Costa Stavrianidis Homework 3

In this homework, the objectives are to

- 1. Use R to examine and preprocess a dataset
- 2. Implement Unsupervised learning methods in a real-world scenario, including: Principal Component Analysis, Hierarchical Clustering, and K-means Clustering in R
- 3. Visualize and understand how to employ Principal Components, Hierarchical Clustering Dendrograms, and K-means Clustering in R

Please make sure to print your knitted .html file into a pdf before you submit it to the Gradescope, and you may only submit your .rmd file to Sakai. (Since Gradescope only allow you to upload pdf file, while sometimes students have problems in knitting pdf directly, hence please knit your rmd files as a html and print the html file as pdf.) 5 points will be deducted for every assignment submission that does not include either the RMarkdown file or the knitted html file. Your code should be adequately commented to clearly explain the steps you used to produce the analyses. RMarkdown homework files should be uploaded to Sakai with the naming convention date_lastname_firstname_HW[X].Rmd. For example, my first homework assignment would be named 20220830_Dunn_Jessilyn_HW1.Rmd. It is important to note that 5 points will be deducted for every assignment that is named improperly. Please add your answer to each question directly after the question prompt in the homework .Rmd file template provided below.

```
library(tidyverse)
library(ggplot2)
library(lubridate)
library(patchwork)
library(gridExtra)
library(psych)
library(corrplot)
library(ggfortify)
library(factoextra)
```

Dataset

Breast Cancer Prediction from Cytopathology Data https://www.kaggle.com/code/gpreda/breast-cancer-prediction-from-cytopathology-data/data (https://www.kaggle.com/code/gpreda/breast-cancer-prediction-from-cytopathology-data/data)

Data Preparation (30 points)

Download the cancer data titled "Breast_Cytopatholgy.csv" from Sakai and import it into R. Look at the
first 5 lines of the data to learn about the dataset. The "diagnosis" field shows whether the patient was
diagnosed with a benign or malignant tumor. Please read additional information about each column
online with the link above.

```
cancer <- read_csv("Breast_Cytopatholgy.csv")</pre>
```

```
## Rows: 569 Columns: 32
## — Column specification
## Delimiter: ","
## chr (1): diagnosis
## dbl (31): id, radius_mean, texture_mean, perimeter_mean, area_mean, smoothne...
##

## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
head(cancer, n=5)
```

```
## # A tibble: 5 × 32
##
         id diagn...1 radiu...2 textu...3 perim...4 area ...5 smoot...6 compa...7 conca...8 conca...9
##
      <dbl> <chr>
                       <dbl>
                               <dbl>
                                        <dbl>
                                                <dbl>
                                                        <dbl>
                                                                 <dbl>
                                                                         <dbl>
                                                                                  <dbl>
                                                                        0.300
## 1 8.42e5 M
                        18.0
                                10.4
                                        123.
                                                1001
                                                       0.118
                                                                0.278
                                                                                 0.147
## 2 8.43e5 M
                        20.6
                                17.8
                                        133.
                                                1326
                                                       0.0847 0.0786 0.0869
                                                                                 0.0702
## 3 8.43e7 M
                                                1203
                        19.7
                                21.2
                                        130
                                                       0.110
                                                                0.160
                                                                        0.197
                                                                                 0.128
## 4 8.43e7 M
                        11.4
                                20.4
                                        77.6
                                                 386.
                                                       0.142
                                                                0.284
                                                                        0.241
                                                                                 0.105
## 5 8.44e7 M
                        20.3
                                14.3
                                        135.
                                                1297
                                                       0.100
                                                                0.133
                                                                        0.198
                                                                                 0.104
## # ... with 22 more variables: symmetry mean <dbl>, fractal dimension mean <dbl>,
       radius_se <dbl>, texture_se <dbl>, perimeter_se <dbl>, area_se <dbl>,
## #
## #
       smoothness se <dbl>, compactness se <dbl>, concavity se <dbl>,
## #
       `concave points se` <dbl>, symmetry se <dbl>, fractal dimension se <dbl>,
       radius worst <dbl>, texture worst <dbl>, perimeter worst <dbl>,
## #
       area worst <dbl>, smoothness worst <dbl>, compactness worst <dbl>,
##
## #
       concavity worst <dbl>, `concave points worst` <dbl>, ...
```

- 2. Answer the following questions by using the summary function or other methods of your choice:
- a. How many observations are there in total?

```
nrow(cancer)
```

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

There are 569.

b. How many independent variables are there?

```
ncol(cancer) - 2
```

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

There are 30, because in the context of the problem, we are considering the "Diagnosis" variable to be dependent.

c. Is there any column with missing values? If yes, how many values are missing?

```
colSums(is.na(cancer))
```

radius_mean	diagnosis	id	##
_ 0	0	0	##
area_mean	perimeter_mean	texture_mean	##
0	0	0	##
concavity_mean	compactness_mean	smoothness_mean	##
0	0	0	##
<pre>fractal_dimension_mean</pre>	symmetry_mean	concave points_mean	##
6	0	0	##
perimeter_se	texture_se	radius_se	##
0	0	0	##
compactness_se	smoothness_se	area_se	##
0	0	0	##
symmetry_se	concave points_se	concavity_se	##
0	0	0	##
texture_worst	radius_worst	fractal_dimension_se	##
0	0	0	##
smoothness_worst	area_worst	perimeter_worst	##
0	0	0	##
concave points_worst	concavity_worst	compactness_worst	##
0	0	0	##
	fractal_dimension_worst	symmetry_worst	##
	0	0	##

Yes, there are 6 missing values in the 'fractal_dimension_mean' column.

d. How many observations are there with a malignant diagnosis and how many are there with a benign diagnosis?

```
sum(cancer$diagnosis == "M")
```

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

```
sum(cancer$diagnosis == "B")
```

```
## [1] 357
```

212 malignant, 357 benign.

