class09

Wanning Cui

```r
fna.data <- "WisconsinCancer.csv"
```

```r
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
```

```r
skimr::skim(wisc.df)
```

Table 1: Data summary

Name	wisc.df
Number of rows	569
Number of columns	31
Column type frequency:	
character	1

numeric	30
Group variables	None

Variable type: character

skim_variable	n_missing	complete_rate	min	max	empty	n_unique	whitespace
diagnosis	0	1	1	1	0	2	0

Variable type: numeric

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
radius_mean	0	1	14.13	3.52	6.98	11.70	13.37	15.78	28.11	
texture_mean	0	1	19.29	4.30	9.71	16.17	18.84	21.80	39.28	
perimeter_mean	0	1	91.97	24.30	43.79	75.17	86.24	104.10	188.50	
area_mean	0	1	654.89	351.91	143.50	420.30	551.10	782.70	2501.00	
smoothness_mean	0	1	0.10	0.01	0.05	0.09	0.10	0.11	0.16	
compactness_mean	0	1	0.10	0.05	0.02	0.06	0.09	0.13	0.35	
concavity_mean	0	1	0.09	0.08	0.00	0.03	0.06	0.13	0.43	
concave.points_mean	0	1	0.05	0.04	0.00	0.02	0.03	0.07	0.20	
symmetry_mean	0	1	0.18	0.03	0.11	0.16	0.18	0.20	0.30	
fractal_dimension_mean	0	1	0.06	0.01	0.05	0.06	0.06	0.07	0.10	
radius_se	0	1	0.41	0.28	0.11	0.23	0.32	0.48	2.87	
texture_se	0	1	1.22	0.55	0.36	0.83	1.11	1.47	4.88	
perimeter_se	0	1	2.87	2.02	0.76	1.61	2.29	3.36	21.98	
area_se	0	1	40.34	45.49	6.80	17.85	24.53	45.19	542.20	
smoothness_se	0	1	0.01	0.00	0.00	0.01	0.01	0.01	0.03	
compactness_se	0	1	0.03	0.02	0.00	0.01	0.02	0.03	0.14	
concavity_se	0	1	0.03	0.03	0.00	0.02	0.03	0.04	0.40	
concave.points_se	0	1	0.01	0.01	0.00	0.01	0.01	0.01	0.05	
symmetry_se	0	1	0.02	0.01	0.01	0.02	0.02	0.02	0.08	
fractal_dimension_se	0	1	0.00	0.00	0.00	0.00	0.00	0.00	0.03	
radius_worst	0	1	16.27	4.83	7.93	13.01	14.97	18.79	36.04	
texture_worst	0	1	25.68	6.15	12.02	21.08	25.41	29.72	49.54	
perimeter_worst	0	1	107.26	33.60	50.41	84.11	97.66	125.40	251.20	
area_worst	0	1	880.58	569.36	185.20	515.30	686.50	1084.00	4254.00	
smoothness_worst	0	1	0.13	0.02	0.07	0.12	0.13	0.15	0.22	
compactness_worst	0	1	0.25	0.16	0.03	0.15	0.21	0.34	1.06	
concavity_worst	0	1	0.27	0.21	0.00	0.11	0.23	0.38	1.25	

skim_variable	n_missing	complete_rate	mean	sd	p0	p25	p50	p75	p100	hist
concave.points_worst	0	1	0.11	0.07	0.00	0.06	0.10	0.16	0.29	
symmetry_worst	0	1	0.29	0.06	0.16	0.25	0.28	0.32	0.66	
fractal_dimension_worst	0	1	0.08	0.02	0.06	0.07	0.08	0.09	0.21	

Store diagnosis column for later use we will exclude this from our dataset for analysis

```
#CREATE DIAGNOSIS VECTOR FOR LATER
diagnosis <- as.factor (wisc.df$diagnosis)
wisc.data <- wisc.df[,-1]
```

> Q1. How many observations are in the dataset?

```
nrow(wisc.df)
```

```
[1] 569
```

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

```
sum(wisc.df$diagnosis=="M")
```

```
[1] 212
```

```
table(wisc.df$diagnosis)
```

```

  B   M 
357 212 
```

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

```
grep("_mean",colnames(wisc.df),value=T)
```

```
 [1] "radius_mean"            "texture_mean"           "perimeter_mean"        
 [4] "area_mean"              "smoothness_mean"        "compactness_mean"      
 [7] "concavity_mean"         "concave.points_mean"    "symmetry_mean"         
[10] "fractal_dimension_mean"
```

```
#colnames(wisc.df)
```

#2. Principal Component Analysis

We need to use `scale=True` here as shown above with our `skim()` report. We could also look at the sd and mean of our columns and see they are on very different scales.

```
# Check column means and standard deviations
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
```

```r
# Perform PCA on wisc.data by completing the following code
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)?

