Lab 8: Breast Cancer Mini Project

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Table of contents

Background

This mini-project explores unsupervised learning techniques applied to the Wisconsin Breast Cancer Diagnostic Data Set, which contains measurements of human breast mass cell nuclei. The project guides the user through exploratory data analysis, performing and interpreting Principal Component Analysis (PCA) to reduce the dimensionality of the data while retaining variance, and applying hierarchical clustering with different linkage methods. It also includes an optional section on K-means clustering for comparison. The ultimate goal is to combine PCA and clustering to better separate benign and malignant cell samples, evaluating the results using metrics like sensitivity and specificity, and finally demonstrating how to predict the classification of new samples using the developed PCA model.

Data Import

Our data come from the U. of Wisconsin Medical Center

```
wisc.df <-read.csv("WisconsinCancer.csv", row.names=1)
```

Q. How many patients/samples are in this dataset?

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

```
[1] 569
```

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

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

```

  B   M 
357 212 
```

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

```
length(grep("mean",colnames(wisc.df),value =TRUE))
```

```
[1] 10
```

There is a diagnosis column that is the clinician consensus that I want to exclude from any further analysis. We will come back later and compare our results to this diagnosis.

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

```
[1] M M M M M M
Levels: B M
```

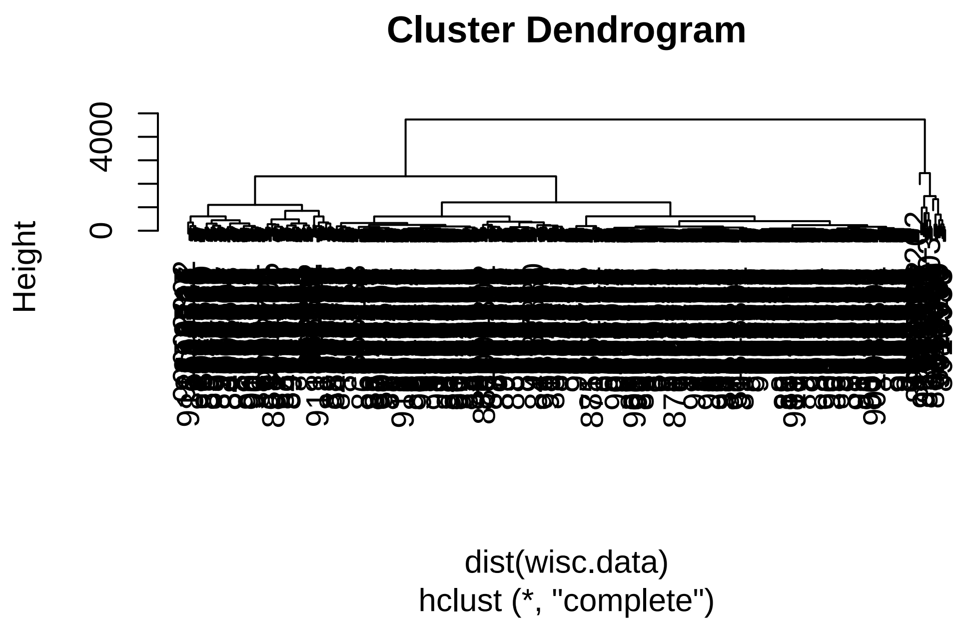
Now we can remove it from the `wisc.df`

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

Clustering

Let's try a `hclust()`

```r
hc <- hclust(dist(wisc.data))
plot(hc)
```



We can extract clusters from this rather poor dendrogram/tree with the `cutree()`

```r
groups <- cutree(hc, k=2)
```

How many individuals in each cluster?

```r
table(groups)
```

```
groups
  1   2 
549  20 
```

```r
table(diagnosis)
```

```
diagnosis
  B   M 
357 212 
```

We can generate a cross-table that compares our cluster `groups` vector with our `diagnosis` vector values.

```
table(diagnosis, groups)
```

```
         groups
diagnosis   1   2
        B 357   0
        M 192  20
```

Principal Component Analysis

The importance of data scaling

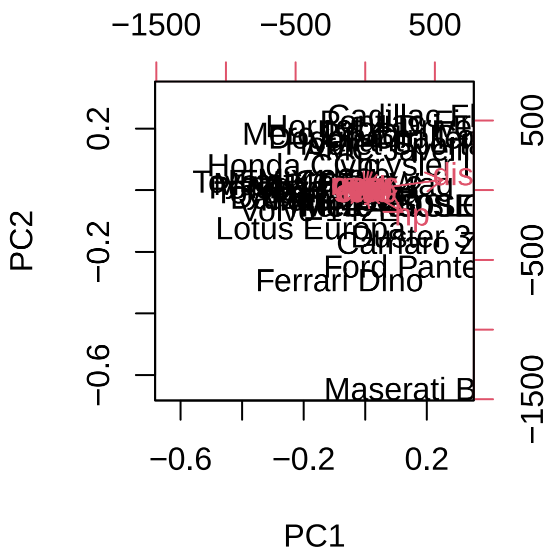
The main function for PCA in base R is `prcomp()` it has a default input parameter of `scale=FALSE`.

```
#prcomp()
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

We could do a PCA of this data as is and it could be mis-leading…

```
pc <-prcomp(mtcars)
biplot(pc)
```



Let's look at the mean values of each column and their standard deviation.

```
colMeans(mtcars)
```

```
       mpg        cyl       disp         hp       drat         wt       qsec
 20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750
        vs         am       gear       carb
  0.437500   0.406250   3.687500   2.812500
```

```
apply(mtcars, 2, sd)
```

```
        mpg         cyl        disp          hp        drat          wt
  6.0269481   1.7859216 123.9386938  68.5628685   0.5346787   0.9784574
       qsec          vs          am        gear        carb
  1.7869432   0.5040161   0.4989909   0.7378041   1.6152000
```

We can "scale" this data before PCA to get a much better representation and analysis of all the columns.

