08_mini_project

Sam Altshuler (PID: A59010373)

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Exploratory Data Analysis

Preparing the data

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

# Complete the following code to input the data and store as wisc.df
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
```

Remove the diagnosis column and save as a new df to not overwrite original data.

```
wisc.data <- wisc.df[,-1]
# Diagnosis vector with original data diagnosis
diagnosis <- wisc.df$diagnosis
```

Exploratory data analysis

- Q1. How many observations are in this dataset?

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

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

- There are 569 separate observations
- Q2. How many of the observations have a malignant diagnosis?

```
length(diagnosis[diagnosis == "M"])
```

```
## [1] 212
```

- There are 212 observations with a malignant diagnosis
- Q3. How many variables/features in the data are suffixed with _mean?

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

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

- There are 10 variables that are suffixed with "_mean".

Principal Component Analysis

Next step in the analysis is to perform a PCA on `wisc.data`. Data needs to be rescaled if: * The input variables use different units of measurement * The input variables have significantly different variances

```r
# Check column means and standards 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
```

```r
# apply standard deviation function to every column in the dataframe
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
```

Based on the means and standard deviations, it appears that the dataset has very different variances and likely different units of measurement (for example smoothness and symmetry are likely not in the same units). PCA with scaling:

```
wisc.pr <- prcomp(wisc.data, scale. = TRUE)
# summary of the results
summary(wisc.pr)
```

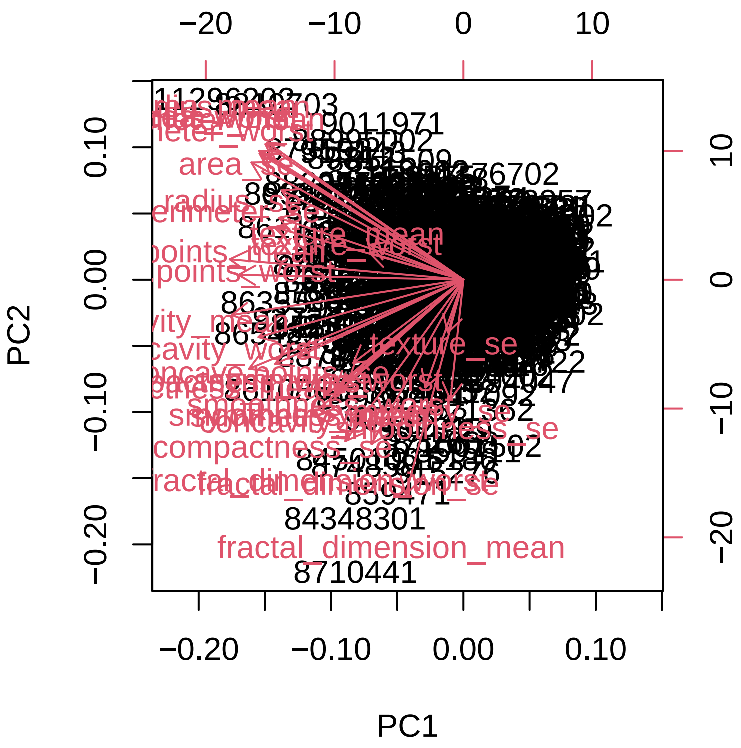
```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion  0.4427 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)?
  - PC1 captures 44.27% of the original variance.
- Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?
  - You need to include the first three PCs (1-3) in order to describe at least 70% of the original variance.
- Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?
  - At least 7 principal components are needed to describe >90% of the original variance.