```r
v <- summary(wisc.pr)
pcvar <- v$importance[3,]
pcvar ["PC1"]
```

```
    PC1 
0.44272 
```

0.4427

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

```r
which(pcvar >= 0.7)[1]
```

```
PC3 
  3 
```

3 PCs

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

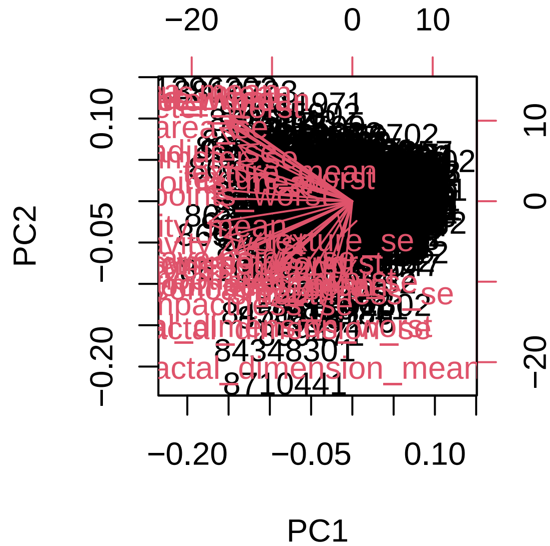
```r
which(pcvar >= 0.9)[1]
```

```
PC7 
  7 
```

7 PCs

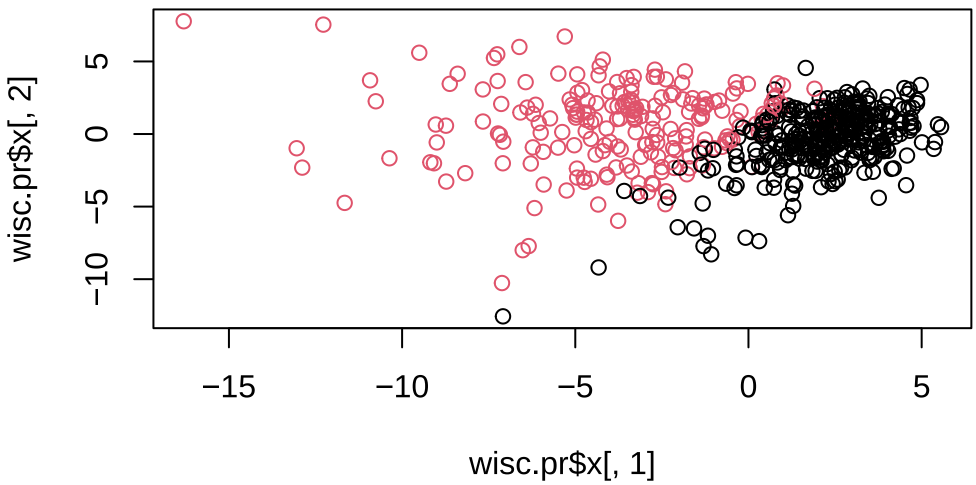
> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

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



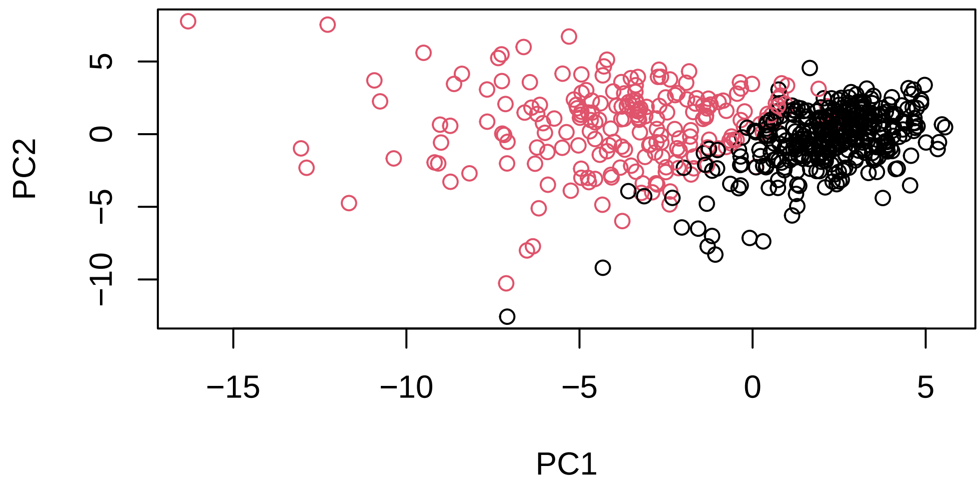
This is not easy to understand because the relationship is not clear at all and the data is hard to interpret.

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



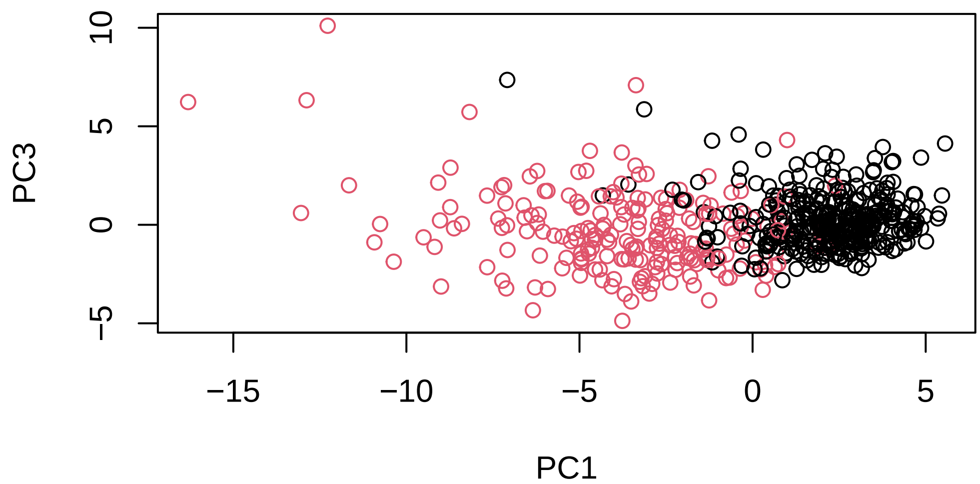
Most red points (malignant diagnosis) are on one side whereas the black points are clustered more tightly on the other side. There seem to be a more positive correlation between PC1 and PC2.

