# mini-project

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#### Unsupervised Learning

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

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)
```

Q1. How many observations are in this dataset? Q2. How many of the observations have a malignant diagnosis? Q3. How many variables/features in the data are suffixed with \_mean? The functions dim(), nrow(), table(), length() and grep() may be useful for answering the first 3 questions above.

```
# How many observations are in this dataset?
nrow(wisc.data)
```

## [1] 569

```
# How many of the observations have a malignant diagnosis?
sum(diagnosis=="M")
```

## [1] 212

```
# How many variables/features in the data are suffixed with _mean?
length(grep("_mean$", colnames(wisc.data)))
```

## [1] 10

#### 2. Principal Component Analysis

Performing PCA The next step in your analysis is to perform principal component analysis (PCA) on wisc.data.

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.

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

```
##
                                                               perimeter_mean
               radius_mean
                                        texture_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
                                                                  radius_worst
##
                symmetry_se
                               fractal_dimension_se
##
              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
##
                                        2.542650e-01
              1.323686e-01
                                                                  2.721885e-01
##
      concave.points_worst
                                      symmetry_worst fractal_dimension_worst
##
              1.146062e-01
                                        2.900756e-01
                                                                  8.394582e-02
##
                          X
##
                         NA
```

#### 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
##
##
##
                         NΑ
```

```
# Perform PCA on wisc.data by completing the following code
wisc.data = subset (wisc.data, select = -X)
wisc.pr <- prcomp(wisc.data , scale. = TRUE)
summary(wisc.pr)</pre>
```

```
## Importance of components:
                             PC1
                                             PC3
                                                     PC4
                                                             PC5
                                                                     PC6
##
                                    PC2
                                                                             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
## 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
                          0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
## Standard deviation
## Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
                          0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
## Cumulative Proportion
                             PC29
                                     PC30
## Standard deviation
                          0.02736 0.01153
## Proportion of Variance 0.00002 0.00000
## Cumulative Proportion 1.00000 1.00000
```

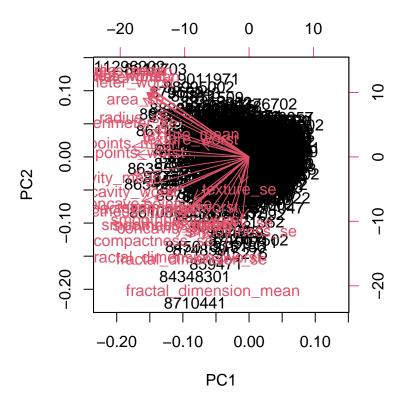
Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)? A: 0.4427 Q5. How many principal components (PCs) are required to describe at least 70% of the original variance in the data? A: 3 Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data? A: 7

## Interpreting PCA results

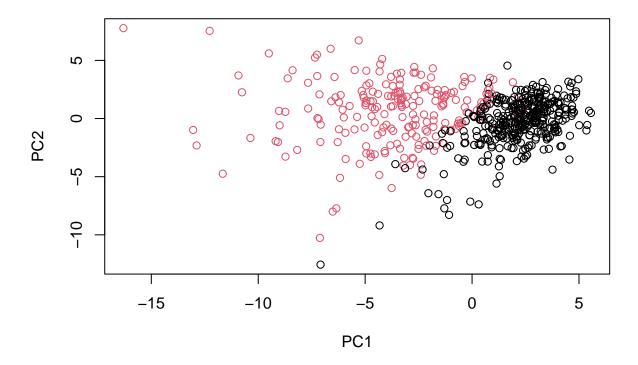
Now you will use some visualizations to better understand your PCA model. A common visualization for PCA results is the so-called biplot.

However, you will often run into some common challenges with using biplots on real-world data containing a non-trivial number of observations and variables. Here we will need to look at some alternative visualizations. You are encouraged to experiment with additional visualizations before moving on to the next section

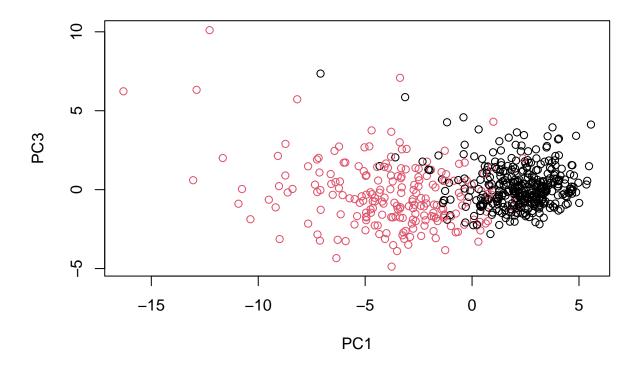
Create a biplot of the wisc.pr using the biplot() function.



