# class 08

Yinuo Song

4/28/23

### Input the data

```
fna.data <- "WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)</pre>
```

|          | diagnosis | radius_m  | nean  | texture_mean   | perimeter_mean | area_mean  | ı            |
|----------|-----------|-----------|-------|----------------|----------------|------------|--------------|
| 842302   | M         | I 17      | 7.99  | 10.38          | 122.80         | 1001.0     | )            |
| 842517   | M         | 1 20      | .57   | 17.77          | 132.90         | 1326.0     | )            |
| 84300903 | M         | 19        | 69.69 | 21.25          | 130.00         | 1203.0     | )            |
| 84348301 | M         | [ 11      | .42   | 20.38          | 77.58          | 386.1      | 1            |
| 84358402 | M         | 1 20      | .29   | 14.34          | 135.10         | 1297.0     | )            |
| 843786   | M         | [ 12      | 2.45  | 15.70          | 82.57          | 477.1      | 1            |
|          | smoothnes | s_mean co | mpac  | ctness_mean co | ncavity_mean o | oncave.po  | ints_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 frac | tal_  | _dimension_mea | n radius_se te | xture_se p | perimeter_se |
| 842302   | 0.        | 2419      |       | 0.0787         | 1 1.0950       | 0.9053     | 8.589        |
| 842517   | 0.        | 1812      |       | 0.0566         | 7 0.5435       | 0.7339     | 3.398        |
| 84300903 | 0.        | 2069      |       | 0.0599         | 9 0.7456       | 0.7869     | 4.585        |
| 84348301 | 0.        | 2597      |       | 0.0974         | 4 0.4956       | 1.1560     | 3.445        |
| 84358402 | 0.        | 1809      |       | 0.0588         | 3 0.7572       | 0.7813     | 5.438        |
| 843786   | 0.        | 2087      |       | 0.0761         | 3 0.3345       | 0.8902     | 2.217        |
|          | area_se s | moothness | s_se  | compactness_s  | e concavity_se | concave.   | points_se    |
| 842302   | 153.40    | 0.006     | 399   | 0.0490         | 4 0.05373      | }          | 0.01587      |
| 842517   | 74.08     | 0.005     | 225   | 0.0130         | 8 0.01860      | 1          | 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_dimen  | sion_se rad: | ius_worst text | ure_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_wor | rst area_wors  | t smoothnes: | s_worst compac | tness_worst |
| 842302   | 184           | .60 2019.0     | 0            | 0.1622         | 0.6656      |
| 842517   | 158           | .80 1956.0     | 0            | 0.1238         | 0.1866      |
| 84300903 | 152           | .50 1709.0     | 0            | 0.1444         | 0.4245      |
| 84348301 | 98            | .87 567.       | 7            | 0.2098         | 0.8663      |
| 84358402 | 152           | .20 1575.0     | 0            | 0.1374         | 0.2050      |
| 843786   | 103           | .40 741.6      | 6            | 0.1791         | 0.5249      |
|          | concavity_wor | rst concave.po | oints_worst  | symmetry_wors  | t           |
| 842302   | 0.73          | 119            | 0.2654       | 0.460          | 1           |
| 842517   | 0.24          | 116            | 0.1860       | 0.275          | 0           |
| 84300903 | 0.49          | 504            | 0.2430       | 0.361          | 3           |
| 84348301 | 0.68          | 369            | 0.2575       |                |             |
| 84358402 | 0.40          | 000            | 0.1625       | 0.236          | 4           |
| 843786   | 0.53          | 355            | 0.1741       | 0.398          | 5           |
|          | fractal_dimen | _              |              |                |             |
| 842302   |               | 0.11890        |              |                |             |
| 842517   |               | 0.08902        |              |                |             |
| 84300903 |               | 0.08758        |              |                |             |
| 84348301 |               | 0.17300        |              |                |             |
| 84358402 |               | 0.07678        |              |                |             |
| 843786   |               | 0.12440        |              |                |             |