```
mtscale <-scale(mtcars)
mtscale
```

	mpg	cyl	disp	hp	drat
Mazda RX4	0.15088482	-0.1049878	-0.57061982	-0.53509284	0.56751369
Mazda RX4 Wag	0.15088482	-0.1049878	-0.57061982	-0.53509284	0.56751369
Datsun 710	0.44954345	-1.2248578	-0.99018209	-0.78304046	0.47399959
Hornet 4 Drive	0.21725341	-0.1049878	0.22009369	-0.53509284	-0.96611753
Hornet Sportabout	-0.23073453	1.0148821	1.04308123	0.41294217	-0.83519779
Valiant	-0.33028740	-0.1049878	-0.04616698	-0.60801861	-1.56460776
Duster 360	-0.96078893	1.0148821	1.04308123	1.43390296	-0.72298087
Merc 240D	0.71501778	-1.2248578	-0.67793094	-1.23518023	0.17475447
Merc 230	0.44954345	-1.2248578	-0.72553512	-0.75387015	0.60491932
Merc 280	-0.14777380	-0.1049878	-0.50929918	-0.34548584	0.60491932
Merc 280C	-0.38006384	-0.1049878	-0.50929918	-0.34548584	0.60491932
Merc 450SE	-0.61235388	1.0148821	0.36371309	0.48586794	-0.98482035
Merc 450SL	-0.46302456	1.0148821	0.36371309	0.48586794	-0.98482035
Merc 450SLC	-0.81145962	1.0148821	0.36371309	0.48586794	-0.98482035
Cadillac Fleetwood	-1.60788262	1.0148821	1.94675381	0.85049680	-1.24665983
Lincoln Continental	-1.60788262	1.0148821	1.84993175	0.99634834	-1.11574009
Chrysler Imperial	-0.89442035	1.0148821	1.68856165	1.21512565	-0.68557523
Fiat 128	2.04238943	-1.2248578	-1.22658929	-1.17683962	0.90416444
Honda Civic	1.71054652	-1.2248578	-1.25079481	-1.38103178	2.49390411
Toyota Corolla	2.29127162	-1.2248578	-1.28790993	-1.19142477	1.16600392
Toyota Corona	0.23384555	-1.2248578	-0.89255318	-0.72469984	0.19345729
Dodge Challenger	-0.76168319	1.0148821	0.70420401	0.04831332	-1.56460776
AMC Javelin	-0.81145962	1.0148821	0.59124494	0.04831332	-0.83519779
Camaro Z28	-1.12671039	1.0148821	0.96239618	1.43390296	0.24956575
Pontiac Firebird	-0.14777380	1.0148821	1.36582144	0.41294217	-0.96611753
Fiat X1-9	1.19619000	-1.2248578	-1.22416874	-1.17683962	0.90416444
Porsche 914-2	0.98049211	-1.2248578	-0.89093948	-0.81221077	1.55876313
Lotus Europa	1.71054652	-1.2248578	-1.09426581	-0.49133738	0.32437703
Ford Pantera L	-0.71190675	1.0148821	0.97046468	1.71102089	1.16600392
Ferrari Dino	-0.06481307	-0.1049878	-0.69164740	0.41294217	0.04383473
Maserati Bora	-0.84464392	1.0148821	0.56703942	2.74656682	-0.10578782
Volvo 142E	0.21725341	-1.2248578	-0.88529152	-0.54967799	0.96027290

	wt	qsec	vs	am	gear
Mazda RX4	-0.610399567	-0.77716515	-0.8680278	1.1899014	0.4235542
Mazda RX4 Wag	-0.349785269	-0.46378082	-0.8680278	1.1899014	0.4235542
Datsun 710	-0.917004624	0.42600682	1.1160357	1.1899014	0.4235542
Hornet 4 Drive	-0.002299538	0.89048716	1.1160357	-0.8141431	-0.9318192
Hornet Sportabout	0.227654255	-0.46378082	-0.8680278	-0.8141431	-0.9318192
Valiant	0.248094592	1.32698675	1.1160357	-0.8141431	-0.9318192
Duster 360	0.360516446	-1.12412636	-0.8680278	-0.8141431	-0.9318192
Merc 240D	-0.027849959	1.20387148	1.1160357	-0.8141431	0.4235542
Merc 230	-0.068730634	2.82675459	1.1160357	-0.8141431	0.4235542

Merc 280	0.227654255	0.25252621	1.1160357	-0.8141431	0.4235542
Merc 280C	0.227654255	0.58829513	1.1160357	-0.8141431	0.4235542
Merc 450SE	0.871524874	-0.25112717	-0.8680278	-0.8141431	-0.9318192
Merc 450SL	0.524039143	-0.13920420	-0.8680278	-0.8141431	-0.9318192
Merc 450SLC	0.575139986	0.08464175	-0.8680278	-0.8141431	-0.9318192
Cadillac Fleetwood	2.077504765	0.07344945	-0.8680278	-0.8141431	-0.9318192
Lincoln Continental	2.255335698	-0.01608893	-0.8680278	-0.8141431	-0.9318192
Chrysler Imperial	2.174596366	-0.23993487	-0.8680278	-0.8141431	-0.9318192
Fiat 128	-1.039646647	0.90727560	1.1160357	1.1899014	0.4235542
Honda Civic	-1.637526508	0.37564148	1.1160357	1.1899014	0.4235542
Toyota Corolla	-1.412682800	1.14790999	1.1160357	1.1899014	0.4235542
Toyota Corona	-0.768812180	1.20946763	1.1160357	-0.8141431	-0.9318192
Dodge Challenger	0.309415603	-0.54772305	-0.8680278	-0.8141431	-0.9318192
AMC Javelin	0.222544170	-0.30708866	-0.8680278	-0.8141431	-0.9318192
Camaro Z28	0.636460997	-1.36476075	-0.8680278	-0.8141431	-0.9318192
Pontiac Firebird	0.641571082	-0.44699237	-0.8680278	-0.8141431	-0.9318192
Fiat X1-9	-1.310481114	0.58829513	1.1160357	1.1899014	0.4235542
Porsche 914-2	-1.100967659	-0.64285758	-0.8680278	1.1899014	1.7789276
Lotus Europa	-1.741772228	-0.53093460	1.1160357	1.1899014	1.7789276
Ford Pantera L	-0.048290296	-1.87401028	-0.8680278	1.1899014	1.7789276
Ferrari Dino	-0.457097039	-1.31439542	-0.8680278	1.1899014	1.7789276
Maserati Bora	0.360516446	-1.81804880	-0.8680278	1.1899014	1.7789276
Volvo 142E	-0.446876870	0.42041067	1.1160357	1.1899014	0.4235542

	carb
Mazda RX4	0.7352031
Mazda RX4 Wag	0.7352031
Datsun 710	-1.1221521
Hornet 4 Drive	-1.1221521
Hornet Sportabout	-0.5030337
Valiant	-1.1221521
Duster 360	0.7352031
Merc 240D	-0.5030337
Merc 230	-0.5030337
Merc 280	0.7352031
Merc 280C	0.7352031
Merc 450SE	0.1160847
Merc 450SL	0.1160847
Merc 450SLC	0.1160847
Cadillac Fleetwood	0.7352031
Lincoln Continental	0.7352031
Chrysler Imperial	0.7352031
Fiat 128	-1.1221521
Honda Civic	-0.5030337

