Machine Learning 1

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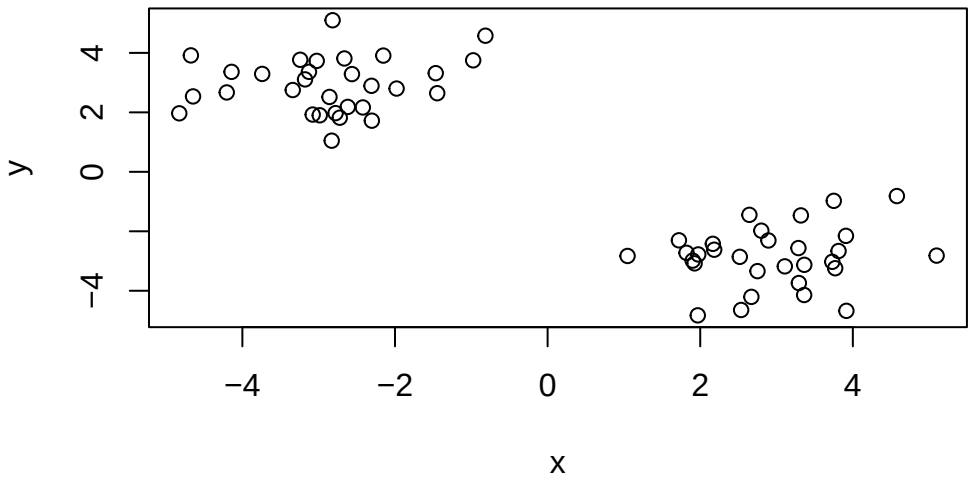
First up kmeans()

Demo of using kmeans() function in base R. First make up some data with a known structure.

```
tmp <- c( rnorm(30, -3), rnorm(30, 3))
x <- cbind(x=tmp,y= rev(tmp))
plot(x)
```



Now we have some made up data in `x` let's see how kmeans works with this data

```
k <- kmeans(x, centers = 2, nstart = 20)
k
```

```
K-means clustering with 2 clusters of sizes 30, 30

Cluster means:
          x         y
1 -2.864525  2.927095
2  2.927095 -2.864525

Clustering vector:
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2

Within cluster sum of squares by cluster:
[1] 53.95309 53.95309
 (between_SS / total_SS =  90.3 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

Q. How many points are in each cluster?

```
k$size
```

```
[1] 30 30
```

Q. How do we get to the cluster membership/assignment?

```
k$cluster
```

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

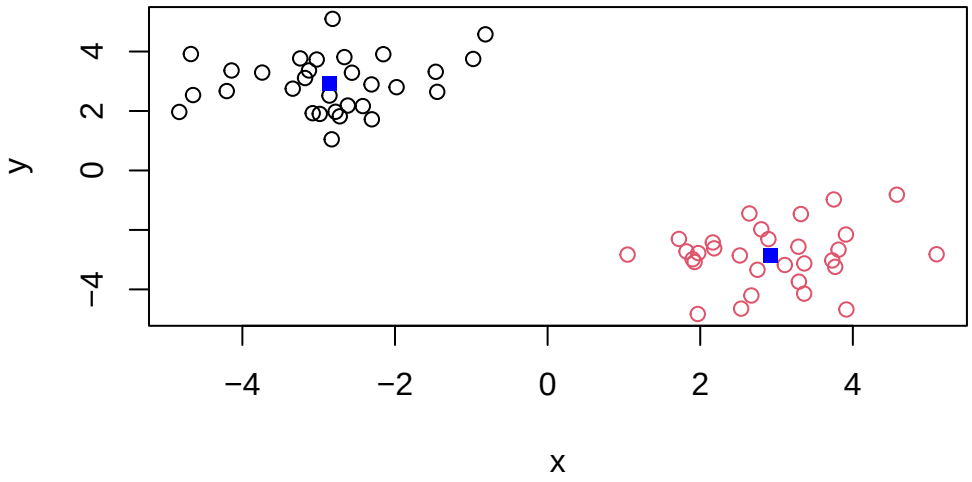
Q. What about cluster centers?

