Class 08: Breast Cancer Analysis Mini Project

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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 class. You'll 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 <- read.csv(file="WisconsinCancer (1).csv")
```

```
wisc.df <- data.frame(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
```

The first column `diagnosis` is the expert opinion on the sample(i.e patient FNA)

```
wisc.df$diagnosis
```

```
  [1] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [19] "M" "B" "B" "B" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M"
 [37] "M" "B" "M" "M" "M" "M" "M" "M" "M" "M" "B" "M" "B" "B" "B" "B" "B" "M"
 [55] "M" "B" "M" "M" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B" "M" "B"
 [73] "M" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "B"
 [91] "B" "M" "B" "B" "M" "M" "B" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[109] "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B"
[127] "M" "M" "B" "M" "B" "M" "M" "B" "M" "M" "B" "B" "M" "B" "B" "M" "B" "B"
[145] "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "M"
[163] "M" "B" "M" "B" "B" "M" "M" "B" "B" "M" "M" "B" "B" "B" "B" "M" "B" "B"
[181] "M" "M" "M" "B" "M" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "M" "M"
[199] "M" "M" "B" "M" "M" "M" "B" "M" "B" "M" "B" "B" "M" "B" "M" "M" "M" "M"
[217] "B" "B" "M" "M" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "B" "M"
[235] "B" "B" "M" "M" "B" "M" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "M" "B"
[253] "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "M" "B" "B" "B" "B"
```

```
[271] "B" "B" "M" "B" "M" "B" "B" "M" "B" "B" "M" "B" "M" "M" "B" "B" "B" "B"
[289] "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "B"
[307] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "M"
[325] "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "M" "B" "M" "B" "M" "B" "B"
[343] "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "M" "M" "B" "B" "B" "B" "B" "B"
[361] "B" "B" "B" "B" "B" "M" "M" "B" "M" "M" "M" "B" "M" "M" "B" "B" "B" "B"
[379] "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "B" "M" "B" "B" "M" "M" "B" "B"
[397] "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B"
[415] "M" "B" "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B"
[433] "M" "M" "B" "M" "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "B" "M"
[451] "B" "M" "B" "B" "B" "B" "B" "B" "B" "B" "M" "M" "B" "B" "B" "B" "B" "B"
[469] "M" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "B" "B" "B" "B" "B"
[487] "B" "M" "B" "M" "B" "B" "M" "B" "B" "B" "B" "B" "M" "M" "B" "M" "B" "M"
[505] "B" "B" "B" "B" "B" "M" "B" "B" "M" "B" "M" "B" "M" "M" "B" "B" "B" "M"
[523] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "M" "B" "M" "M" "B" "B" "B"
[541] "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B" "B"
[559] "B" "B" "B" "B" "M" "M" "M" "M" "M" "M" "B"
```

Remove the diagnosis from data for subsequent analysis

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

```
[1] 569  30
```

Store the diagnosis as a vector for later use when we compare our results to those from experts in the field.

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

> Q1. How many observations are in this dataset?

There are 569 observations in the dataset.

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

```
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

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

```
sum(grepl("_mean$", names(wisc.data)))
```

```
[1] 10
```

Performing PCA

The `prcomp()` function to do PCA has a `scale=FALSE` default. In general we nearly always want to set this to TRUE so our analysis is not dominated by columns/variables in our data set that have high standard deviation and mean when compared to others just because the units of measurement are on different units/scales

```
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
```