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



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

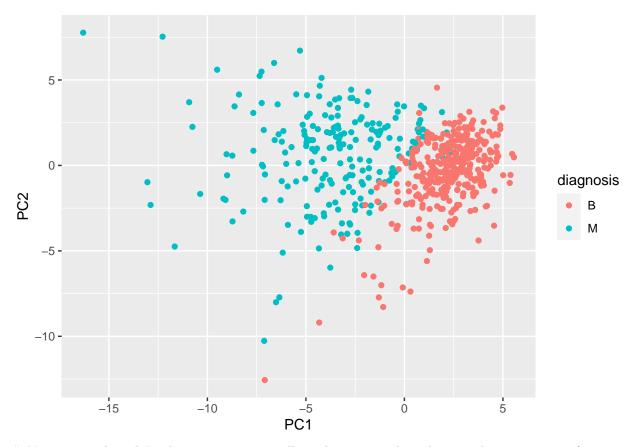


Overall, the plots indicate that principal component 1 is capturing a separation of malignant (red) from benign (black) samples. This is an important and interesting result worthy of further exploration - as we will do in the next sections!

```
# 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 In this exercise, you will produce scree plots showing the proportion of variance explained as the number of principal components increases. The data from PCA must be prepared for these plots, as there is not a built-in function in base R to create them directly from the PCA model.

As you look at these plots, ask yourself if there's an 'elbow' in the amount of variance explained that might lead you to pick a natural number of principal components. If an obvious elbow does not exist, as is typical in some real-world datasets, consider how else you might determine the number of principal components to retain based on the scree plot.

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

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

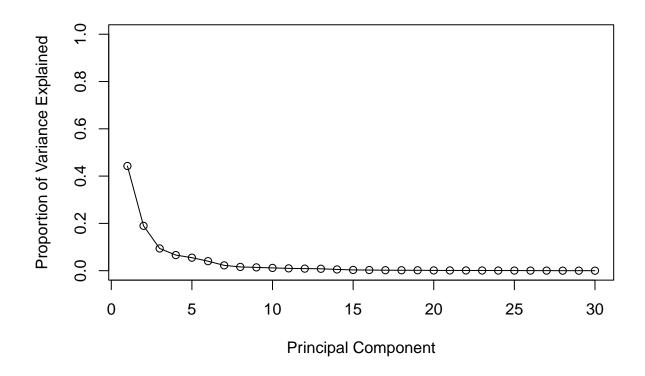
```
## [1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357
```

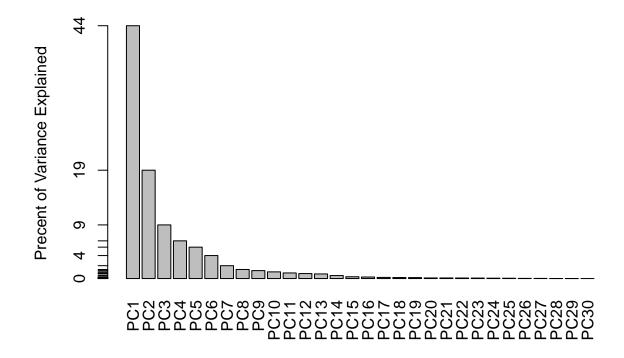
Calculate the variance explained by each principal component by dividing by the total variance explained of all principal components. Assign this to a variable called pve and create a plot of variance explained for each principal component.