```
k$centers
```

```
          x         y
1 -2.864525  2.927095
2  2.927095 -2.864525
```

Now we got to the main results, let's use them to plot our data with the kmeans results.

```r
plot(x, col=k$cluster)
points(k$centers, col="blue", pch=15)
```



Now for hclust()

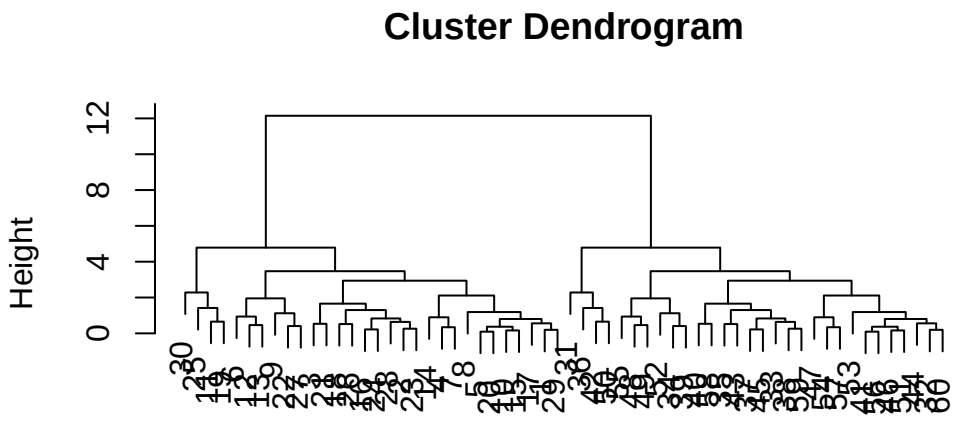
We will the same data `x` with the `hclust()`. In this case, `hclust()` requires a distance matrix as input.

```r
hc <- hclust(dist(x))
hc
```

```
Call:
hclust(d = dist(x))

Cluster method   : complete
Distance         : euclidean
Number of objects: 60
```

Let's plot our hclust result

```
plot(hc)
```



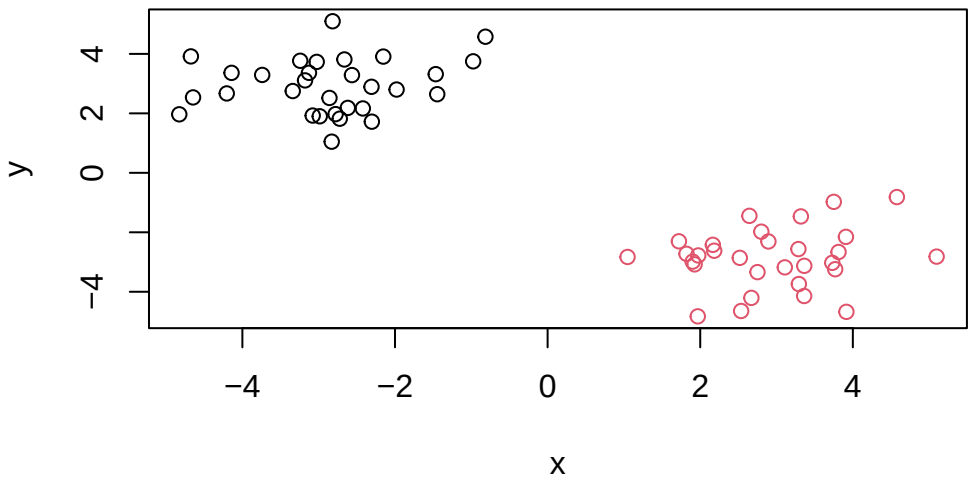
To get our cluster membership vector we need to "cut" the tree with the `cutree()`.

