# Class 08 Mini Project

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In today's mini-project we will explore a complete analysis using unsupervised learning techniques – clustering and PCA.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set FNA breast biopsy data

## **Data Import**

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

Remove the first column:

```
# We can use -1 here to remove the first column
wisc.data <- wisc.df[,-1]
head(wisc.data)</pre>
```

	radius_mean te	xture_mean	perimet	er_mean	${\tt area\_mean}$	${\tt smoothness\_mean}$
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	0.10030
843786	12.45	15.70		82.57	477.1	0.12780
	compactness_me	an concavit	y_mean	concave	points_mea	an symmetry_mean
842302	0.277	60	0.3001		0.1471	.0 0.2419
842517	0.078	64	0.0869		0.0701	.7 0.1812
84300903	0.159	90	0.1974		0.1279	0.2069

84348301       0.28390       0.2414       0.10520       0.2597         84358402       0.13280       0.1980       0.10430       0.1809         843786       0.17000       0.1578       0.08089       0.2087	9					
843786 0.17000 0.1578 0.08089 0.2087						
	7					
<pre>fractal_dimension_mean radius_se texture_se perimeter_se area_se</pre>						
842302 0.07871 1.0950 0.9053 8.589 153.40						
842517 0.05667 0.5435 0.7339 3.398 74.08						
84300903 0.05999 0.7456 0.7869 4.585 94.03						
84348301 0.09744 0.4956 1.1560 3.445 27.23						
84358402 0.05883 0.7572 0.7813 5.438 94.44						
843786 0.07613 0.3345 0.8902 2.217 27.19						
<pre>smoothness_se compactness_se concavity_se concave.points_se</pre>						
842302 0.006399 0.04904 0.05373 0.01587						
842517 0.005225 0.01308 0.01860 0.01340						
84300903 0.006150 0.04006 0.03832 0.02058						
84348301 0.009110 0.07458 0.05661 0.01867						
84358402 0.011490 0.02461 0.05688 0.01885						
843786 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						
<pre>perimeter_worst area_worst smoothness_worst compactness_worst</pre>						
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

Creating a vector diagnosis that has the diagnosis data.

# Create diagnosis vector for later
diagnosis <- wisc.df\$diagnosis
diagnosis</pre>

Q1. How many observations are in this dataset?

There are 569 observations/patients in the data set.

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

#### [1] 569

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

There are 212 observations with a malignant diagnosis. This was found by using grep() function to see which elements in diagnosis vector have malignant ("M") diagnosis.

#grep to look for matches with malignant diagnoses and length to see how many matches in t length(grep("M", diagnosis))

#### [1] 212

```
#or can use table() function to count up the malignant diagnoses
table(diagnosis)
```

#### diagnosis

B M

357 212

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

Let's look at the column names first:

#### 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"
```

The grep() function helps us to look for the column names containing "\_mean". The length() function will show the results of the vector.

```
#look through column names to find ones with "mean" with the grep function
#use length to find the number of column names with the key word
matches <- (grep("_mean", colnames(wisc.data)))
length(matches)</pre>
```

[1] 10

There are 10 variables/features suffixed with \_mean.

Q. How many dimensions are in this dataset?

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

Г1] 30

## **Principal Component Analysis (PCA)**

Let's check the mean and standard deviation:

```
# Check column means and standard deviations
colMeans(wisc.data)
```

perimeter_mean	texture_mean	radius_mean
9.196903e+01	1.928965e+01	1.412729e+01
compactness_mean	smoothness_mean	area_mean
1.043410e-01	9.636028e-02	6.548891e+02
symmetry_mean	concave.points_mean	concavity_mean
1.811619e-01	4.891915e-02	8.879932e-02
texture_se	radius se	fractal dimension mean

```
6.279761e-02
                                 4.051721e-01
                                                          1.216853e+00
        perimeter_se
                                      area_se
                                                         smoothness_se
        2.866059e+00
                                 4.033708e+01
                                                         7.040979e-03
                                 concavity_se
      compactness_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))

radius_mean	texture_mean	perimeter_mean
4	4	24
area_mean	${\tt smoothness\_mean}$	${\tt compactness\_mean}$
352	0	0
concavity_mean	concave.points_mean	${\tt symmetry\_mean}$
0	0	0
${\tt fractal\_dimension\_mean}$	radius_se	texture_se
0	0	1
perimeter_se	area_se	smoothness_se
2	45	0
compactness_se	concavity_se	concave.points_se
0	0	0
symmetry_se	fractal_dimension_se	radius_worst
0	0	5
texture_worst	perimeter_worst	area_worst
6	34	569
smoothness_worst	compactness_worst	concavity_worst
0	0	0
concave.points_worst	symmetry_worst	${\tt fractal\_dimension\_worst}$
0	0	0

