Lab08 Mini Project

Elsa Quillin (PID: A69043008

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Background

The goal of this mini-project is for you to explore a complete analysis using the unsupervised learning techniques covered in the last class. We will extend what you've learned by combining PCA as a preprocessing step to clustering using data that consist of measurements of cell nuclei of human breast masses. This expands on our RNA-Seq analysis from last day.

The data itself comes from the Wisconsin Breast Cancer Diagnostic Data Set first reported by K. P. Benne and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets".

Values in this data set describe characteristics of the cell nuclei present in digitized images of a fine needle aspiration (FNA) of a breast mass.

Data import

```
fna.data <- "https://bioboot.github.io/bimm143_S20/class-material/WisconsinCancer.csv"
wisc.df <- read.csv(fna.data, row.names = 1)
head(wisc.df)
```

```
         diagnosis radius_mean texture_mean perimeter_mean area_mean
842302           M       17.99        10.38         122.80    1001.0
842517           M       20.57        17.77         132.90    1326.0
84300903         M       19.69        21.25         130.00    1203.0
84348301         M       11.42        20.38          77.58     386.1
84358402         M       20.29        14.34         135.10    1297.0
843786           M       12.45        15.70          82.57     477.1
         smoothness_mean compactness_mean concavity_mean concave.points_mean
842302           0.11840          0.27760         0.3001             0.14710
842517           0.08474          0.07864         0.0869             0.07017
84300903         0.10960          0.15990         0.1974             0.12790
84348301         0.14250          0.28390         0.2414             0.10520
84358402         0.10030          0.13280         0.1980             0.10430
843786           0.12780          0.17000         0.1578             0.08089
         symmetry_mean fractal_dimension_mean radius_se texture_se perimeter_se
842302          0.2419                0.07871    1.0950     0.9053        8.589
842517          0.1812                0.05667    0.5435     0.7339        3.398
84300903        0.2069                0.05999    0.7456     0.7869        4.585
84348301        0.2597                0.09744    0.4956     1.1560        3.445
84358402        0.1809                0.05883    0.7572     0.7813        5.438
843786          0.2087                0.07613    0.3345     0.8902        2.217
         area_se smoothness_se compactness_se concavity_se concave.points_se
842302    153.40      0.006399        0.04904      0.05373           0.01587
842517     74.08      0.005225        0.01308      0.01860           0.01340
84300903   94.03      0.006150        0.04006      0.03832           0.02058
84348301   27.23      0.009110        0.07458      0.05661           0.01867
84358402   94.44      0.011490        0.02461      0.05688           0.01885
843786     27.19      0.007510        0.03345      0.03672           0.01137
         symmetry_se fractal_dimension_se radius_worst texture_worst
842302       0.03003             0.006193        25.38         17.33
842517       0.01389             0.003532        24.99         23.41
84300903     0.02250             0.004571        23.57         25.53
84348301     0.05963             0.009208        14.91         26.50
84358402     0.01756             0.005115        22.54         16.67
843786       0.02165             0.005082        15.47         23.75
         perimeter_worst area_worst smoothness_worst compactness_worst
842302            184.60     2019.0           0.1622            0.6656
842517            158.80     1956.0           0.1238            0.1866
84300903          152.50     1709.0           0.1444            0.4245
84348301           98.87      567.7           0.2098            0.8663
84358402          152.20     1575.0           0.1374            0.2050
843786            103.40      741.6           0.1791            0.5249
         concavity_worst concave.points_worst symmetry_worst
```

```
842302            0.7119             0.2654          0.4601
842517            0.2416             0.1860          0.2750
84300903          0.4504             0.2430          0.3613
84348301          0.6869             0.2575          0.6638
84358402          0.4000             0.1625          0.2364
843786            0.5355             0.1741          0.3985
         fractal_dimension_worst
842302                   0.11890
842517                   0.08902
84300903                 0.08758
84348301                 0.17300
84358402                 0.07678
843786                   0.12440
```