```
grps <- cutree(hc, h=8)
grps
```

```
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2
[39] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

Now plot our data with the hclust() results.

```
plot(x, col=grps)
```



Principal Component Analysis (PCA)

PCA of UK food data

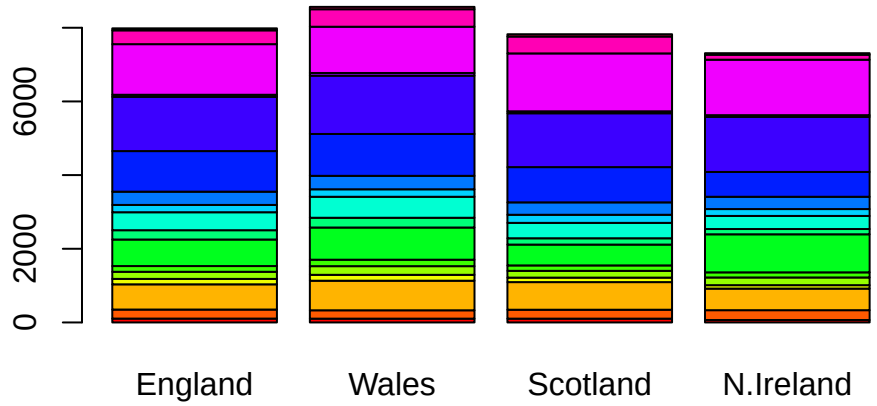
Read data from website and try a few visualization

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names = 1)
x
```

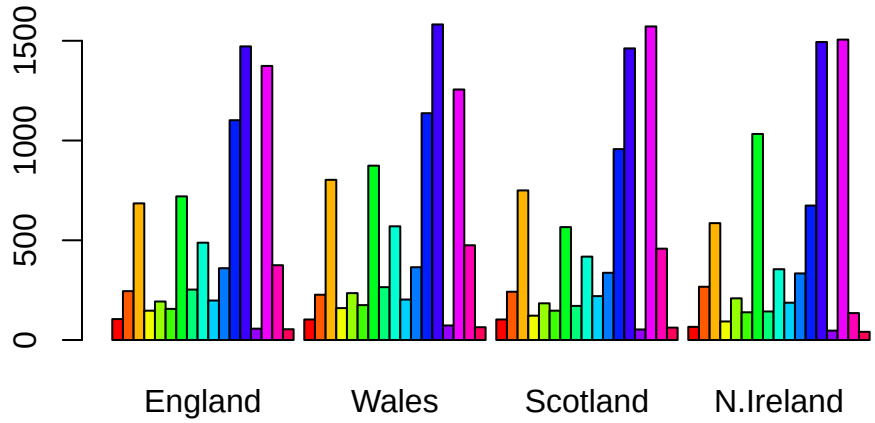
	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass_meat	245	227	242	267
Other_meat	685	803	750	586
Fish	147	160	122	93
Fats_and_oils	193	235	184	209
Sugars	156	175	147	139
Fresh_potatoes	720	874	566	1033
Fresh_Veg	253	265	171	143
Other_Veg	488	570	418	355
Processed_potatoes	198	203	220	187

Processed_Veg	360	365	337	334
Fresh_fruit	1102	1137	957	674
Cereals	1472	1582	1462	1494
Beverages	57	73	53	47
Soft_drinks	1374	1256	1572	1506
Alcoholic_drinks	375	475	458	135
Confectionery	54	64	62	41

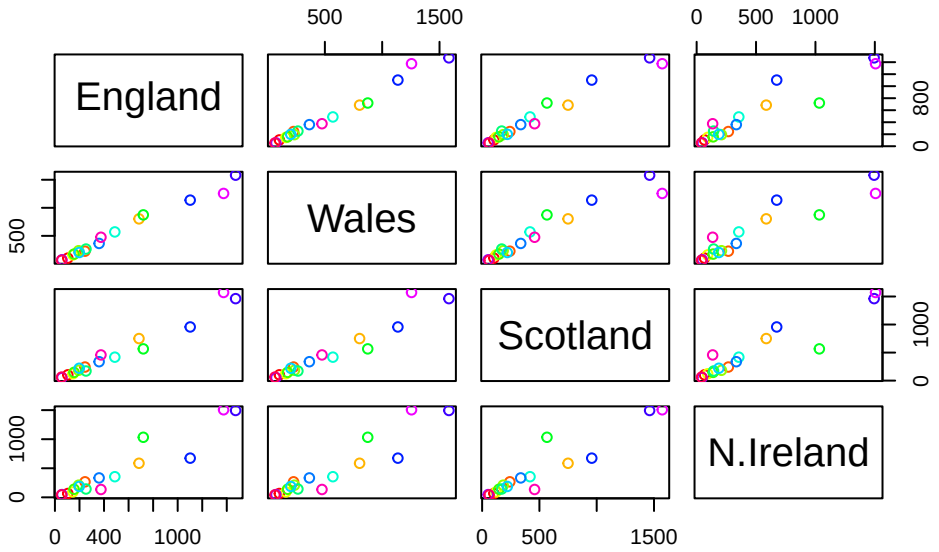
```
cols <- rainbow(nrow(x))
barplot(as.matrix(x), col=cols)
```