The data above is not standardized at all. First we need to scale the data with prcomp().

```
# Perform PCA on wisc.data by completing the following code
wisc.pr <- prcomp(wisc.data, scale = TRUE)</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
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
                       0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
Cumulative Proportion
                                   PC23
                                          PC24
                                                  PC25
                                                          PC26
                          PC22
                                                                  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 covers 44.27% of the original variance of the whole data set. This makes sense because PC1 covers the most and the subsequent PCs start covering less.

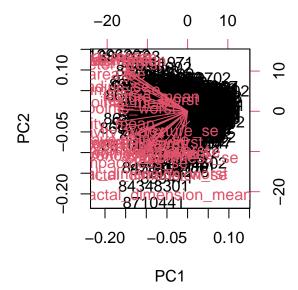
Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data?

We look at the cumulative proportion of the components, and see that three PCs are needed to describe at least 70% of the original variance. Three of them show 72.6% of the original variance.

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

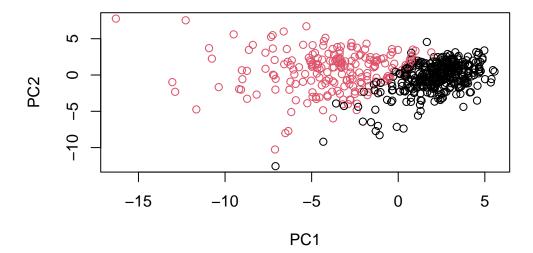
Seven PCs describe at least 90% of the original variance.

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

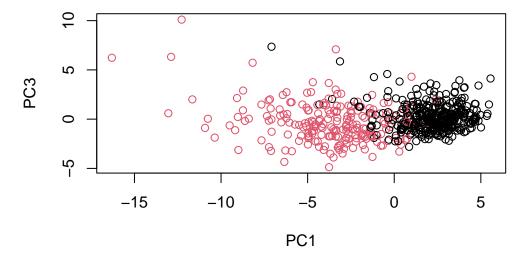


This plot is very cluttered and hard to understand. It uses rownames as plotting characters and makes it hard to distinguish any trend with the eye.

Let's make a standard scatter plot of PC1 vs PC2.



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



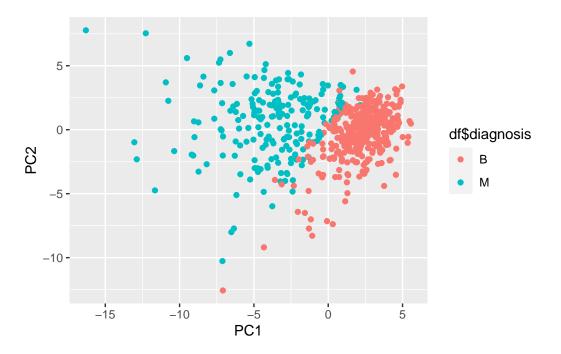
The separation between the two groups are less distinct than PC1 vs PC2 since they have better proportion of original variance than PC3.

Use ggplot to make a better visualization plot.

```
# 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=df$diagnosis) +
   geom_point()</pre>
```



#### **Scree Plots**

Scree plots are used to show the proportion of variance. They have 'elbows' where you can figure out number of principal components by eye more naturally.

We will begin by calculating te variance of each principal component. To do this, we sequare the sdev of wisc.pr

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

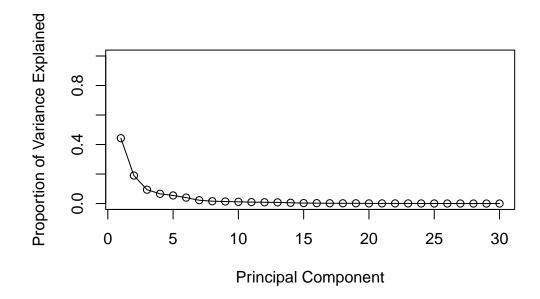
```
[1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357
```

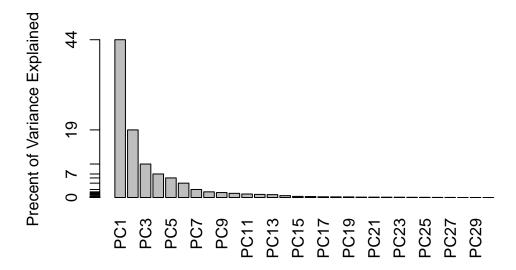
Now we will calculate the variance given by each principal component. We will divide the variance from each PC by the total variance.