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

```
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
         compactness_mean concavity_mean concave.points_mean symmetry_mean
842302            0.27760         0.3001             0.14710         0.2419
842517            0.07864         0.0869             0.07017         0.1812
84300903          0.15990         0.1974             0.12790         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
         fractal_dimension_mean radius_se texture_se perimeter_se area_se
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
         smoothness_se compactness_se concavity_se concave.points_se
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
          perimeter_worst area_worst smoothness_worst compactness_worst
842302             184.60     2019.0           0.1622             0.6656
842517             158.80     1956.0           0.1238             0.1866
84300903           152.50     1709.0           0.1444             0.4245
84348301            98.87      567.7           0.2098             0.8663
84358402           152.20     1575.0           0.1374             0.2050
843786             103.40      741.6           0.1791             0.5249
          concavity_worst concave.points_worst symmetry_worst
842302             0.7119               0.2654         0.4601
842517             0.2416               0.1860         0.2750
84300903           0.4504               0.2430         0.3613
84348301           0.6869               0.2575         0.6638
84358402           0.4000               0.1625         0.2364
843786             0.5355               0.1741         0.3985
          fractal_dimension_worst
842302                    0.11890
842517                    0.08902
84300903                  0.08758
84348301                  0.17300
84358402                  0.07678
843786                    0.12440
```

```
diagnosis <- as.factor(wisc.df$diagnosis)
```

Q1. How many observations are in this dataset?

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

```
[1] 569  30
```

There are 30 observations for each sample

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

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

```
[1] 212
```

212 of the observations have a malignant diagnosis, so 357 are benign

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

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

```
[1] 10
```

There are 10 columns that are suffixed with "_mean"

Principal Component Analysis

The main function in base R for PCA is called `prcomp()`. An optional argument `scale()` should nearly always be switched to `scale=TRUE` for this function.

```
colMeans(wisc.data)
```

```
            radius_mean            texture_mean          perimeter_mean
           1.412729e+01            1.928965e+01            9.196903e+01
              area_mean         smoothness_mean        compactness_mean
           6.548891e+02            9.636028e-02            1.043410e-01
         concavity_mean      concave.points_mean           symmetry_mean
           8.879932e-02            4.891915e-02            1.811619e-01
 fractal_dimension_mean               radius_se              texture_se
           6.279761e-02            4.051721e-01            1.216853e+00
           perimeter_se                 area_se           smoothness_se
           2.866059e+00            4.033708e+01            7.040979e-03
         compactness_se            concavity_se       concave.points_se
           2.547814e-02            3.189372e-02            1.179614e-02
            symmetry_se     fractal_dimension_se            radius_worst
           2.054230e-02            3.794904e-03            1.626919e+01
          texture_worst         perimeter_worst              area_worst
           2.567722e+01            1.072612e+02            8.805831e+02
       smoothness_worst        compactness_worst         concavity_worst
```

```
          1.323686e-01            2.542650e-01            2.721885e-01
  concave.points_worst          symmetry_worst fractal_dimension_worst
          1.146062e-01            2.900756e-01            8.394582e-02
```

```
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
```

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

```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                          PC8    PC9    PC10   PC11    PC12    PC13    PC14
Standard deviation     0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
Cumulative Proportion  0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
                          PC15    PC16    PC17    PC18    PC19    PC20   PC21
Standard deviation     0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
```

```
Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
Cumulative Proportion  0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                          PC22    PC23   PC24    PC25    PC26    PC27    PC28
Standard deviation     0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
Cumulative Proportion  0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
                          PC29    PC30
Standard deviation     0.02736 0.01153
Proportion of Variance 0.00002 0.00000
Cumulative Proportion  1.00000 1.00000
```

> Q4. From your results, what proportion of the original variance is captured by the first principal components (PC1)?

PC1 captures 0.4427 of the variance (44.27%).

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

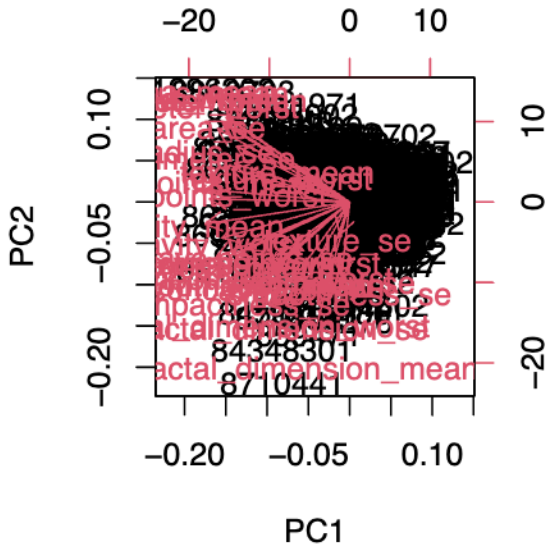
Three PCAs are required to get to at least 70% of the variance.