```
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?

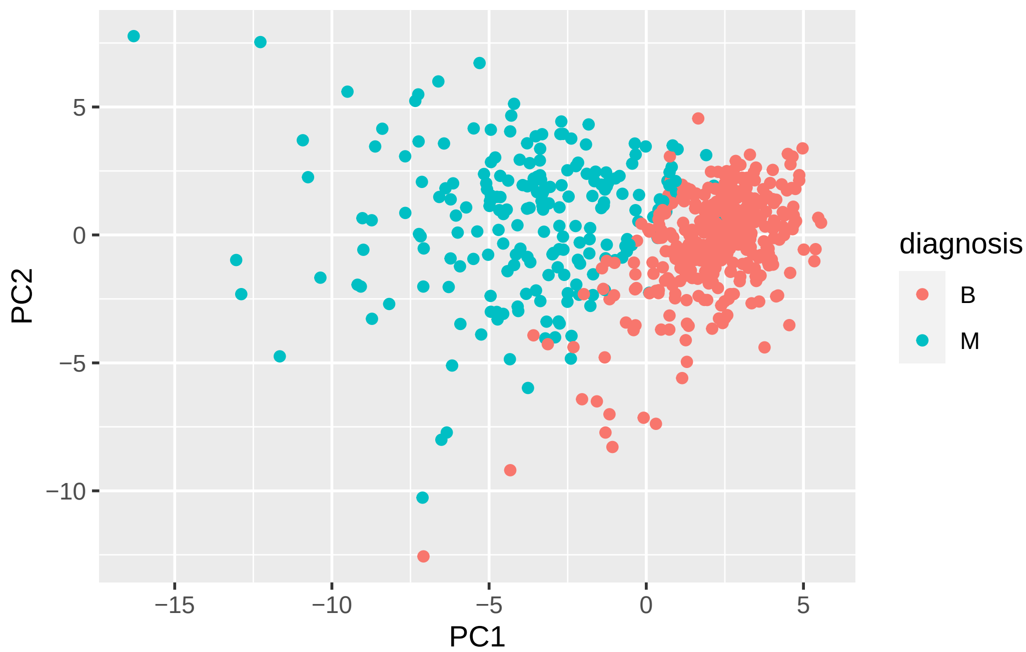
```
plot(wisc.pr$x[,1], wisc.pr$x[,3],col = diagnosis,
     xlab = "PC1", ylab = "PC3")
```




```
# Create a data.frame for ggplot
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

