

# Class08

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## Save Input Data File

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

## Storing

```
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              |                  |                   |                   |         |

## Remove 1st Column

```
wisc.data <- wisc.df[,-1]
```

## Diagnosis Vector

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

```
[1] "M" "M" "M" "M" "M" "M"
```

## Benign v Malignant Count

```
table(diagnosis)
```

```
diagnosis  
  B    M  
357 212
```

## Q1. How Many Observations in this Dataset?

569 Observations

## Q2. How many Malignant?

212 Cases

## Q3. How many Variables in Data are Suffixed with '\_mean'?

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

```
[1] 10
```

## Checking Column Means and SD

```
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            |

## PCA

```
wisc.pr <- prcomp(wisc.data, scale=T)
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. What proportion of the original variance is captured by the first principal components (PC1)?**

.4427

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

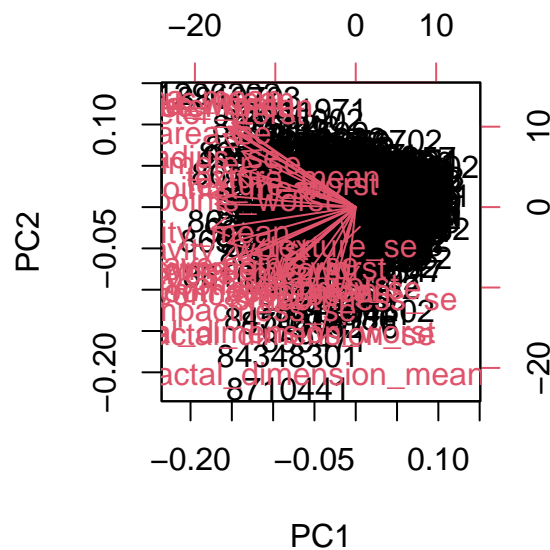
Cumulative proportion exceeds 70% at PC3 (0.72636). Therefore, three principal components (PC1, PC2, and PC3) are required to explain at least 70% of the original variance in the data.

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

Cumulative proportion exceeds 90% at PC7 (0.91010). Therefore, seven principal components (PC1-PC7) are required to explain at least 90% of the original variance in the data

## Biplot

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

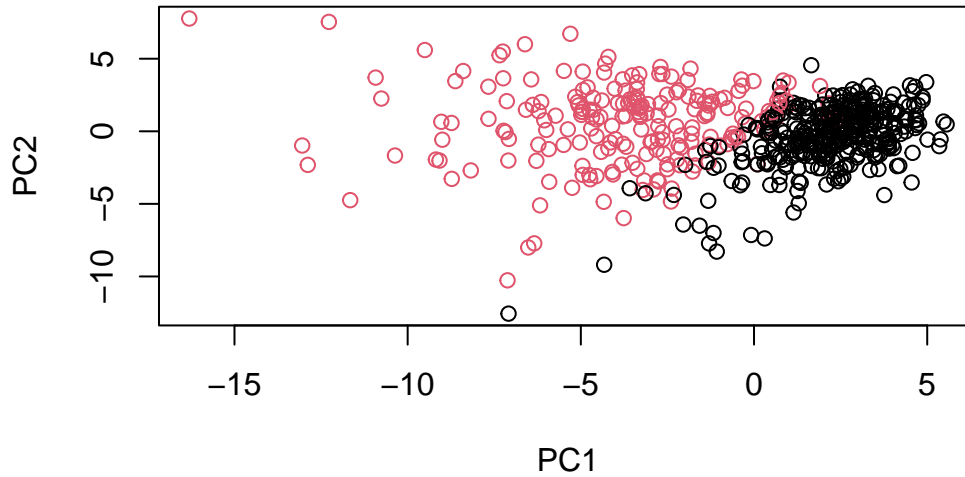


**Q7. What stands out to you about this plot? Is it easy or difficult to understand? Why?**

This plot is a hot mess, need to generate our own plots for better understanding.

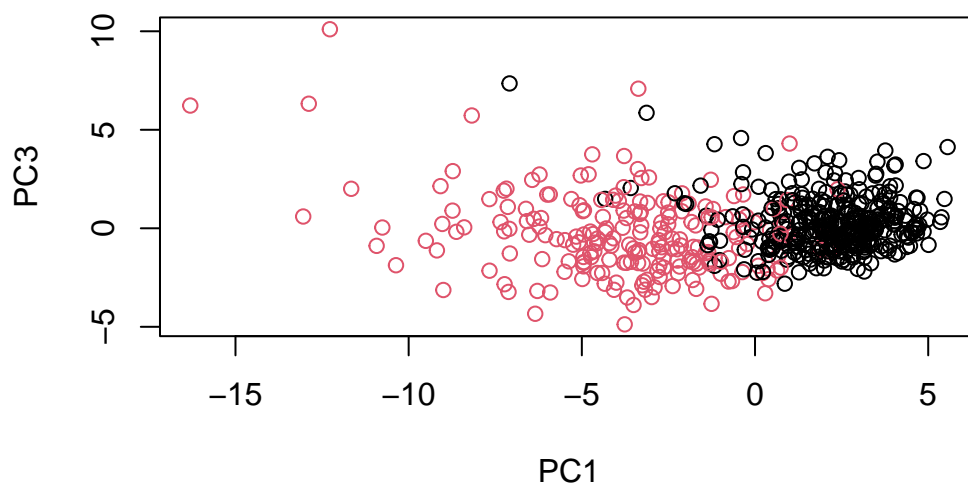
**Main “PC Score Plot”, “PC1vPC2 Plot”**