```
Toyota Corolla      -1.1221521
Toyota Corona       -1.1221521
Dodge Challenger    -0.5030337
AMC Javelin         -0.5030337
Camaro Z28           0.7352031
Pontiac Firebird    -0.5030337
Fiat X1-9           -1.1221521
Porsche 914-2       -0.5030337
Lotus Europa        -0.5030337
Ford Pantera L       0.7352031
Ferrari Dino         1.9734398
Maserati Bora        3.2116766
Volvo 142E          -0.5030337
attr(,"scaled:center")
       mpg        cyl       disp         hp       drat         wt       qsec 
 20.090625   6.187500 230.721875 146.687500   3.596563   3.217250  17.848750 
        vs         am       gear       carb 
  0.437500   0.406250   3.687500   2.812500 
attr(,"scaled:scale")
        mpg         cyl        disp          hp        drat          wt 
  6.0269481   1.7859216 123.9386938  68.5628685   0.5346787   0.9784574 
       qsec          vs          am        gear        carb 
  1.7869432   0.5040161   0.4989909   0.7378041   1.6152000 
```

```r
round(colMeans(mtscale))
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   0    0    0    0    0    0    0    0    0    0    0 
```

```r
apply(mtscale,2,sd)
```

```
 mpg  cyl disp   hp drat   wt qsec   vs   am gear carb 
   1    1    1    1    1    1    1    1    1    1    1 
```

```r
pc.scale <-prcomp(mtscale)
pc.scale
```

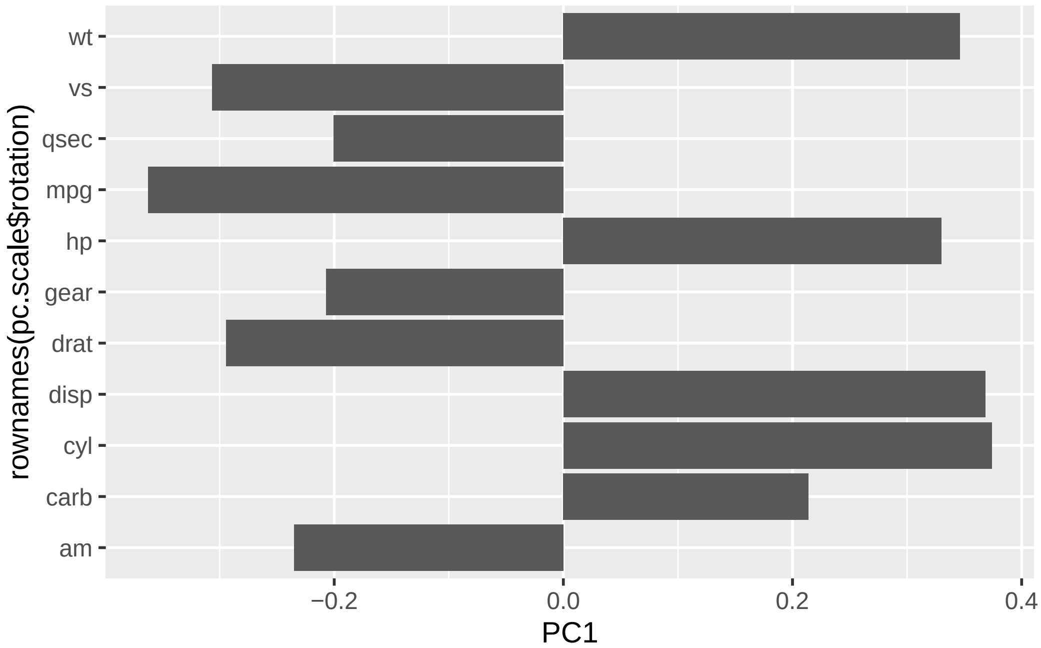
```
Standard deviations (1, .., p=11):
 [1] 2.5706809 1.6280258 0.7919579 0.5192277 0.4727061 0.4599958 0.3677798
 [8] 0.3505730 0.2775728 0.2281128 0.1484736
```

```
Rotation (n x k) = (11 x 11):
            PC1         PC2         PC3          PC4         PC5         PC6
mpg  -0.3625305  0.01612440 -0.22574419 -0.022540255 -0.10284468 -0.10879743
cyl   0.3739160  0.04374371 -0.17531118 -0.002591838 -0.05848381  0.16855369
disp  0.3681852 -0.04932413 -0.06148414  0.256607885 -0.39399530 -0.33616451
hp    0.3300569  0.24878402  0.14001476 -0.067676157 -0.54004744  0.07143563
drat -0.2941514  0.27469408  0.16118879  0.854828743 -0.07732727  0.24449705
wt    0.3461033 -0.14303825  0.34181851  0.245899314  0.07502912 -0.46493964
qsec -0.2004563 -0.46337482  0.40316904  0.068076532  0.16466591 -0.33048032
vs   -0.3065113 -0.23164699  0.42881517 -0.214848616 -0.59953955  0.19401702
am   -0.2349429  0.42941765 -0.20576657 -0.030462908 -0.08978128 -0.57081745
gear -0.2069162  0.46234863  0.28977993 -0.264690521 -0.04832960 -0.24356284
carb  0.2140177  0.41357106  0.52854459 -0.126789179  0.36131875  0.18352168
              PC7          PC8          PC9        PC10         PC11
mpg   0.367723810  0.754091423 -0.235701617 -0.13928524 -0.124895628
cyl   0.057277736  0.230824925 -0.054035270  0.84641949 -0.140695441
disp  0.214303077 -0.001142134 -0.198427848 -0.04937979  0.660606481
hp   -0.001495989  0.222358441  0.575830072 -0.24782351 -0.256492062
drat  0.021119857 -0.032193501  0.046901228  0.10149369 -0.039530246
wt   -0.020668302  0.008571929 -0.359498251 -0.09439426 -0.567448697
qsec  0.050010522  0.231840021  0.528377185  0.27067295  0.181361780
vs   -0.265780836 -0.025935128 -0.358582624  0.15903909  0.008414634
am   -0.587305101  0.059746952  0.047403982  0.17778541  0.029823537
gear  0.605097617 -0.336150240  0.001735039  0.21382515 -0.053507085
carb -0.174603192  0.395629107 -0.170640677 -0.07225950  0.319594676
```

We can look at the two main results figures from PCA - the “PC plot” (a.k.a. score plot, ordination plot, or PC1 vs PC2 plot). The “loadings plot” how the original variables contribute to the new PCs

A loadings plot of the unscalled PCA results

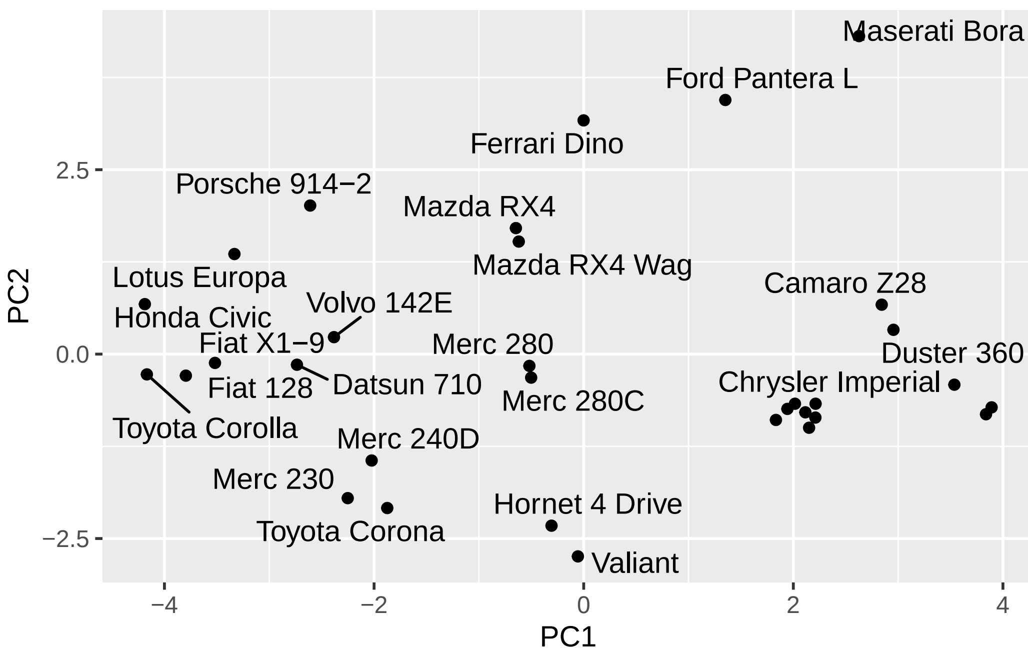
```r
library(ggplot2)
ggplot(pc.scale$rotation)+
  aes(PC1, rownames(pc.scale$rotation))+
  geom_col()
```



PC plot of scaled PCA results

