Class 8 | Breast Cancer Mini-Project

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Background Information

This source provides materials for a class mini-project focused on unsupervised learning analysis of human breast cancer cell data. Students will conduct principal component analysis (PCA) for dimensionality reduction and then apply hierarchical and k-means clustering techniques.

The project involves exploratory data analysis, interpreting PCA results, evaluating clustering performance by comparing cluster assignments to actual diagnoses, and optionally combining PCA with clustering. The goal is to identify potential groupings within the cell data based on their characteristics without prior knowledge of malignancy, and the project concludes with an application of the PCA model to classify new patient samples.

Data Import

Our data comes from the U.Wisconsin Medical Center, and we will import this `.csv` document from our class website.

```
# We do NOT want patient ID data, so we will manually remove it.
wisc.df <- read.csv("WisconsinCancer.csv", row.names = 1)
```

> (Q1) How many patients are in this dataset?

```
# Considering that each row designates one patient...
nrow(wisc.df)
```

```
[1] 569
```

> (Q2) How many patients were given a malignant diagnosis?

```
# We can create a table here!
table(wisc.df$diagnosis)
```

```
  B   M
357 212
```

> (Q3) How many variables/features in the data are suffixed with `_mean`?

```
# This tells us which columns have `_means`...
# And we can use `length()` to determine the number.
length(grep("_mean", colnames(wisc.df), value = TRUE))
```

```
[1] 10
```

There is also a diagnosis column that is the clinician consensus—I want to exclude this column from further analysis. We will come back later and compare our results to this diagnosis.

```
# This first part creates a factor...
diagnosis <- as.factor(wisc.df$diagnosis)
head(diagnosis)
```

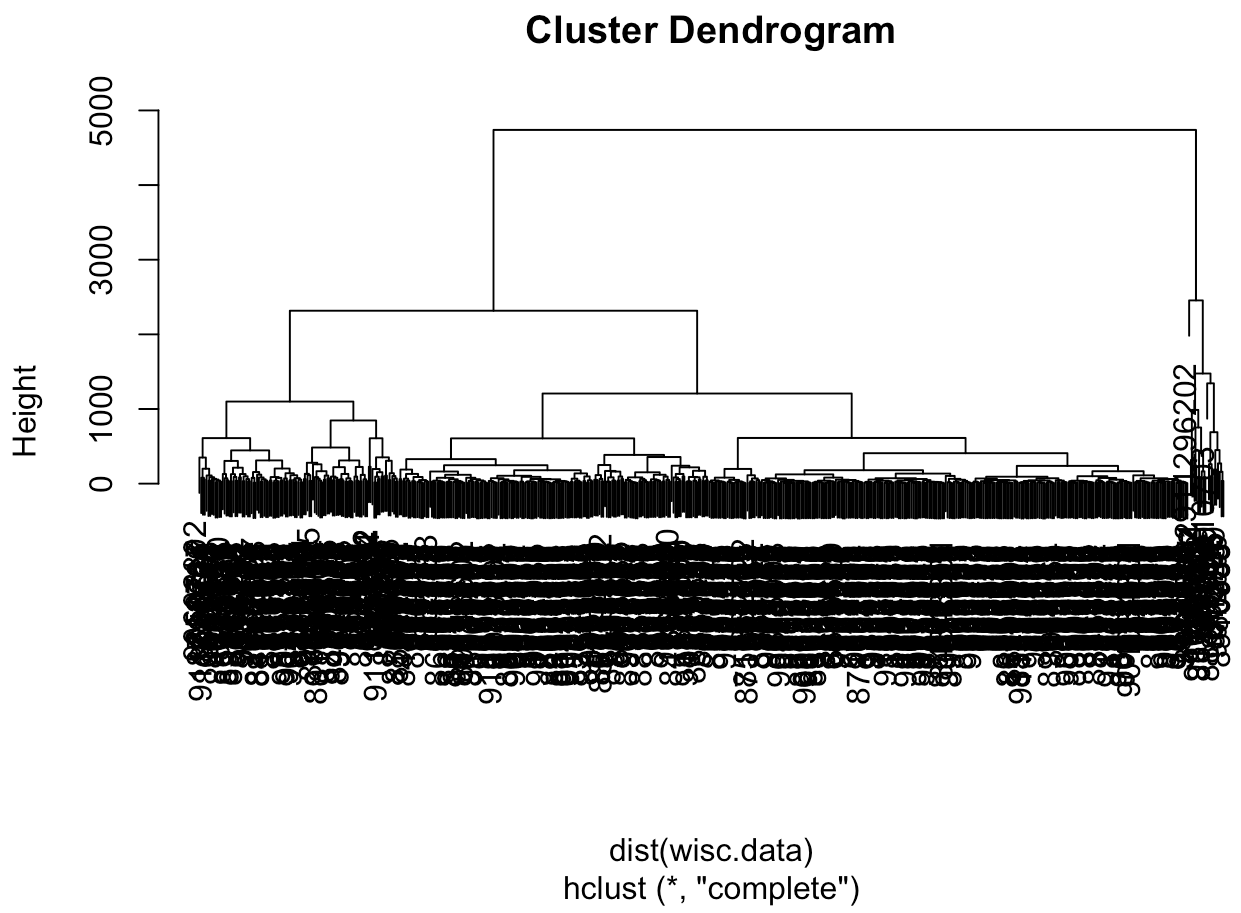
```
[1] M M M M M M
Levels: B M
```

```
# And here we can remove it from `wisc.df`.
wisc.data <- wisc.df[,-1]
```

Clustering

Let's try clustering with `hclust()`. But, results are quite messy, so we will move on to PCA later.

```
# Here is what a hierarchical clustering would look like:
hc <- hclust(dist(wisc.data))
plot(hc)
```




```
# And we can try to extract clusters with membership:
grps <- cutree(hc, k=2)

# And how many we have in each group?
table(diagnosis, grps)
```