```
plot(wisc.pr$x[,1], wisc.pr$x[,2], col=as.factor(diagnosis), xlab="PC1", ylab="PC2")
```



**Q8. Generating PC1 and PC3 Plot**

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



This plot is not as clearly separated as PC1 vs PC2

## Creating Data.Frame for ggplot

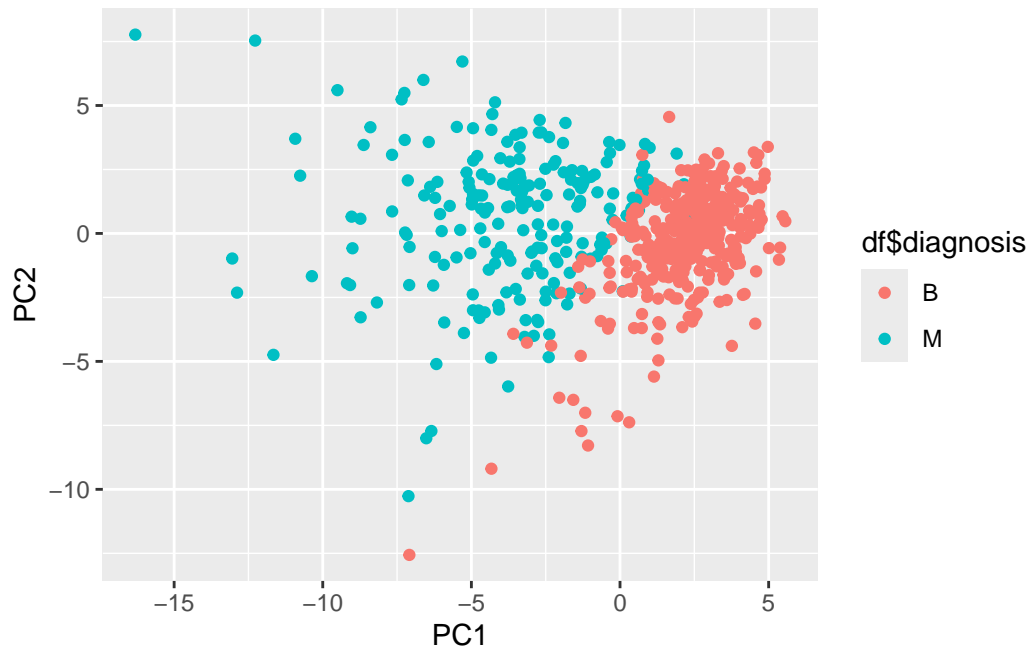
```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis
```

## Making Scatterplot using ggplot2

```
library(ggplot2)
ggplot(df) +
  aes(PC1, PC2, col=df$diagnosis) +
  geom_point()
```

Warning: Use of `df\$diagnosis` is discouraged.  
i Use `diagnosis` instead.





## Calculating Variance of Each Component

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