```
library(ggrepel)
ggplot(pc.scale$x)+
  aes(PC1,PC2, label=rownames(pc.scale$x))+
  geom_point()+
  geom_text_repel()
```

```
Warning: ggrepel: 9 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```



> **Key point**: In general we will set `scale=TRUE` when we do PCA. This is not the default but probably should be…

We can check the SD and mean of the different columns in `wisc.data` to see if we need to scale - hint: we do!

PCA of wisc.data

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

```
Standard deviations (1, .., p=30):
 [1] 3.64439401 2.38565601 1.67867477 1.40735229 1.28402903 1.09879780
 [7] 0.82171778 0.69037464 0.64567392 0.59219377 0.54213992 0.51103950
[13] 0.49128148 0.39624453 0.30681422 0.28260007 0.24371918 0.22938785
[19] 0.22243559 0.17652026 0.17312681 0.16564843 0.15601550 0.13436892
[25] 0.12442376 0.09043030 0.08306903 0.03986650 0.02736427 0.01153451

Rotation (n x k) = (30 x 30):
                                PC1          PC2          PC3          PC4
radius_mean             -0.21890244  0.233857132 -0.008531243  0.041408962
```

texture_mean	-0.10372458	0.059706088	0.064549903	-0.603050001
perimeter_mean	-0.22753729	0.215181361	-0.009314220	0.041983099
area_mean	-0.22099499	0.231076711	0.028699526	0.053433795
smoothness_mean	-0.14258969	-0.186113023	-0.104291904	0.159382765
compactness_mean	-0.23928535	-0.151891610	-0.074091571	0.031794581
concavity_mean	-0.25840048	-0.060165363	0.002733838	0.019122753
concave.points_mean	-0.26085376	0.034767500	-0.025563541	0.065335944
symmetry_mean	-0.13816696	-0.190348770	-0.040239936	0.067124984
fractal_dimension_mean	-0.06436335	-0.366575471	-0.022574090	0.048586765
radius_se	-0.20597878	0.105552152	0.268481387	0.097941242
texture_se	-0.01742803	-0.089979682	0.374633665	-0.359855528
perimeter_se	-0.21132592	0.089457234	0.266645367	0.088992415
area_se	-0.20286964	0.152292628	0.216006528	0.108205039
smoothness_se	-0.01453145	-0.204430453	0.308838979	0.044664180
compactness_se	-0.17039345	-0.232715896	0.154779718	-0.027469363
concavity_se	-0.15358979	-0.197207283	0.176463743	0.001316880
concave.points_se	-0.18341740	-0.130321560	0.224657567	0.074067335
symmetry_se	-0.04249842	-0.183848000	0.288584292	0.044073351
fractal_dimension_se	-0.10256832	-0.280092027	0.211503764	0.015304750
radius_worst	-0.22799663	0.219866379	-0.047506990	0.015417240
texture_worst	-0.10446933	0.045467298	-0.042297823	-0.632807885
perimeter_worst	-0.23663968	0.199878428	-0.048546508	0.013802794
area_worst	-0.22487053	0.219351858	-0.011902318	0.025894749
smoothness_worst	-0.12795256	-0.172304352	-0.259797613	0.017652216
compactness_worst	-0.21009588	-0.143593173	-0.236075625	-0.091328415
concavity_worst	-0.22876753	-0.097964114	-0.173057335	-0.073951180
concave.points_worst	-0.25088597	0.008257235	-0.170344076	0.006006996
symmetry_worst	-0.12290456	-0.141883349	-0.271312642	-0.036250695
fractal_dimension_worst	-0.13178394	-0.275339469	-0.232791313	-0.077053470