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

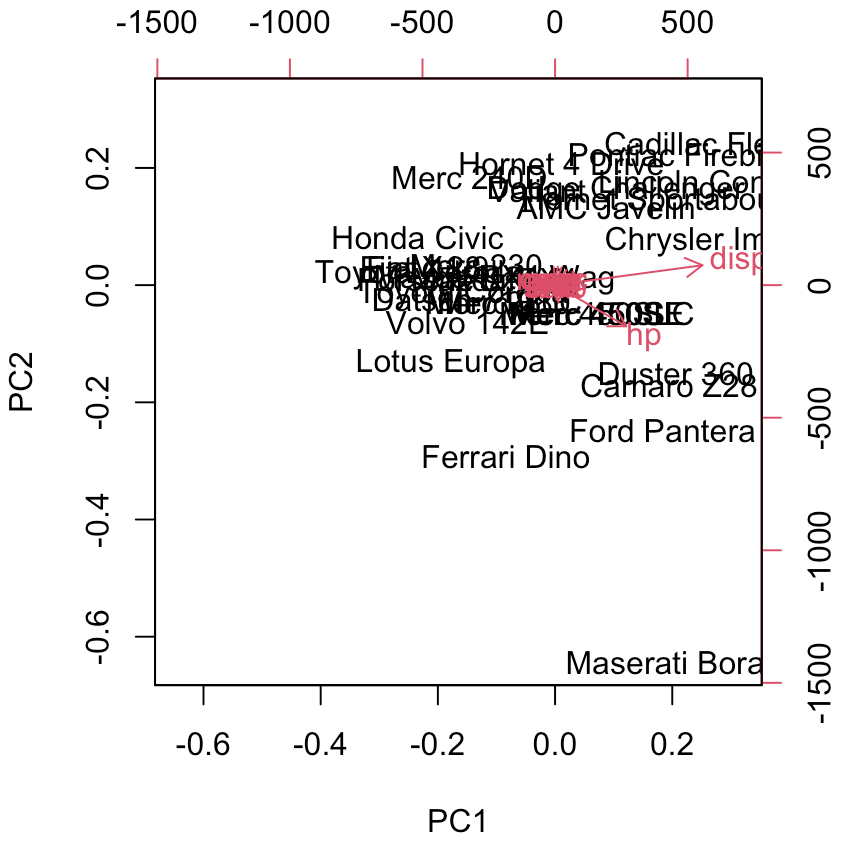
The results here show us that there are 20 outliers, all of which are within the “malignant” diagnostic group.

Principal Component Analyses

Principal Component Analysis | `mtcars`

The main function for PCA in base R is `prcomp()`, where it has a default input parameter of `scale=FALSE`.

```
# Here, we try out the function.
pc <- prcomp(mtcars, scale=F)
biplot(pc)
```



Let's check out the mean values of each column and their standard deviation.

```
# `colMeans()` will return the means.
colMeans(mtcars)
```

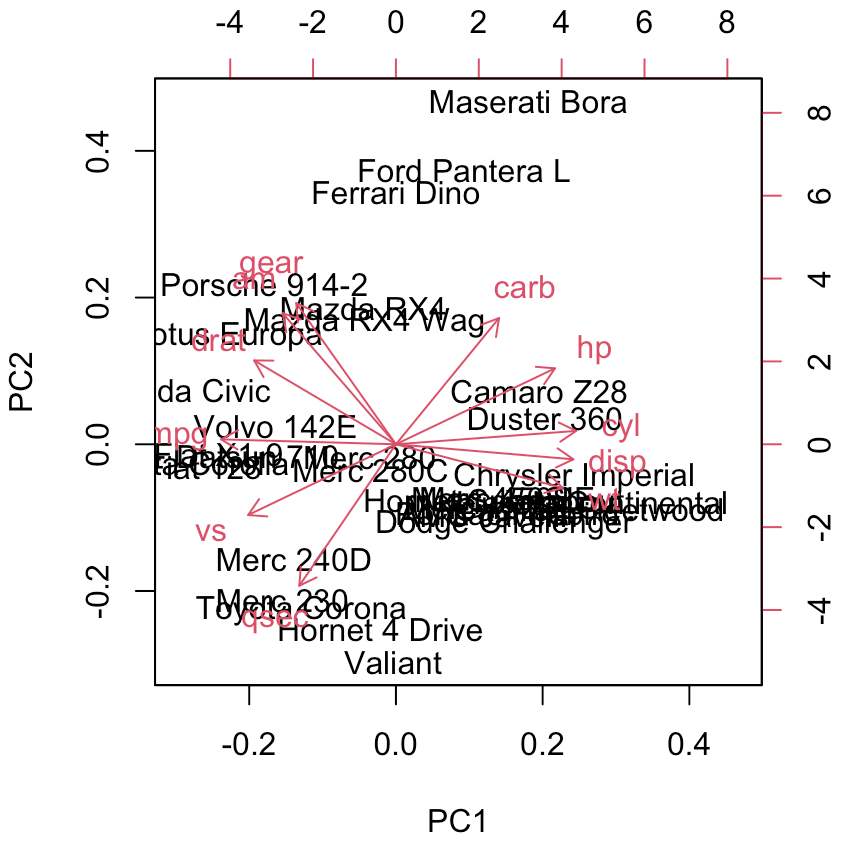
```
      mpg       cyl      disp        hp      drat        wt      qsec
20.090625  6.187500 230.721875 146.687500  3.596563  3.217250 17.848750
       vs        am      gear      carb
 0.437500  0.406250  3.687500  2.812500
```

```
# We can use `apply()` to find the standard deviation.
apply(mtcars, 2, sd)
```

```
       mpg        cyl       disp         hp       drat         wt
 6.0269481  1.7859216 123.9386938 68.5628685  0.5346787  0.9784574
      qsec         vs         am       gear       carb
 1.7869432  0.5040161  0.4989909  0.7378041  1.6152000
```