```
[1] 3.644394 2.385656 1.678675 1.407352 1.284029 1.098798
```

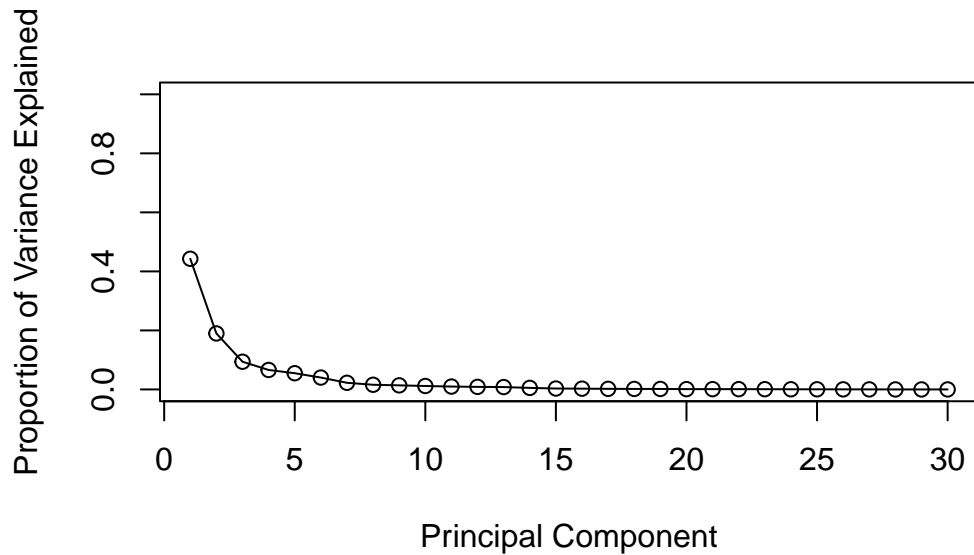
## Variance Explained by Each Principal Component: pve

```
pr.var <- wisc.pr$sdev^2
pve <- pr.var/sum(pr.var)
pve
```

```
[1] 4.427203e-01 1.897118e-01 9.393163e-02 6.602135e-02 5.495768e-02
[6] 4.024522e-02 2.250734e-02 1.588724e-02 1.389649e-02 1.168978e-02
[11] 9.797190e-03 8.705379e-03 8.045250e-03 5.233657e-03 3.137832e-03
[16] 2.662093e-03 1.979968e-03 1.753959e-03 1.649253e-03 1.038647e-03
```

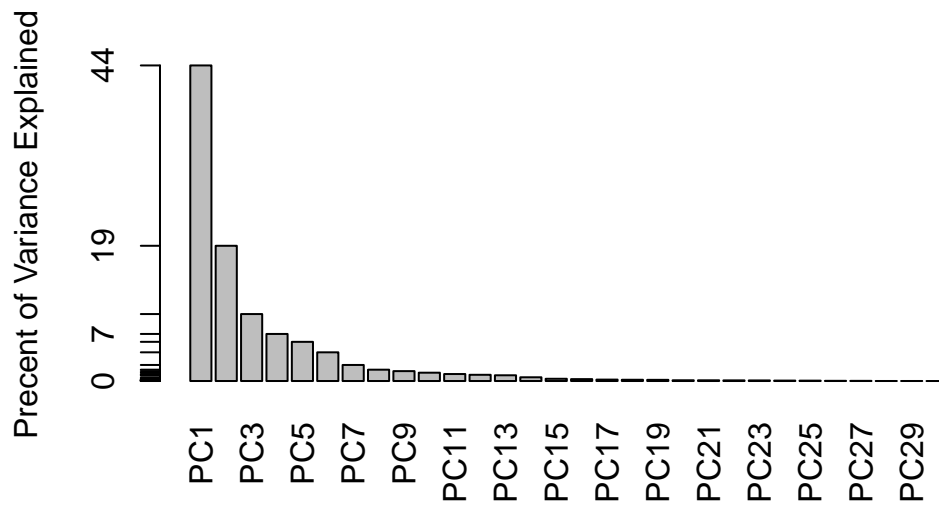
```
[21] 9.990965e-04 9.146468e-04 8.113613e-04 6.018336e-04 5.160424e-04
[26] 2.725880e-04 2.300155e-04 5.297793e-05 2.496010e-05 4.434827e-06
```

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



## Alternative Scree Plot of Same Data

```
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 )
```



**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`?**

```
loadings <- wisc.pr$rotation[, 1]
concave_points_loading <- loadings[names(wisc.data) == "concave.points_mean"]
head(concave_points_loading)
```