	PC5	PC6	PC7	PC8
radius_mean	-0.037786354	0.0187407904	-0.1240883403	0.007452296
texture_mean	0.049468850	-0.0321788366	0.0113995382	-0.130674825
perimeter_mean	-0.037374663	0.0173084449	-0.1144770573	0.018687258
area_mean	-0.010331251	-0.0018877480	-0.0516534275	-0.034673604
smoothness_mean	0.365088528	-0.2863744966	-0.1406689928	0.288974575
compactness_mean	-0.011703971	-0.0141309489	0.0309184960	0.151396350
concavity_mean	-0.086375412	-0.0093441809	-0.1075204434	0.072827285
concave.points_mean	0.043861025	-0.0520499505	-0.1504822142	0.152322414
symmetry_mean	0.305941428	0.3564584607	-0.0938911345	0.231530989
fractal_dimension_mean	0.044424360	-0.1194306679	0.2957600240	0.177121441
radius_se	0.154456496	-0.0256032561	0.3124900373	-0.022539967
texture_se	0.191650506	-0.0287473145	-0.0907553556	0.475413139
perimeter_se	0.120990220	0.0018107150	0.3146403902	0.011896690

area_se	0.127574432	-0.0428639079	0.3466790028	-0.085805135
smoothness_se	0.232065676	-0.3429173935	-0.2440240556	-0.573410232
compactness_se	-0.279968156	0.0691975186	0.0234635340	-0.117460157
concavity_se	-0.353982091	0.0563432386	-0.2088237897	-0.060566501
concave.points_se	-0.195548089	-0.0312244482	-0.3696459369	0.108319309
symmetry_se	0.252868765	0.4902456426	-0.0803822539	-0.220149279
fractal_dimension_se	-0.263297438	-0.0531952674	0.1913949726	-0.011168188
radius_worst	0.004406592	-0.0002906849	-0.0097099360	-0.042619416
texture_worst	0.092883400	-0.0500080613	0.0098707439	-0.036251636
perimeter_worst	-0.007454151	0.0085009872	-0.0004457267	-0.030558534
area_worst	0.027390903	-0.0251643821	0.0678316595	-0.079394246
smoothness_worst	0.324435445	-0.3692553703	-0.1088308865	-0.205852191
compactness_worst	-0.121804107	0.0477057929	0.1404729381	-0.084019659
concavity_worst	-0.188518727	0.0283792555	-0.0604880561	-0.072467871
concave.points_worst	-0.043332069	-0.0308734498	-0.1679666187	0.036170795
symmetry_worst	0.244558663	0.4989267845	-0.0184906298	-0.228225053
fractal_dimension_worst	-0.094423351	-0.0802235245	0.3746576261	-0.048360667