```
library(ggplot2)
```

```
ggplot(df) +
  aes(PC1, PC2, col=diagnosis) +
  geom_point()
```



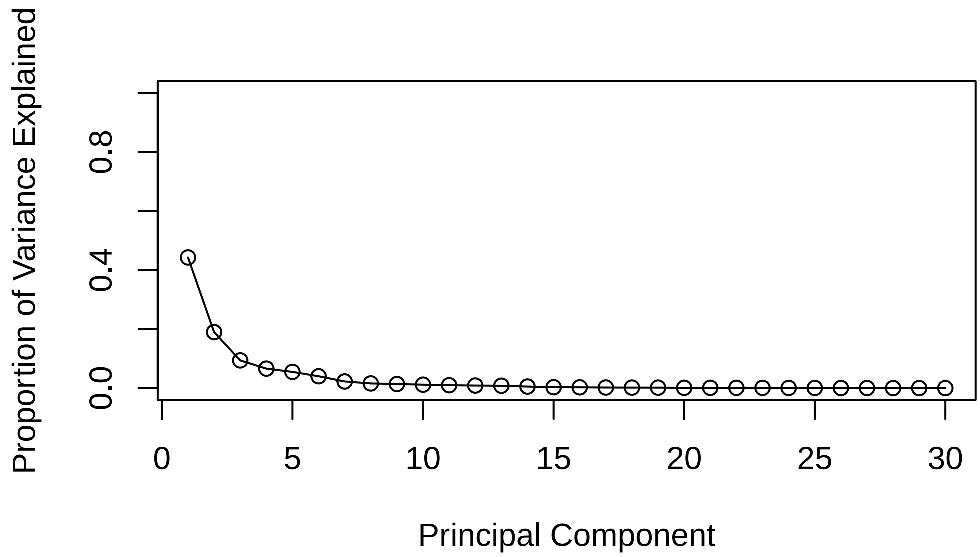
#Variance explained

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

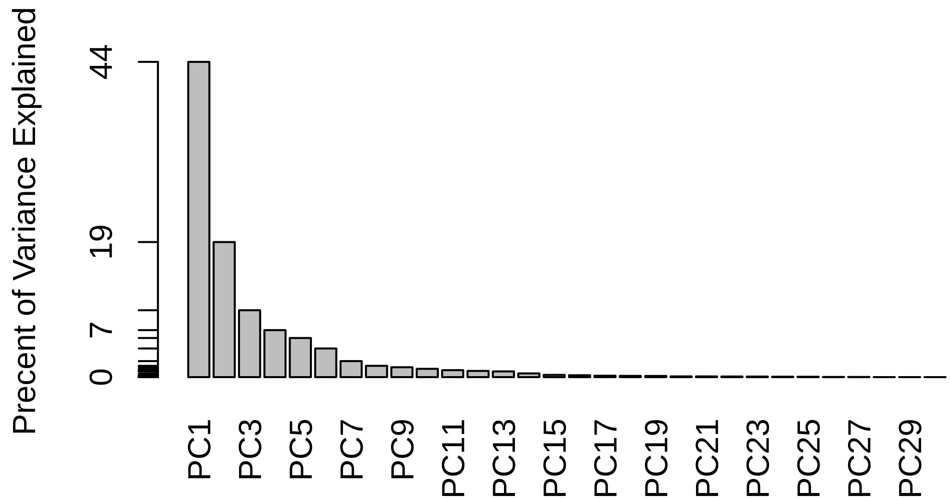
```
[1] 13.281608  5.691355  2.817949  1.980640  1.648731  1.207357
```

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



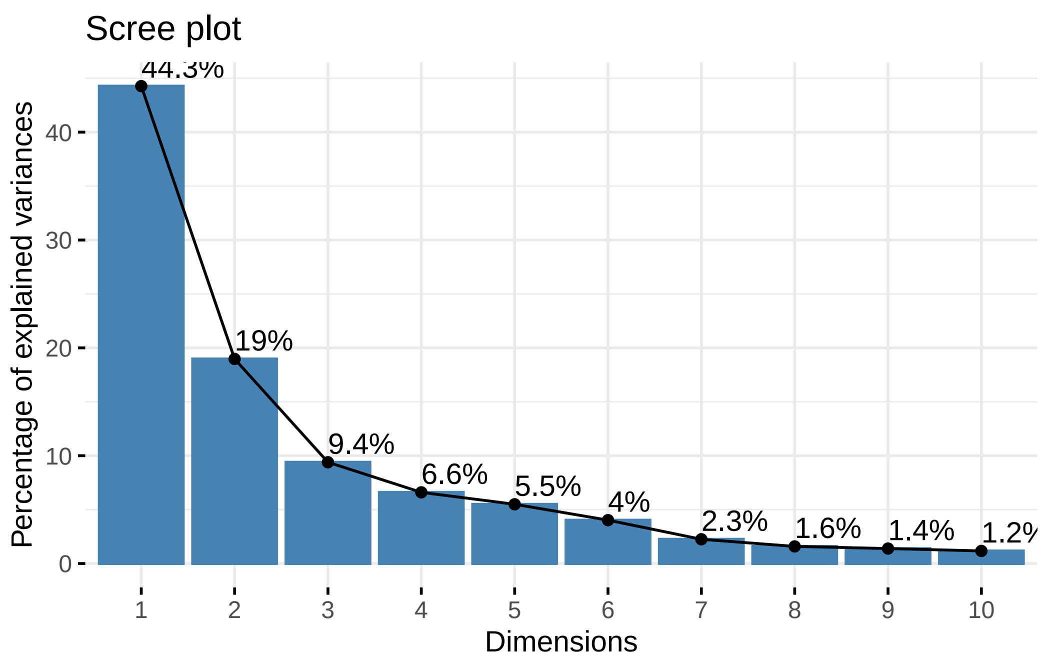