```
# Variance explained by each principal component: pve
pve <- pr.var / sum(pr.var)

# Plot variance explained for each principal component
plot(pve, xlab = "Principal Component",</pre>
```

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



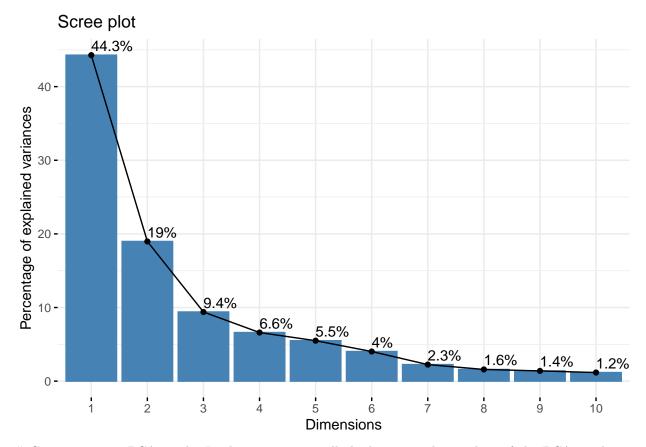


OPTIONAL: There are quite a few CRAN packages that are helpful for PCA. This includes the factoextra package. Feel free to explore this package. For example:

```
## ggplot based graph
#install.packages("factoextra")
library(factoextra)

## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa

fviz_eig(wisc.pr, addlabels = TRUE)
```



# Communicating PCA results In this section we will check your understanding of the PCA results, in particular the loadings and variance explained. The loadings, represented as vectors, explain the mapping from the original features to the principal components. The principal components are naturally ordered from the most variance explained to the least variance explained.

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? A: -0.2608538

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

```
## concave.points_mean
## -0.2608538
```

Q10. What is the minimum number of principal components required to explain 80% of the variance of the data? A: 5

#### 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
                                                            PC12
##
                              PC8
                                      PC9
                                             PC10
                                                    PC11
                                                                    PC13
## 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
                                                              PC19
##
                             PC15
                                     PC16
                                             PC17
                                                      PC18
                                                                      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
## 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
```

#### 3. Hierarchical clustering

The goal of this section is to do hierarchical clustering of the original data. Recall from class that this type of clustering does not assume in advance the number of natural groups that exist in the data.

As part of the preparation for hierarchical clustering, the distance between all pairs of observations are computed. Furthermore, there are different ways to link clusters together, with single, complete, and average being the most common linkage methods.

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>
```

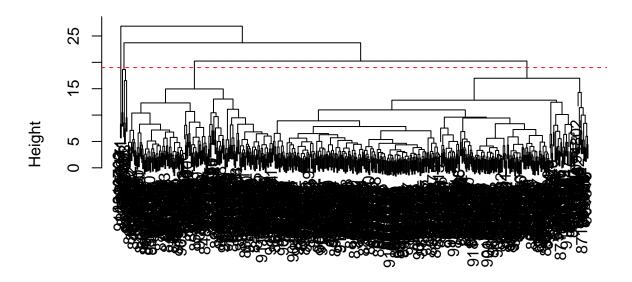
### Results of hierarchical clustering

Let's use the hierarchical clustering model you just created to determine a height (or distance between clusters) where a certain number of clusters exists.

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

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

### **Cluster Dendrogram**



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

# Selecting number of clusters In this section, you will compare the outputs from your hierarchical clustering model to the actual diagnoses. Normally when performing unsupervised learning like this, a target variable (i.e. known answer or labels) isn't available. We do have it with this dataset, however, so it can be used to check the performance of the clustering model.

When performing supervised learning - that is, when you're trying to predict some target variable of interest and that target variable is available in the original data - using clustering to create new features may or may not improve the performance of the final model.

This exercise will help you determine if, in this case, hierarchical clustering provides a promising new feature.

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)
table(wisc.hclust.clusters, diagnosis)</pre>
```

##		diagr	nosis
##	wisc.hclust.clusters	В	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).

Before moving on, explore how different numbers of clusters affect the ability of the hierarchical clustering to separate the different diagnoses.