Perform PCA on wisc.data by completing the following code

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

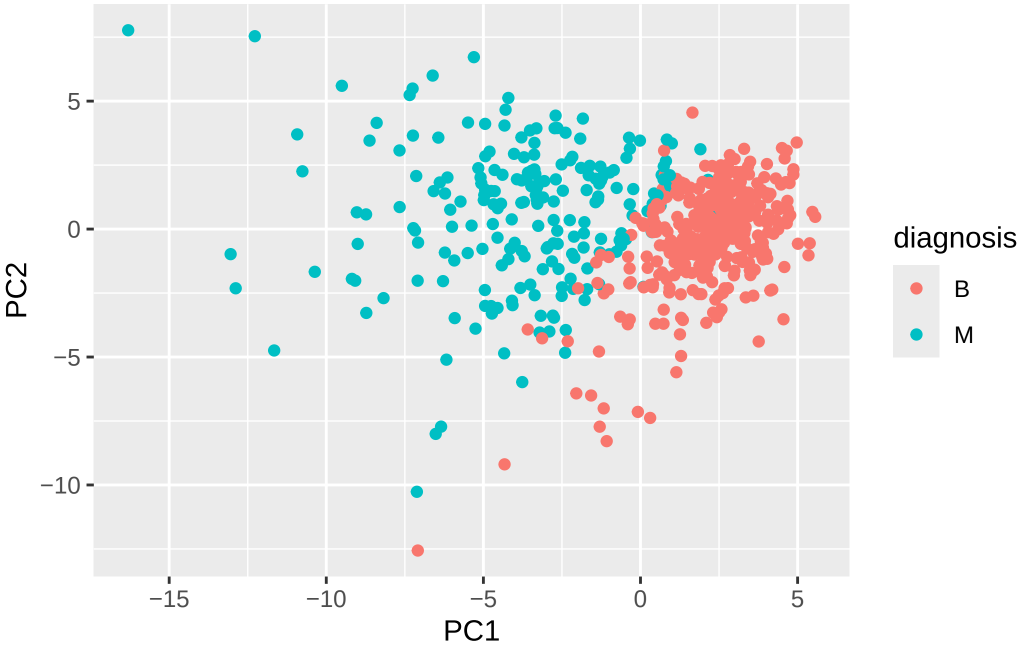
```
Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6     PC7
Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
Cumulative Proportion  0.4427 0.6324 0.72636 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
```

The main PC result figure is called a "score plot" or "PC Plot"

```
library(ggplot2)

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



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

44.2%

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

3 PCs

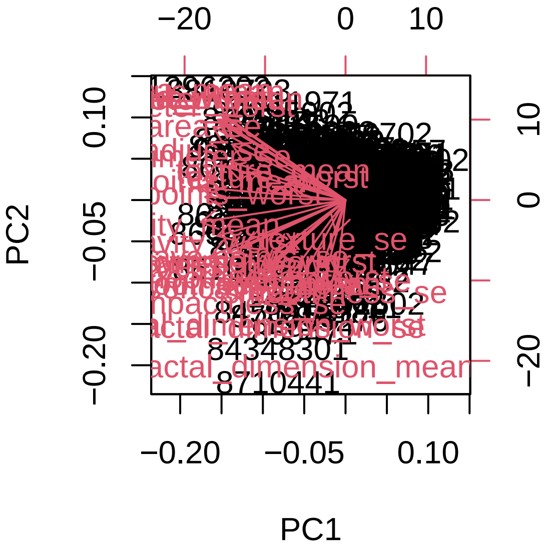
> Q6. How many principal components (PCs) are required to describe at least 90% of the original variance in the data?

7 PCs

Interpreting PCA results

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

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

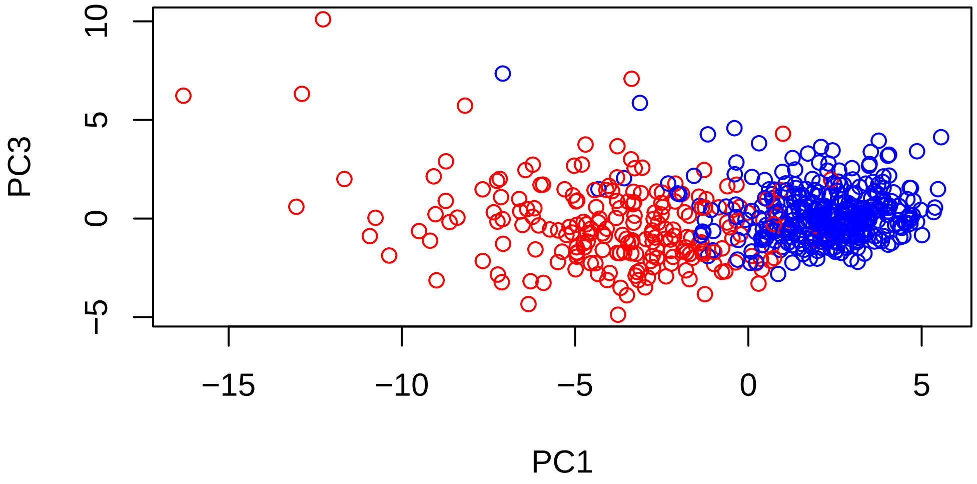


> Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?

The biplot is difficult to interpret because too many variables and data points overlap, making it hard to distinguish which features contribute to which principal components

> 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 = ifelse(diagnosis == "M", "red", "blue"),
     xlab = "PC1", ylab = "PC3")
```