For this question, please type your answers in full sentences outside of R chunks. Do not just show the output of running your code.

3. Change the "id" column into the index column (i.e. turn the ID values into row names) and delete the "id" column. Use str() to display the resulting dataframe. (5 points)

```
rownames(cancer) <- cancer$id
```

```
## Warning: Setting row names on a tibble is deprecated.
```

```
cancer <- cancer %>% subset(select=-id)
```

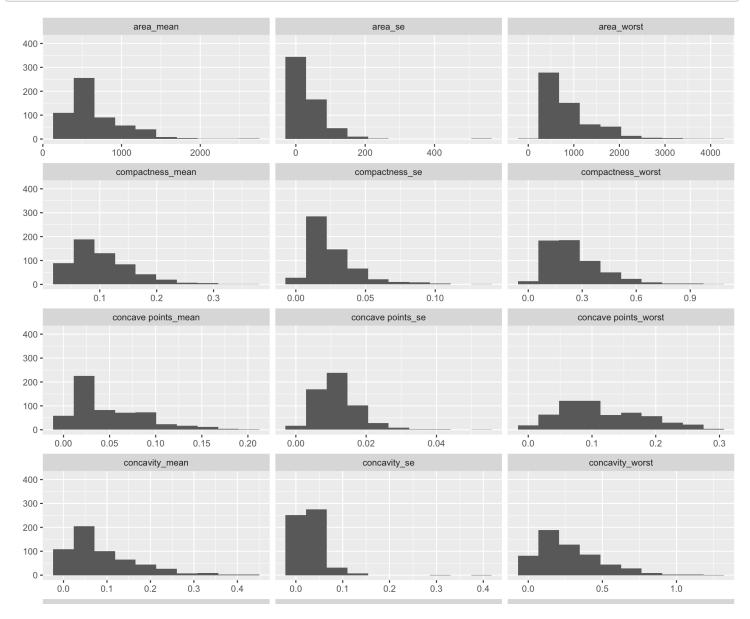
4. In this dataset, there isn't any column with a very large number of missing values. For the column(s) with some missing values, let's impute these missing values by mean substitution. Keep in mind that if it is reasonable to assume that the observations with missing values could have different distributions and characteristics for the two different diagnosis groups, imputation must be performed separately for the two different diagnosis groups.

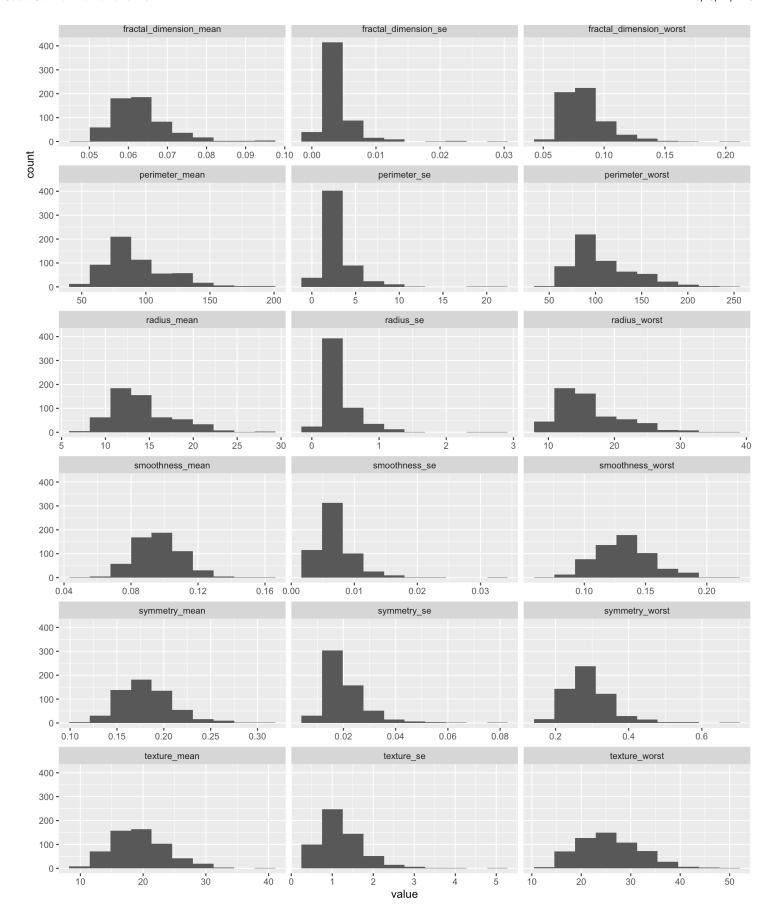
```
# Calculate means for different outcome groups
mean m <- cancer %>% filter(diagnosis == "M" & !is.na(fractal dimension mean)) %>%
  pull(fractal dimension mean) %>%
  mean
mean b <- cancer %>% filter(diagnosis == "B" & !is.na(fractal dimension mean)) %>%
  pull(fractal dimension mean) %>%
  mean
# Set empty values in variable to mean
cancer <- cancer %>%
  mutate(fractal_dimension_mean = ifelse(diagnosis == "M" & is.na(fractal_dimension_m
ean),
                                     mean m, fractal dimension mean)) %>%
  mutate(fractal_dimension_mean = ifelse(diagnosis == "B" & is.na(fractal_dimension_m
ean),
                                     mean b, fractal dimension mean))
sum(is.na(cancer$fractal dimension mean))
```