```
# 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",</pre>
```

```
ylab = "Proportion of Variance Explained",
ylim = c(0, 1), type = "o")
```





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? We can see this through \$rotation.

## head(wisc.pr\$rotation)

	PC1	PC2	PC3	PC4	PC5
radius_mean	-0.2189024	0.23385713	-0.008531243	0.04140896 -0	.03778635
texture_mean	-0.1037246	0.05970609	0.064549903 -	-0.60305000 0	.04946885
perimeter_mean	-0.2275373	0.21518136	-0.009314220	0.04198310 -0	.03737466
area_mean	-0.2209950	0.23107671	0.028699526	0.05343380 -0	.01033125
${\tt smoothness\_mean}$	-0.1425897	-0.18611302	-0.104291904	0.15938277 0	.36508853
compactness_mean	-0.2392854	-0.15189161	-0.074091571	0.03179458 -0	.01170397
	PO	C6 PC	7 PC8	PC9	PC10
radius_mean	0.01874079	90 -0.1240883	4 0.007452296	5 -0.223109764	0.09548644
texture_mean	-0.03217883	37 0.0113995	4 -0.130674825	0.112699390	0.24093407
perimeter_mean	0.01730844	15 -0.1144770	6 0.018687258	3 -0.223739213	0.08638562
area_mean	-0.00188774	18 -0.0516534	3 -0.034673604	1 -0.195586014	0.07495649
${\tt smoothness\_mean}$	-0.28637449	97 -0.1406689	9 0.288974575	0.006424722	-0.06929268
compactness_mean	-0.01413094	19 0.0309185	0 0.151396350	0.167841425	0.01293620
	PC1:	PC12	PC13	PC14	PC15

```
-0.04147149 0.05106746 0.01196721 0.059506135 -0.05111877
radius_mean
texture_mean
                0.30224340 \quad 0.25489642 \ 0.20346133 \ -0.021560100 \ -0.10792242
               -0.01678264 0.03892611 0.04410950 0.048513812 -0.03990294
perimeter_mean
area_mean
               -0.11016964 0.06543751 0.06737574 0.010830829 0.01396691
smoothness mean
                0.13702184  0.31672721  0.04557360  0.445064860  -0.11814336
compactness_mean 0.30800963 -0.10401704 0.22928130 0.008101057 0.23089996
                     PC16
                                PC17
                                            PC18
                                                       PC19
radius_mean
               -0.1505839 0.20292425 0.146712338 0.22538466 -0.04969866
texture mean
               -0.1578420 -0.03870612 -0.041102985
                                                 0.02978864 -0.24413499
perimeter_mean
               -0.1144540 0.19482131 0.158317455
                                                 0.23959528 -0.01766501
area_mean
               -0.2046132 \quad 0.16792991 \ -0.352226802 \ -0.16456584 \quad 0.01710096
smoothness_mean
compactness_mean 0.1701784 -0.02030771 0.007794138 0.28422236
                                                            0.48868633
                                 PC22
                      PC21
                                              PC23
                                                         PC24
                                                                    PC25
radius_mean
               -0.06857001 -0.07292890 -0.0985526942 -0.18257944 -0.01922650
                0.44836947 -0.09480063 -0.0005549975 0.09878679
texture_mean
                                                              0.08474593
perimeter_mean
               -0.06976904 -0.07516048 -0.0402447050 -0.11664888
                                                              0.02701541
               -0.01844328 -0.09756578 0.0077772734 0.06984834 -0.21004078
area_mean
               -0.11949175 -0.06382295 -0.0206657211 0.06869742
smoothness_mean
                                                              0.02895489
compactness mean 0.19262140 0.09807756 0.0523603957 -0.10413552
                                                              0.39662323
                      PC26
                                 PC27
                                              PC28
                                                          PC29
radius mean
               -0.12947640 -0.13152667 2.111940e-01 0.211460455
texture_mean
               -0.02455666 -0.01735731 -6.581146e-05 -0.010533934
               -0.12525595 -0.11541542 8.433827e-02 0.383826098
perimeter_mean
area_mean
                -0.03700369 0.06968992 1.479269e-03 -0.003434667
smoothness_mean
                compactness_mean
                       PC30
radius_mean
                0.702414091
texture_mean
                0.000273661
perimeter_mean
               -0.689896968
area_mean
               -0.032947348
smoothness_mean
               -0.004847458
compactness_mean 0.044674186
```

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

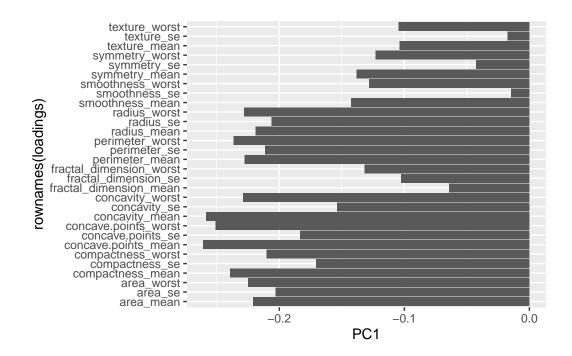
#### [1] -0.2608538

The component of the loading vector for concave.points\_mean is -0.26085376.

There is a complicated mix of variables that go together to make up PC1 - i.e. there are many of the original variables that together contribute highly to PC1.

