Class 08: Mini Project

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1. Exploratory Data Analysis

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

```
Q1. How many observations are in this dataset?
nrow(wisc.data)
```

```
[1] 569
```

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

```
mal <- "M"
sum(diagnosis == "M")</pre>
```

[1] 212

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

```
all_col_names <- colnames(wisc.df)
mean <- "mean"

mean_suffix <- grep(mean,all_col_names,value ="TRUE")
mean_suffix</pre>
```

```
[1] "radius_mean" "texture_mean" "perimeter_mean" [4] "area_mean" "smoothness_mean" "compactness_mean"
```

^{[7] &}quot;concavity_mean" "concave.points_mean" "symmetry_mean"

^{[10] &}quot;fractal_dimension_mean"

2. Principal Component Analysis

colMeans(wisc.data)

radius_mean	texture_mean	perimeter_mean
1.412729e+01	1.928965e+01	9.196903e+01
area_mean	${\tt smoothness_mean}$	compactness_mean
6.548891e+02	9.636028e-02	1.043410e-01
${\tt concavity_mean}$	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	<pre>fractal_dimension_worst</pre>
1.146062e-01	2.900756e-01	8.394582e-02

apply(wisc.data,2,sd)

texture_mean	perimeter_mean
4.301036e+00	2.429898e+01
smoothness_mean	compactness_mean
1.406413e-02	5.281276e-02
concave.points_mean	symmetry_mean
3.880284e-02	2.741428e-02
radius_se	texture_se
2.773127e-01	5.516484e-01
area_se	smoothness_se
4.549101e+01	3.002518e-03
concavity_se	concave.points_se
3.018606e-02	6.170285e-03
fractal_dimension_se	radius_worst
	4.301036e+00 smoothness_mean 1.406413e-02 concave.points_mean 3.880284e-02 radius_se 2.773127e-01 area_se 4.549101e+01 concavity_se 3.018606e-02

```
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)
summary(wisc.pr)</pre>
```

Importance of components:

```
PC2
                                             PC4
                       PC1
                                      PC3
                                                    PC5
                                                           PC6
                                                                PC7
Standard deviation
                   666.170 85.49912 26.52987 7.39248 6.31585 1.73337 1.347
Proportion of Variance
                     0.982 0.01618 0.00156 0.00012 0.00009 0.00001 0.000
                     0.982 0.99822 0.99978 0.99990 0.99999 0.99999 1.000
Cumulative Proportion
                      PC8
                            PC9
                                 PC10
                                       PC11
                                              PC12
                                                     PC13
                                                            PC14
Standard deviation
                   0.6095 0.3944 0.2899 0.1778 0.08659 0.05623 0.04649
Proportion of Variance 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000
                   1.0000 1.0000 1.0000 1.0000 1.00000 1.00000
Cumulative Proportion
                      PC15
                            PC16
                                   PC17
                                          PC18
                                                 PC19
                                                        PC20
                                                               PC21
Standard deviation
                   0.03642 0.0253 0.01936 0.01534 0.01359 0.01281 0.008838
Cumulative Proportion
                   1.00000 1.0000 1.00000 1.00000 1.00000 1.00000 1.000000
                      PC22
                              PC23
                                      PC24
                                             PC25
                                                     PC26
                                                             PC27
                   0.00759 0.005909 0.005329 0.004018 0.003534 0.001918
Standard deviation
1.00000 1.000000 1.000000 1.000000 1.000000
Cumulative Proportion
                       PC28
                               PC29
                                       PC30
Standard deviation
                   0.001688 0.001416 0.0008379
Proportion of Variance 0.000000 0.000000 0.0000000
Cumulative Proportion 1.000000 1.000000 1.0000000
```

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

44.27%

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

3 PCs

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

7 PCs

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

Warning in arrows (0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows (0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

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Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

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Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

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Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows (0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