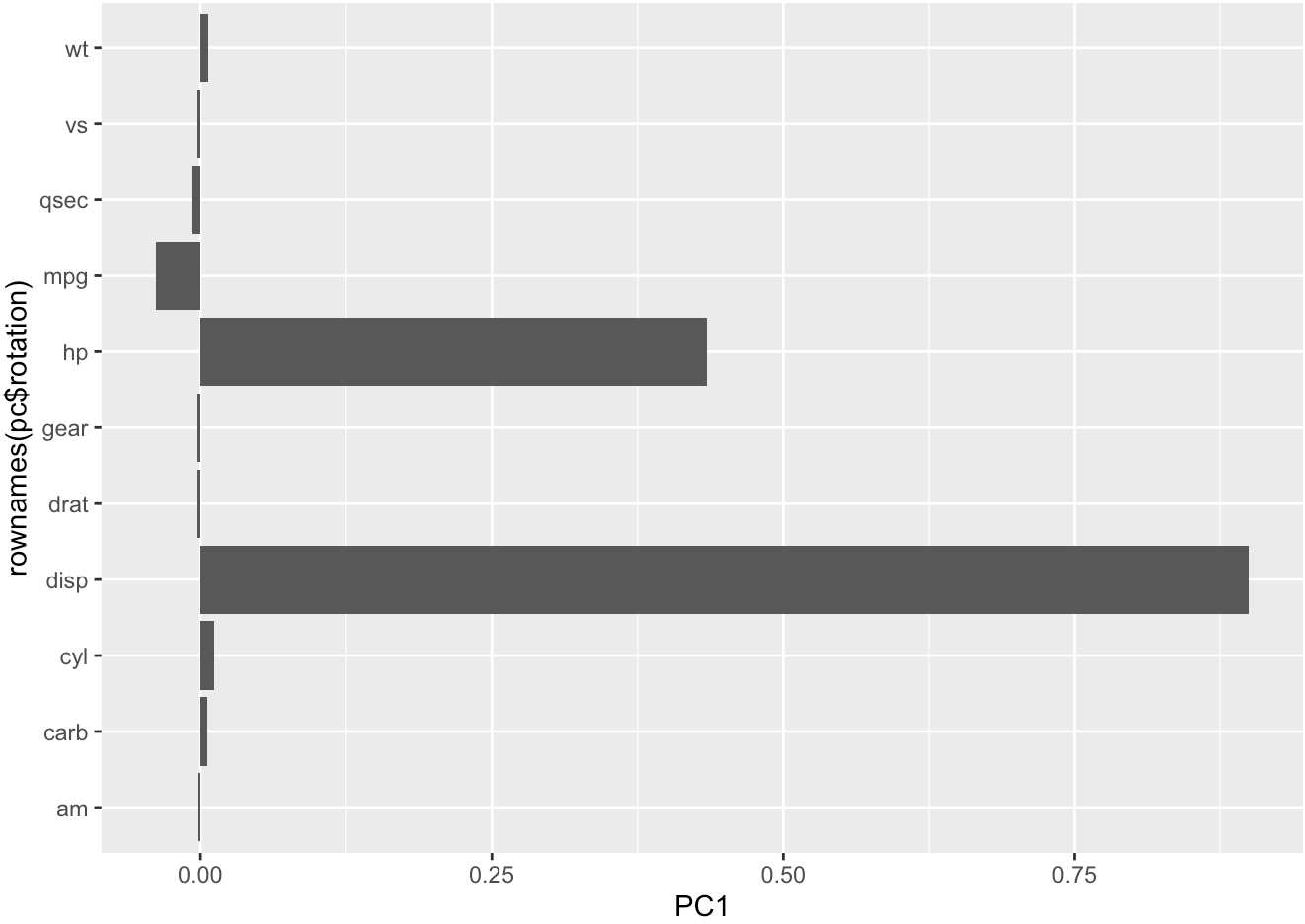
By looking at these results, we see that many of these are on different scales, so we can set `scale=TRUE` within `prcomp()` to account for these differences.

```
# Using mtscale will have the exact same effect.
pc.scale <- prcomp(mtcars, scale=TRUE)
biplot(pc.scale)
```



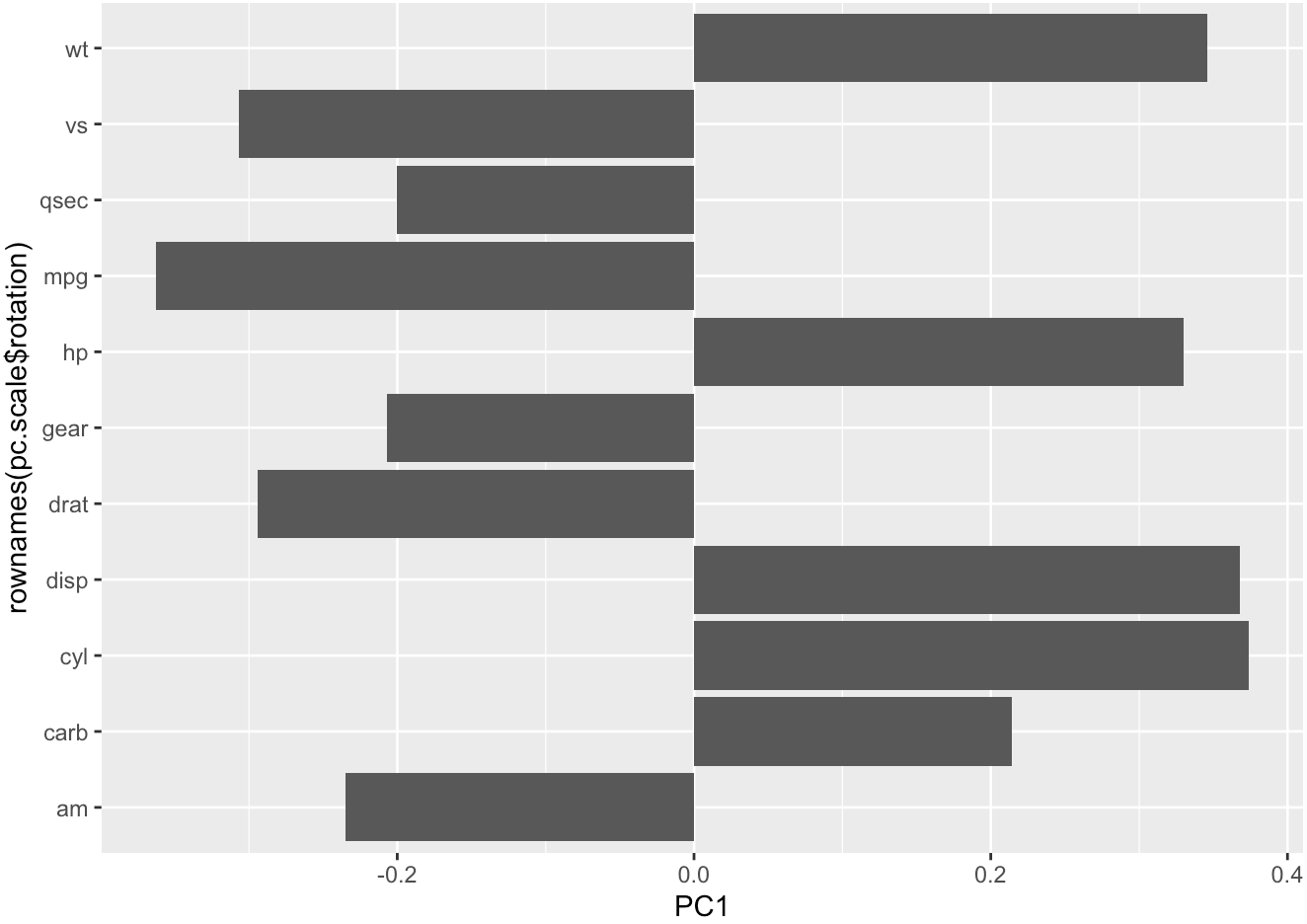
We can also use a “loadings plot” to compare how the original variables contribute to the new PCs.

```
# 'hp' and 'disp' are shown to have the greatest effect.
library(ggplot2)
ggplot(pc$rotation) +
  aes(PC1, rownames(pc$rotation)) +
  geom_col()
```