[1] 0

5. After imputation, use "ggplot" and "facet_wrap" to plot a 10 x 3 grid of histograms to explore the data shape and distribution of all the independent variables in this dataset. The dataset has 10 sets of independent variables, and each set consists of the mean, standard error and worst value of a particular cell measurement. For example, "area_se" is the standard error of area measurements from a particular patient in this study. Remember to select a reasonable number of bins when plotting and add legends and labels when appropriate. Adjust the size of the plot display so that you can see all the facets clearly when you knit.

```
cancer_plot <- cancer %>% subset(select=-diagnosis) %>% gather()
plot1 <- ggplot(cancer_plot, aes(value)) + geom_histogram(bins = 10) +
  facet_wrap(~key, scales = 'free_x', ncol = 3)
plot1</pre>
```





6. If you observe the independent variable distributions closely, groups of variables that start with "area",

"compactness" and "concavity" are consistently strongly skewed to the right. Apply log transform using formula log(x+1) to these 9 variables.

7. The pre-processed dataset needs to be scaled before performing PCA. Can you give a brief explanation as to why that is the case? Standardize the dataset. Use summary() again to show that your dataset has been properly standardized by checking the means and range of values of the variables.

```
# Create function for standardization
scale2 <- function(x) ((x - mean(x)) / sd(x))

# Apply function to every independent variable
cancer <- cancer %>% mutate_at(vars(-("diagnosis")), scale2)
summary(cancer)
```

```
##
     diagnosis
                        radius mean
                                                             perimeter_mean
                                           texture_mean
##
    Length:569
                       Min.
                               :-2.0279
                                          Min.
                                                  :-2.2273
                                                             Min.
                                                                    :-1.9828
                                                             1st Qu.:-0.6913
##
    Class :character
                       1st Ou.:-0.6888
                                          1st Qu.:-0.7253
##
    Mode :character
                       Median :-0.2149
                                          Median :-0.1045
                                                             Median :-0.2358
##
                        Mean
                               : 0.0000
                                                  : 0.0000
                                                                    : 0.0000
                                          Mean
                                                             Mean
##
                        3rd Ou.: 0.4690
                                          3rd Qu.: 0.5837
                                                             3rd Qu.: 0.4992
                               : 3.9678
##
                       Max.
                                          Max.
                                                  : 4.6478
                                                             Max.
                                                                    : 3.9726
##
      area mean
                      smoothness mean
                                          compactness mean
                                                             concavity mean
           :-2.8860
##
    Min.
                      Min.
                              :-3.10935
                                          Min.
                                                  :-1.6925
                                                             Min.
                                                                    :-1.1774
    1st Qu.:-0.6672
##
                      1st Ou.:-0.71034
                                          1st Qu.:-0.7556
                                                             1st Ou.:-0.7619
    Median :-0.1065
                      Median :-0.03486
                                          Median : -0.2049
##
                                                             Median :-0.3256
         : 0.0000
                             : 0.00000
##
    Mean
                      Mean
                                          Mean
                                                : 0.0000
                                                             Mean
                                                                    : 0.0000
    3rd Qu.: 0.6198
                       3rd Qu.: 0.63564
                                          3rd Qu.: 0.5237
##
                                                             3rd Qu.: 0.5746
##
           : 3.0268
                              : 4.76672
                                                  : 4.2564
                                                                    : 3.8920
    Max.
                      Max.
                                                             Max.
##
    concave points mean symmetry mean
                                            fractal_dimension_mean
##
    Min.
           :-1.2607
                        Min.
                                :-2.74171
                                            Min.
                                                    :-1.8259
##
    1st Ou.:-0.7373
                                            1st Ou.:-0.7205
                        1st Ou.:-0.70262
    Median :-0.3974
                        Median :-0.07156
                                            Median :-0.1620
##
   Mean
           : 0.0000
                        Mean : 0.00000
                                            Mean : 0.0000
##
    3rd Qu.: 0.6464
##
                         3rd Qu.: 0.53031
                                            3rd Qu.: 0.4735
##
    Max.
           : 3.9245
                        Max.
                                : 4.48081
                                            Max.
                                                    : 4.9554
```

```
##
      radius se
                                            perimeter se
                          texture se
                                                                 area se
##
            :-1.0590
                               :-1.5529
                                           Min.
                                                   :-1.0431
    Min.
                       Min.
                                                              Min.
                                                                      :-1.9362
                       1st Ou.:-0.6942
##
    1st Ou.:-0.6230
                                           1st Ou.:-0.6232
                                                              1st Ou.:-0.6865
##
    Median : -0.2920
                       Median :-0.1973
                                           Median :-0.2864
                                                              Median :-0.2568
##
    Mean
            : 0.0000
                       Mean
                               : 0.0000
                                           Mean
                                                   : 0.0000
                                                              Mean
                                                                      : 0.0000
##
    3rd Qu.: 0.2659
                       3rd Qu.: 0.4661
                                           3rd Qu.: 0.2428
                                                              3rd Qu.: 0.5832