```
barplot(as.matrix(x), col=cols, beside=TRUE)
```




```
pairs(x, col=cols)
```



PCA to the rescue!! The main base R PCA function is called `prcomp()` and we will need to give it the transpose of our input data!

```
pca <- prcomp( t(x) )
```

There is a nice summary of how well PCA is doing

```
summary(pca)
```

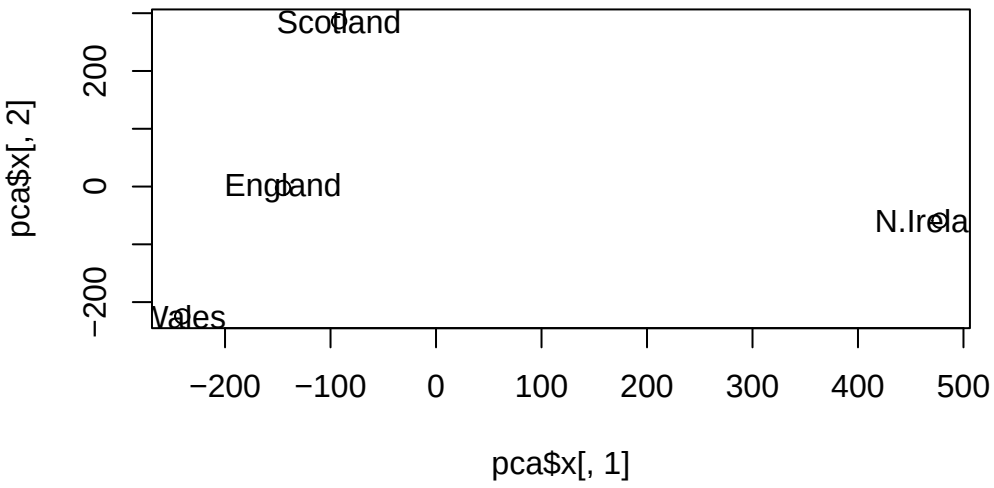
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
attributes(pca)
```

```
$names
[1] "sdev"     "rotation" "center"   "scale"    "x"

$class
[1] "prcomp"
```