What about for the scaled data?

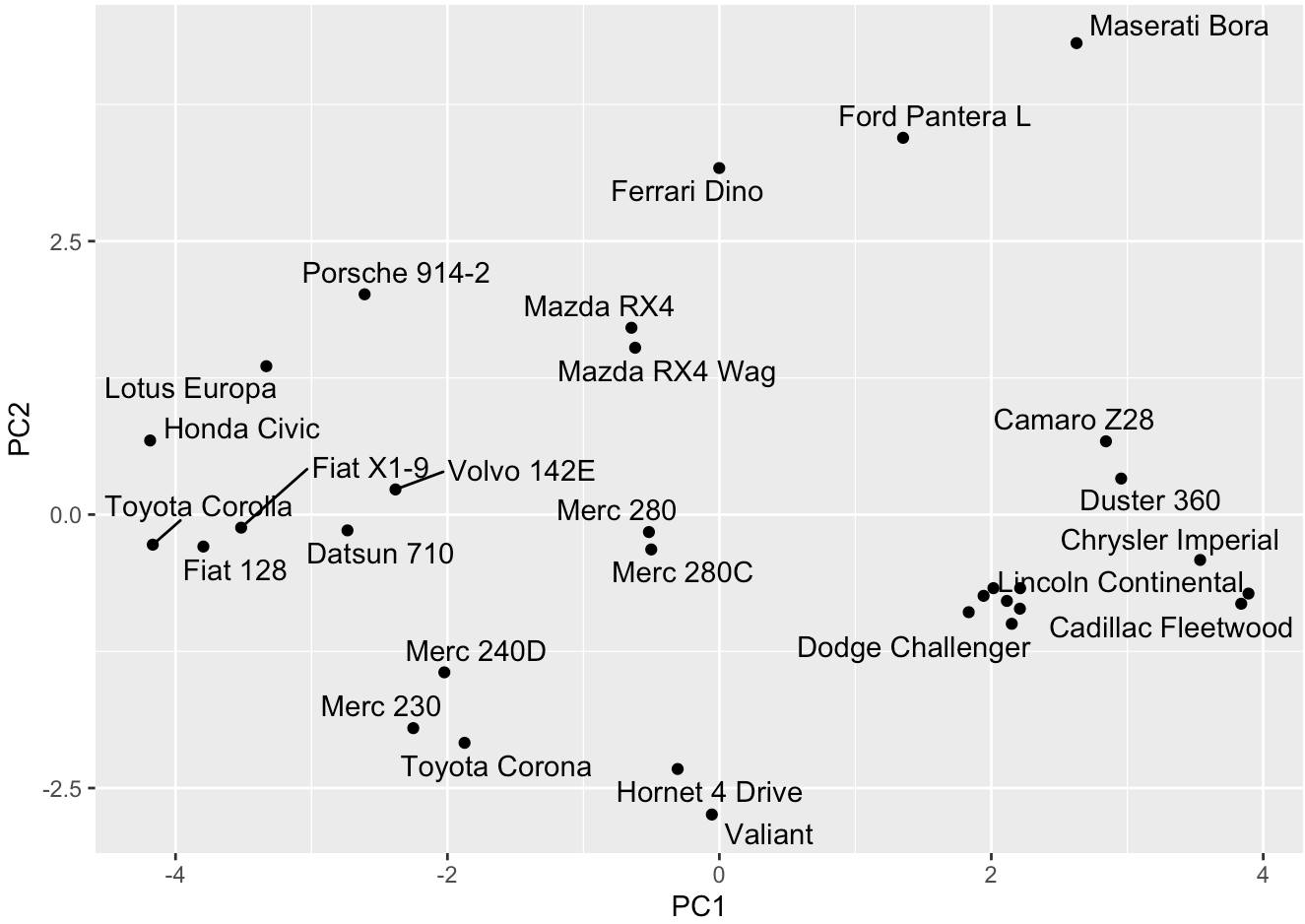
```
# We see that most variables have a similar effect.
library(ggplot2)
ggplot(pc.scale$rotation) +
  aes(PC1, rownames(pc.scale$rotation)) +
  geom_col()
```



