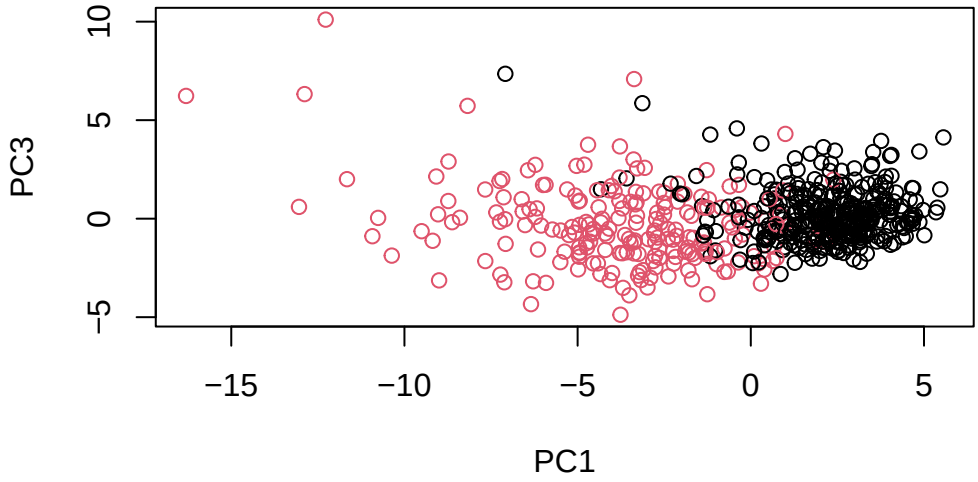
Let's generate a more standard scatter plot of each observation along the principal components.

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



Q3. 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")
```



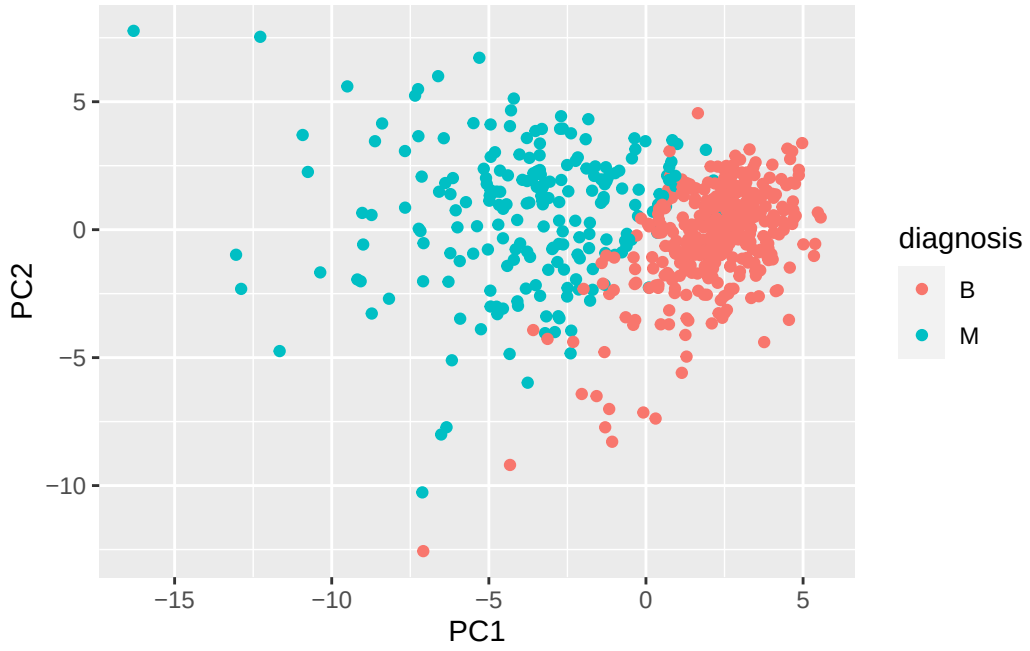
There are less overlapping values in the PC1/PC2 plot, compared to the PC1/PC3 plot.

Let's see if we can use the **ggplot2** package to make a more fancy figure of these results. Remember that ggplot requires a data.frame as input and we will also need to add our `diagnosis` vector as a column if we want to use it for mapping to the plot color aesthetic.