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

Seven PCAs are required to get to at least 90% of variance.

Let's make our main result figure-the "PC plot", or "score plot", or "ordienation plot"

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

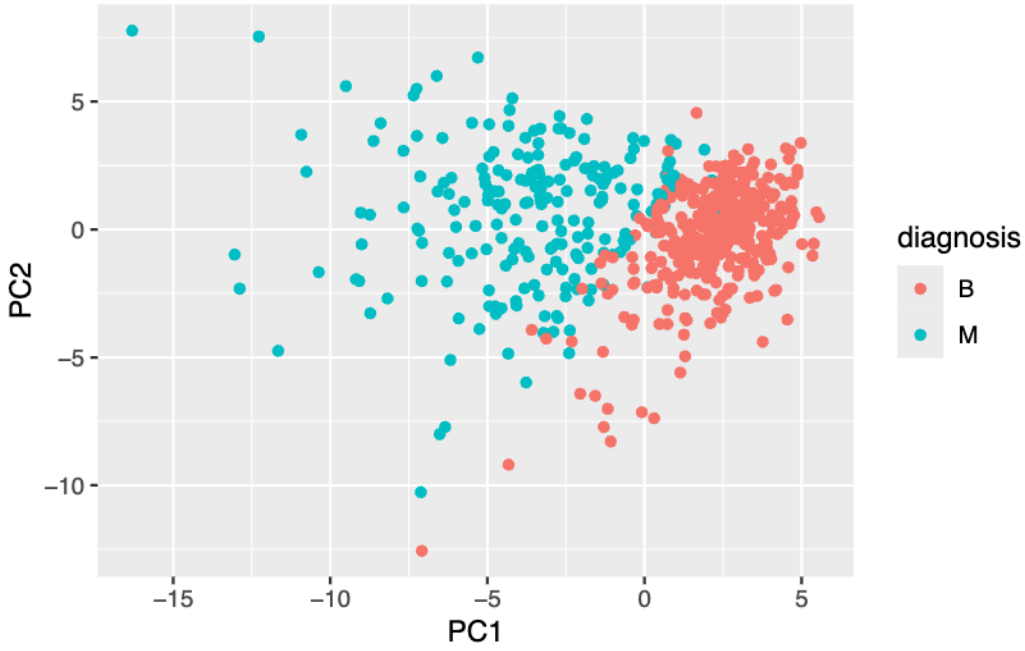


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

This plot is very messy and impossible to read since there is so much overlap

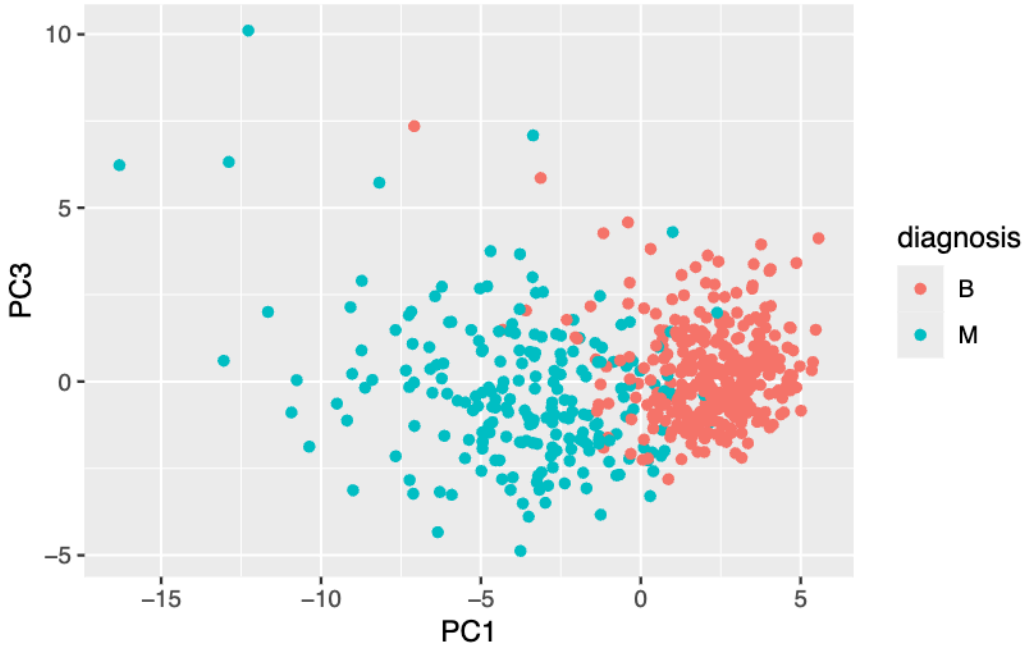
```
library(ggplot2)

ggplot(wisc.pr$x)+
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



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