And finally, let's create a more understandable PC plot of our scaled PCA results. We can use a `geom_point()` plot and call upon the `ggrepel` library for better labeling.

```
# We can add a few settings to make a nicer plot.
library(ggrepel)
ggplot(pc.scale$x) +
  aes(PC1, PC2, label=rownames(pc.scale$x)) +
  geom_point() +
  geom_text_repel()
```

```
Warning: ggrepel: 6 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```

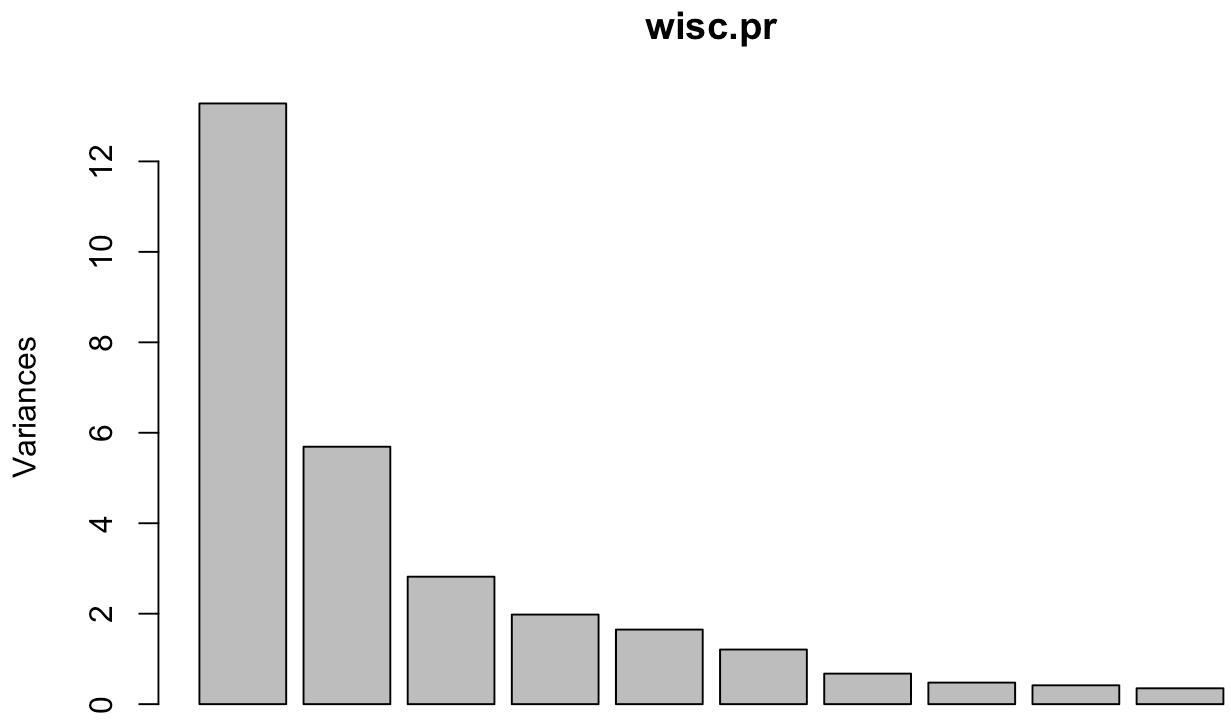


> **Key point:** In general, we will set `scale=TRUE` when we do PCA. This is not the default, but probably should be...

Principal Component Analysis | `wisc.data`

Let's begin to do the same with our `wisc.data` dataset.

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



To see how well PCA is doing here in terms of capturing the variance, we can use the `summary()` function.

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

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

```
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

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

Thanks to `summary()`, we know that answer is **44.7%**.

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

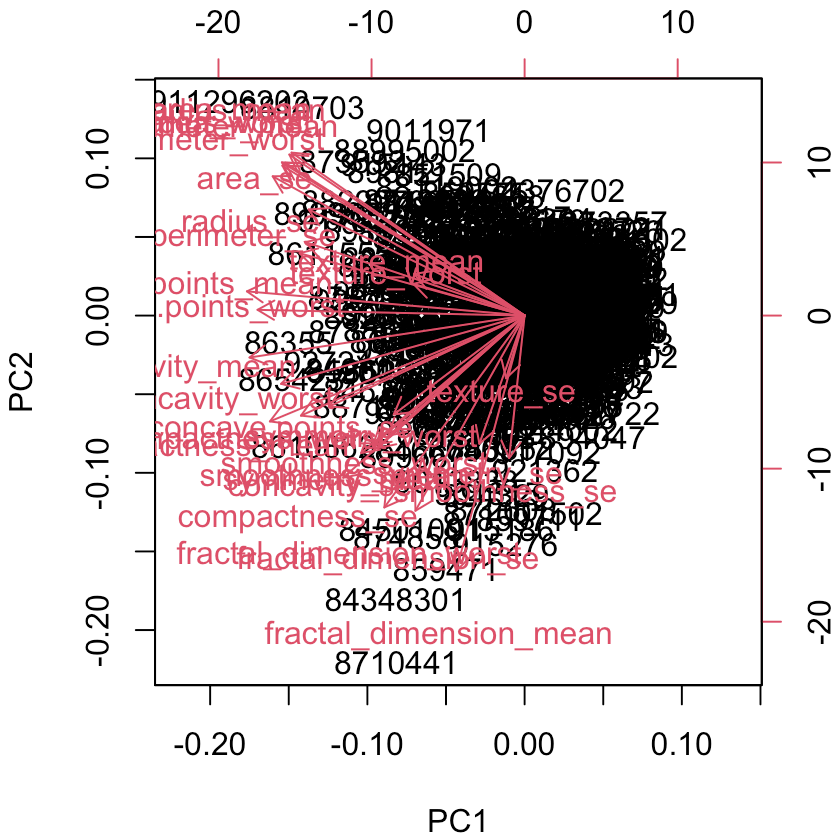
Using up to **PC3** will cover ~72% of the variance in our data.