WE can use -1 to remove the 1st column.

```
wisc.data <- wisc.df[,-1]
head(wisc.data)</pre>
```

|          | 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      |        | 0.14230 |
| 843786   | 12.45            | 15.70     |          | 82.57      | 477.1       |        | 0.10030 |
|          | ompactness_mean  |           | waan d   |            |             | Simmo  |         |
| 842302   | 0.27760          |           | 0.3001   | Joneave.po | 0.14710     | •      | 0.2419  |
| 842517   | 0.07864          |           | 0.0869   |            | 0.07017     |        | 0.1812  |
| 84300903 | 0.15990          |           | 0.1974   |            | 0.12790     |        | 0.1012  |
| 84348301 | 0.28390          |           | 0.1374   |            | 0.12730     |        | 0.2597  |
| 84358402 | 0.13280          |           | 0.1980   |            | 0.10020     |        | 0.1809  |
| 843786   | 0.17000          |           | 0.1578   |            | 0.08089     |        | 0.2087  |
|          | ractal_dimension |           |          | texture s  |             |        |         |
| 842302   |                  | .07871    | 1.0950   | 0.90       | -           | 8.589  | 153.40  |
| 842517   |                  | .05667    | 0.5435   | 0.73       |             | 3.398  | 74.08   |
| 84300903 |                  | .05999    | 0.7456   |            |             | 4.585  |         |
| 84348301 |                  | .09744    | 0.4956   |            |             | 3.445  |         |
| 84358402 |                  | .05883    | 0.7572   |            |             | 5.438  |         |
| 843786   |                  | .07613    | 0.3345   | 0.890      |             | 2.217  | 27.19   |
|          | noothness_se co  |           |          |            |             |        |         |
| 842302   | 0.006399         | 0.04      |          | 0.05373    |             | 0.015  |         |
| 842517   | 0.005225         | 0.01      |          | 0.01860    |             | 0.013  |         |
| 84300903 | 0.006150         | 0.04      |          | 0.03832    |             | 0.020  |         |
| 84348301 | 0.009110         | 0.07      |          | 0.05661    |             | 0.018  |         |
| 84358402 | 0.011490         | 0.02      |          | 0.05688    |             | 0.018  |         |
| 843786   | 0.007510         | 0.03      |          | 0.03672    |             | 0.011  |         |
|          | ymmetry_se frac  |           |          |            | orst textu  |        |         |
| 842302   | 0.03003          | 0         | .006193  | 25         | 5.38        | 17.    | 33      |
| 842517   | 0.01389          | 0         | .003532  | 24         | 1.99        | 23.    | 41      |
| 84300903 | 0.02250          | 0         | .004571  | 23         | 3.57        | 25.    | 53      |
| 84348301 | 0.05963          | 0         | .009208  | 14         | 1.91        | 26.    | 50      |
| 84358402 | 0.01756          | 0         | .005115  | 22         | 2.54        | 16.    | 67      |
| 843786   | 0.02165          | 0         | .005082  | 15         | 5.47        | 23.    | 75      |
| pe       | erimeter_worst   | area_wors | t smootl | ness_wor   | st compact: | ness_w | orst    |
| 842302   | 184.60           | 2019.     | 0        | 0.163      | 22          | 0.     | 6656    |
| 842517   | 158.80           | 1956.     | 0        | 0.123      | 38          | 0.     | 1866    |
| 84300903 | 152.50           | 1709.     | 0        | 0.14       | 14          | 0.     | 4245    |
| 84348301 | 98.87            | 567.      | 7        | 0.209      | 98          | 0.     | 8663    |
| 84358402 | 152.20           | 1575.     | 0        | 0.13       | 74          | 0.     | 2050    |
| 843786   | 103.40           | 741.      | 6        | 0.179      | 91          | 0.     | 5249    |
| C        | oncavity_worst   | concave.p | oints_w  | orst symme | etry_worst  |        |         |
| 842302   | 0.7119           |           | 0.5      | 2654       | 0.4601      |        |         |
| 842517   | 0.2416           |           | 0.3      | 1860       | 0.2750      |        |         |
| 84300903 | 0.4504           |           | 0.3      | 2430       | 0.3613      |        |         |
| 84348301 | 0.6869           |           | 0.3      | 2575       | 0.6638      |        |         |