```
# Alternative scree plot of the same data, note data driven y-axis
barplot(pve, ylab = "Precent of Variance Explained",
     names.arg=paste0("PC",1:length(pve)), las=2, axes = FALSE)
axis(2, at=pve, labels=round(pve,2)*100 )
```




```r
library(factoextra)
```

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

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



#Communicating PCA results >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
```

The component is -0.26085376

#3. Hierarchical clustering

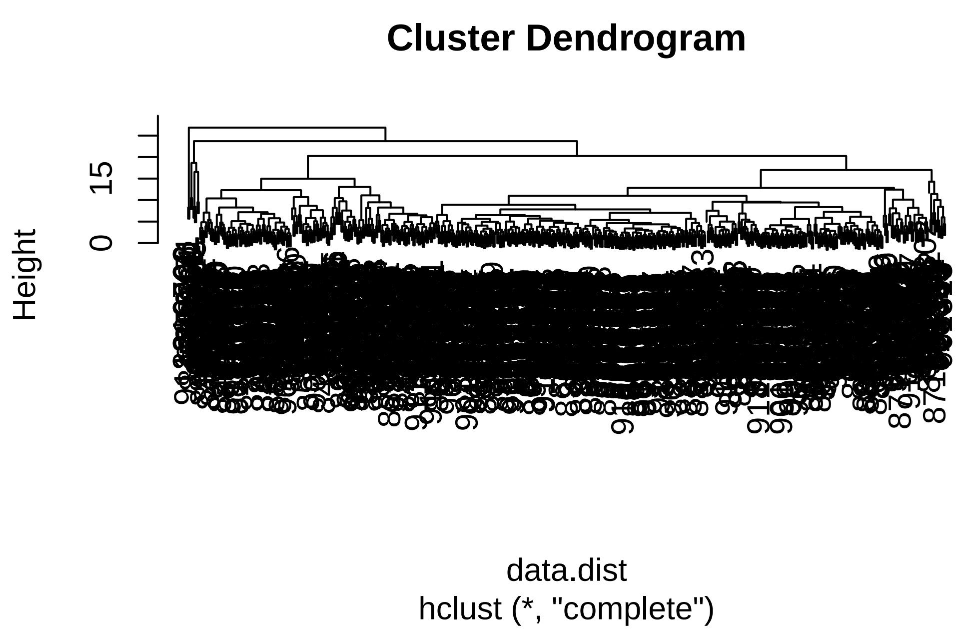
```r
# Scale the wisc.data data using the "scale()" function
data.scaled <- scale(wisc.data)
```

```r
data.dist <-dist(data.scaled)
```

```r
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?

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



The height is 20