The clusters of malignant and benign samples are still fairly distinct, though less clearly separated than in the PC1 vs PC2 plot. This suggests that PC3 still captures some biologically meaningful variation, but not as much as PC2.

> 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?

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

```
[1] -0.2608538
```

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

```
pr.var <- wisc.pr$sdev^2
pve <- pr.var / sum(pr.var)
cumulative_pve <- cumsum(pve)
which(cumulative_pve >= 0.80)[1]
```

```
[1] 5
```

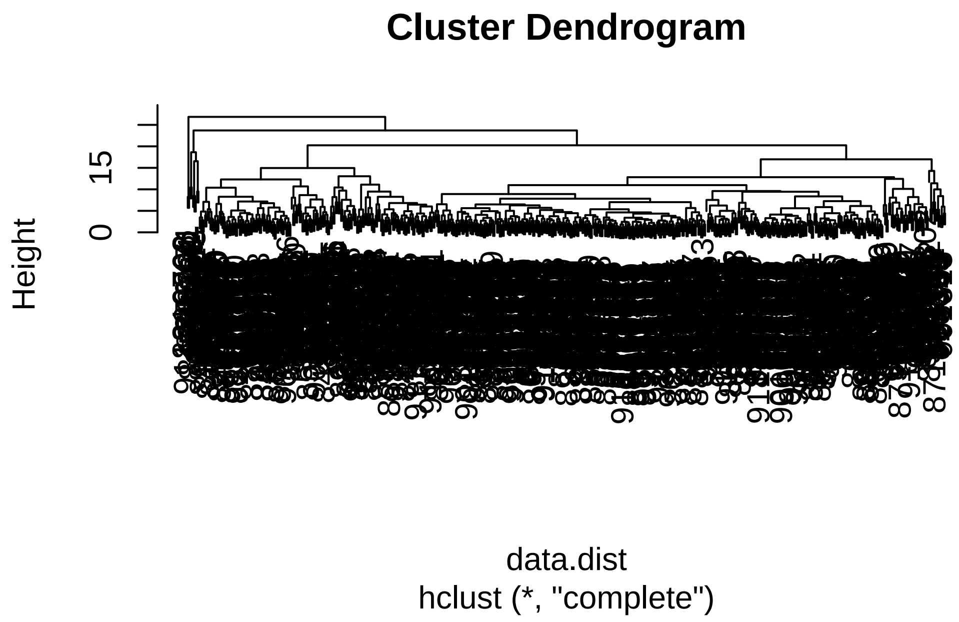
Hierarchial Clustering

Just clustering the original data is not very informative or helpful.

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

View the clustering dendogram result

```
plot(wisc.hclust)
```



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

```
wisc.hclust.clusters
  1   2   3   4
177   7 383   2
```