| 84358402 | 0.4000                            | 0.1625 | 0.2364 |
|----------|-----------------------------------|--------|--------|
| 843786   | 0.5355                            | 0.1741 | 0.3985 |
|          | ${\tt fractal\_dimension\_worst}$ |        |        |
| 842302   | 0.11890                           |        |        |
| 842517   | 0.08902                           |        |        |
| 84300903 | 0.08758                           |        |        |
| 84348301 | 0.17300                           |        |        |
| 84358402 | 0.07678                           |        |        |
| 843786   | 0.12440                           |        |        |

Setup a separate new 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.

```
diagnosis <- factor(wisc.df$diagnosis)
diagnosis</pre>
```

```
[556] B B B B B B B M M M M M M B
Levels: B M
```

#### **Exploratory data analysis**

Q1. How many observations are in this dataset?

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

#### [1] 569

There are 569 observations.

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

```
summary(diagnosis)

B M
357 212

212 observations have a malignant diagnosis.
```

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

```
A=colnames(wisc.data)
  Α
 [1] "radius_mean"
                                "texture_mean"
 [3] "perimeter_mean"
                                "area_mean"
 [5] "smoothness_mean"
                                "compactness_mean"
 [7] "concavity_mean"
                                "concave.points_mean"
                                "fractal_dimension_mean"
 [9] "symmetry_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"
  grep("_mean",A)
 [1] 1 2 3 4 5 6 7 8 9 10
  length(grep("_mean",A))
```

10 variables are suffixed with \_mean.

## **Principal Component Analysis**

### **Performing PCA**

It is important to check if the data need to be scaled before performing PCA. Recall two common reasons for scaling data include:

- The input variables use different units of measurement.
- The input variables have significantly different variances.

Check the mean and standard deviation of the features (i.e. columns) of the wisc.data to determine if the data should be scaled. Use the colMeans() and apply() functions like you've done before.

#### colMeans(wisc.data)

| radius_mean               | texture_mean                   | perimeter_mean                    |
|---------------------------|--------------------------------|-----------------------------------|
| 1.412729e+01              | 1.928965e+01                   | 9.196903e+01                      |
| area_mean                 | ${\tt smoothness\_mean}$       | 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               | ${\tt fractal\_dimension\_se}$ | 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                      |
| ${\tt smoothness\_worst}$ | ${\tt compactness\_worst}$     | concavity_worst                   |
| 1.323686e-01              | 2.542650e-01                   | 2.721885e-01                      |
| concave.points_worst      | symmetry_worst                 | ${\tt fractal\_dimension\_worst}$ |
| 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
                                                            3.002518e-03
          2.021855e+00
                                   4.549101e+01
        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
                                perimeter_worst
         texture_worst
                                                              area_worst
          6.146258e+00
                                   3.360254e+01
                                                            5.693570e+02
                              compactness_worst
      smoothness_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
```

```
wisc.pr <- prcomp(wisc.data,scale=TRUE )
summary(wisc.pr)</pre>
```

#### 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 0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624 Standard deviation 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)?

44.3% of the original variance is captured by the first principal components

```
PC1 <- wisc.pr$x[,1]
PC2 <- wisc.pr$x[,2]
```

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