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10? A: 4 and 5 both looks good

```
print(i)
  wisc.hclust.clusters <- cutree(wisc.hclust, k=i)</pre>
  print(table(wisc.hclust.clusters, diagnosis))
## [1] 2
                         diagnosis
##
## wisc.hclust.clusters
                            В
                                 М
                        1 357 210
##
##
                        2
                             0
                                 2
##
   [1] 3
##
                         diagnosis
## wisc.hclust.clusters
                            В
                        1 355 205
##
##
                             2
                                 5
                             0
                                 2
##
                        3
## [1] 4
##
                         diagnosis
## wisc.hclust.clusters
                            В
                                 М
##
                        1
                           12 165
##
                        2
                             2
                                 5
##
                        3 343
                                40
                                 2
##
                             0
   [1] 5
##
##
                         diagnosis
   wisc.hclust.clusters
                             В
##
                        1
                           12 165
                        2
##
                             0
                                 5
                        3 343
                                40
##
##
                             2
                                 0
                        5
                             0
                                 2
##
##
   [1] 6
##
                         diagnosis
##
   wisc.hclust.clusters
                            В
                                 М
##
                        1
                           12 165
##
                        2
                             0
                                 5
                        3 331
##
                                39
##
                        4
                             2
                                 0
                        5
##
                           12
                                 1
                             0
                                 2
##
   [1] 7
##
##
                         diagnosis
##
   wisc.hclust.clusters
                            В
##
                           12 165
                        1
##
                        2
                             0
                                 3
                        3 331
##
                                39
##
                        4
                            2
                                 0
                        5
                           12
##
                                 1
##
                        6
                            0
                                 2
                                 2
##
                        7
                             0
```

for (i in 2:10){

```
## [1] 8
##
                            diagnosis
##
   wisc.hclust.clusters
                               В
                                    Μ
                              12
##
                                   86
##
                           2
                               0
                                   79
                           3
                               0
                                    3
##
                           4
                             331
                                   39
##
                           5
##
                               2
                                    0
##
                           6
                              12
                                    1
                           7
                               0
                                    2
##
##
                           8
                               0
                                    2
   [1] 9
##
##
                            diagnosis
##
   wisc.hclust.clusters
                               В
                              12
##
                                   86
                           2
##
                               0
                                   79
                           3
                               0
                                    3
##
##
                           4
                             331
                                   39
##
                          5
                                    0
                               2
##
                           6
                              12
                                    0
##
                           7
                               0
                                    2
##
                           8
                               0
                                    2
                           9
                               0
                                    1
##
   [1] 10
##
##
                            diagnosis
##
   wisc.hclust.clusters
                               В
                                    Μ
##
                              12
                                   86
                         2
                               0
                                   59
##
                         3
##
                               0
                                    3
##
                         4
                             331
                                   39
##
                         5
                                   20
##
                         6
                               2
                                    0
                         7
##
                              12
                                    0
##
                         8
                               0
                                    2
                                    2
##
                         9
                               0
##
                         10
                               0
                                    1
```

# Using different methods

As we discussed in our last class videos 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".

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

A: I think complete and Ward.D2 are both much better than the other methods because they have much clear separation of the diagnoses at each cluster than the rest.

```
wisc.hclust_single <- hclust(data.dist, method = "single")
wisc.hclust.clusters <- cutree(wisc.hclust_single, k=4)
table(wisc.hclust.clusters, diagnosis)</pre>
```

## diagnosis

```
## wisc.hclust.clusters
                            В
##
                        1 356 209
##
                            1
                                0
                                2
##
                        3
                            0
##
                            0
wisc.hclust_avg <- hclust(data.dist, method = "average")</pre>
wisc.hclust.clusters <- cutree(wisc.hclust avg, k=4)
table(wisc.hclust.clusters, diagnosis)
##
                         diagnosis
  wisc.hclust.clusters
                            В
                                М
##
                        1 355 209
                            2
                                0
##
                        3
                            0
##
                                1
##
                            0
                                2
wisc.hclust_ward <- hclust(data.dist, method = "ward.D2")</pre>
wisc.hclust.clusters <- cutree(wisc.hclust_ward, k=4)</pre>
table(wisc.hclust.clusters, diagnosis)
##
                         diagnosis
##
  wisc.hclust.clusters
                            В
                                М
```

### 4. OPTIONAL: K-means clustering

2

3 337

0 115

48

1

6 48

14

K-means clustering and comparing results In class we discussed two main types of clustering: hierarchical and k-means.

In this optional section, you will create a k-means clustering model on the Wisconsin breast cancer data and compare the results to the actual diagnoses and the results of your hierarchical clustering model. Take some time to see how each clustering model performs in terms of separating the two diagnoses and how the clustering models compare to each other.