```
wisc.hclust.clusters <- cutree(wisc.hclust, k=4, h=NULL)
```

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

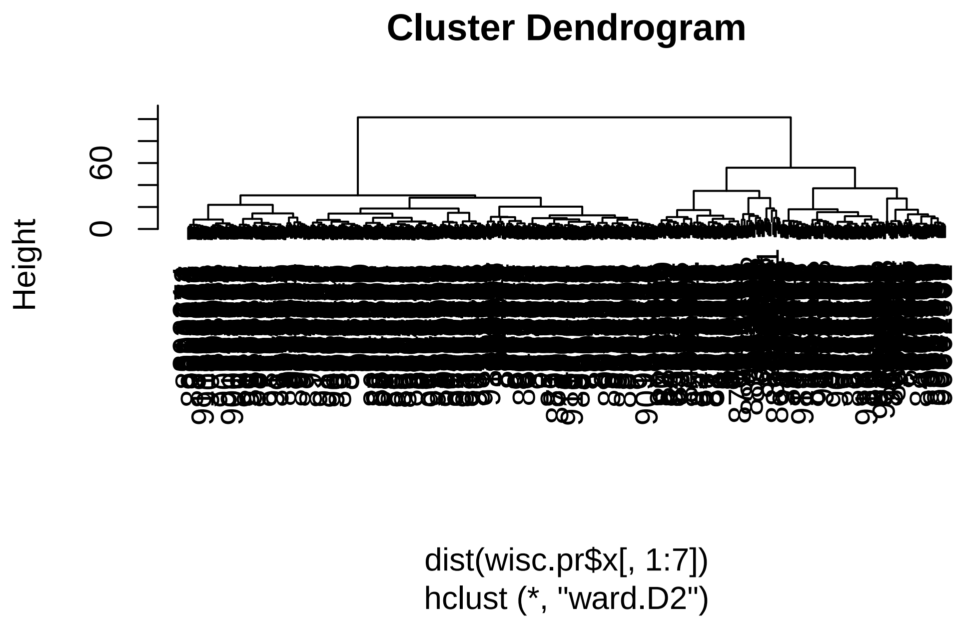
```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  12 165
                   2   2   5
                   3 343  40
                   4   0   2
```

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

I also prefer the "ward.D2" method because it results in minimal variance from different clusters.

#4. Combining methods

```
wisc.pr.hclust <- hclust (dist(wisc.pr$x[,1:7]),method="ward.D2")
plot(wisc.pr.hclust)
abline(wisc.pr.hclust, col="red", lty=2)
```



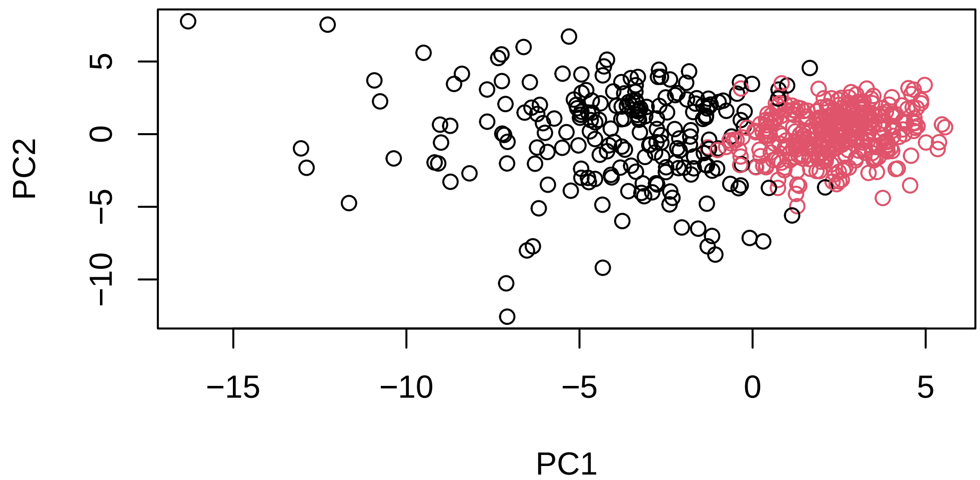