	PC9	PC10	PC11	PC12
radius_mean	-0.223109764	0.095486443	-0.04147149	0.051067457
texture_mean	0.112699390	0.240934066	0.30224340	0.254896423
perimeter_mean	-0.223739213	0.086385615	-0.01678264	0.038926106
area_mean	-0.195586014	0.074956489	-0.11016964	0.065437508
smoothness_mean	0.006424722	-0.069292681	0.13702184	0.316727211
compactness_mean	-0.167841425	0.012936200	0.30800963	-0.104017044
concavity_mean	0.040591006	-0.135602298	-0.12419024	0.065653480
concave.points_mean	-0.111971106	0.008054528	0.07244603	0.042589267
symmetry_mean	0.256040084	0.572069479	-0.16305408	-0.288865504
fractal_dimension_mean	-0.123740789	0.081103207	0.03804827	0.236358988
radius_se	0.249985002	-0.049547594	0.02535702	-0.016687915
texture_se	-0.246645397	-0.289142742	-0.34494446	-0.306160423
perimeter_se	0.227154024	-0.114508236	0.16731877	-0.101446828
area_se	0.229160015	-0.091927889	-0.05161946	-0.017679218
smoothness_se	-0.141924890	0.160884609	-0.08420621	-0.294710053
compactness_se	-0.145322810	0.043504866	0.20688568	-0.263456509
concavity_se	0.358107079	-0.141276243	-0.34951794	0.251146975
concave.points_se	0.272519886	0.086240847	0.34237591	-0.006458751
symmetry_se	-0.304077200	-0.316529830	0.18784404	0.320571348
fractal_dimension_se	-0.213722716	0.367541918	-0.25062479	0.276165974
radius_worst	-0.112141463	0.077361643	-0.10506733	0.039679665
texture_worst	0.103341204	0.029550941	-0.01315727	0.079797450
perimeter_worst	-0.109614364	0.050508334	-0.05107628	-0.008987738
area_worst	-0.080732461	0.069921152	-0.18459894	0.048088657
smoothness_worst	0.112315904	-0.128304659	-0.14389035	0.056514866

```
compactness_worst       -0.100677822 -0.172133632  0.19742047 -0.371662503
concavity_worst          0.161908621 -0.311638520 -0.18501676 -0.087034532
concave.points_worst     0.060488462 -0.076648291  0.11777205 -0.068125354
symmetry_worst           0.064637806 -0.029563075 -0.15756025  0.044033503
fractal_dimension_worst -0.134174175  0.012609579 -0.11828355 -0.034731693
                               PC13         PC14         PC15        PC16
radius_mean              0.01196721  0.059506135 -0.051118775 -0.15058388
texture_mean             0.20346133 -0.021560100 -0.107922421 -0.15784196
perimeter_mean           0.04410950  0.048513812 -0.039902936 -0.11445396
area_mean                0.06737574  0.010830829  0.013966907 -0.13244803
smoothness_mean          0.04557360  0.445064860 -0.118143364 -0.20461325
compactness_mean         0.22928130  0.008101057  0.230899962  0.17017837
concavity_mean           0.38709081 -0.189358699 -0.128283732  0.26947021
concave.points_mean      0.13213810 -0.244794768 -0.217099194  0.38046410
symmetry_mean            0.18993367  0.030738856 -0.073961707 -0.16466159
fractal_dimension_mean   0.10623908 -0.377078865  0.517975705 -0.04079279
radius_se               -0.06819523  0.010347413 -0.110050711  0.05890572
texture_se              -0.16822238 -0.010849347  0.032752721 -0.03450040
perimeter_se            -0.03784399 -0.045523718 -0.008268089  0.02651665
area_se                  0.05606493  0.083570718 -0.046024366  0.04115323
smoothness_se            0.15044143 -0.201152530  0.018559465 -0.05803906
compactness_se           0.01004017  0.491755932  0.168209315  0.18983090
concavity_se             0.15878319  0.134586924  0.250471408 -0.12542065
concave.points_se       -0.49402674 -0.199666719  0.062079344 -0.19881035
symmetry_se              0.01033274 -0.046864383 -0.113383199 -0.15771150
fractal_dimension_se    -0.24045832  0.145652466 -0.353232211  0.26855388
radius_worst            -0.13789053  0.023101281  0.166567074 -0.08156057
texture_worst           -0.08014543  0.053430792  0.101115399  0.18555785
perimeter_worst         -0.09696571  0.012219382  0.182755198 -0.05485705
area_worst              -0.10116061 -0.006685465  0.314993600 -0.09065339
smoothness_worst        -0.20513034  0.162235443  0.046125866  0.14555166
compactness_worst        0.01227931  0.166470250 -0.049956014 -0.15373486
concavity_worst          0.21798433 -0.066798931 -0.204835886 -0.21502195
concave.points_worst    -0.25438749 -0.276418891 -0.169499607  0.17814174
symmetry_worst          -0.25653491  0.005355574  0.139888394  0.25789401
fractal_dimension_worst -0.17281424 -0.212104110 -0.256173195 -0.40555649
                                PC17          PC18        PC19         PC20
radius_mean              0.202924255  0.1467123385  0.22538466 -0.049698664
texture_mean            -0.038706119 -0.0411029851  0.02978864 -0.244134993
perimeter_mean           0.194821310  0.1583174548  0.23959528 -0.017665012
area_mean                0.255705763  0.2661681046 -0.02732219 -0.090143762
smoothness_mean          0.167929914 -0.3522268017 -0.16456584  0.017100960
compactness_mean        -0.020307708  0.0077941384  0.28422236  0.488686329
```

```
concavity_mean         -0.001598353 -0.0269681105  0.00226636 -0.033387086
concave.points_mean     0.034509509 -0.0828277367 -0.15497236 -0.235407606
symmetry_mean          -0.191737848  0.1733977905 -0.05881116  0.026069156
fractal_dimension_mean  0.050225246  0.0878673570 -0.05815705 -0.175637222
radius_se              -0.139396866 -0.2362165319  0.17588331 -0.090800503
texture_se              0.043963016 -0.0098586620  0.03600985 -0.071659988
perimeter_se           -0.024635639 -0.0259288003  0.36570154 -0.177250625
area_se                 0.334418173  0.3049069032 -0.41657231  0.274201148
smoothness_se           0.139595006 -0.2312599432 -0.01326009  0.090061477
compactness_se         -0.008246477  0.1004742346 -0.24244818 -0.461098220
concavity_se            0.084616716 -0.0001954852  0.12638102  0.066946174
concave.points_se       0.108132263  0.0460549116 -0.01216430  0.068868294
symmetry_se            -0.274059129  0.1870147640 -0.08903929  0.107385289
fractal_dimension_se   -0.122733398 -0.0598230982  0.08660084  0.222345297
radius_worst           -0.240049982 -0.2161013526  0.01366130 -0.005626909
texture_worst           0.069365185  0.0583984505 -0.07586693  0.300599798
perimeter_worst        -0.234164147 -0.1885435919  0.09081325  0.011003858
area_worst             -0.273399584 -0.1420648558 -0.41004720  0.060047387
smoothness_worst       -0.278030197  0.5015516751  0.23451384 -0.129723903
compactness_worst      -0.004037123 -0.0735745143  0.02020070  0.229280589
concavity_worst        -0.191313419 -0.1039079796 -0.04578612 -0.046482792
concave.points_worst   -0.075485316  0.0758138963 -0.26022962  0.033022340
symmetry_worst          0.430658116 -0.2787138431  0.11725053 -0.116759236
fractal_dimension_worst 0.159394300  0.0235647497 -0.01149448 -0.104991974
                                PC21        PC22          PC23        PC24
radius_mean            -0.0685700057 -0.07292890 -0.0985526942 -0.18257944
texture_mean            0.4483694667 -0.09480063 -0.0005549975  0.09878679
perimeter_mean         -0.0697690429 -0.07516048 -0.0402447050 -0.11664888
area_mean              -0.0184432785 -0.09756578  0.0077772734  0.06984834
smoothness_mean        -0.1194917473 -0.06382295 -0.0206657211  0.06869742
compactness_mean        0.1926213963  0.09807756  0.0523603957 -0.10413552
concavity_mean          0.0055717533  0.18521200  0.3248703785  0.04474106
concave.points_mean    -0.0094238187  0.31185243 -0.0514087968  0.08402770
symmetry_mean          -0.0869384844  0.01840673 -0.0512005770  0.01933947
fractal_dimension_mean -0.0762718362 -0.28786888 -0.0846898562 -0.13326055
radius_se               0.0863867747  0.15027468 -0.2641253170 -0.55870157
texture_se              0.2170719674 -0.04845693 -0.0008738805  0.02426730
perimeter_se           -0.3049501584 -0.15935280  0.0900742110  0.51675039
area_se                 0.1925877857 -0.06423262  0.0982150746 -0.02246072
smoothness_se          -0.0720987261 -0.05054490 -0.0598177179  0.01563119
compactness_se         -0.1403865724  0.04528769  0.0091038710 -0.12177779
concavity_se            0.0630479298  0.20521269 -0.3875423290  0.18820504
concave.points_se       0.0343753236  0.07254538  0.3517550738 -0.10966898
```

```
symmetry_se             -0.0976995265  0.08465443 -0.0423628949  0.00322620
fractal_dimension_se     0.0628432814 -0.24470508  0.0857810992  0.07519442
radius_worst             0.0072938995  0.09629821 -0.0556767923 -0.15683037
texture_worst           -0.5944401434  0.11111202 -0.0089228997 -0.11848460
perimeter_worst         -0.0920235990 -0.01722163  0.0633448296  0.23711317
area_worst               0.1467901315  0.09695982  0.1908896250  0.14406303
smoothness_worst         0.1648492374  0.06825409  0.0936901494 -0.01099014
compactness_worst        0.1813748671 -0.02967641 -0.1479209247  0.18674995
concavity_worst         -0.1321005945 -0.46042619  0.2864331353 -0.28885257
concave.points_worst     0.0008860815 -0.29984056 -0.5675277966  0.10734024
symmetry_worst           0.1627085487 -0.09714484  0.1213434508 -0.01438181
fractal_dimension_worst -0.0923439434  0.46947115  0.0076253382  0.03782545
                               PC25         PC26         PC27          PC28
radius_mean             -0.01922650 -0.129476396 -0.131526670  2.111940e-01
texture_mean             0.08474593 -0.024556664 -0.017357309 -6.581146e-05
perimeter_mean           0.02701541 -0.125255946 -0.115415423  8.433827e-02
area_mean               -0.21004078  0.362727403  0.466612477 -2.725083e-01
smoothness_mean          0.02895489 -0.037003686  0.069689923  1.479269e-03
compactness_mean         0.39662323  0.262808474  0.097748705 -5.462767e-03
concavity_mean          -0.09697732 -0.548876170  0.364808397  4.553864e-02
concave.points_mean     -0.18645160  0.387643377 -0.454699351 -8.883097e-03
symmetry_mean           -0.02458369 -0.016044038 -0.015164835  1.433026e-03
fractal_dimension_mean  -0.20722186 -0.097404839 -0.101244946 -6.311687e-03
radius_se               -0.17493043  0.049977080  0.212982901 -1.922239e-01
texture_se               0.05698648 -0.011237242 -0.010092889 -5.622611e-03
perimeter_se             0.07292764  0.103653282  0.041691553  2.631919e-01
area_se                  0.13185041 -0.155304589 -0.313358657 -4.206811e-02
smoothness_se            0.03121070 -0.007717557 -0.009052154  9.792963e-03
compactness_se           0.17316455 -0.049727632  0.046536088 -1.539555e-02
concavity_se             0.01593998  0.091454968 -0.084224797  5.820978e-03
concave.points_se       -0.12954655 -0.017941919 -0.011165509 -2.900930e-02
symmetry_se             -0.01951493 -0.017267849 -0.019975983 -7.636526e-03
fractal_dimension_se    -0.08417120  0.035488974 -0.012036564  1.975646e-02
radius_worst             0.07070972 -0.197054744 -0.178666740  4.126396e-01
texture_worst           -0.11818972  0.036469433  0.021410694 -3.902509e-04
perimeter_worst          0.11803403 -0.244103670 -0.241031046 -7.286809e-01
area_worst              -0.03828995  0.231359525  0.237162466  2.389603e-01
smoothness_worst        -0.04796476  0.012602464 -0.040853568 -1.535248e-03
compactness_worst       -0.62438494 -0.100463424 -0.070505414  4.869182e-02
concavity_worst          0.11577034  0.266853781 -0.142905801 -1.764090e-02
concave.points_worst     0.26319634 -0.133574507  0.230901389  2.247567e-02
symmetry_worst           0.04529962  0.028184296  0.022790444  4.920481e-03
fractal_dimension_worst  0.28013348  0.004520482  0.059985998 -2.356214e-02
```

```
                                 PC29          PC30
radius_mean              2.114605e-01  0.7024140910
texture_mean            -1.053393e-02  0.0002736610
perimeter_mean           3.838261e-01 -0.6898969685
area_mean               -4.227949e-01 -0.0329473482
smoothness_mean         -3.434667e-03 -0.0048474577
compactness_mean        -4.101677e-02  0.0446741863
concavity_mean          -1.001479e-02  0.0251386661
concave.points_mean     -4.206949e-03 -0.0010772653
symmetry_mean           -7.569862e-03 -0.0012803794
fractal_dimension_mean   7.301433e-03 -0.0047556848
radius_se                1.184421e-01 -0.0087110937
texture_se              -8.776279e-03 -0.0010710392
perimeter_se            -6.100219e-03  0.0137293906
area_se                 -8.592591e-02  0.0011053260
smoothness_se            1.776386e-03 -0.0016082109
compactness_se           3.158134e-03  0.0019156224
concavity_se             1.607852e-02 -0.0089265265
concave.points_se       -2.393779e-02 -0.0021601973
symmetry_se             -5.223292e-03  0.0003293898
fractal_dimension_se    -8.341912e-03  0.0017989568
radius_worst            -6.357249e-01 -0.1356430561
texture_worst            1.723549e-02  0.0010205360
perimeter_worst          2.292180e-02  0.0797438536
area_worst               4.449359e-01  0.0397422838
smoothness_worst         7.385492e-03  0.0045832773
compactness_worst        3.566904e-06 -0.0128415624
concavity_worst         -1.267572e-02  0.0004021392
concave.points_worst     3.524045e-02 -0.0022884418
symmetry_worst           1.340423e-02  0.0003954435
fractal_dimension_worst  1.147766e-02  0.0018942925
```