                               : 6.6494
##
    Max.
            : 8.8991
                       Max.
                                           Max.
                                                   : 9.4537
                                                              Max.
                                                                      : 4.0749
##
    smoothness se
                       compactness se
                                            concavity_se
                                                              concave points se
##
            :-1.7745
                               :-1.3241
                                                   :-1.1284
                                                                      :-1.9118
    Min.
                       Min.
                                           Min.
                                                              Min.
##
    1st Ou.:-0.6235
                       1st Ou.:-0.6989
                                           1st Ou.:-0.5833
                                                              1st Ou.:-0.6739
    Median : -0.2201
                       Median :-0.2773
                                           Median :-0.1981
                                                              Median :-0.1404
##
##
    Mean
           : 0.0000
                       Mean
                               : 0.0000
                                           Mean
                                                   : 0.0000
                                                              Mean
                                                                      : 0.0000
                       3rd Qu.: 0.4028
                                           3rd Qu.: 0.3708
##
    3rd Ou.: 0.3680
                                                              3rd Qu.: 0.4722
##
    Max.
            : 8.0229
                       Max.
                               : 5.9323
                                           Max.
                                                   :11.0139
                                                              Max.
                                                                      : 6.6438
##
     symmetry se
                       fractal dimension se radius worst
                                                                 texture worst
##
    Min.
            :-1.5315
                               :-1.0960
                                                      :-1.7254
                                                                         :-2.22204
                       Min.
                                              Min.
                                                                 Min.
##
    1st Ou.:-0.6511
                       1st Ou.:-0.5846
                                              1st Ou.:-0.6743
                                                                  1st Ou.:-0.74797
    Median :-0.2192
                       Median :-0.2297
                                              Median :-0.2688
                                                                 Median :-0.04348
##
            : 0.0000
                                                      : 0.0000
##
    Mean
                       Mean
                               : 0.0000
                                              Mean
                                                                 Mean
                                                                         : 0.00000
##
    3rd Qu.: 0.3554
                       3rd Qu.: 0.2884
                                              3rd Qu.: 0.5216
                                                                  3rd Qu.: 0.65776
    Max.
            : 7.0657
                               : 9.8429
                                              Max.
                                                      : 4.0906
                                                                         : 3.88249
##
                       Max.
                                                                 Max.
    perimeter worst
                                           smoothness worst
##
                          area worst
                                                              compactness worst
##
    Min.
            :-1.6919
                       Min.
                               :-2.5092
                                           Min.
                                                  :-2.6803
                                                              Min.
                                                                      :-1.6394
    1st Qu.:-0.6890
                       1st Qu.:-0.6689
                                           1st Qu.:-0.6906
##
                                                              1st Qu.:-0.6990
    Median :-0.2857
                       Median :-0.1521
                                           Median :-0.0468
                                                              Median :-0.2316
##
##
    Mean
           : 0.0000
                       Mean
                               : 0.0000
                                                  : 0.0000
                                                                      : 0.0000
                                           Mean
                                                              Mean
                       3rd Qu.: 0.6712
##
    3rd Ou.: 0.5398
                                           3rd Qu.: 0.5970
                                                              3rd Qu.: 0.6186
##
    Max.
            : 4.2836
                               : 3.1371
                                           Max.
                                                   : 3.9519
                                                              Max.
                                                                      : 4.2793
                       Max.
    concavity worst
##
                       concave points worst symmetry worst
                               :-1.7435
##
    Min.
            :-1.4782
                       Min.
                                              Min.
                                                      :-2.1591
##
    1st Qu.:-0.7766
                       1st Qu.:-0.7557
                                              1st Qu.:-0.6413
    Median :-0.1557
                       Median :-0.2233
                                              Median :-0.1273
##
##
    Mean
            : 0.0000
                               : 0.0000
                                                      : 0.0000
                       Mean
                                              Mean
##
    3rd Qu.: 0.6201
                       3rd Qu.: 0.7119
                                              3rd Qu.: 0.4497
##
            : 3.7763
                               : 2.6835
                                              Max.
                                                      : 6.0407
    Max.
                       Max.
##
    fractal dimension worst
           :-1.6004
##
    Min.
    1st Qu.:-0.6913
##
##
    Median :-0.2163
            : 0.0000
##
    Mean
##
    3rd Qu.: 0.4504
##
            : 6.8408
    Max.
```

PCA is looking for the sequence of linear combinations of the variables that have maximal variance. Since it is trying to maximize variance, the variables will have different variances depending on their individual scales. If you change one variable's scale from kg to g, it will then have more variance. Since the scale clearly matters for PCA, we must standardize the different variables to put them on the same scale beforehand.