```
ggplot(wisc.pr$x)+
  aes(PC1, PC3, col=diagnosis) +
  geom_point()
```

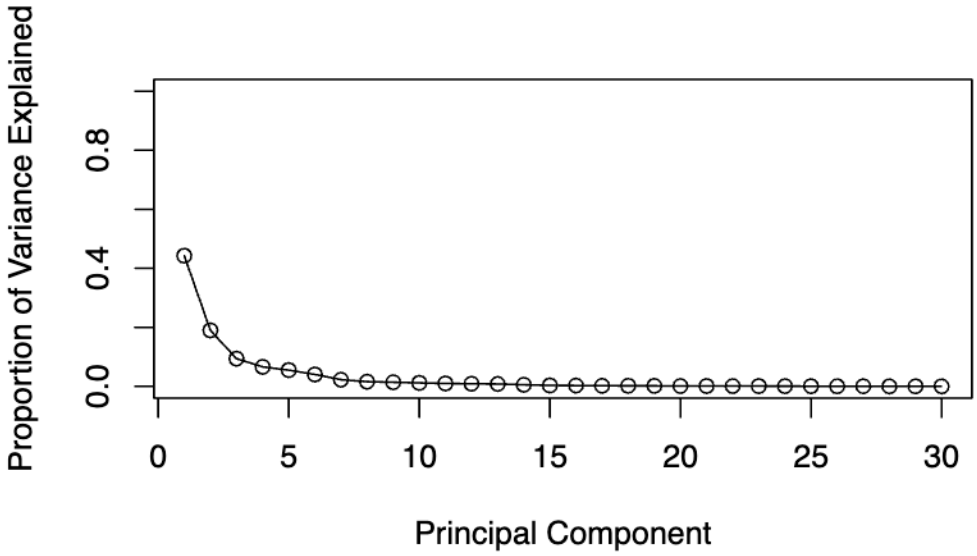