```r
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
```

```
grps
  1   2
216 353
```

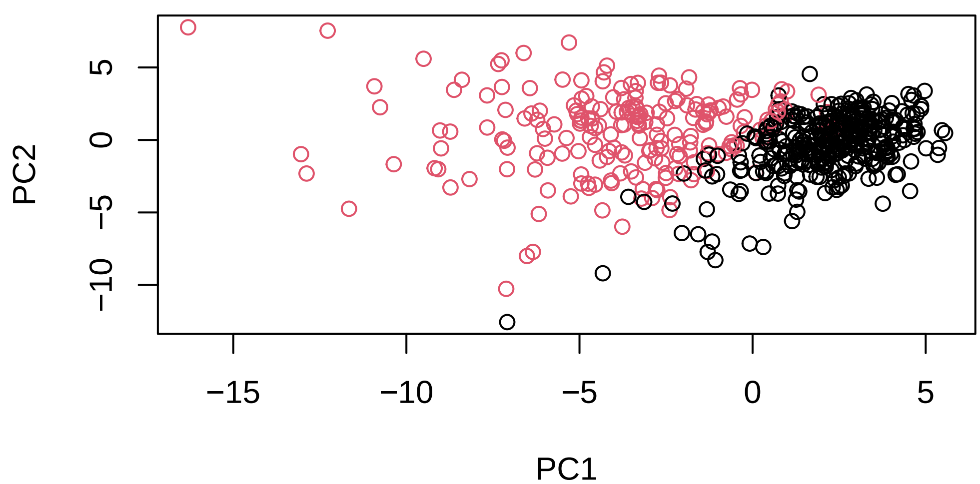
```r
table(grps, diagnosis)
```

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

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




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



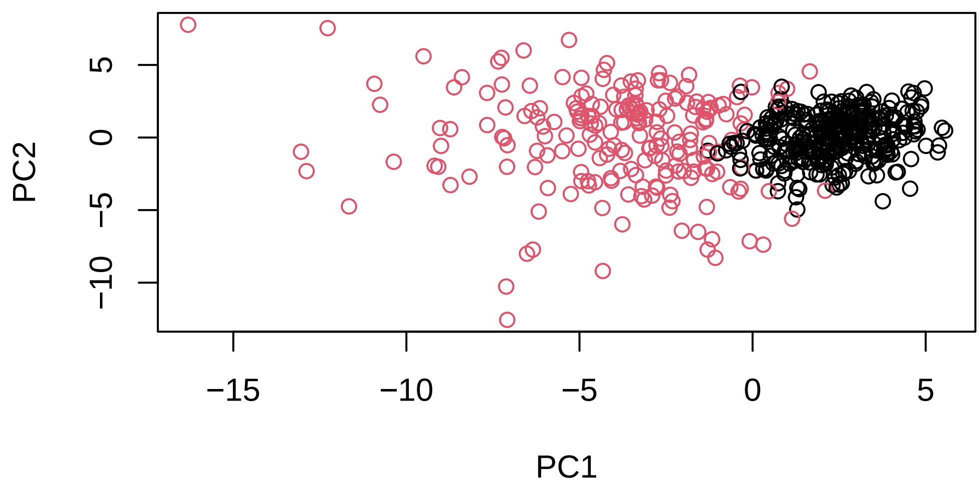
```
g <- as.factor(grps)
levels(g)
```

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

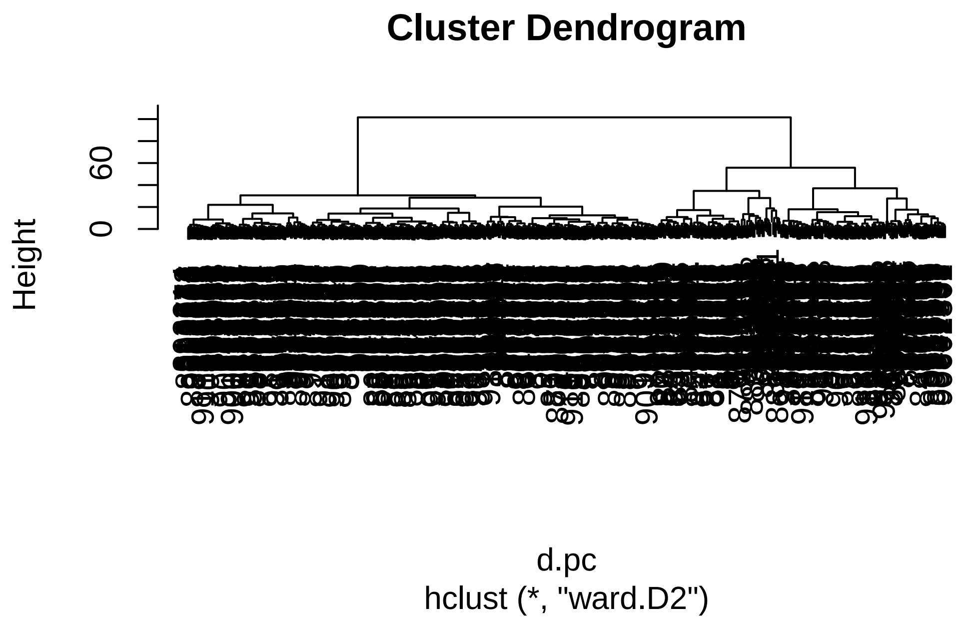
```
g <- relevel(g,2)
levels(g)
```

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

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




```
## Use the distance along the first 7 PCs for clustering i.e. wisc.pr$x[, 1:7]
d.pc <- dist(wisc.pr$x[,1:7])
wisc.pr.hc <- hclust(d.pc, method="ward.D2")
plot(wisc.pr.hc)
```




```r
wisc.pr.hclust.clusters <- cutree(wisc.pr.hc, k=4)
table(wisc.pr.hclust.clusters, diagnosis)
```

```
                       diagnosis
wisc.pr.hclust.clusters   B   M
                      1   0  45
                      2   2  77
                      3  26  66
                      4 329  24
```

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

```
         wisc.pr.hclust.clusters
diagnosis   1   2   3   4
        B   0   2  26 329
        M  45  77  66  24
```

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

It does not help with separating the diagnoses because the false positive or non-significant results are not removed.

> 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.