```
# 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 the variance of each principal component by squaring the sdev component of `wisc.pr` (i.e. `wisc.pr$sdev^2`). Save the result as an object called `pr.var`.

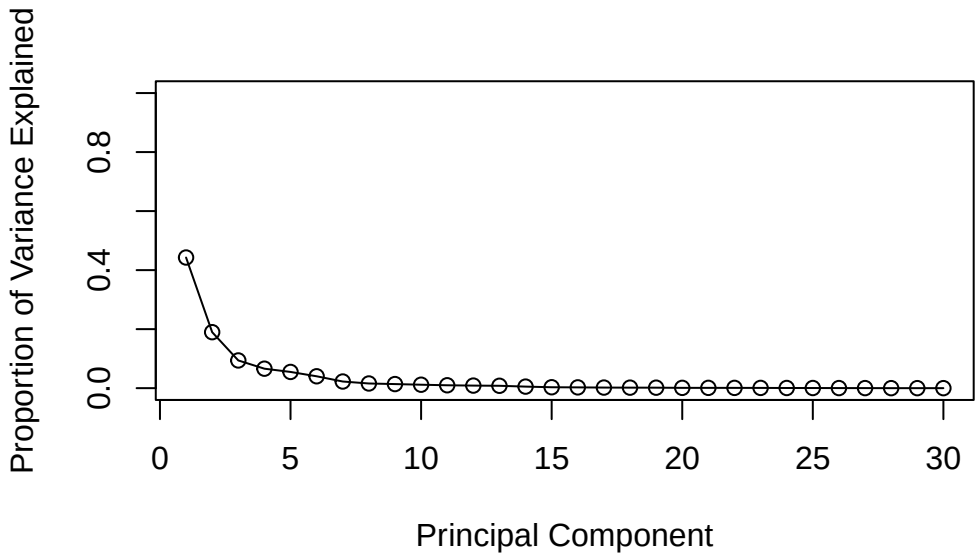
```
# Calculate the variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

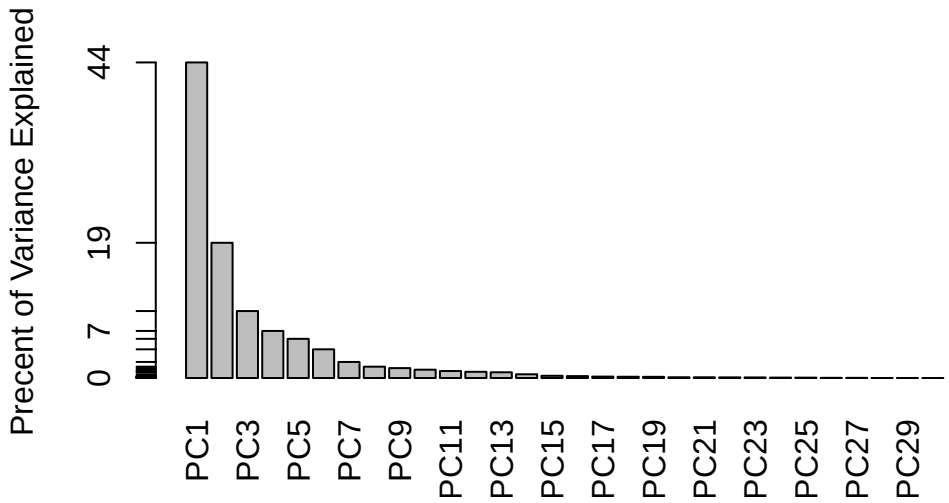
Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components. Assign this to a variable called `pve` and create a plot of variance explained for each principal component.