```
pr.var <- wisc.pr$sdev^2
head(pr.var)
```

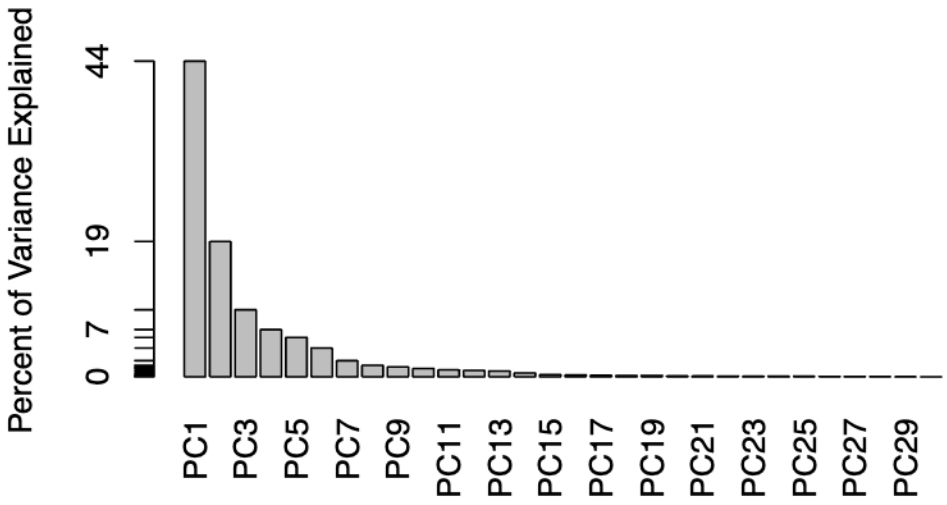
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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

plot(pve, xlab = "Principal Component",
     ylab = "Proportion of Variance Explained",
     ylim = c(0, 1), type = "o")
```




```
barplot(pve, ylab = "Percent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```

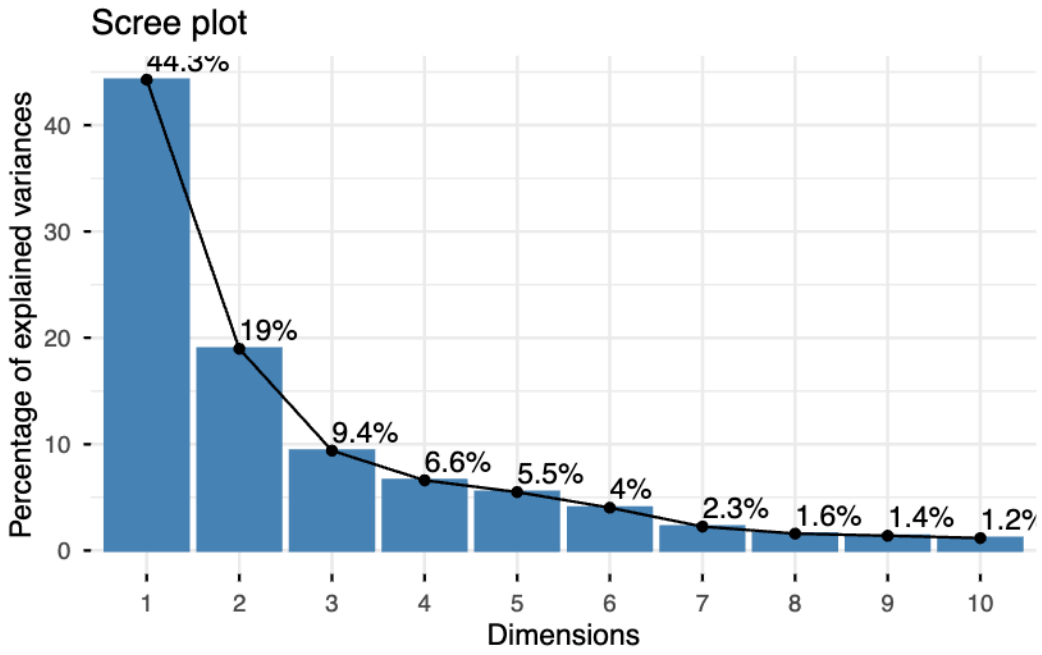


```
library(factoextra)
```

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

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

```
Warning in geom_bar(stat = "identity", fill = barfill, color = barcolor, :
Ignoring empty aesthetic: `width`.
```



Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr$rotation[,1]) for the feature concave.points_mean? This tells us how much this original feature contributes to the first PC.

```
wisc.pr$rotation[,1]
```

```
    radius_mean    texture_mean  perimeter_mean
     -0.21890244      -0.10372458      -0.22753729
      area_mean  smoothness_mean  compactness_mean
     -0.22099499      -0.14258969      -0.23928535
 concavity_mean concave.points_mean   symmetry_mean
```

```
           -0.25840048            -0.26085376            -0.13816696
fractal_dimension_mean              radius_se             texture_se
           -0.06436335            -0.20597878            -0.01742803
         perimeter_se                 area_se          smoothness_se
           -0.21132592            -0.20286964            -0.01453145
       compactness_se           concavity_se      concave.points_se
           -0.17039345            -0.15358979            -0.18341740
          symmetry_se    fractal_dimension_se            radius_worst
           -0.04249842            -0.10256832            -0.22799663
        texture_worst         perimeter_worst              area_worst
           -0.10446933            -0.23663968            -0.22487053
      smoothness_worst       compactness_worst         concavity_worst
           -0.12795256            -0.21009588            -0.22876753
  concave.points_worst          symmetry_worst fractal_dimension_worst
           -0.25088597            -0.12290456            -0.13178394
```

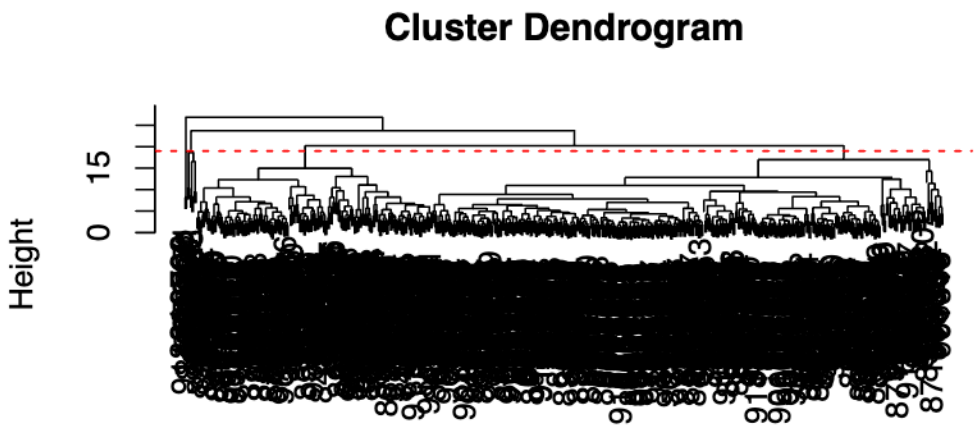
-0.26085376

Hierarchical Clustering

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist, method = "complete")
```