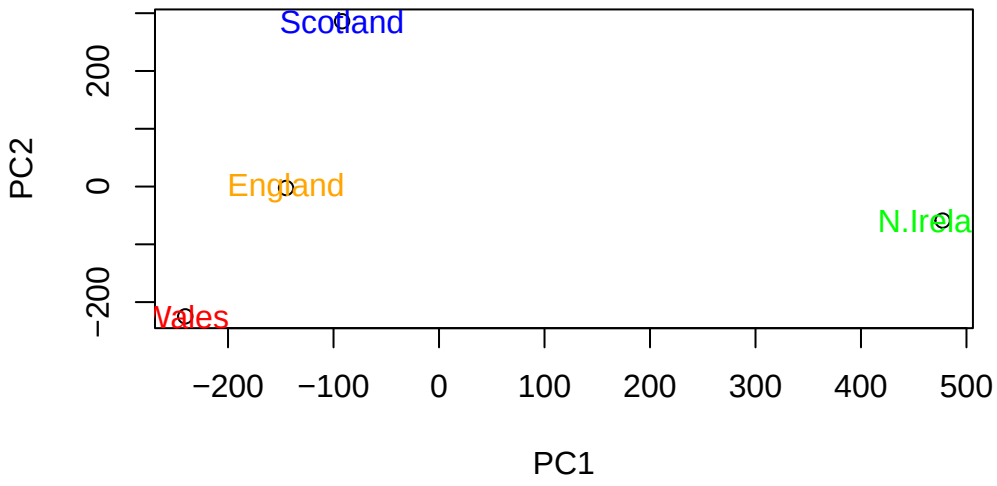
To make our new PCA plot (aka PCA score plot) we access `pca$x`

```
plot(pca$x[,1], pca$x[,2])
text(pca$x[,1], pca$x[,2], colnames(x))
```



Color up the plot

```
country_cols <- c("orange", "red", "blue", "green")
plot(pca$x[,1], pca$x[,2], xlab = "PC1", ylab = "PC2")
text(pca$x[,1], pca$x[,2], colnames(x), col = country_cols)
```



PCA of RNA-Seq data

Read in data from website

```
url2 <- "https://tinyurl.com/expression-CSV"
rna.data <- read.csv(url2, row.names=1)
head(rna.data)
```

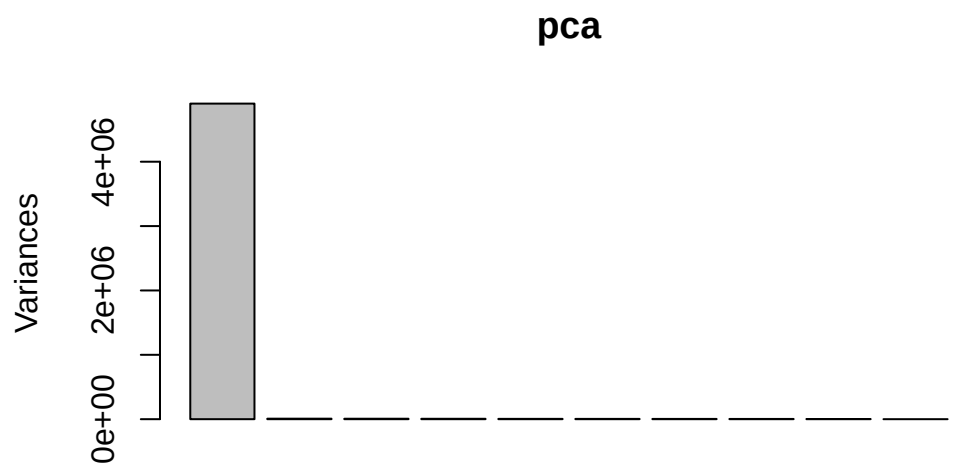
```
       wt1 wt2  wt3  wt4 wt5 ko1 ko2 ko3 ko4 ko5
gene1  439 458  408  429 420  90  88  86  90  93
gene2  219 200  204  210 187 427 423 434 433 426
gene3 1006 989 1030 1017 973 252 237 238 226 210
gene4  783 792  829  856 760 849 856 835 885 894
gene5  181 249  204  244 225 277 305 272 270 279
gene6  460 502  491  491 493 612 594 577 618 638
```