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

Using up to **PC7** will cover ~91% of the variance in our data.

Now, if we were to create a biplot of the data, it would be hard to distinguish many results.

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

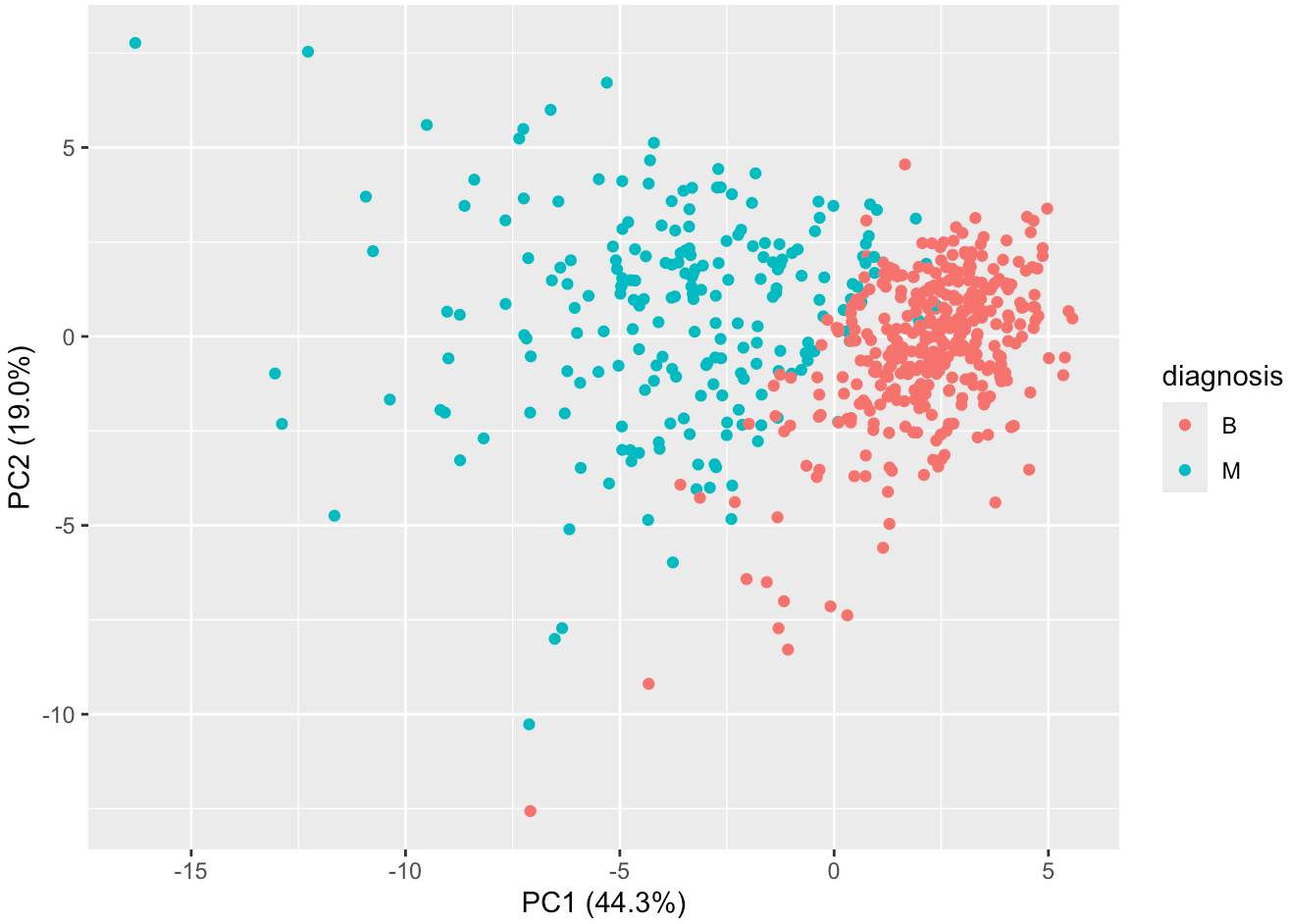


> (Q7) What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is quite difficult to understand, and it is very cramped, preventing any real conclusions from being drawn.

Let's also create the main PC1 vs. PC2 figure, which according to `summary()`, will capture 63.2% of the variance in our data.