```
concave.points_mean
-0.2608538
```

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

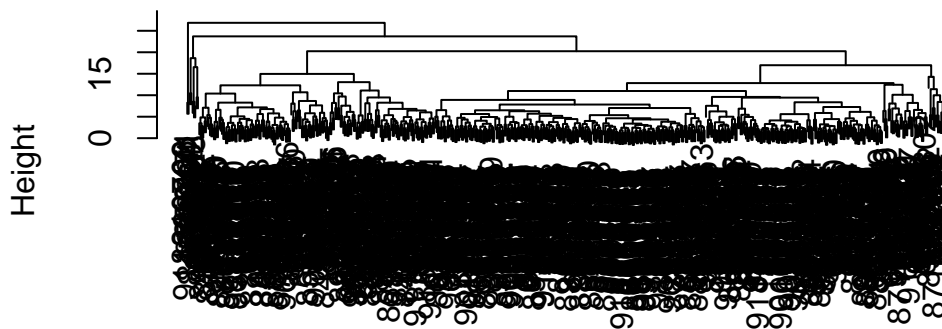
Cumulative proportion exceeds 80% at PC5 (0.84734). Therefore, seven principal components (PC1-PC5) are required to explain at least 80% of the original variance in the data.

# Hierarchical Clustering

## Scale Function

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

### Cluster Dendrogram

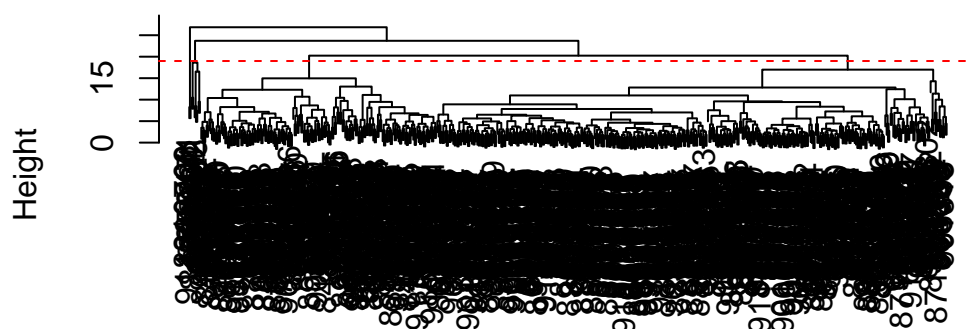


data.dist  
hclust (\*, "complete")

**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)
```

## Cluster Dendrogram



```
data.dist  
hclust (*, "complete")
```

$h = 19$

## Selecting Number of Clusters

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

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

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

```
wisc.hclust.clusters2 <- cutree(wisc.hclust, k=2)
table(wisc.hclust.clusters2, diagnosis)
```

```
      diagnosis
wisc.hclust.clusters2  B  M
1 357 210
2   0   2
```

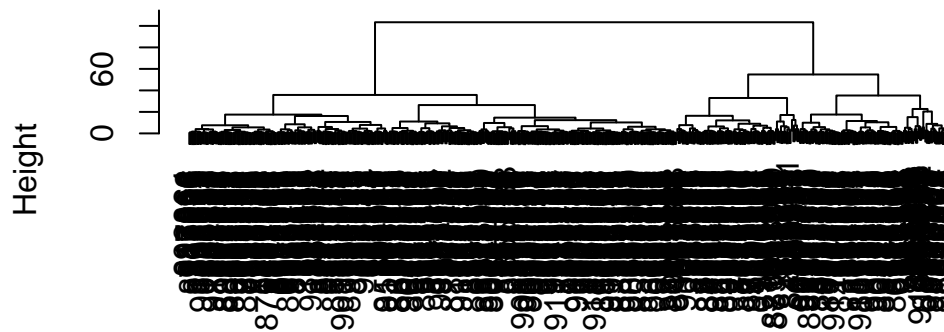
```
wisc.hclust.clusters10 <- cutree(wisc.hclust, k=10)
table(wisc.hclust.clusters10, diagnosis)
```

```
      diagnosis
wisc.hclust.clusters10  B  M
1    12 86
2     0 59
3     0  3
4   331 39
5     0 20
6     2  0
7    12  0
8     0  2
9     0  2
10    0  1
```