Q10. 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)
```

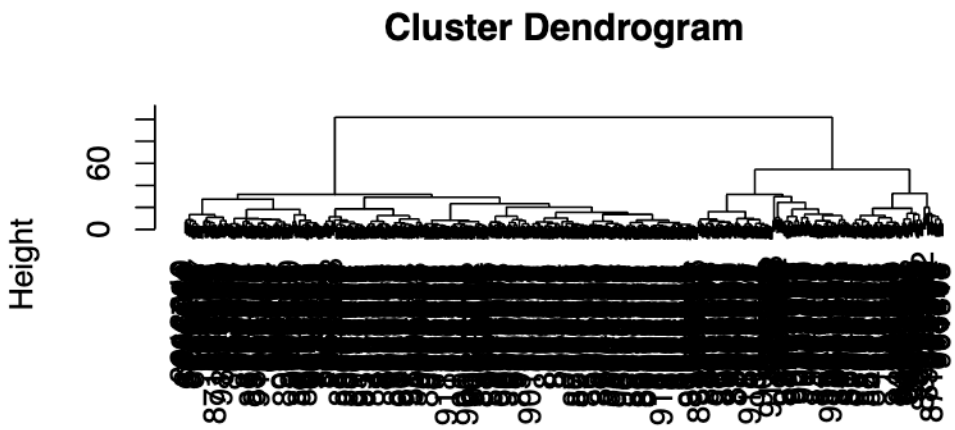



```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
table(wisc.hclust.clusters, diagnosis)
```

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

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