Another PCA summary

```
summary(pca)
```

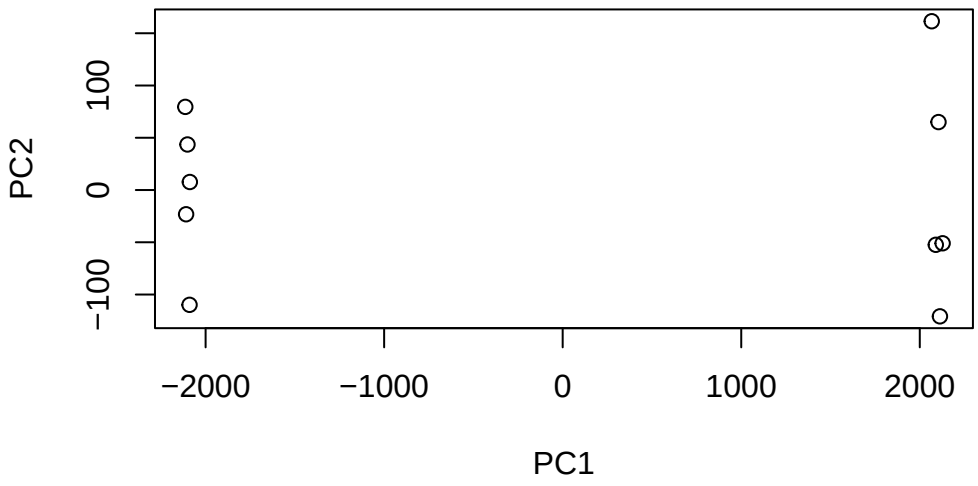
```
Importance of components:
                            PC1      PC2      PC3       PC4
Standard deviation     324.1502 212.7478 73.87622 3.176e-14
Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
pca <- prcomp( t(rna.data))
plot(pca)
```