Create a k-means model on wisc.data, assigning the result to wisc.km. Be sure to create 2 clusters, corresponding to the actual number of diagnosis. Also, remember to scale the data (with the scale() function and repeat the algorithm 20 times (by setting setting the value of the nstart argument appropriately). Running multiple times such as this will help to find a well performing model.

```
wisc.km <- kmeans(scale(wisc.data), centers= 2, nstart= 20)</pre>
```

Use the table() function to compare the cluster membership of the k-means model (wisc.km\$cluster) to the actual diagnoses contained in the diagnosis vector.

```
table(wisc.km$cluster, diagnosis)
```

```
## diagnosis
## B M
## 1 343 37
## 2 14 175
```

##

##

##

##

Q14. How well does k-means separate the two diagnoses? How does it compare to your helust results? diagnosis B M 1 14 175 2 343 37 TP:175, FP:14 TN:343, FN:37 **Accuracy**, essentially how many did we get correct? **Sensitivity**: TP/(TP+FN) **Specificity**: TN/(TN+FN) A: kmeans has better separation for diagnosis because it has less false classification when it has 2 clusters compared with heluster when we cut the tree to less or equal to 4 groups

Use the table() function to compare the cluster membership of the k-means model (wisc.km\$cluster) to your hierarchical clustering model from above (wisc.hclust.clusters). Recall the cluster membership of the hierarchical clustering model is contained in wisc.hclust.clusters object.

#### table(wisc.hclust.clusters,wisc.km\$cluster)

Looking at the second table you generated, it looks like clusters 1, 2, and 4 from the hierarchical clustering model can be interpreted as the cluster 1 equivalent from the k-means algorithm, and cluster 3 can be interpreted as the cluster 2 equivalent.

### 5. Combining methods

### Clustering on PCA results

In this final section, you will put together several steps you used earlier and, in doing so, you will experience some of the creativity and open endedness that is typical in unsupervised learning.

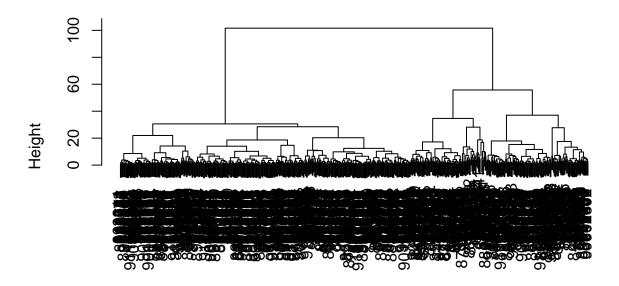
Recall from earlier sections that the PCA model required significantly fewer features to describe 70%, 80% and 95% of the variability of the data. In addition to normalizing data and potentially avoiding over-fitting, PCA also uncorrelates the variables, sometimes improving the performance of other modeling techniques.

Let's see if PCA improves or degrades the performance of hierarchical clustering.

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)</pre>
```

# **Cluster Dendrogram**



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

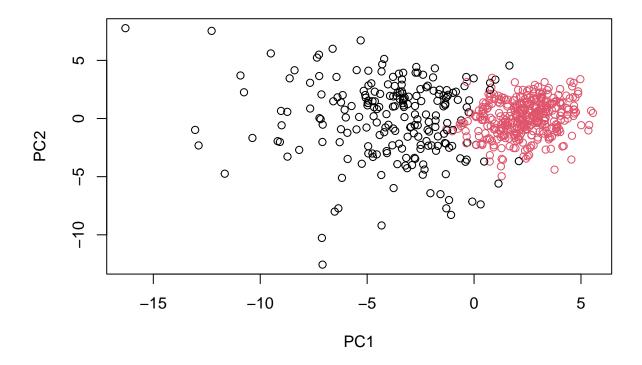
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)

## grps
## 1 2
## 216 353

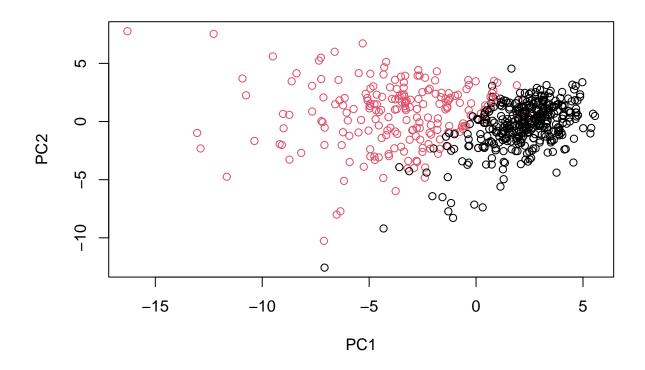
table(grps, diagnosis)

## diagnosis
## grps B M
## 1 28 188
## 2 329 24

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



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



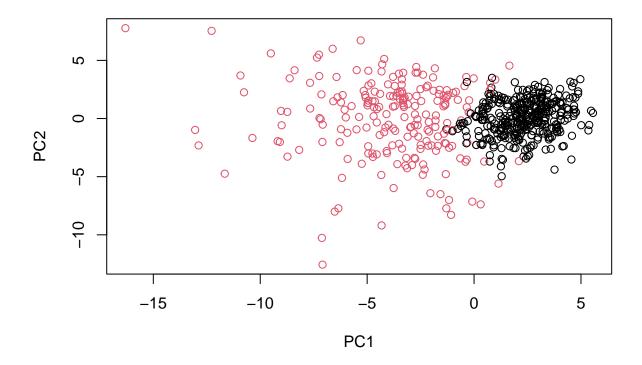
```
g <- as.factor(grps)
levels(g)