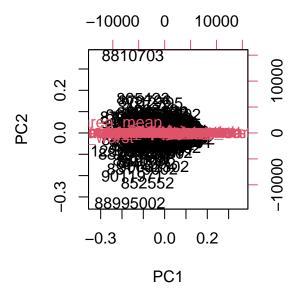
Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows (0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

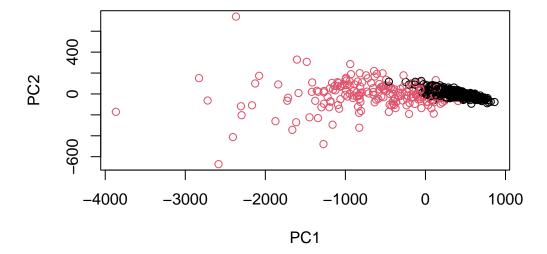
Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length = arrow.len): zero-length arrow is of indeterminate angle and so skipped

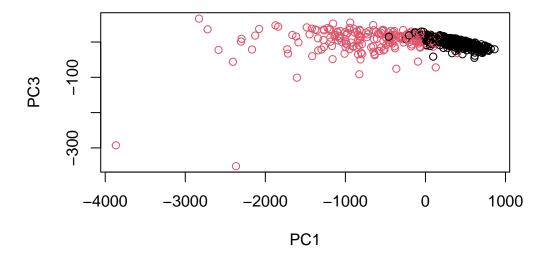


Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

It has 4 axes, everything is large but the plot si small so there is much overlap which makes it hard to understand.



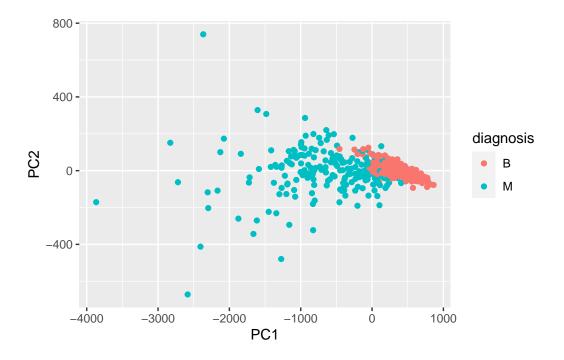
Q8. Generate a similar plot for principal components 1 and 3. What do you notice about these plots?



When PC1 is plotted against PC3 rather than PC2, it leans higher on the y axis. THey are also both skewed to the right of the plot a lot. They also both separate benign form malignant diagnoses.

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis

ggplot(df) +
   aes(PC1, PC2, col=diagnosis) +
   geom_point()</pre>
```



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

- [1] 4.437826e+05 7.310100e+03 7.038337e+02 5.464874e+01 3.989002e+01
- [6] 3.004588e+00

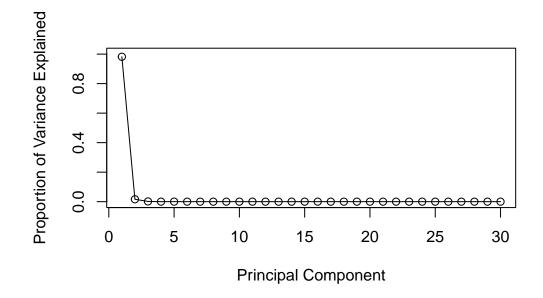
```
total_var <- sum(wisc.pr$sdev^2)
total_var</pre>
```

[1] 451896.6

```
pve <- (wisc.pr$sdev^2) / total_var
pve</pre>
```

- [1] 9.820447e-01 1.617649e-02 1.557511e-03 1.209320e-04 8.827245e-05
- [6] 6.648840e-06 4.017137e-06 8.220172e-07 3.441353e-07 1.860187e-07
- [11] 6.994732e-08 1.659089e-08 6.996416e-09 4.783183e-09 2.935492e-09
- [16] 1.416849e-09 8.295777e-10 5.204059e-10 4.084640e-10 3.633134e-10
- [21] 1.728497e-10 1.274875e-10 7.726830e-11 6.283577e-11 3.573023e-11
- [26] 2.763960e-11 8.144523e-12 6.302115e-12 4.436669e-12 1.553447e-12

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



Q9. For the first principal component, what is the component of the loading vector (i.e. wisc.pr\$rotation[,1]) for the feature concave.points_mean?

-4.778078e-05

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