```
# 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 )
```

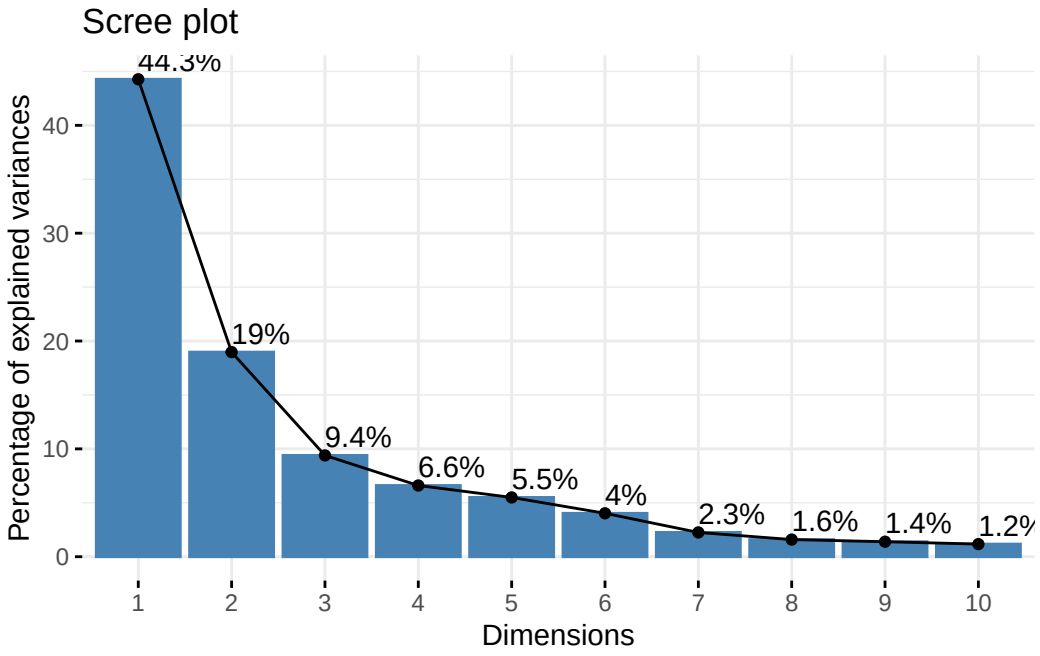


OPTIONAL: There are quite a few CRAN packages that are helpful for PCA. This includes the **factoextra** package. Feel free to explore this package. For example:

```
## 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`?

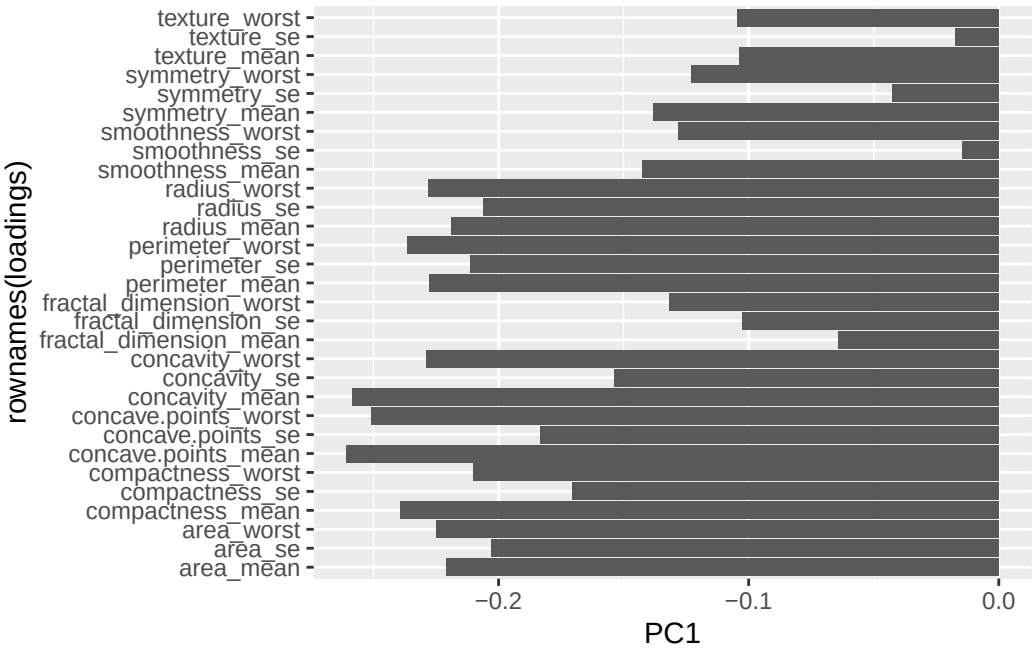
How much do the original variables contribute to the new PCs that we have calculated? Look at the `$rotation` component of the returned PCA object.