## [1] "1" "2"

g <- relevel(g,2)
levels(g)

## [1] "2" "1"

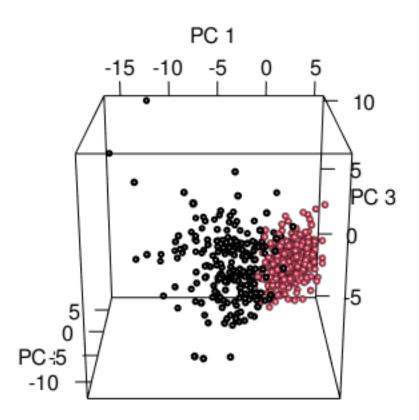
# Plot using our re-ordered factor
plot(wisc.pr$x[,1:2], col=g)</pre>
```



#### install.packages("rgl")

```
library(rgl)
plot3d(wisc.pr$x[,1:3], xlab="PC 1", ylab="PC 2", zlab="PC 3", cex=1.5, size=1, type="s", col=grps)
rglwidget(width = 400, height = 400)
```

## Warning in snapshot3d(scene = x, width = width, height = height): webshot = TRUE
## requires the webshot2 package; using rgl.snapshot() instead



To include the

interactive rgl plot in your HTML renderd lab report (not PDF) you can add the R code rglwidget(width = 400, height = 400) after you call the plot3d() function. It will look just like the plot above. Try rotating and zooming on this 3D plot.

```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method="ward.D2")</pre>
# Cut this hierarchical clustering model into 2 clusters and assign the results to wisc.pr.hclust.clust
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)</pre>
# Compare to actual diagnoses
table(wisc.pr.hclust.clusters, diagnosis)
```

```
##
                           diagnosis
## wisc.pr.hclust.clusters
                              В
                                  Μ
##
                            28 188
##
                          2 329
```

accuracy for PCA

```
(188+329)/569
```

```
## [1] 0.9086116
```

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. A: Kmeans is better at clustering this dataset

```
table(wisc.km$cluster, diagnosis)
```

```
## diagnosis
## B M
## 1 343 37
## 2 14 175
```

table(wisc.hclust.clusters, diagnosis)

```
## diagnosis
## wisc.hclust.clusters B M
## 1 0 115
## 2 6 48
## 3 337 48
## 4 14 1
```

B M 1 14 175 2 343 37 TP:175, FP:14 TN:343, FN:37 Sensitivity: TP/(TP+FN) Specificity: TN/(TN+FN) A: kmeans accuracy:

```
km_acc = (175+343)/569
km_sens = 175/(175+37)
km_spec = 343/(343+37)
cat(km_acc,km_sens,km_spec)
```

## 0.9103691 0.8254717 0.9026316

hcluster accuracy: diagnosis wisc.hclust.clusters B M 1 0 115 3 337 48