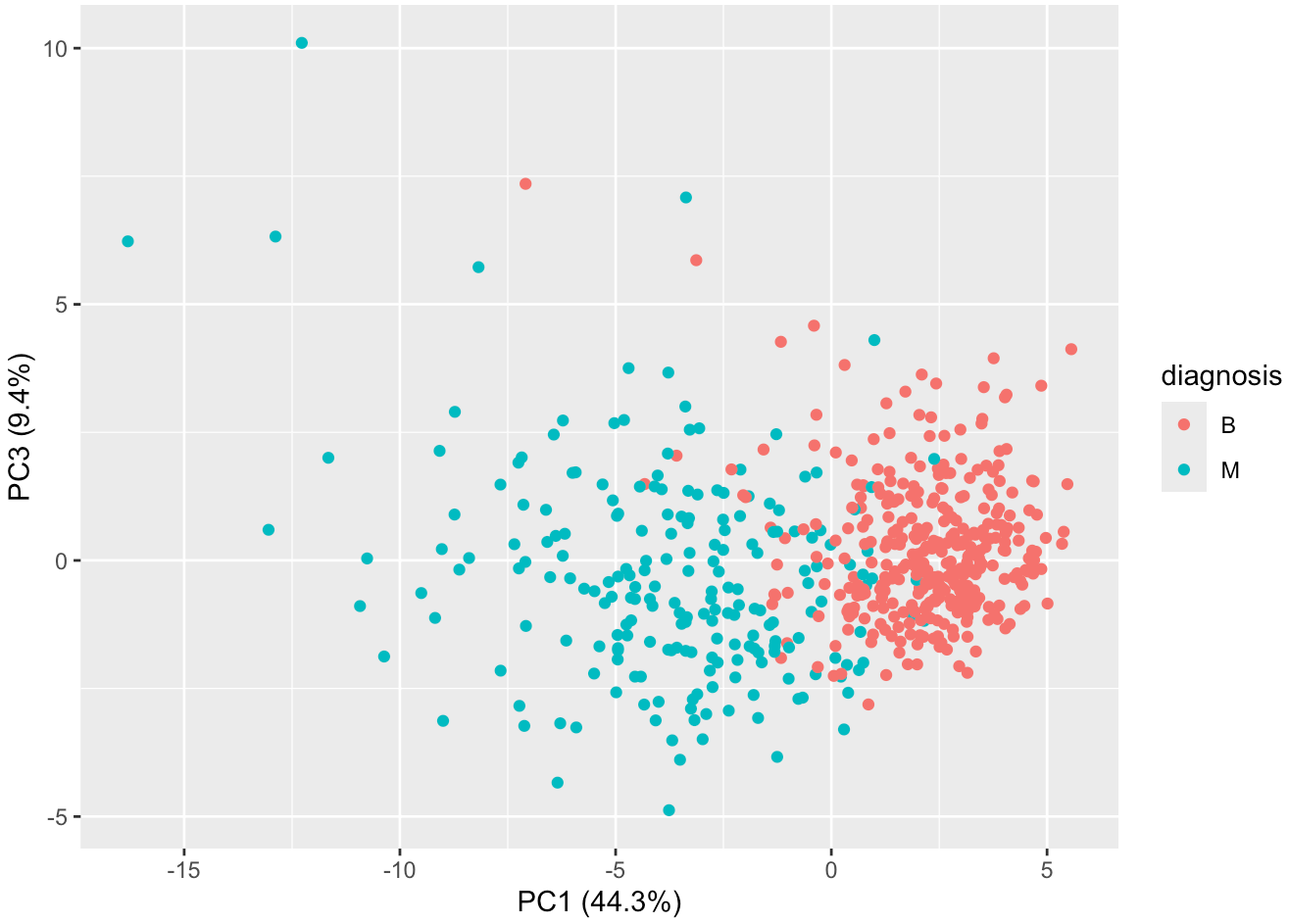
```
# There's a separation between malignant and benign!
ggplot(wisc.pr$x) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point() +
  xlab("PC1 (44.3%)") +
  ylab("PC2 (19.0%)")
```



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

```
# There's still a separation between malignant and benign!
ggplot(wisc.pr$x) +
  aes(PC1, PC3, col=diagnosis) +
```

```
  geom_point() +
  xlab("PC1 (44.3%)") +
  ylab("PC3 (9.4%)")
```



There is still a significant separation between malignant and benign samples, but the graph is oriented differently.

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[,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
```

The component of the loading vector for `concave.points_mean` is -0.26085376.

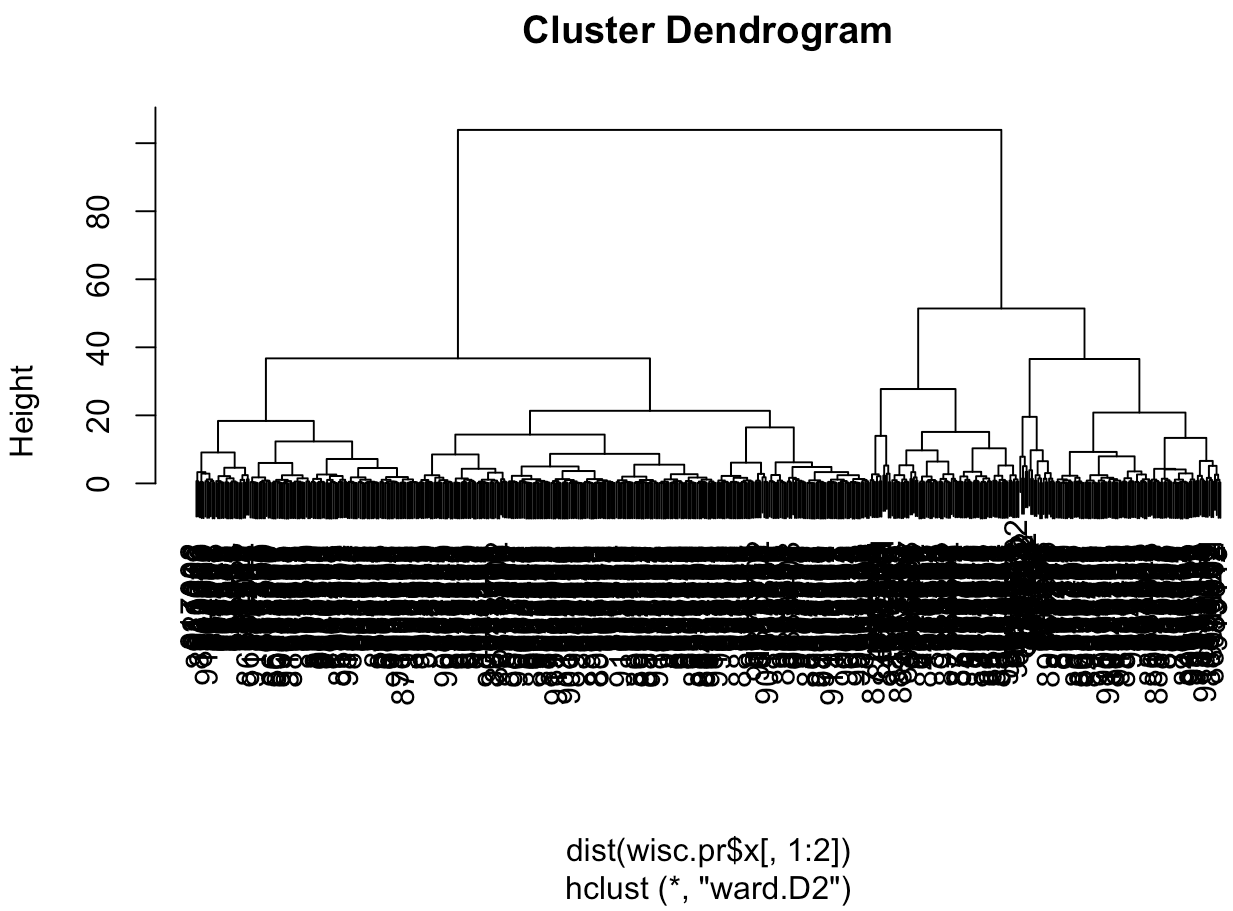
> (Q10) What is the minimum number of principal components required to explain 80% of the variance of the data?

Once again, with the help of `summary()`, we can determine that up to **PC5** is needed to explain 80% of the variance in the data (specifically, ~84%).

Combining Methods

We can take our PCA results and use them as a "basis set" for other analyses such as clustering.