Interpreting PCA results

Visualize the PCA using a biplot

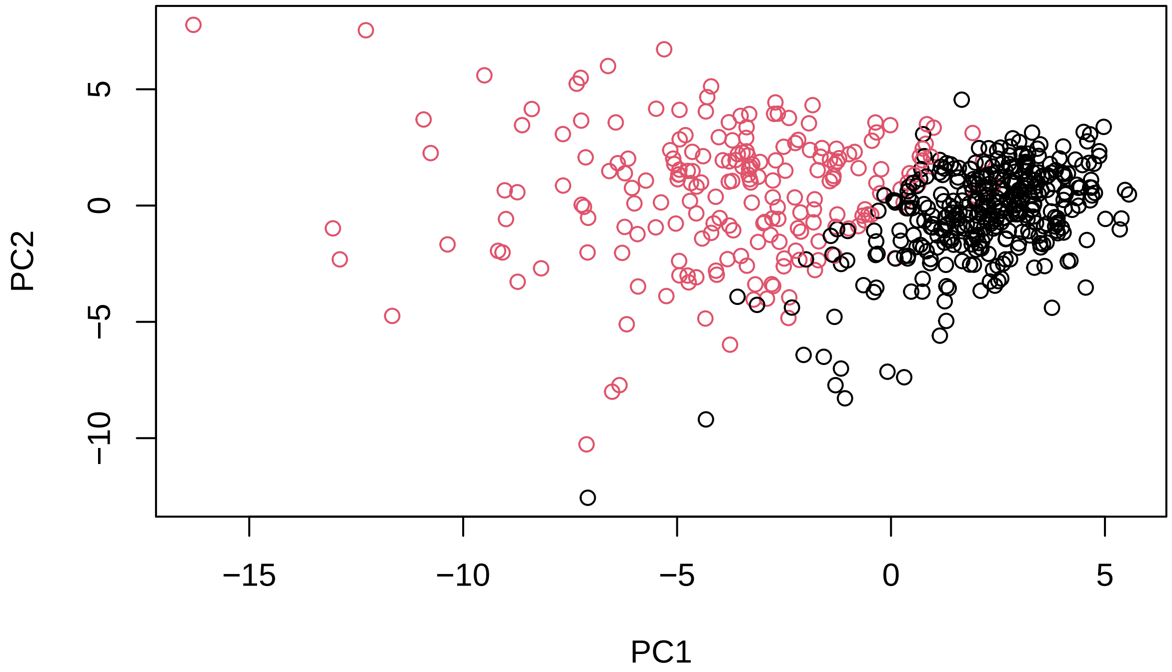
```r
biplot(wisc.pr)
```



- Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?
  - This plot is very hard to read, you cannot even separate out the observations into readable labels. There is just too much crowding.

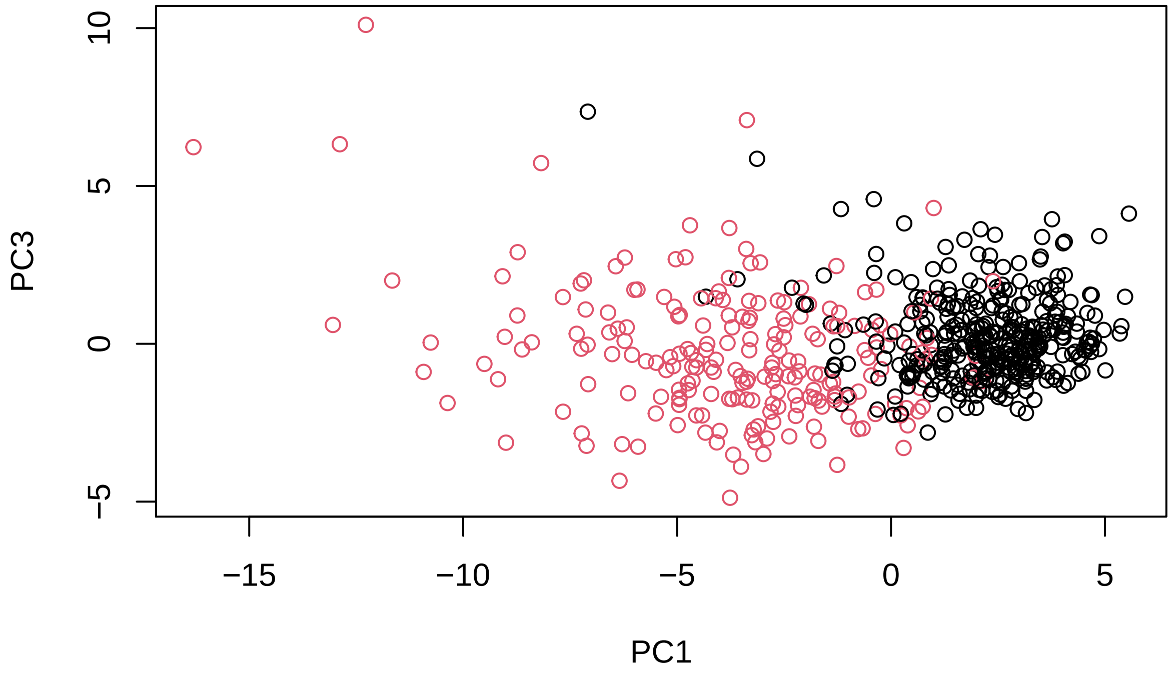
Let's create a standard scatter plot using PC1 as the x and PC2 as the y axis.

```r
plot(wisc.pr$x,
     col = as.factor(diagnosis),
     xlab = "PC1",
     ylab = "PC2")
```