```
loadings <- as.data.frame(wisc.pr$rotation)

ggplot(loadings) +
  aes(PC1, rownames(loadings)) +
  geom_col()</pre>
```



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

There are a minimum of 23 PCs required for 80% of the variance.

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

#### Importance of components:

PC1 PC2 PC3 PC4 PC5 PC6 PC7 Standard deviation 1.37000 1.02185 1.01192 1.01122 1.00434 1.0025 1.00234 Proportion of Variance 0.06256 0.03481 0.03413 0.03409 0.03362 0.0335 0.03349 Cumulative Proportion 0.06256 0.09737 0.13150 0.16559 0.19921 0.2327 0.26620

```
PC8
                                   PC9
                                          PC10
                                                  PC11
                                                          PC12
                                                                  PC13
                                                                          PC14
Standard deviation
                       1.00214 1.00143 1.00089 1.00070 1.00047 1.00039 1.00035
Proportion of Variance 0.03348 0.03343 0.03339 0.03338 0.03336 0.03336 0.03336
Cumulative Proportion
                       0.29968 0.33311 0.36650 0.39988 0.43324 0.46660 0.49996
                          PC15
                                  PC16
                                          PC17
                                                  PC18
                                                          PC19
                                                                  PC20
                                                                          PC21
Standard deviation
                       1.00018 1.00016 1.00009 1.00008 1.00005 1.00003 1.00001
Proportion of Variance 0.03335 0.03334 0.03334 0.03334 0.03334 0.03333
Cumulative Proportion
                       0.53330 \ 0.56665 \ 0.59999 \ 0.63333 \ 0.66666 \ 0.70000 \ 0.73333
                          PC22
                                  PC23
                                          PC24
                                                  PC25
                                                          PC26
                                                                  PC27
Standard deviation
                       1.00001 1.00000 1.00000 1.00000 1.00000 1.00000
Proportion of Variance 0.03333 0.03333 0.03333 0.03333 0.03333 0.03333
Cumulative Proportion
                       0.76667 0.80000 0.83333 0.86667 0.90000 0.93333 0.96667
                          PC29
                                    PC30
Standard deviation
                       1.00000 6.075e-16
Proportion of Variance 0.03333 0.000e+00
Cumulative Proportion 1.00000 1.000e+00
```

### **Hierarchical Clustering**

Hierarchical clustering computes the distances between all pairs of observations.

We will start by scaling the data.

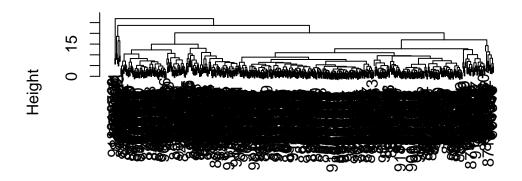
```
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)</pre>
```

Calculate the Euclidean distances between all pairs of observations from the scaled data.

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

Now create a hierarchical clustering

```
wisc.hclust <- hclust(data.dist)
plot(wisc.hclust)</pre>
```

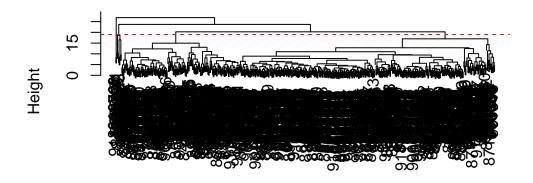


data.dist hclust (\*, "complete")

Q11. Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters?

The clustering model has 4 clusters at h=19.

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



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

Cut this tree with cutree() function.