## Combining PCA and Clustering

```
d <- dist(wisc.pr$x[,1:3])
hc <- hclust(d, method="ward.D2")
plot(hc)
```

## Cluster Dendrogram

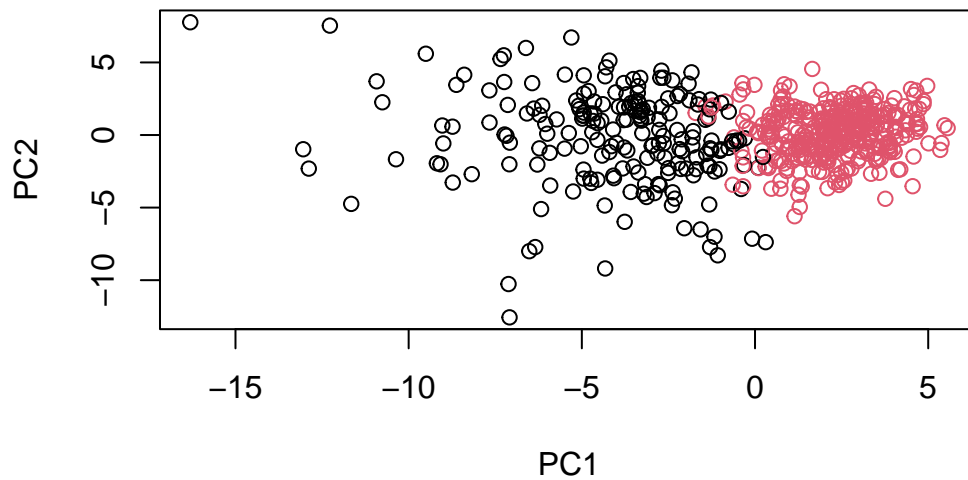


d  
hclust (\*, "ward.D2")

## Cutree into 2 groups/branches

```
grps <- cutree(hc,k=2)
```

```
plot(wisc.pr$x, col=grps)
```



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

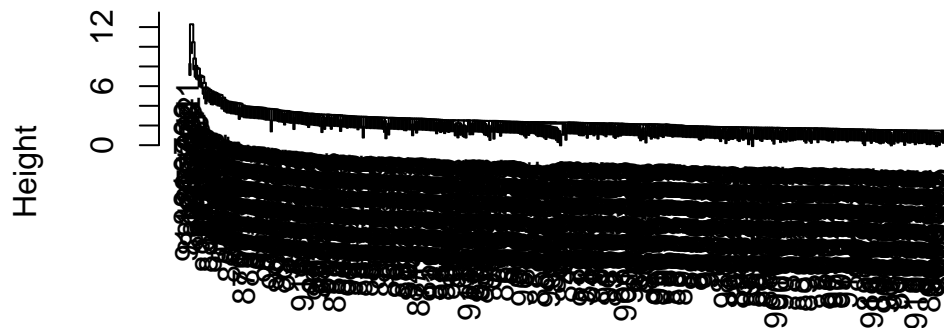
My favorite is ward.d2 it produces the cleanest and most balanced clustering.

Single

```
wist.single.clust <- hclust(data.dist, method="single")  
plot(wist.single.clust)
```



## Cluster Dendrogram

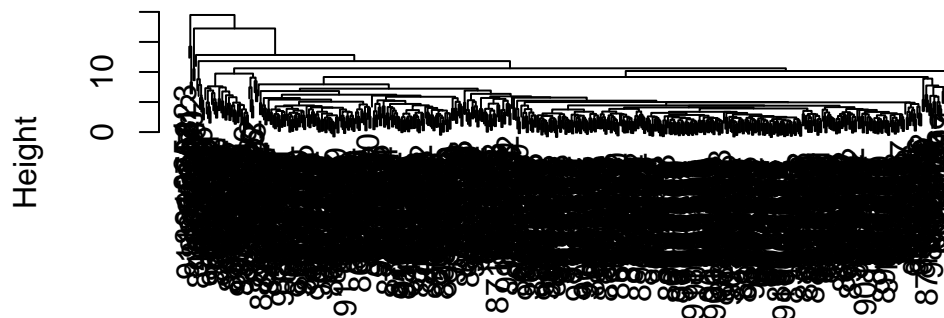


```
data.dist  
hclust (*, "single")
```

Average

```
wist.average.clust <- hclust(data.dist, method="average")  
plot(wist.average.clust)
```

## Cluster Dendrogram



```
data.dist  
hclust (*, "average")
```

Ward.D2

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