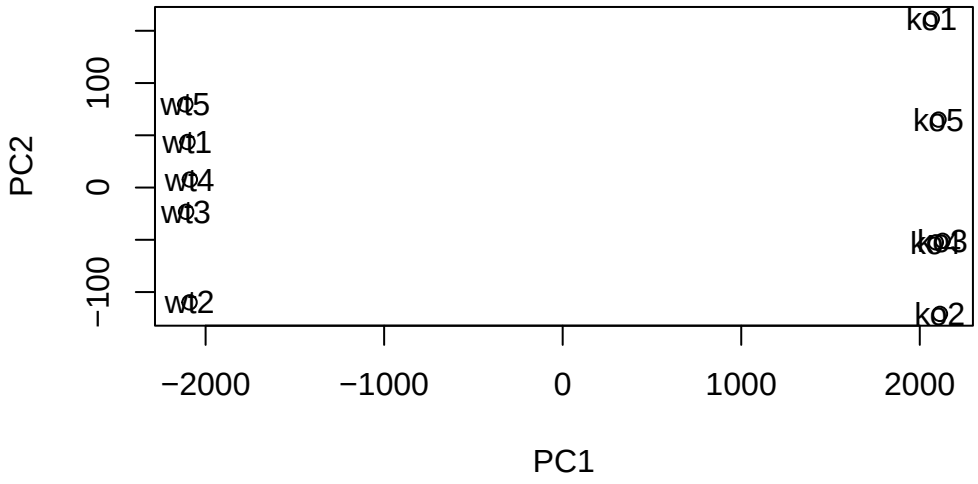


Do our PCA plot of this RNA-Seq data

```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```

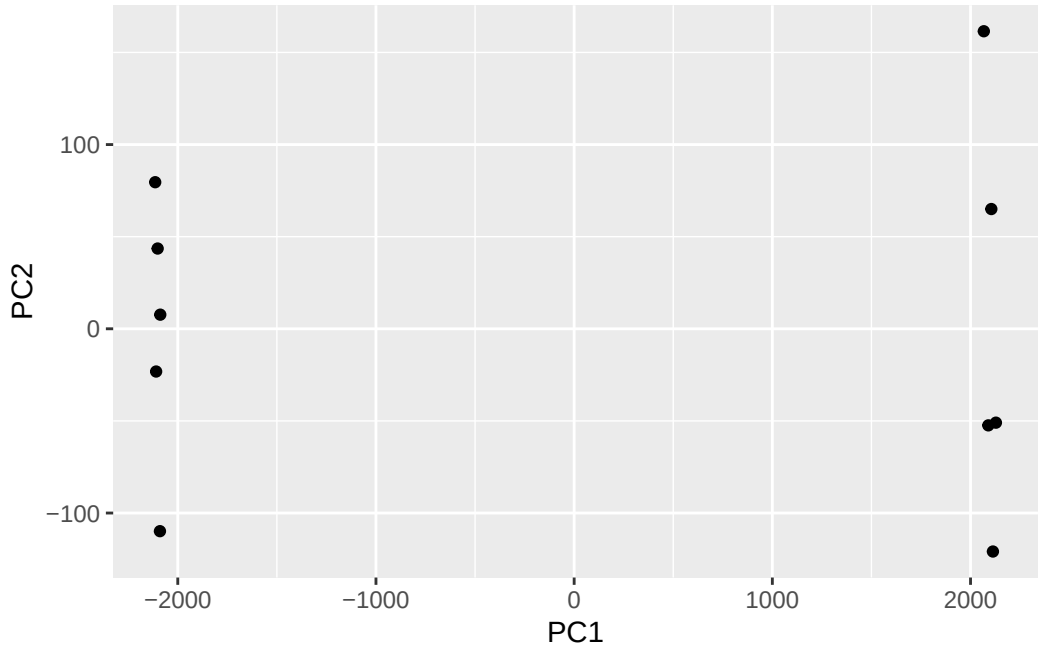



```
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2",
     text(pca$x[,1], pca$x[,2], colnames(rna.data)))
```



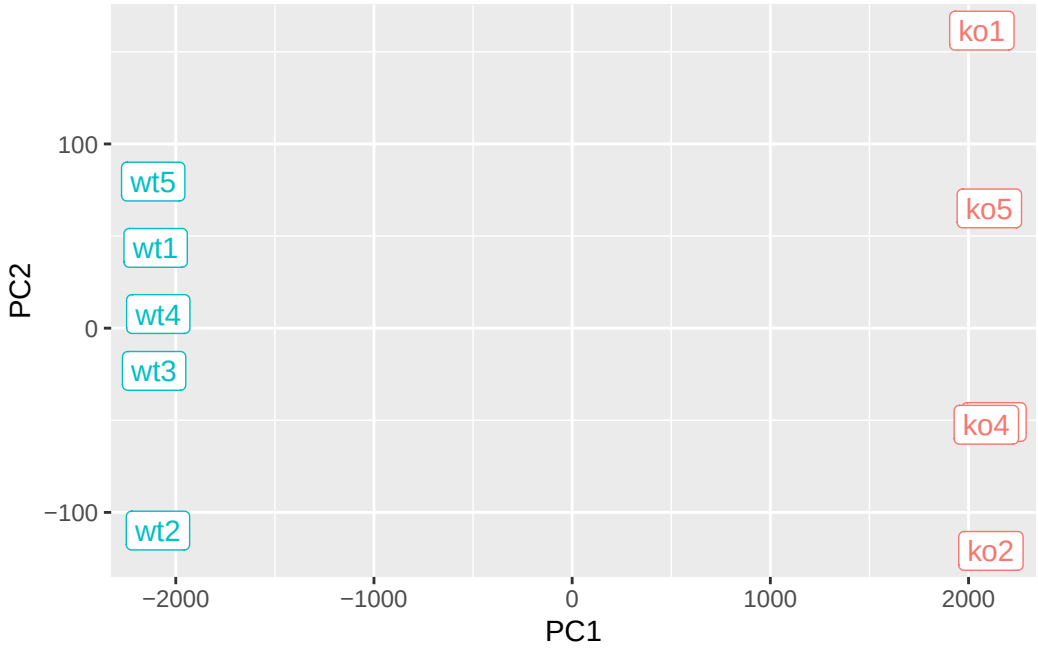
Using ggplot to make the graph look a bit different