To see how well PCA is doing here in terms of capturing the variance (or spread) in the data we can use the `summary()` function.

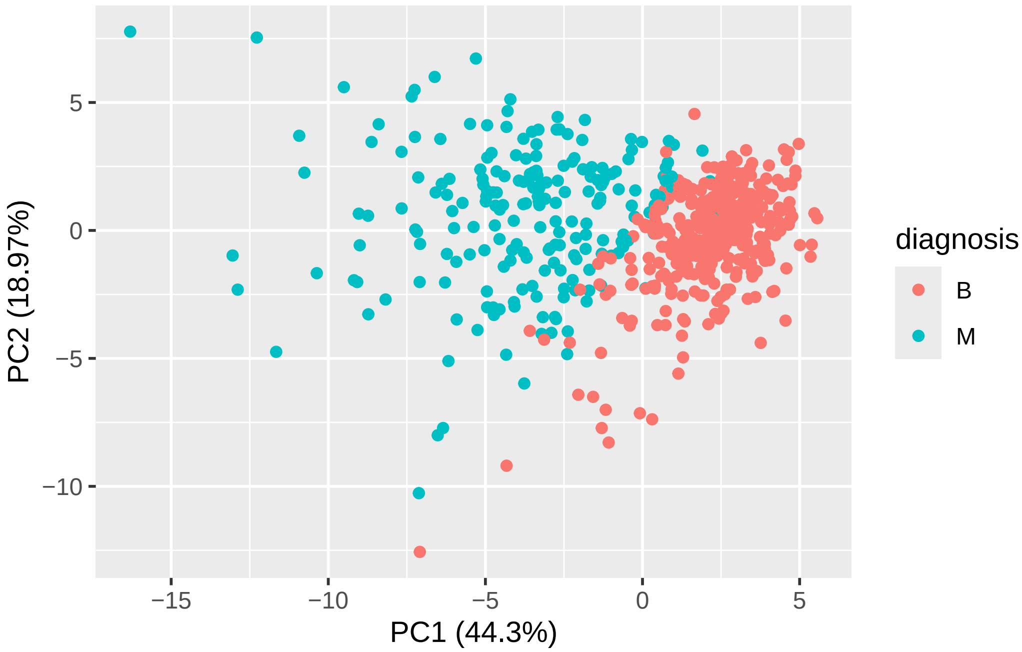
```r
summary(wisc.pr)
```

```
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
```

Let’s make the main PC1 vs PC2 plot

```
ggplot(wisc.pr$x)+
  aes(PC1,PC2, col=diagnosis)+
  geom_point()+
  xlab("PC1 (44.3%)")+
  ylab("PC2 (18.97%)")
```



> 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?