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

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



+ These plots seem relatively similar, however that is likely because PC1 explains much of the variance. However, the plot comparing PC1 v PC2 has a more clean line between the benign and malignant cells since together they explain 63% of the total variance while PC1 and PC3 only explain 55%. This is seen by the overlap in colors around PC1 = 0 in the PC1 v PC3 graph.

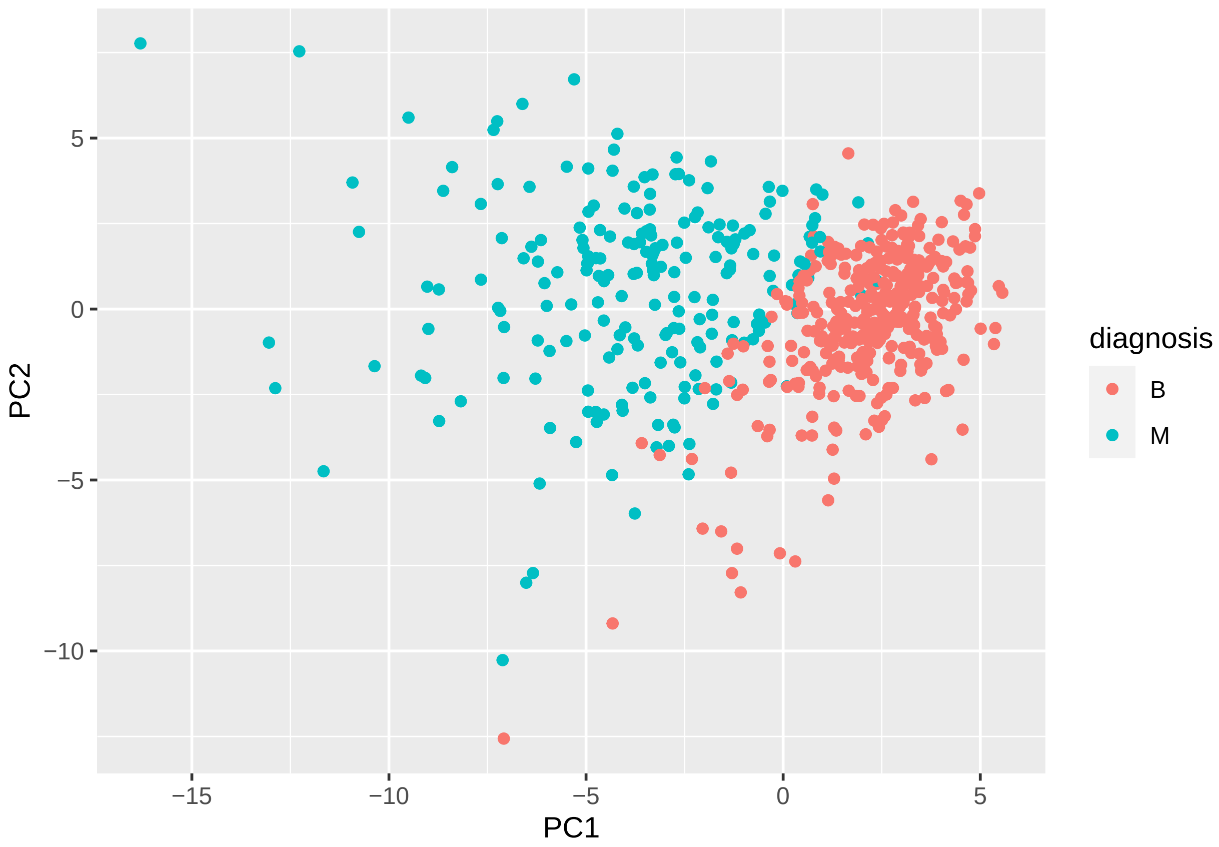
Use ggplot2 to create some better looking figures.

```
# load in the package
library(ggplot2)
```

```
## Warning: package 'ggplot2' was built under R version 4.0.3
```

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

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



Variance Explained

Produce the scree plots to show proportion of variance explained as number of PCs increases.