PCA (25 points)

8. Calculate the principal components using the function princomp() and print the summary of the results.

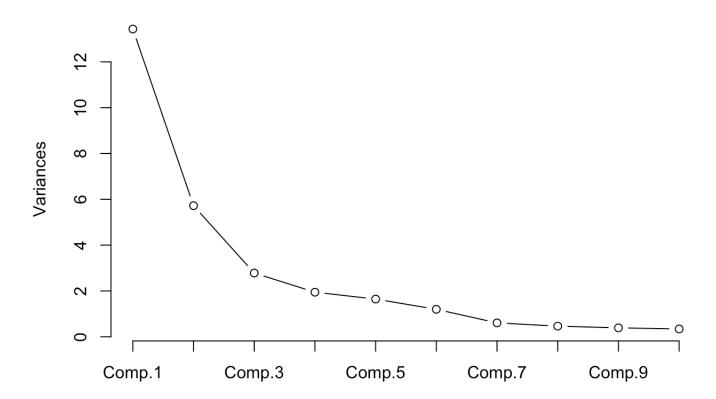
```
pca_cancer <- princomp(cancer[,-1])
pca_sum <- summary(pca_cancer)
pca_sum</pre>
```

```
##
   Importance of components:
                                                              Comp.4
##
                              Comp.1
                                        Comp.2
                                                   Comp.3
                                                                          Comp.5
                          3.6649813 2.3922560 1.66811749 1.39504520 1.28282751
## Standard deviation
  Proportion of Variance 0.4485245 0.1910988 0.09291716 0.06498591 0.05495146
                          0.4485245 0.6396234 0.73254052 0.79752643 0.85247789
  Cumulative Proportion
##
                                          Comp.7
                                                     Comp.8
                              Comp.6
                                                                Comp.9
                                                                           Comp.10
## Standard deviation
                          1.09535614 0.77911399 0.68072240 0.62488147 0.58480539
## Proportion of Variance 0.04006391 0.02026958 0.01547329 0.01303881 0.01141998
  Cumulative Proportion
                           0.89254180 0.91281138 0.92828467 0.94132348 0.95274347
##
                              Comp.11
                                           Comp.12
                                                       Comp.13
## Standard deviation
                          0.527120745 0.496992966 0.480676398 0.401643553
  Proportion of Variance 0.009278182 0.008247896 0.007715219 0.005386718
##
  Cumulative Proportion
                          0.962021648 0.970269544 0.977984763 0.983371481
##
                              Comp.15
                                           Comp.16
                                                       Comp.17
## Standard deviation
                          0.300490558 0.289969850 0.268537964 0.235037574
  Proportion of Variance 0.003015118 0.002807685 0.002407987 0.001844664
  Cumulative Proportion
                          0.986386600 0.989194284 0.991602271 0.993446935
##
##
                              Comp.19
                                           Comp.20
                                                       Comp.21
                                                                    Comp.22
## Standard deviation
                          0.193208881 0.179478677 0.174145056 0.1639589564
  Proportion of Variance 0.001246513 0.001075644 0.001012663 0.0008976623
                          0.994693448 0.995769092 0.996781755 0.9976794170
  Cumulative Proportion
##
                               Comp.23
                                             Comp.24
                                                          Comp.25
                                                                        Comp.26
## Standard deviation
                          0.1475830310 0.1210596744 0.1114839259 0.1055347689
## Proportion of Variance 0.0007273032 0.0004893749 0.0004150182 0.0003719065
## Cumulative Proportion
                          0.9984067203 0.9988960952 0.9993111134 0.9996830199
##
                               Comp.27
                                             Comp.28
                                                          Comp.29
                                                                        Comp.30
## Standard deviation
                          0.0840075545 4.101507e-02 2.477457e-02 1.180696e-02
## Proportion of Variance 0.0002356565 5.617327e-05 2.049533e-05 4.654990e-06
## Cumulative Proportion
                          0.9999186764 9.999748e-01 9.999953e-01 1.000000e+00
```

9. Plot a scree plot using the screeplot() function.

```
screeplot(pca_sum, type = 'lines')
```

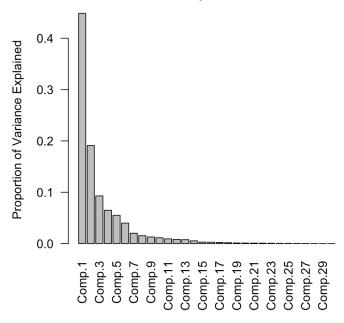




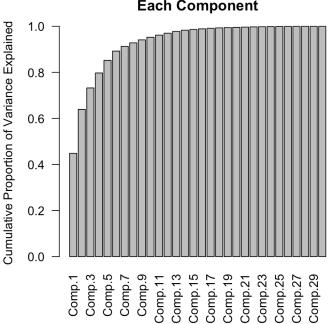
- 10. Plot the following two plots and use patchwork/gridExtra to position the two plots side by side:
- a. proportion of variance explained by the number of principal components
- b. cumulative proportion of variance explained by the number of principal components; draw horizontal lines at 88% of variance and 95% variance.

Note: please remember to clearly label your plots with titles, axis labels and legends when appropriate.