```
wisc.hclust <- hclust(data.dist, method = "ward.D2")
plot(wisc.hclust)
```



I preferred the "ward.D2" method since it was the easiest method to visualize the number of clusters. The other methods ended up being a lot more chaotic (especially "single", yuck!) making it harder to distinguish the branches.

Combining methods

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

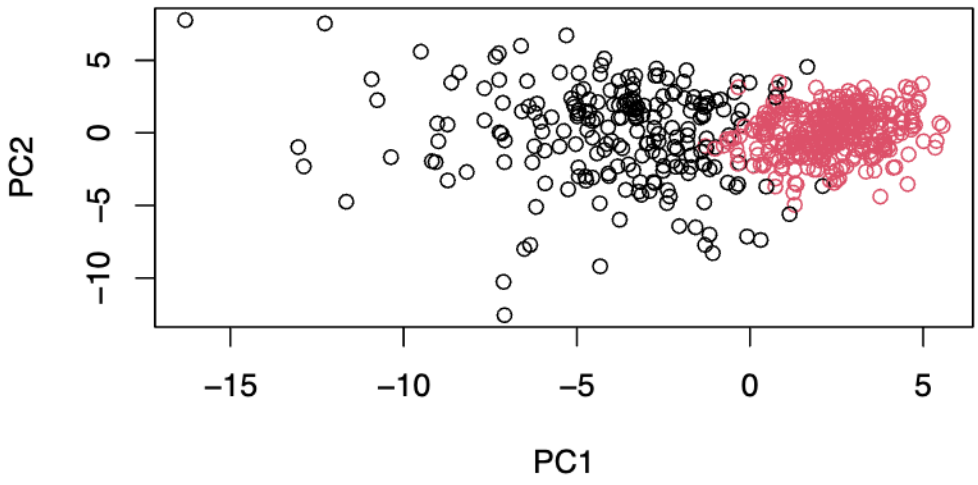
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

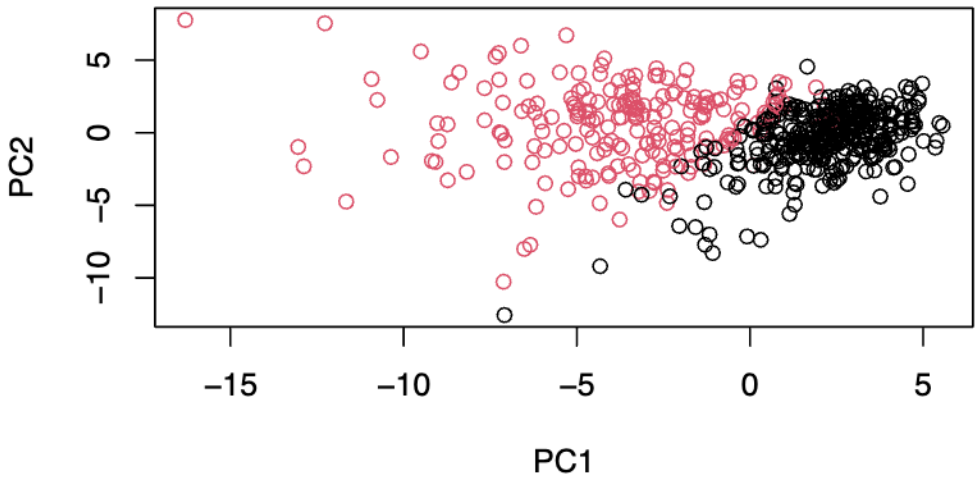
```
table(grps, diagnosis)
```

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

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




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



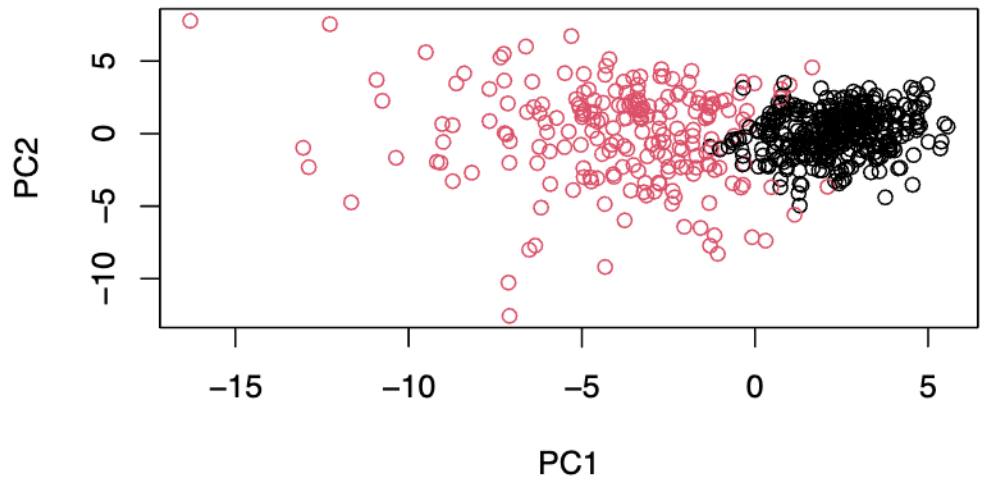
```
g <- as.factor(grps)
levels(g)
```

```
[1] "1" "2"
```

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

```
[1] "2" "1"
```

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




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

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

```
table(wisc.pr.hclust.clusters)
```

```
wisc.pr.hclust.clusters
  1   2
216 353
```

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

```
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.pr.hclust.clusters   B   M
                      1  28 188
                      2 329  24
```

It separates them out pretty well, but not perfectly. It captured 88.7% of the malignant samples, which in a clinical practice seems really low. It captured 92% of the benign tumors which is a little better.

Q14. How well do the hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses? Again, use the table() function to compare the output of each model (wisc.km$cluster and wisc.hclust.clusters) with the vector containing the actual diagnoses.