```
wisc.pr.var.per[1]
```

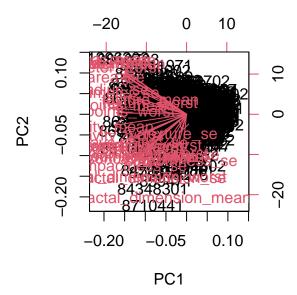
[1] 44.3

```
wisc.pr.var.per[1]+wisc.pr.var.per[2]
[1] 63.3
  wisc.pr.var.per[1]+wisc.pr.var.per[2]+wisc.pr.var.per[3]
[1] 72.7
3 principal components (PCs) are required to describe at least 70% of the original variance in
the data.
Q6. How many principal components (PCs) are required to describe at least 90% of the original
variance in the data?
  wisc.pr.var.per[1]+wisc.pr.var.per[2]+wisc.pr.var.per[3]+wisc.pr.var.per[4]
[1] 79.3
  wisc.pr.var.per[1]+wisc.pr.var.per[2]+wisc.pr.var.per[3]+wisc.pr.var.per[4]+wisc.pr.var.pe
[1] 84.8
  wisc.pr.var.per[1]+wisc.pr.var.per[2]+wisc.pr.var.per[3]+wisc.pr.var.per[4]+wisc.pr.var.pe
[1] 88.8
  wisc.pr.var.per[1]+wisc.pr.var.per[2]+wisc.pr.var.per[3]+wisc.pr.var.per[4]+wisc.pr.var.pe
[1] 91.1
```

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

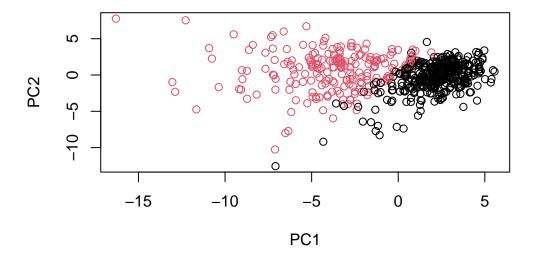
#### Interpreting PCA results

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

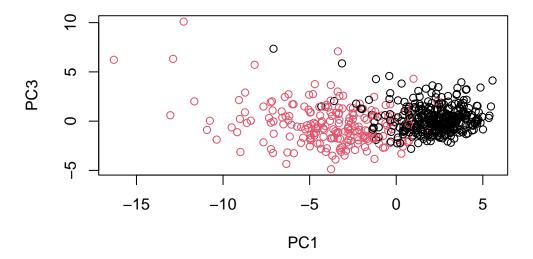


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why? Too much captions. The data has not been filtered and processed.

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



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



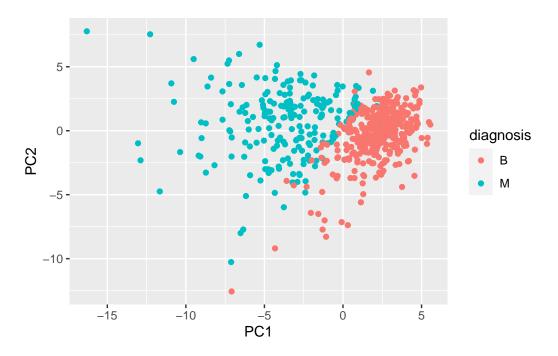
The malignment ones have similar distribution in values of PC 1.

As this is such a striking result let's see if we can use the  $\mathbf{ggplot2}$  package to make a more fancy figure of these results

```
# 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()</pre>
```



#### 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.

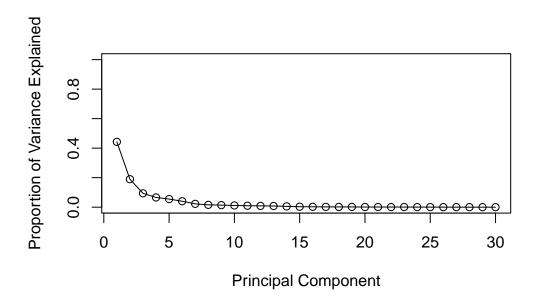
```
pr.var <- wisc.pr$sdev^2
head(pr.var)</pre>
```

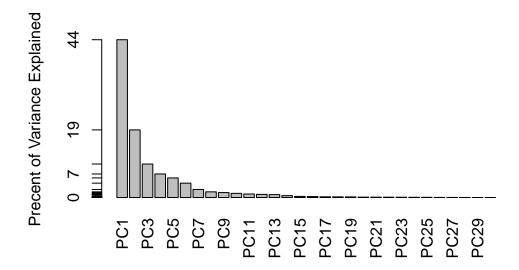
```
[1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357
```

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./