```
TP=115
FP=0
TN=337
FN=48
#Sensitivity
TP/(TP+FN)
```

## [1] 0.7055215

```
#Specificity
TN/(TN+FN)
```

## [1] 0.8753247

```
#accuracy
(TP+TN)/(TP+FP+TN+FN)
```

```
## [1] 0.904
```

##6. Sensitivity/Specificity Sensitivity refers to a test's ability to correctly detect ill patients who do have the condition. In our example here the sensitivity is the total number of samples in the cluster identified as predominantly malignant (cancerous) divided by the total number of known malignant samples. In other words: TP/(TP+FN).

Specificity relates to a test's ability to correctly reject healthy patients without a condition. In our example specificity is the proportion of benign (not cancerous) samples in the cluster identified as predominantly benign that are known to be benign. In other words: TN/(TN+FN).

Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity? A: Kmeans is better in both specificity and sensitivity kmeans specificity: 0.9026316 hclust specificity: 0.8753247 kmeans sensitivity: 0.8254717 hclust sensitivity: 0.7055215

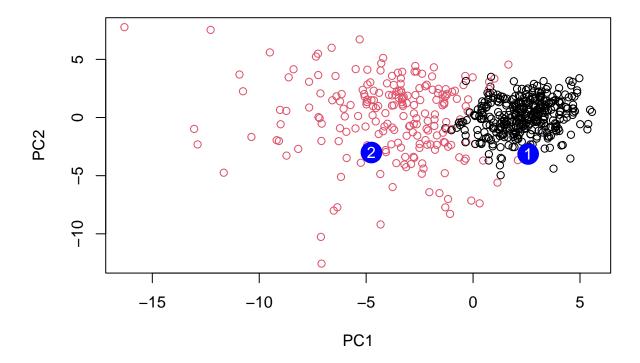
#### 7. Prediction

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
                        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
                                                        PC12
                                                                  PC13
##
                                             PC11
                                                                           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
                        PC16
##
             PC15
                                    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
                         PC22
##
              PC21
                                    PC23
                                               PC24
                                                            PC25
## [1,]
        0.1228233 0.09358453 0.08347651
                                         0.1223396
                                                     0.02124121
##
  [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=g)
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? A: patient 2 #About this document Here we use the sessionInfo() function to report on our R systems setup at the time of document execution.

#### sessionInfo()

```
## R version 4.1.1 (2021-08-10)
## Platform: x86 64-apple-darwin17.0 (64-bit)
## Running under: macOS Big Sur 10.16
## Matrix products: default
           /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
##
  [1] stats
                 graphics grDevices utils
                                               datasets
                                                         methods
                                                                    base
##
## other attached packages:
## [1] rgl_0.107.14
                        factoextra_1.0.7 ggplot2_3.3.5
##
## loaded via a namespace (and not attached):
   [1] tidyselect_1.1.1 xfun_0.27
                                            purrr_0.3.4
                                                               haven 2.4.3
                          colorspace_2.0-2 vctrs_0.3.8
   [5] carData_3.0-4
                                                               generics_0.1.1
##
```

```
## [9] htmltools_0.5.2
                          yaml_2.2.1
                                            utf8_1.2.2
                                                               rlang_0.4.12
## [13] pillar_1.6.4
                          ggpubr_0.4.0
                                            foreign_0.8-81
                                                               glue_1.4.2
## [17] withr_2.4.2
                          readxl_1.3.1
                                            lifecycle_1.0.1
                                                               stringr_1.4.0
## [21] cellranger_1.1.0
                          munsell_0.5.0
                                            ggsignif_0.6.3
                                                               gtable_0.3.0
## [25] zip_2.2.0
                          htmlwidgets_1.5.4 evaluate_0.14
                                                               labeling_0.4.2
                                                               fastmap_1.1.0
## [29] knitr_1.36
                          rio_0.5.27
                                            forcats_0.5.1
## [33] curl_4.3.2
                          fansi 0.5.0
                                            highr_0.9
                                                               broom 0.7.9
## [37] Rcpp_1.0.7
                          scales_1.1.1
                                            backports_1.3.0
                                                               jsonlite_1.7.2
                          farver_2.1.0
                                                               digest_0.6.28
## [41] abind_1.4-5
                                            hms 1.1.1
## [45] stringi_1.7.5
                          openxlsx_4.2.4
                                            rstatix_0.7.0
                                                               dplyr_1.0.7
## [49] ggrepel_0.9.1
                          grid_4.1.1
                                            tools_4.1.1
                                                               magrittr_2.0.1
## [53] tibble_3.1.5
                          crayon_1.4.1
                                            tidyr_1.1.4
                                                               car_3.0-11
## [57] pkgconfig_2.0.3
                          ellipsis_0.3.2
                                            data.table_1.14.2 rmarkdown_2.11
## [61] R6_2.5.1
                          compiler_4.1.1
```