```
grps <- cutree(wisc.hclust,h=19)
# a table of groups and their diagnoses
table(grps, diagnosis)</pre>
```

## diagnosis grps 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?

Yes, we can do this with the cutree() function.

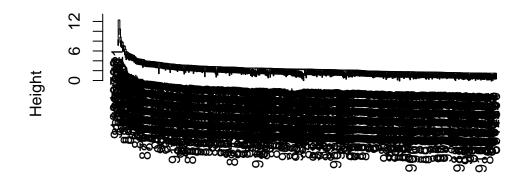
```
wisc.hclust.clusters <- cutree(wisc.hclust, h=20)
table(wisc.hclust.clusters, diagnosis)</pre>
```

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

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

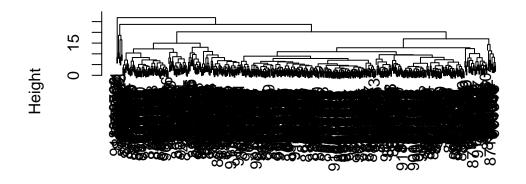
```
plot(hclust(data.dist, "single"))
```

# **Cluster Dendrogram**



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

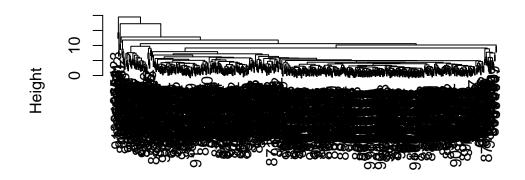
```
plot(hclust(data.dist, "complete"))
```



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

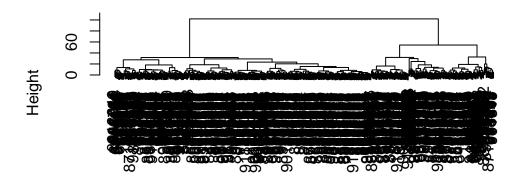
plot(hclust(data.dist, "average"))

# **Cluster Dendrogram**



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

```
plot(hclust(data.dist, "ward.D2"))
```

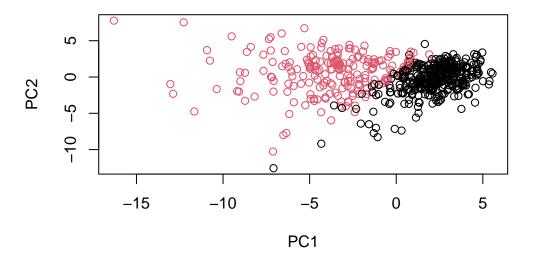


data.dist hclust (\*, "ward.D2")

My favorite is ward.D2 as it shows the clusters better visually and it is easier to identify where the clusters are, especially at the top. It is more spaced out with the clusters.

## Combine Methods: PCA and HCLUST

My PCA results interestingly showed a separation of M and B samples along PC1.

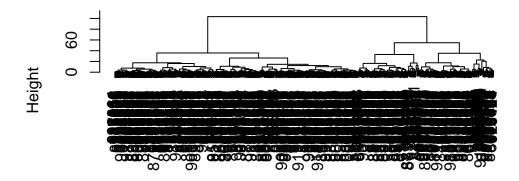


I want to cluster my PCA results - that is use wisc.pr\$x as input to hclust(). Try clustering in 3 PCs, that is PC1, PC2, PC3.

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

Tree result figure:

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



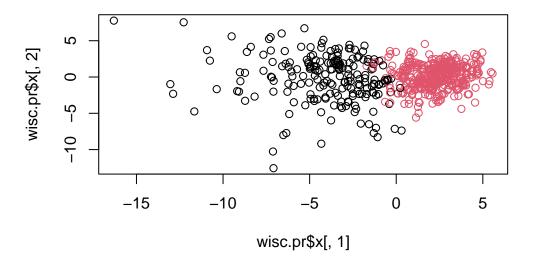
d hclust (\*, "ward.D2")

Let's cut this tree into two groups/clusters

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

grps
1    2
203 366

plot(wisc.pr$x[,1], wisc.pr$x[,2], col = grps)</pre>
```



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

How well do the clusters separate the M and B diagnoses?

```
table(grps, diagnosis)

diagnosis
grps B M
    1 24 179
    2 333 33

(179+333)/nrow(wisc.data)

[1] 0.8998243
```