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

```
[1] -0.2608538
```

There is a complicated mix of variables that make up PC1.

```
loadings <- as.data.frame(wisc.pr$rotation)
ggplot(loadings) +
  aes(PC1, rownames(loadings)) +
  geom_col()
```



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

You need 5 principal components to explain 80% of the variance in the data.

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 data set and assign the result to `data.dist`.

```
data.dist <- dist(data.scaled)
```

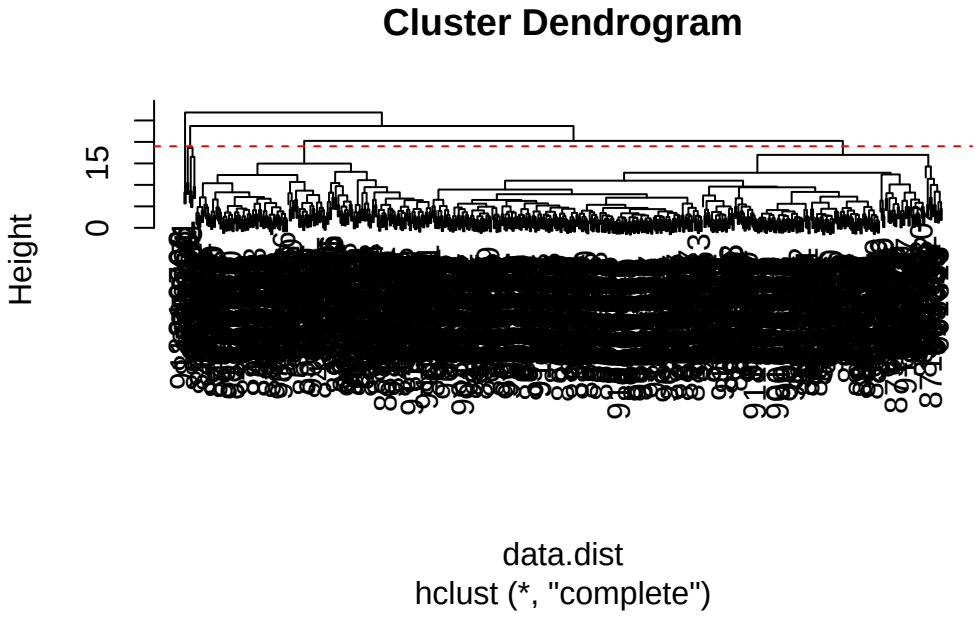
Calculate a hierarchical clustering model using complete linkage. Manually specify the method argument to `hclust()` and assign the results to `wisc.hclust`.

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

Results of hierarchical clustering

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)
```



Selecting number of clusters

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

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

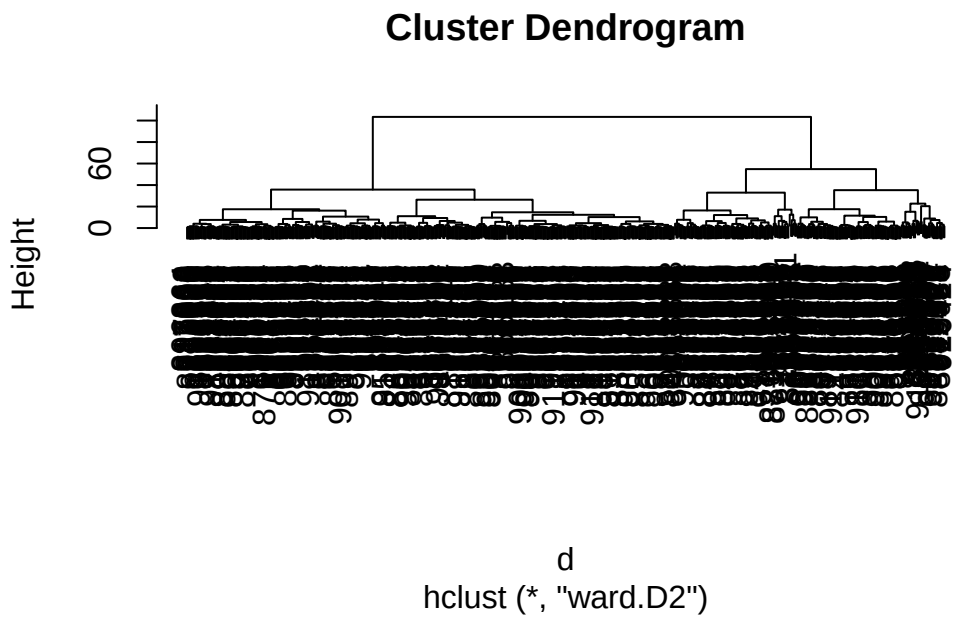
```
                   diagnosis
wisc.hclust.clusters   B   M
                   1 357 210
                   2   0   2
```

Changing the k value doesn't really have an effect on the accuracy matches.

I like the `ward.D2` method, because you can quantify the values between the clusters and diagnosis.

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