```
cumulative_pve <- cumsum(pve)
which(cumulative_pve >= 0.8)[1]
```

[1] 1

3. Hierarchical Clustering

```
scaled <- scale(wisc.data)

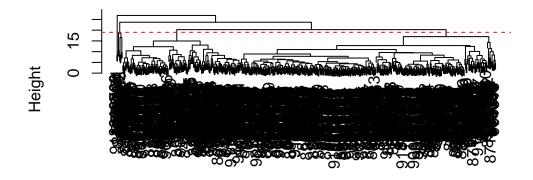
data.dist <- dist(scaled)

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

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)</pre>
```

Cluster Dendrogram



data.dist hclust (*, "complete")

19
 wisc.hclust.clusters <- cutree(wisc.hclust, k = 4)
 table(wisc.hclust.clusters, diagnosis)</pre>

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

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

You can try multiple numbers between 2 and 10 and then decide which one is a better match.

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

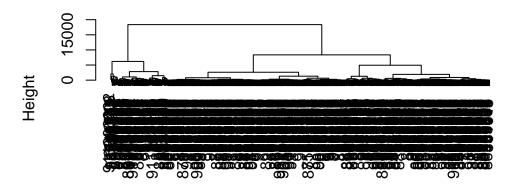
"ward.D2" because it shows the cleanest clusters and is the easiest to interpret for me

5. Combining Methods

```
cum.var <- cumsum(summary(wisc.pr)$importance[2, ])
num.comp <- which.max(cum.var >= 0.9)

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")

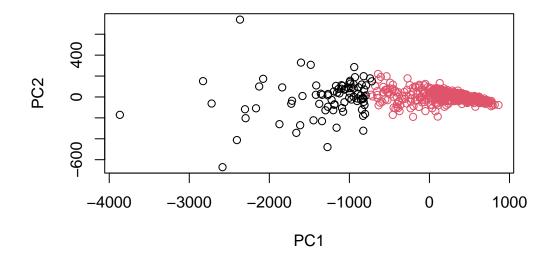
```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)

grps
1    2
86 483

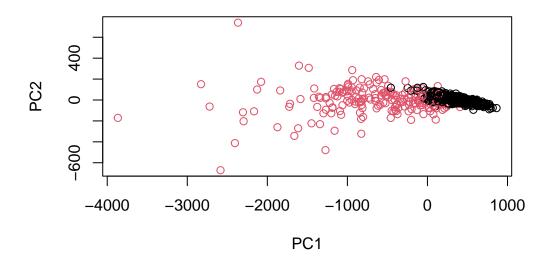
table(grps, diagnosis)

diagnosis
grps    B    M
1    0 86
2 357 126

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



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



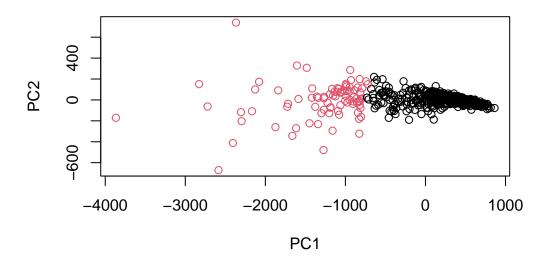
```
g <- as.factor(grps)
levels(g)

[1] "1" "2"

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

[1] "2" "1"

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



```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[, 1:7]), method = "ward.D2")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hclust, k=2)</pre>
```

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

Q17. 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?

The wisc.km\$cluster is better in my opinion because the wisc.hclust.clusters breaks it down into more groups but with less meaning, the numbers for each group are very insignificantly changed from the first.