```
library(ggplot2)

df <- as.data.frame(pca$x)

# Our first basic plot
ggplot(df) +
  aes(PC1, PC2) +
  geom_point()
```



Now adding some color

```
# Add a 'wt' and 'ko' "condition" column
df$samples <- colnames(rna.data)
df$condition <- substr(colnames(rna.data),1,2)

p <- ggplot(df) +
        aes(PC1, PC2, label=samples, col=condition) +
        geom_label(show.legend = FALSE)
p
```

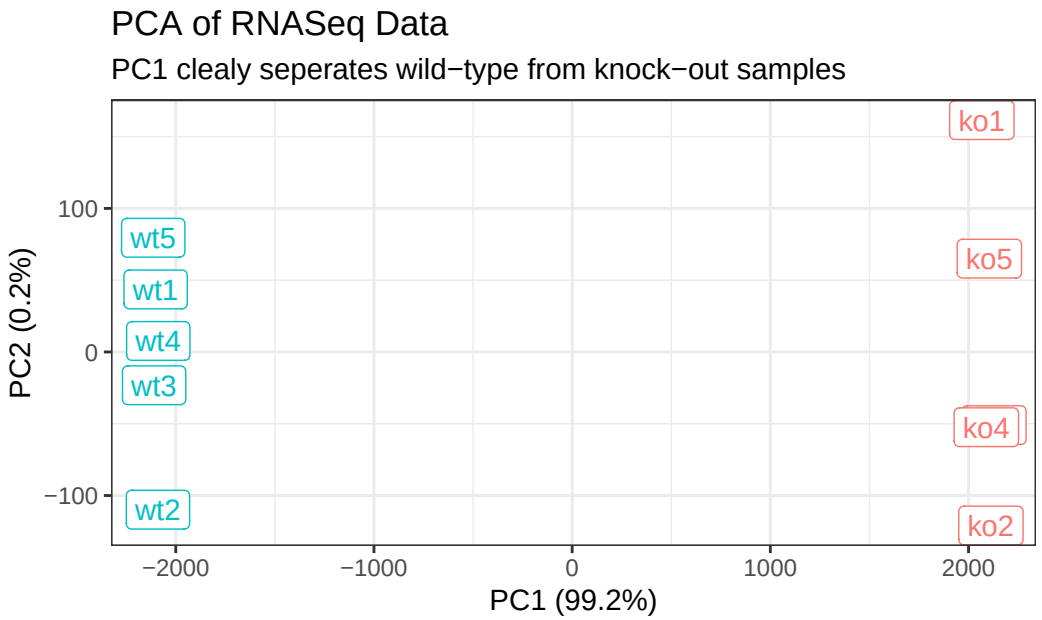


Now just polishing it up...

```
## Variance captured per PC
pca.var <- pca$sdev^2

## Percent variance is often more informative to look at
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)
pca.var.per
```

```
 [1] 99.2  0.2  0.1  0.1  0.1  0.1  0.1  0.1  0.1  0.0
```

```
p + labs(title="PCA of RNASeq Data",
       subtitle = "PC1 clealy seperates wild-type from knock-out samples",
       x=paste0("PC1 (", pca.var.per[1], "%)"),
       y=paste0("PC2 (", pca.var.per[2], "%)"),
       caption="Class example data") +
     theme_bw()
```


PCA of RNASeq Data
PC1 clealy seperates wild−type from knock−out samples
ko1
ko5
ko4
ko2
wt5
wt1
wt4
wt3
wt2
100
0
−100
PC2 (0.2%)
−2000
−1000
0
1000
2000
PC1 (99.2%)
Class example data