```
table(wisc.hclust.clusters, diagnosis)
```

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

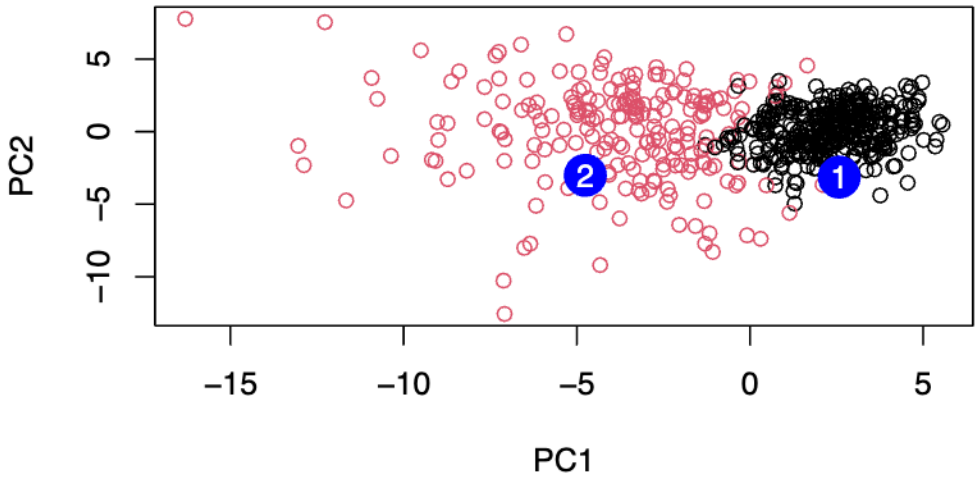
It does a little worse than the previous method in identifying the malignant tumors, but correctly identified more of the benign tumors into one group. So it is identifying more malignant tumors as benign which is more dangerous in practice since people could go untreated if this algorithm was determining their sample results.

Prediction

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

```
          PC1       PC2        PC3        PC4       PC5        PC6        PC7
[1,]  2.576616 -3.135913  1.3990492 -0.7631950  2.781648 -0.8150185 -0.3959098
[2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945  0.8193031
           PC8       PC9       PC10       PC11      PC12       PC13     PC14
[1,] -0.2307350 0.1029569 -0.9272861  0.3411457  0.375921  0.1610764 1.187882
[2,] -0.3307423 0.5281896 -0.4855301  0.7173233 -1.185917  0.5893856 0.303029
          PC15       PC16        PC17        PC18        PC19        PC20
[1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
[2,] 0.1299153  0.1448061 -0.40509706  0.06565549  0.25591230 -0.4289500
          PC21       PC22       PC23       PC24        PC25         PC26
[1,]  0.1228233 0.09358453 0.08347651  0.1223396  0.02124121  0.078884581
[2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
             PC27         PC28          PC29         PC30
[1,]  0.220199544 -0.02946023 -0.015620933  0.005269029
[2,] -0.001134152  0.09638361  0.002795349 -0.019015820
```

```r
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")
```



Q16. Which of these new patients should we prioritize for follow up based on your results?

We should prioritize patients from group 2 for followup since they have been clustered as the malignant group and therefore have sample results that more closely relate to the malignant features.

```
sessionInfo()
```

```
R version 4.5.1 (2025-06-13)
Platform: aarch64-apple-darwin20
Running under: macOS Sequoia 15.6.1

Matrix products: default
BLAS:   /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRblas.0.dylib
LAPACK: /Library/Frameworks/R.framework/Versions/4.5-arm64/Resources/lib/libRlapack.dylib;

locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

time zone: America/Los_Angeles
tzcode source: internal

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

other attached packages:
[1] factoextra_1.0.7 ggplot2_4.0.0

loaded via a namespace (and not attached):
 [1] gtable_0.3.6       jsonlite_2.0.0     dplyr_1.1.4        compiler_4.5.1
 [5] ggsignif_0.6.4     tidyselect_1.2.1   Rcpp_1.1.0         tidyr_1.3.1
 [9] scales_1.4.0       yaml_2.3.10        fastmap_1.2.0      R6_2.6.1
[13] ggpubr_0.6.2       labeling_0.4.3     generics_0.1.4     Formula_1.2-5
[17] knitr_1.50         backports_1.5.0    ggrepel_0.9.6      tibble_3.3.0
[21] car_3.1-3          pillar_1.11.1      RColorBrewer_1.1-3 rlang_1.1.6
[25] broom_1.0.10       xfun_0.53          S7_0.2.0           cli_3.6.5
[29] withr_3.0.2        magrittr_2.0.4     digest_0.6.37      grid_4.5.1
[33] lifecycle_1.0.4    vctrs_0.6.5        rstatix_0.7.3      evaluate_1.0.5
[37] glue_1.8.0         farver_2.1.2       abind_1.4-8        carData_3.0-5
[41] rmarkdown_2.30     purrr_1.1.0        tools_4.5.1        pkgconfig_2.0.3
[45] htmltools_0.5.8.1
```