```
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")</pre>
```





### **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? This tells us how much this original feature contributes to the first PC.

#### wisc.pr\$rotation[,1]

| perimeter_mean    | texture_mean             | radius_mean            |
|-------------------|--------------------------|------------------------|
| -0.22753729       | -0.10372458              | -0.21890244            |
| compactness_mean  | ${\tt smoothness\_mean}$ | area_mean              |
| -0.23928535       | -0.14258969              | -0.22099499            |
| symmetry_mean     | concave.points_mean      | concavity_mean         |
| -0.13816696       | -0.26085376              | -0.25840048            |
| texture_se        | radius_se                | fractal_dimension_mean |
| -0.01742803       | -0.20597878              | -0.06436335            |
| smoothness_se     | area_se                  | perimeter_se           |
| -0.01453145       | -0.20286964              | -0.21132592            |
| concave.points_se | concavity_se             | compactness_se         |
| -0.18341740       | -0.15358979              | -0.17039345            |
| radius_worst      | fractal_dimension_se     | symmetry_se            |
|                   |                          |                        |

```
-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 loading vector (i.e. wisc.pr\$rotation[,1]) for the feature concave.points\_mean is -0.26085376.

### 3. Hierarchical clustering

First scale the wisc.data data and assign the result to data.scaled.

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

Calculate the (Euclidean) distances between all pairs of observations in the new scaled dataset and assign the result to data.dist.

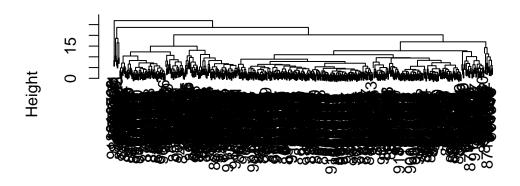
```
data.dist <-dist(data.scaled)</pre>
```

Create 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")</pre>
```

Q10 Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

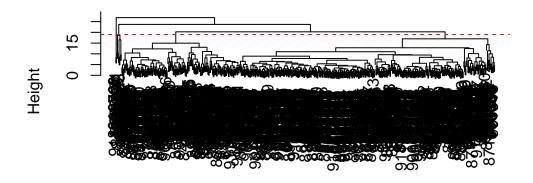
```
plot(wisc.hclust)
```



data.dist hclust (\*, "complete")

```
I choose height =19

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



data.dist hclust (\*, "complete")

#### Selecting number of clusters

Use cutree() to cut the tree so that it has 4 clusters. Assign the output to the variable wisc.hclust.clusters.

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

We can use the table() function to compare the cluster membership to the 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
```

Here we picked four clusters and see that cluster 1 largely corresponds to malignant cells (with diagnosis values of 1) whilst cluster 3 largely corresponds to benign cells (with diagnosis values of 0).

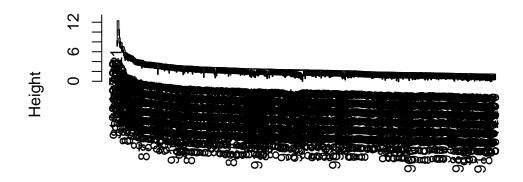
## Using different methods

There are number of different "methods" we can use to combine points during the hierarchical clustering procedure. These include "single", "complete", "average" and (my favorite) "ward.D2"

"single"