Proportion of Variance Explained by Each Component



Cumulative Proportion of Variance Explained by Each Component



11. What proportions of variance are captured from the first, second and third principal components? How many principal components do you need to describe at least 88% and 95% of the variance, respectively?

```
print(c(pov[1], pov[2], pov[3]))
```

```
## Comp.1 Comp.2 Comp.3
## 0.44852454 0.19109881 0.09291716
```

```
pov_cum[pov_cum>.88]
```

```
##
      Comp.6
                Comp. 7
                           Comp.8
                                     Comp.9
                                               Comp.10
                                                         Comp.11
                                                                    Comp.12
                                                                              Comp.13
## 0.8925418 0.9128114 0.9282847 0.9413235 0.9527435 0.9620216 0.9702695 0.9779848
##
     Comp.14
               Comp.15
                          Comp.16
                                    Comp.17
                                               Comp.18
                                                         Comp.19
                                                                    Comp.20
                                                                              Comp.21
## 0.9833715 0.9863866 0.9891943 0.9916023 0.9934469 0.9946934 0.9957691 0.9967818
##
               Comp.23
                                    Comp.25
                                               Comp.26
                                                                    Comp.28
                                                                              Comp.29
     Comp.22
                          Comp.24
                                                         Comp.27
## 0.9976794 0.9984067 0.9988961 0.9993111 0.9996830 0.9999187 0.9999748 0.9999953
##
     Comp.30
## 1.000000
```

```
pov_cum[pov_cum>.95]
```

```
##
     Comp.10
               Comp.11
                          Comp.12
                                    Comp.13
                                               Comp.14
                                                         Comp.15
                                                                    Comp.16
                                                                              Comp.17
## 0.9527435 0.9620216 0.9702695 0.9779848 0.9833715 0.9863866 0.9891943 0.9916023
##
     Comp.18
               Comp.19
                          Comp.20
                                    Comp.21
                                               Comp.22
                                                         Comp.23
                                                                    Comp.24
                                                                              Comp.25
## 0.9934469 0.9946934 0.9957691 0.9967818 0.9976794 0.9984067 0.9988961 0.9993111
##
     Comp.26
               Comp.27
                          Comp.28
                                    Comp.29
                                               Comp.30
## 0.9996830 0.9999187 0.9999748 0.9999953 1.0000000
```

The first, second, and third components capture 0.44852454, 0.19109881, and 0.09291716 of the variance, respectively.

You need 6 principal components to describe at least 88% of the variance, and 10 to capture at least 95% of the variance.

12. Which are the top 2 variables that contribute the most to the variance captured from PC1, PC2, and PC3 respectively? (hint: look at the loadings information)

```
sort(abs(pca_sum$loadings[,2]), decreasing = T)[1:2]
```

```
## fractal_dimension_mean fractal_dimension_se
## 0.3687653 0.2841809
```

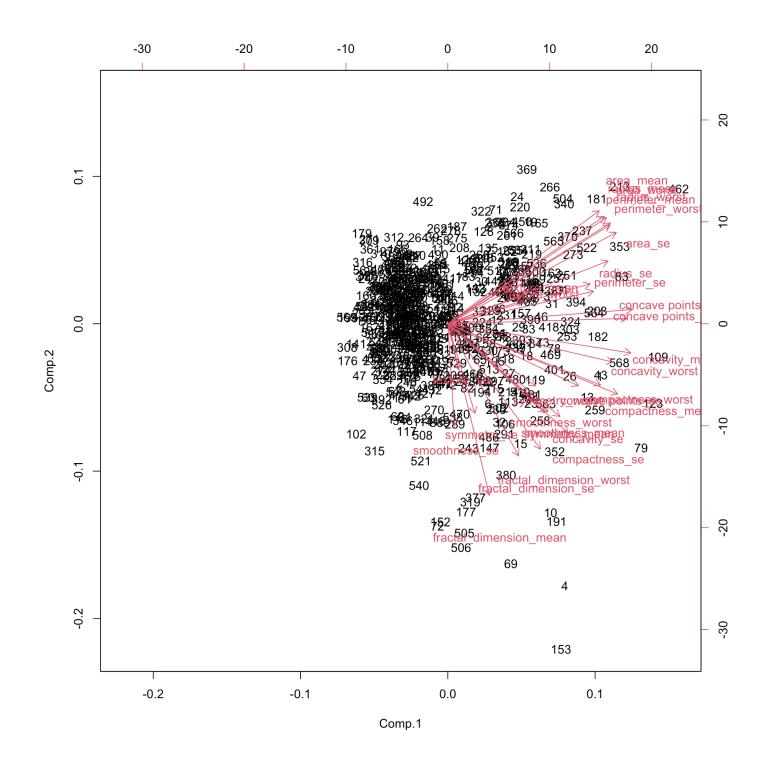
```
sort(abs(pca_sum$loadings[,3]), decreasing = T)[1:2]
```

```
## texture_se smoothness_se
## 0.3936197 0.2929809
```

The top 2 variables for PC1 are concave points_mean and concavity_mean. The top 2 variables for PC2 are fractal_dimension_mean and fractal_dimension_se. The top 2 variables for PC3 are texture_se and smoothness se.