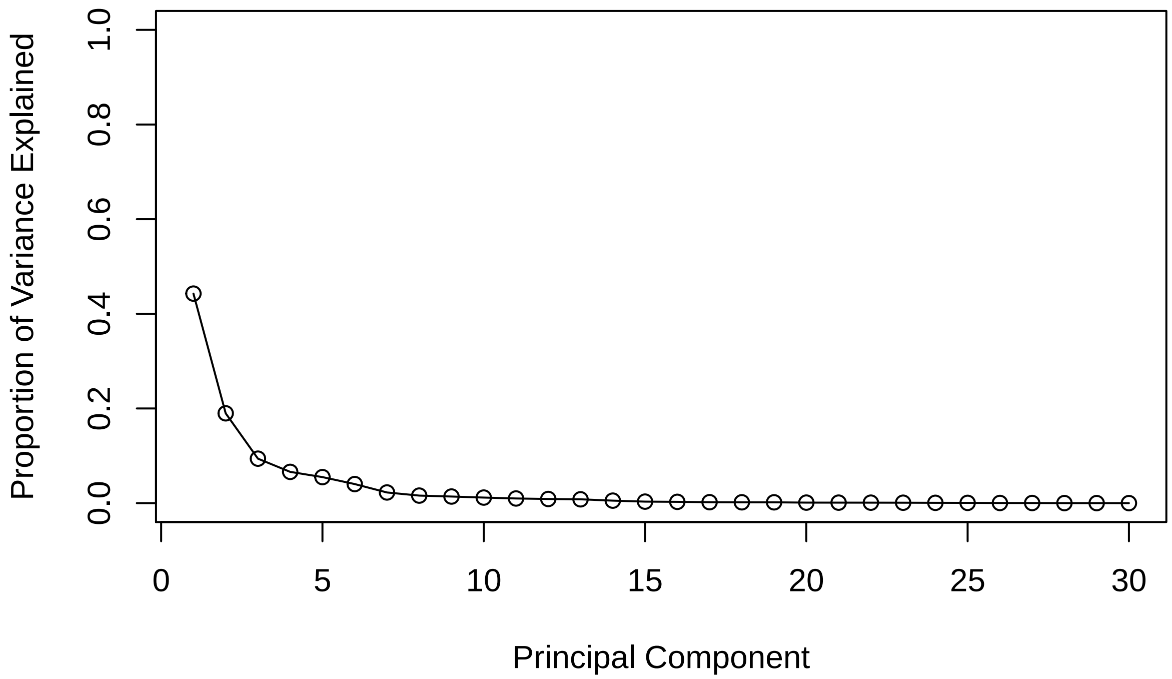
```
# Calculate the variance of each component
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

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

Calculate percent variance to understand the amount of variance that can be explained by each PC.

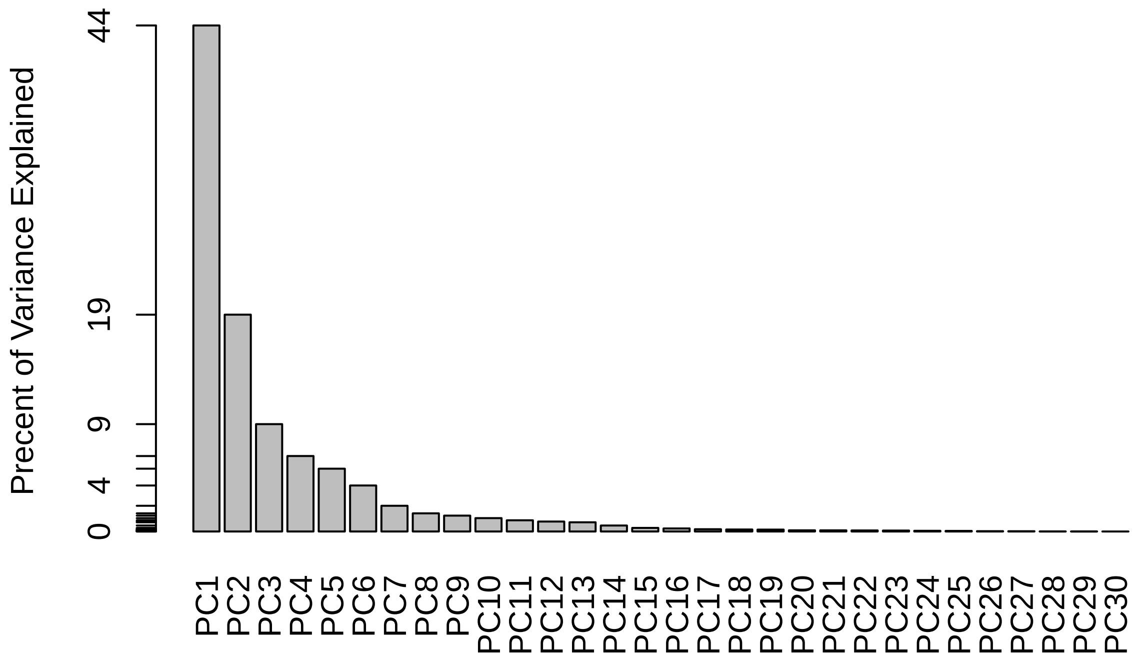
```
pve <- pr.var/sum(pr.var)