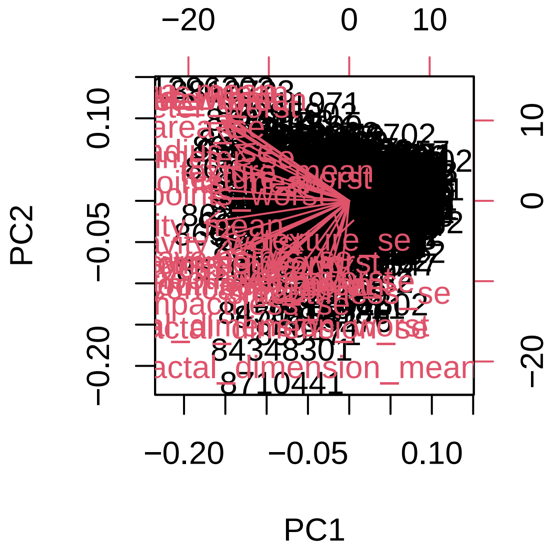
5

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

7

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

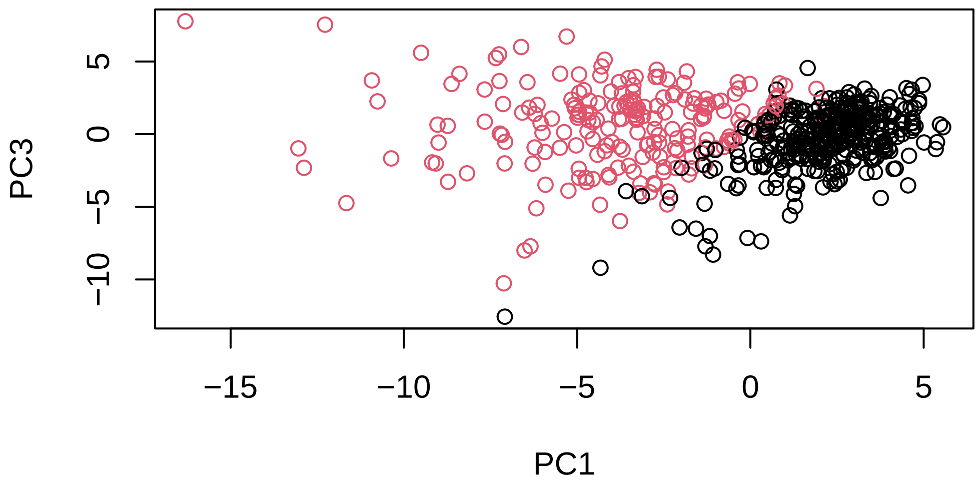
```
biplot(wisc.pr)
```



This plot is very difficult to understand. The agglomeration of the tags and values in this chart makes it difficult to make a proper analysis of what it's been plotted here.

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

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



This plot shows a more comprehensive and easier to visually digest distribution of all the data points in our `wisc.pr` data set.

> 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?

```r
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
```

Value is -0.26085376

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

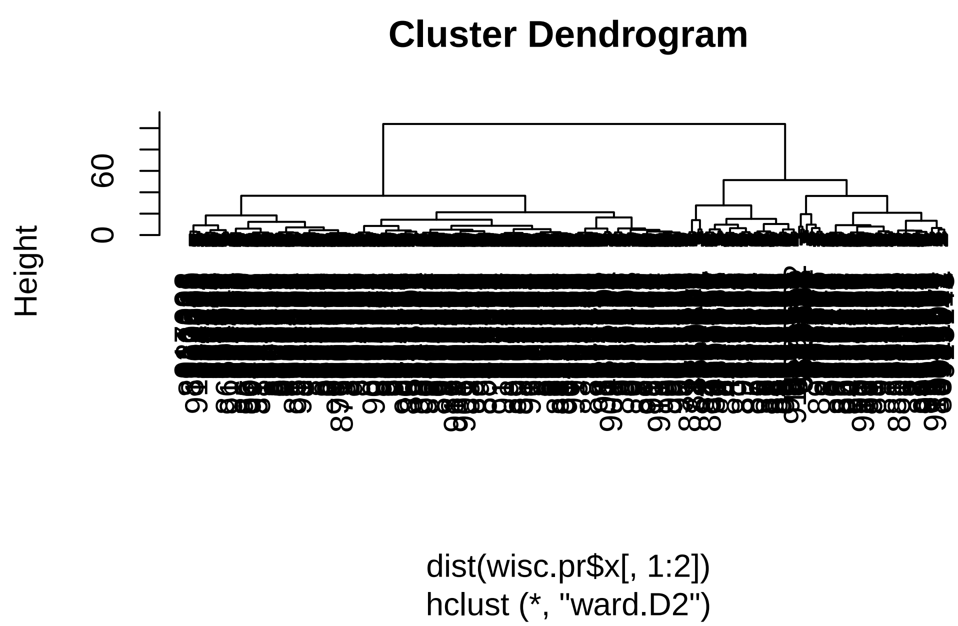
5

Combining Methods

We can take our PCA results and use them as a basis set for other analysis such as clustering.

Clustering on PCA results

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



We can "cut" this tree to yield our clusters (groups)

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

```
pc.groups
  1   2
195 374
```

How do my cluster groups compare to the expert diagnosis

```r
table(diagnosis, pc.groups)
```

```
         pc.groups
diagnosis   1   2
        B  18 339
        M 177  35
```

```r
table (diagnosis)
```

```
diagnosis
  B   M
357 212
```

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

It does a better job, since it's getting more precise. We separated more diagnoses correctly this time.

> 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? 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.

They did really badly. We are doing much better after PCA - the new PCA variables (what we call a basis set) give us much better separation of M and B

7. Prediction

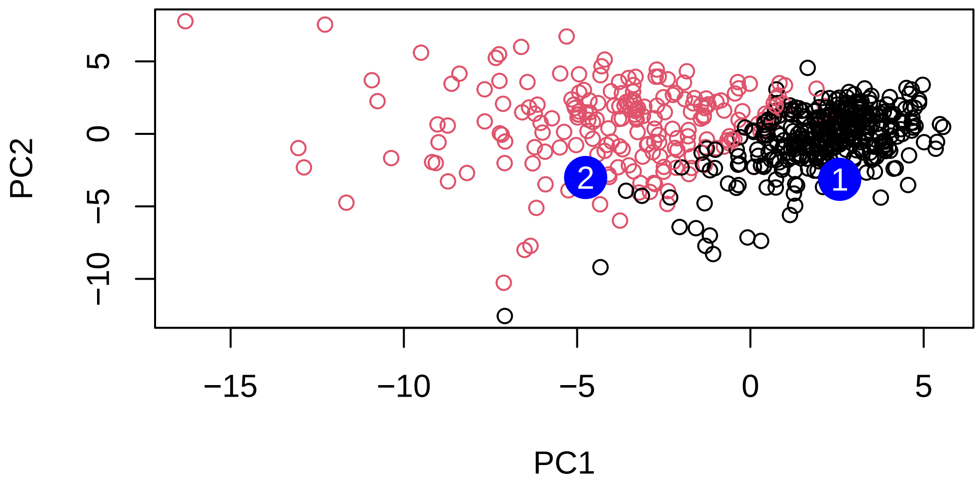
> Q18. Which of these new patients should we prioritize for follow up based on your results?

We can use our PCA model for the analysis of new "unseen" data. In this case from U. Mich.

```
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=diagnosis)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], c(1,2), col="white")
```



Based on this plot patient 2, since he is more likely to have malignant cancer cells based on its position in the PCA distribution.