```
plot(hclust(data.dist, method="single"))
```

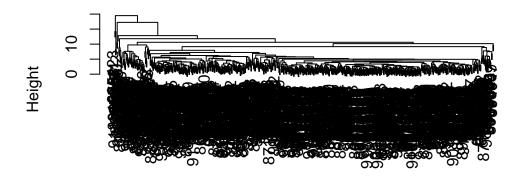
# **Cluster Dendrogram**



data.dist hclust (\*, "single")

"average"

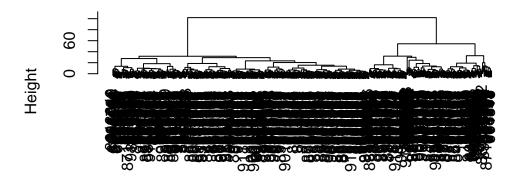
```
plot(hclust(data.dist, method="average"))
```



data.dist hclust (\*, "average")

"ward.D2"

plot(hclust(data.dist, method="ward.D2"))



data.dist hclust (\*, "ward.D2")

Q12 Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

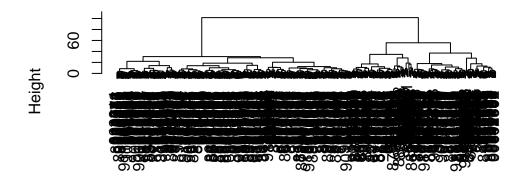
I like ward.D2 the best. It looks more clear and more equally-distributed.

# 4. Combining methods

#### Clustering on PCA results

Using the minimum number of principal components required to describe at least 90% of the variability in the data, create a hierarchical clustering model with the linkage method="ward.D2". We use Ward's criterion here because it is based on multidimensional variance like principal components analysis. Assign the results to wisc.pr.hclust.

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



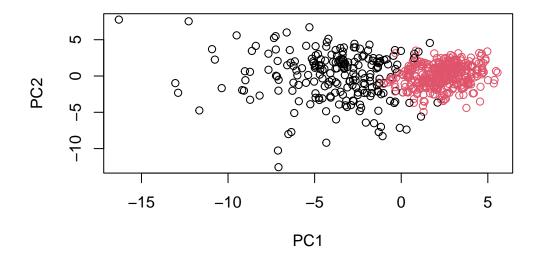
dist(wisc.pr\$x[, 1:7]) hclust (\*, "ward.D2")

This looks much more promising than our previous clustering results on the original scaled data. Note the two main branches of or dendrogram indicating two main clusters - maybe these are malignant and benign.

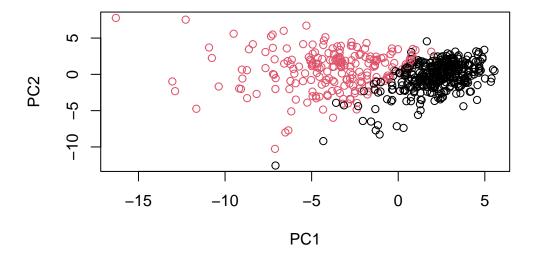
```
table(grps, diagnosis)

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)



Cut this hierarchical clustering model into 2 clusters and assign the results to wisc.pr.hclust.clusters.

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

Q13 How well does the newly created model with four clusters separate out the two diagnoses?

Q14 How well do the 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.

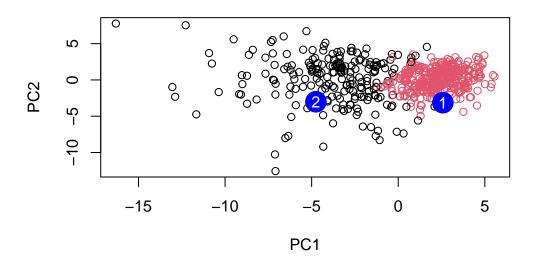
```
diagnosis
wisc.hclust.clusters B M
1 12 165
2 2 5
3 343 40
4 0 2
```

#### 6. Prediction

We will use the predict() function that will take our PCA model from before and new cancer cell data and project that data onto our PCA space.

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

```
PC1
                                PC3
                                           PC4
                                                     PC5
                     PC2
                                                                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
[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
                     PC16
                                 PC17
                                             PC18
                                                         PC19
[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
                      PC22
                                 PC23
                                                        PC25
           PC21
                                            PC24
                                                                     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
     0.220199544 -0.02946023 -0.015620933 0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
  plot(wisc.pr$x[,1:2], col=grps)
  points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
  text(npc[,1], npc[,2], c(1,2), col="white")
```



Black is group 1(M dominant), Red is group 2(B dominant)

Patient 1 should be prioritized.