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



Or this can be shown as a bargraph:

```
# 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 )
```



There isn't an easy elbow to see but I would say the elbow is around PC5.

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?
  - The loading vector shows the covariance between the original value and the scaled principal component. For example, the concave.points_mean loading vector is -0.2608, which means this is the value that is multiplied by the concave.points_mean to determine it's contribution to PC1.
- Q10. What is the minimum number of principal components required to explain 80% of the variance of the data?
  - There is a minimum 5 PCs needed to explain at least 80% of the variance of the data.

Prediction

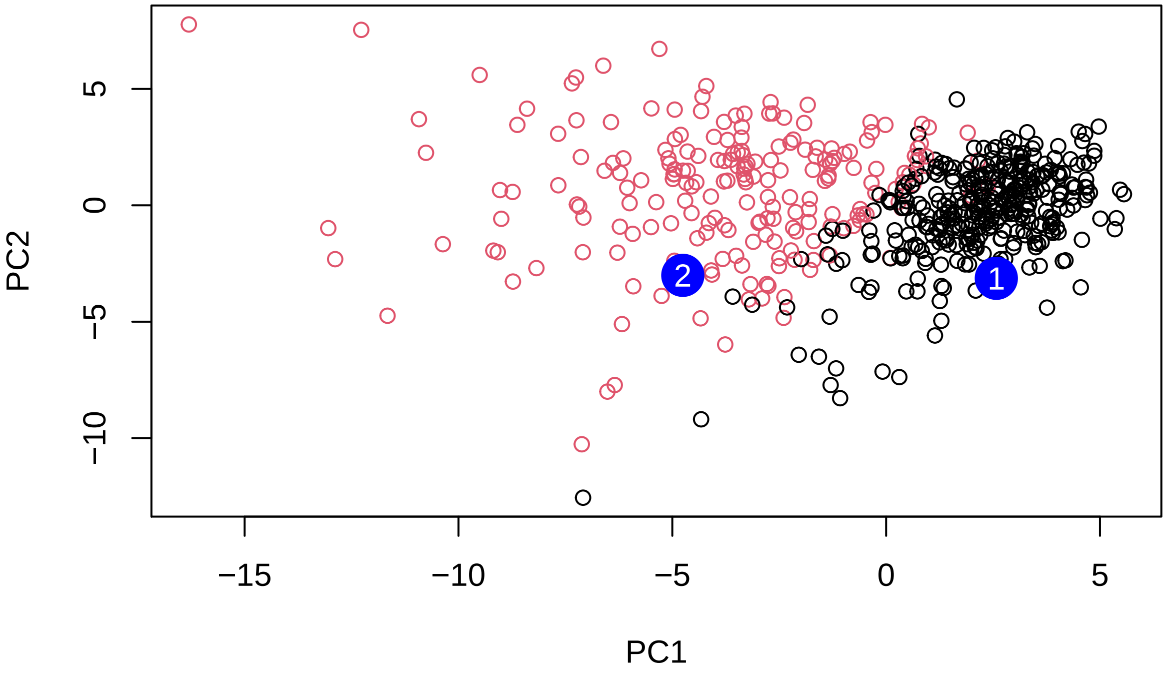
Add in new data

```
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 these predictions on the original PCA data.

```r
plot(wisc.pr$x[,1:2], col=as.factor(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?
    - You should prioritize patient 2 because their data point appears to be within the malignant clusters.