13. Plot a biplot using the biplot() function.

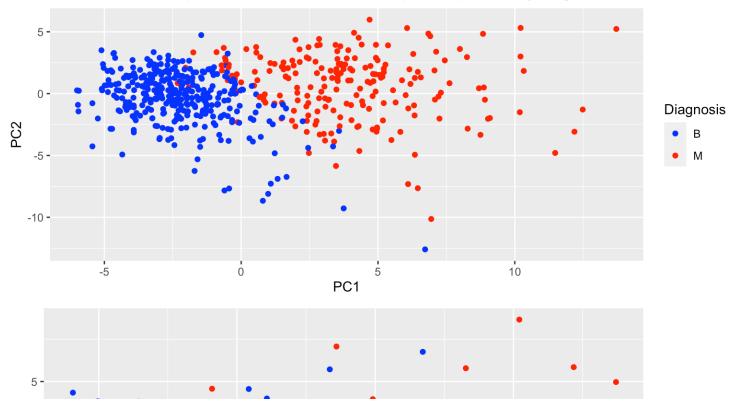
biplot(pca_cancer)

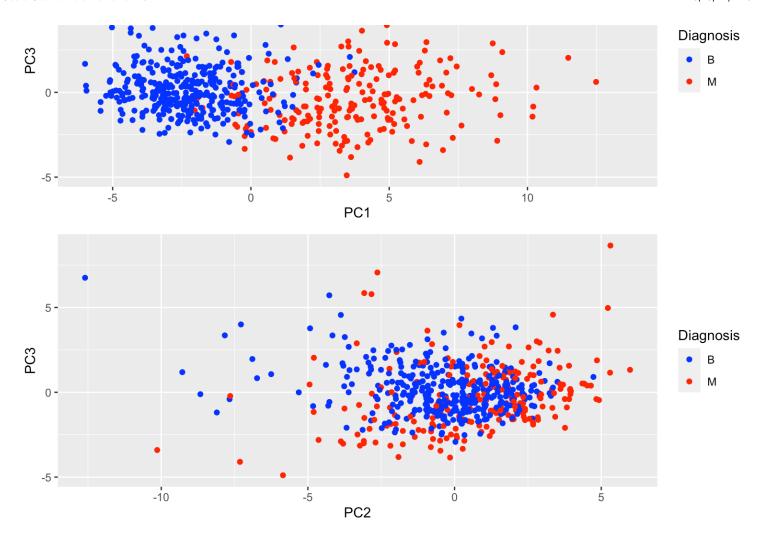


14. Plot a 3 x 1 grid of scatter plots, where each plot is a scatter plot between two of the first 3 principal components, with different colors for each diagnosis group. For example, in grid cell (1,1), you should plot a scatter plot where the x-axis is PC1 and the y-axis is PC2, where red observations correspond to malignant diagnosis and blue observations correspond to the benign diagnosis. Remember to adjust the plot display size so that you can see clearly. Add legends and labels when appropriate.

```
# Create dataframe of principle components with their scores and diagnosis for each
# observation
pc_3 <- pca_cancer$scores[,1:3]</pre>
pc_3_diag <- data.frame(pc_3, as.factor(cancer$diagnosis))</pre>
colnames(pc 3 diag) <- c("PC1", "PC2", "PC3", "Diagnosis")</pre>
# Plot scatterplots
plot1 <- ggplot(pc_3_diag, aes(x = PC1, y = PC2, color = Diagnosis)) + geom_point() +</pre>
  scale_color_manual(values=c("blue", "red"))
plot2 <- ggplot(pc 3 diag, aes(x = PC1, y = PC3, color = Diagnosis)) + geom point() +
  scale_color_manual(values=c("blue", "red"))
plot3 <- ggplot(pc 3 diag, aes(x = PC2, y = PC3, color = Diagnosis)) + geom point() +
  scale color manual(values=c("blue", "red"))
plotlist <- list(plot1, plot2, plot3)</pre>
grid.arrange(grobs = plotlist, ncol = 1,
             top = "Scatterplots Between First Three Principal Components by Diagnosi
s")
```

Scatterplots Between First Three Principal Components by Diagnosis





Hierarchical Clustering (15 points)

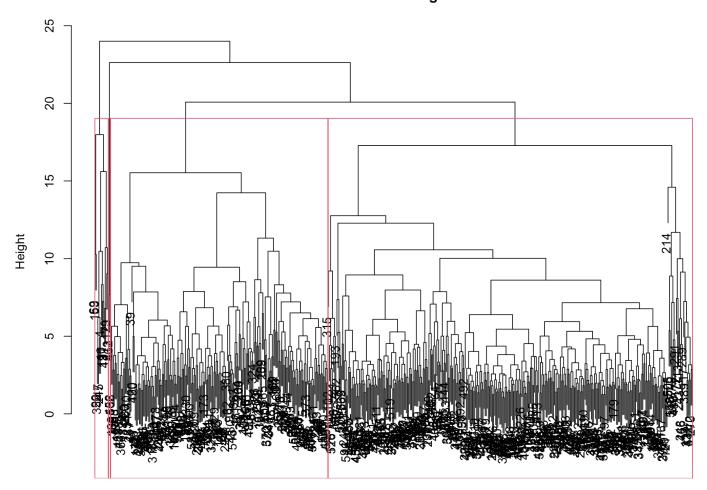
15. Calculate a dissimilarity matrix using Euclidean distance. Compute hierarchical clustering using the complete linkage method and plot the dendrogram. Use the rect.hclust() function to display dividing the dendrogram into 4 branches.

```
# Dissimilarity matrix
dis <- dist(cancer[,-1])

set.seed(20)
# Hierarchical clustering with complete linkage
hc <- hclust(dis, method = 'complete')

# Plotting
plot(hc)
rect.hclust(hc, 4)</pre>
```

Cluster Dendrogram



dis hclust (*, "complete")