```
plot(wisc.pr.hclust)
```



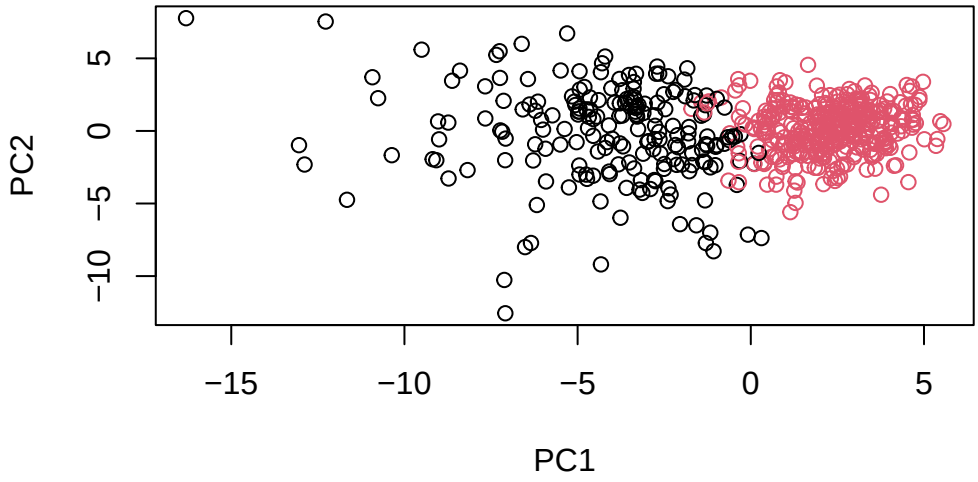

```
grps <- cutree(wisc.pr.hclust, k = 2)
table(grps)
```

```
grps
  1   2
203 366
```

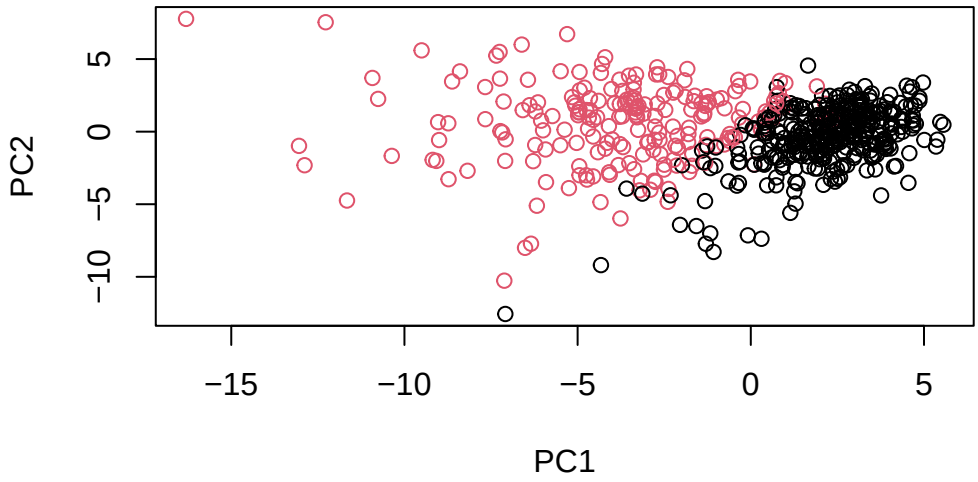
```
table(grps, diagnosis)
```

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

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




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




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

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

```
                        diagnosis
wisc.pr.hclust.clusters   B   M
                      1  24 179
```

```
  2 333  33
```

```
(179 + 333)/569
```

```
[1] 0.8998243
```

The cluster model is about 90% accurate.