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

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

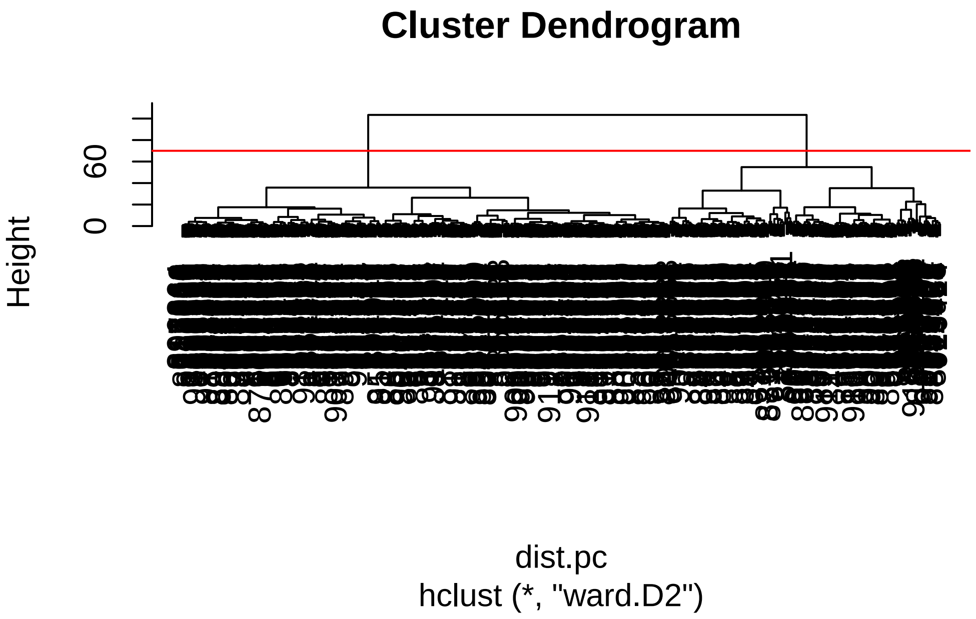
Combining Methods (PCA and Clustering)

Clustering the original data was not very productive. The PCA results looked promising. Here we combine these methods by clustering from our PCA results. In other words "clustering in PC space"...

```
##Take the first 3 PCs
dist.pc <- dist(wisc.pr$x[,1:3])
wisc.pr.hclust <- hclust(dist.pc, method="ward.D2" )
```

View the tree...

```
plot(wisc.pr.hclust)
abline(h=70, col="red")
```



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

At a height of approximately 70, the dendrogram divides the samples into 4 clusters.

Selecting number of clusters

```r
wisc.hclust.clusters <- cutree(wisc.pr.hclust, h = 70)
table(wisc.hclust.clusters, diagnosis)
```

```
                    diagnosis
wisc.hclust.clusters   B   M
                   1  24 179
                   2 333  33
```

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

The best match between clusters and diagnosis typically occurs with 2 clusters, where one corresponds mostly to malignant samples and the other to benign samples.Cutting into more than 2 clusters will split groups unnecessarily or create small mixed clusters.

Using different methods

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

The Ward.D2 method produced the clearest, most balanced clustering. It minimizes within-cluster variance, forming compact, spherical groups that aligned well with malignant vs. benign diagnoses.

> Q14. How well does k-means separate the two diagnoses? How does it compare to your hclust results?

```r
kmeans.results <- kmeans(wisc.pr$x[,1:3], centers = 2)
table(kmeans.results$cluster, diagnosis)
```

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

The k-means model with 2 clusters separates malignant and benign cases reasonably well — one cluster mostly corresponds to malignant samples, and the other to benign. However, hierarchical clustering in PCA space (using Ward.D2) slightly outperformed k-means, producing cleaner separation with fewer mixed samples.

Combining Methods

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

At four clusters, two major groups correspond closely to the malignant and benign diagnoses, while the smaller clusters represent outliers or borderline samples.

To get our clustering membership vector (i.e our main clustering result) we "cut" the tree at a desired height or to yield a desired number of "k" groups.

```r
grps <- cutree(wisc.pr.hclust, h=70)
table(grps)
```

```
grps
  1   2 
203 366 
```

How this clustering grps compares to expert diagnosis

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

```
    diagnosis
grps   B   M
   1  24 179
   2 333  33
```

> Q16. How well do the k-means and hierarchical clustering models you created in previous sections (i.e. before PCA) do in terms of separating the diagnoses?

Before PCA, both k-means and hierarchical clustering performed poorly — the data's high dimensionality and differing scales obscured the structure, resulting in mixed clusters with low separation accuracy. After PCA, clustering performance improved dramatically because noise and redundant dimensions were removed, revealing clearer biological groupings.

Sensitivity/Specificity

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

PCA + Ward.D2 hierarchical clustering correctly identified benign cases with minimal malignant misclassification. k-means on PCA data is slightly better at detecting malignant samples but at the cost of more benign false positives. Overall, PCA + Ward.D2 gave the best trade-off between sensitivity and specificity.

Sensitivity : TP/(TP+FN) Specificity : TN/(TN+FN)

Prediction

We can use our PCA model for prediction with new input patient samples.

> Q18. Which of these new patients should we prioritize for follow up based on your results?

2