```
wisc.pr.hc <- hclust(d.pc, method="single")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hc, k=4)
table(diagnosis,wisc.pr.hclust.clusters)
```

```
         wisc.pr.hclust.clusters
diagnosis   1   2   3   4
        B 356   1   0   0
        M 209   0   2   1
```

```
wisc.pr.hc <- hclust(d.pc, method="average")
wisc.pr.hclust.clusters <- cutree(wisc.pr.hc, k=4)
table(diagnosis,wisc.pr.hclust.clusters)
```

```
         wisc.pr.hclust.clusters
diagnosis   1   2   3   4
        B 355   0   2   0
        M 206   4   0   2
```

There's not much difference among these hierarchical clustering models.

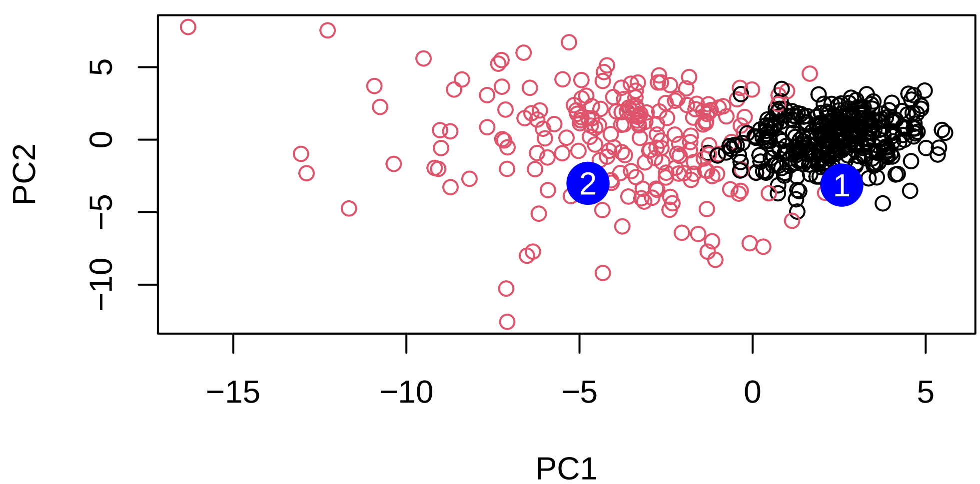
#6. Prediction

```
#url <- "new_samples.csv"
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
```

```
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 the patients with malignant diagnoses from cluster 2.

```
sessionInfo()
```

```
R version 4.3.1 (2023-06-16 ucrt)
Platform: x86_64-w64-mingw32/x64 (64-bit)
Running under: Windows 11 x64 (build 22621)

Matrix products: default


locale:
[1] LC_COLLATE=English_United States.utf8
[2] LC_CTYPE=English_United States.utf8
[3] LC_MONETARY=English_United States.utf8
[4] LC_NUMERIC=C
[5] LC_TIME=English_United States.utf8

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_3.4.4

loaded via a namespace (and not attached):
 [1] gtable_0.3.4      jsonlite_1.8.7    ggsignif_0.6.4    dplyr_1.1.3
 [5] compiler_4.3.1    Rcpp_1.0.11       tidyselect_1.2.0  stringr_1.5.0
 [9] tidyr_1.3.0       scales_1.2.1      yaml_2.3.7        fastmap_1.1.1
[13] ggpubr_0.6.0      R6_2.5.1          labeling_0.4.3    generics_0.1.3
[17] skimr_2.1.5       knitr_1.44        backports_1.4.1   ggrepel_0.9.4
[21] tibble_3.2.1      car_3.1-2         munsell_0.5.0     pillar_1.9.0
[25] rlang_1.1.1       utf8_1.2.3        broom_1.0.5       stringi_1.7.12
[29] repr_1.1.6        xfun_0.40         cli_3.6.1         withr_2.5.1
[33] magrittr_2.0.3    digest_0.6.33     grid_4.3.1        base64enc_0.1-3
[37] lifecycle_1.0.3   vctrs_0.6.3       rstatix_0.7.2     evaluate_0.22
[41] glue_1.6.2        farver_2.1.1      abind_1.4-5       carData_3.0-5
[45] fansi_1.0.5       colorspace_2.1-0  rmarkdown_2.25    purrr_1.0.2
[49] tools_4.3.1       pkgconfig_2.0.3   htmltools_0.5.6.1
```