16. Divide the dendrogram into 4 clusters using cutree() function. Then use the table() function and the diagnosis label to compare the diagnostic composition (benign vs. malignant) of each of the 4 clusters. If you had to choose diagnostic labels for each of the clusters, how would you label each(e.g. cluster 1 is benign or malignant, cluster 2 is ..., etc.)?

```
# Divide into 4 clusters
hc_4 <- cutree(hc, 4)

# Create dataframe with clusters and diagnosis for each observation
diagnosis <- cancer %>% pull(diagnosis)
comp <- data.frame(hc_4, diagnosis)

# Create table of amount of each diagnosis for each cluster
with(comp, table(hc_4, diagnosis))</pre>
```

```
##
        diagnosis
## hc 4
           В
##
      1
          18 189
##
      2
           2
              11
      3 337
##
              10
##
           0
                2
```

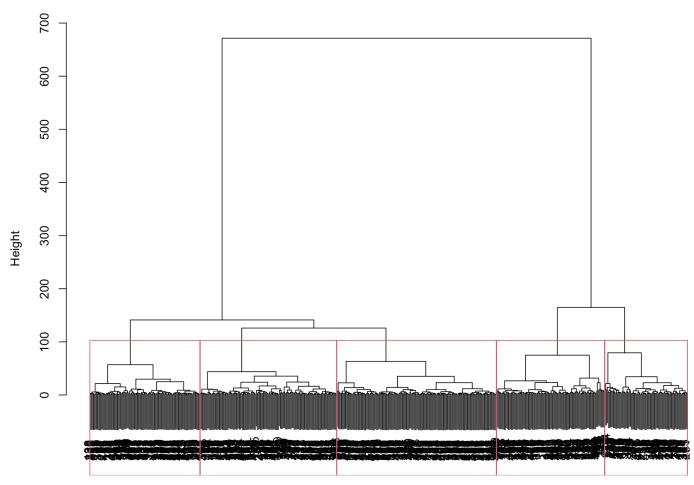
Clusters 1, 2, and 4 I would label as malignant, and Cluster 3 as benign.

17. Now try 5 clusters with and plot dendrograms for hierarchical clustering using Ward's linkage. Then use the table() function to view the clustering result. As in the previous question, how would you label each of these 5 clusters?

```
set.seed(20)
# Hierarchical clustering with Ward's linkage
hc1 <- hclust(dis, method = 'ward.D')

# Plotting
plot(hc1)
rect.hclust(hc1, 5)</pre>
```

Cluster Dendrogram



dis hclust (*, "ward.D")

```
# Labeling 5 clusters
hc_5 <- cutree(hc1, 5)
comp1 <- data.frame(hc_5, diagnosis)
with(comp1, table(hc_5, diagnosis))</pre>
```

```
##
        diagnosis
## hc_5
           В
                М
##
           0 103
       1
##
       2
          19
               60
##
       3
          63
               42
##
       4 127
                3
##
                4
       5 148
```

I would label Clusters 1 and 2 as malignant, and Clusters 3, 4, and 5 as benign.

K-Means Clustering (15 points)

18. Perform k-means clustering on this dataset using the kmeans() function with K=2. Then use the table() function and the diagnosis label to compare the diagnostic composition (benign vs. malignant) of each of the 2 clusters (hint: the cluster information from k-means is stored in the \$cluster attribute of the k-means result.)

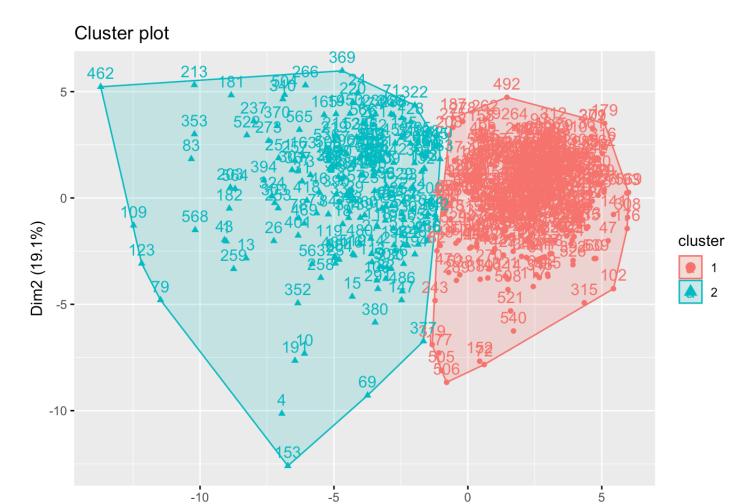
```
set.seed(20)
# Perform Kmeans clustering and create table of amount of diagnoses per cluster
km <- kmeans(cancer[,-1], 2, nstart = 20)
comp2 <- data.frame(km$cluster, diagnosis)
with(comp2, table(km$cluster, diagnosis))</pre>
```

```
## diagnosis
## B M
## 1 346 33
## 2 11 179
```

Cluster 1 I would label as benign and Cluster 2 as malignant.

19. Visualize the clusters using the fviz_cluster() function from the factoextra package.

```
fviz_cluster(km, data = cancer[,-1])
```



20. What is the benefit of hierarchical clustering over k-means based on the example problem we have just explored? The benefit is that you do not have to pre-specify how many clusters you want as you do with K-means. Choosing the correct number of clusters can be difficult when using K-means. With Hierarchical, you take a bottom-up approach, and begin with each data point as its own cluster and you merge clusters together. You can then choose how many clusters you'd like after viewing the dendrogram.

Dim1 (44.9%)