```
# Let's create another hclust(), but what's the difference?
wisc.hc<- hclust(dist(wisc.pr$x[,1:2]), method="ward.D2")
plot(wisc.hc)
```



Despite the data still being quite compact in this plot, we can see that there are two major clusters. We can also "cut" this tree to yield our clusters in this way:

```
pc.grps <- cutree(wisc.hc, k=2)
table(pc.grps)
```

```
pc.grps
  1   2
195 374
```

How do my cluster `grps` compare to the clinician diagnoses?

Clustering on PCA Results

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

```
table(diagnosis, pc.grps)
```

```
         pc.grps
diagnosis   1   2
        B  18 339
        M 177  35
```

What this is telling us is that the vast majority of malignant samples reside in cluster 1, and the majority of benign samples reside in cluster 2. It separates the two diagnoses quite well—certainly better than before.

> (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.

First, let's do both a K-means clustering and `hclust()` to store new objects.

```
# Here, we define the two objects for older clustering methods.
wisc.km <- kmeans(wisc.data, centers=2)
wisc.hclust.clusters <- cutree(wisc.hc, k=4)
```

If we return `table()`s here with the results from those clustering models...

```
# These are the K-means and H-clustering tables.
table(wisc.km$cluster, diagnosis)
```

```
   diagnosis
      B   M
  1 356  82
  2   1 130
```

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

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1   0 112
                   2  18  65
                   3 232  18
                   4 107  17
```

We see that the number of samples situated in the non-majority clusters is much larger, which proves that PCA separates the diagnoses much more accurately.

Prediction

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

We can use our PCA model for the analysis of new "unseen" data. In this case from U.Michigan...

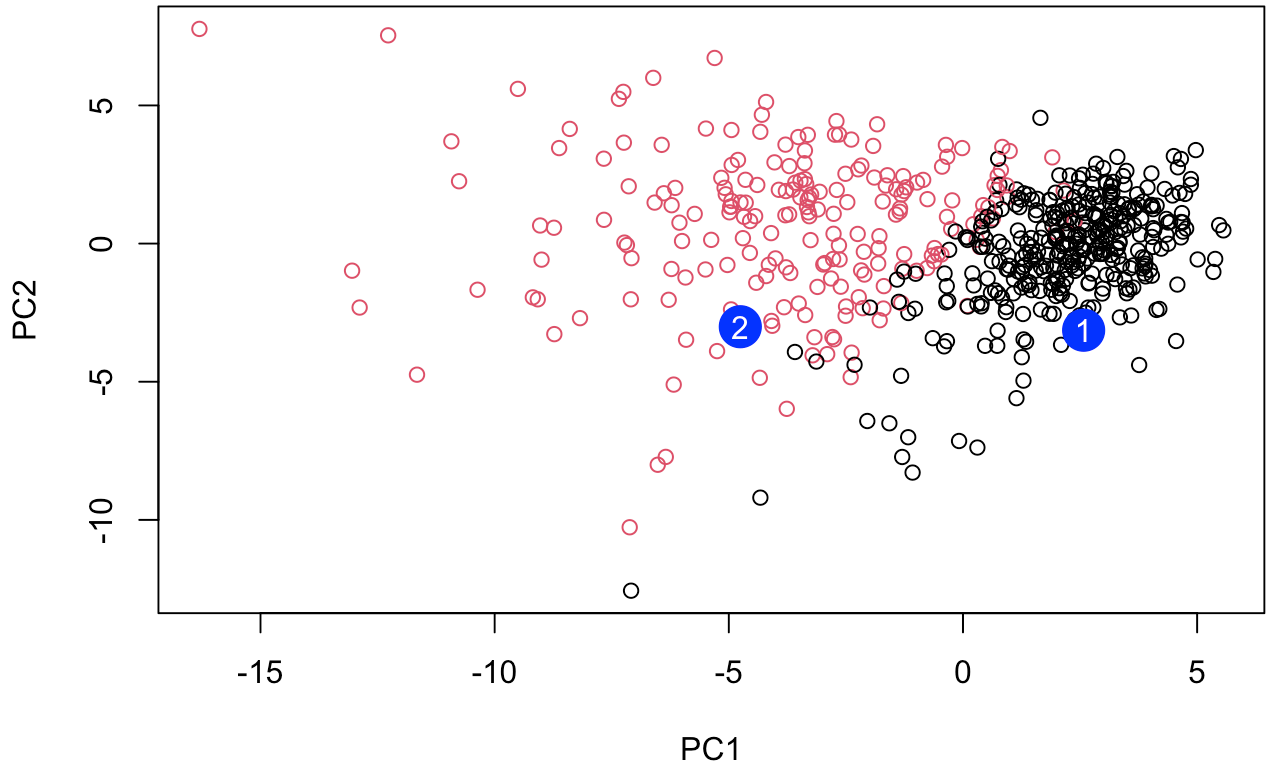
```
#url <- "new_samples.csv"
url <- "https://tinyurl.com/new-samples-CSV"
new <- read.csv(url)
```

```
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
```

If we plot our two new patients along with what we have...

```
# Here, we are instead using a "base R" function as provided from the lab sheet.
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")
```



...we see that patient 1 sits firmly within the benign group, but patient 2 is clearly past the separation between benign and malignant diagnoses. Therefore, we should prioritize **Patient 2** for follow-up, as the statistics point towards the growth being malignant.