6. Sensitivity/Specificity

Q17. Which of your analysis procedures resulted in a clustering model with the best specificity? How about sensitivity?

```
#K-Means

#Sensitivity:
    37 / (37 + 175)

[1] 0.1745283

#Specificity:
    14 / (14 + 343)

[1] 0.03921569

#Hierarchical

# Sensitivity:
    5 / (5 + 165)
```

[1] 0.02941176

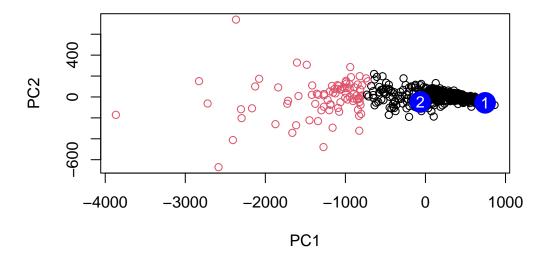
```
# Specificity:
12 / (12 + 343)
```

[1] 0.03380282

K-means for both.

7. Prediction

```
#url <- "new_samples.csv"</pre>
  url <- "https://tinyurl.com/new-samples-CSV"</pre>
  new <- read.csv(url)</pre>
  npc <- predict(wisc.pr, newdata=new)</pre>
  npc
          PC1
                   PC2
                             PC3
                                       PC4
                                                           PC6
                                                                    PC7
                                                 PC5
[1,] 745.60081 -56.16454 -21.15609 -3.330663 9.355518 2.317462 -1.147268
[2,] -64.40839 -48.46996 -15.93413 12.089591 -4.636008 -1.045210 -0.295228
           PC8
                       PC9
                                 PC10
                                           PC11
                                                       PC12
[1,] -0.7644759   0.11704582   0.06401851   0.1191717   -0.05611973   -0.040020096
[2,] -0.7454142 -0.09167106 -0.76173550 0.3206674 0.02602751 0.005023528
           PC14
                        PC15
                                   PC16
                                               PC17
                                                           PC18
                                                                       PC19
[1,] 0.01354667 -0.018755904 -0.01050870 -0.01183961 0.020946097 0.030567858
PC21
                                    PC22
                                                 PC23
            PC20
[1,] -0.007960122 -0.003773165 0.018561168 0.0001875602 -0.005463212
[2,] 0.007001178 -0.022182056 0.008725155 0.0075849336 0.004619616
            PC25
                        PC26
                                    PC27
                                                 PC28
[1,] -0.005992320 0.005357732 4.550233e-05 0.003252776 0.0012510265
[2,] 0.002804663 0.003229335 1.977351e-03 -0.002261832 0.0009130702
             PC30
[1,] -0.0009794321
[2,] -0.0009078383
  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?

The ones labeled in red.

sessionInfo()

R version 4.3.2 (2023-10-31)

Platform: aarch64-apple-darwin20 (64-bit)

Running under: macOS Ventura 13.5

Matrix products: default

BLAS: /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRblas.0.dylib LAPACK: /Library/Frameworks/R.framework/Versions/4.3-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] ggplot2_3.4.4

loaded via a namespace (and not attached):

[1]	vctrs_0.6.5	cli_3.6.2	knitr_1.45	rlang_1.1.3
[5]	xfun_0.41	generics_0.1.3	jsonlite_1.8.8	labeling_0.4.3
[9]	glue_1.7.0	<pre>colorspace_2.1-0</pre>	htmltools_0.5.7	scales_1.3.0
[13]	fansi_1.0.6	rmarkdown_2.25	grid_4.3.2	evaluate_0.23
[17]	munsell_0.5.0	tibble_3.2.1	fastmap_1.1.1	yaml_2.3.8
[21]	lifecycle_1.0.4	compiler_4.3.2	dplyr_1.1.4	pkgconfig_2.0.3
[25]	farver_2.1.1	digest_0.6.34	R6_2.5.1	tidyselect_1.2.0
[29]	utf8_1.2.4	pillar_1.9.0	magrittr_2.0.3	withr_3.0.0
[33]	tools_4.3.2	gtable_0.3.4		