class07 (Machine Learning 1)

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PCA of UK food data

Read data from website, and try some visualizations

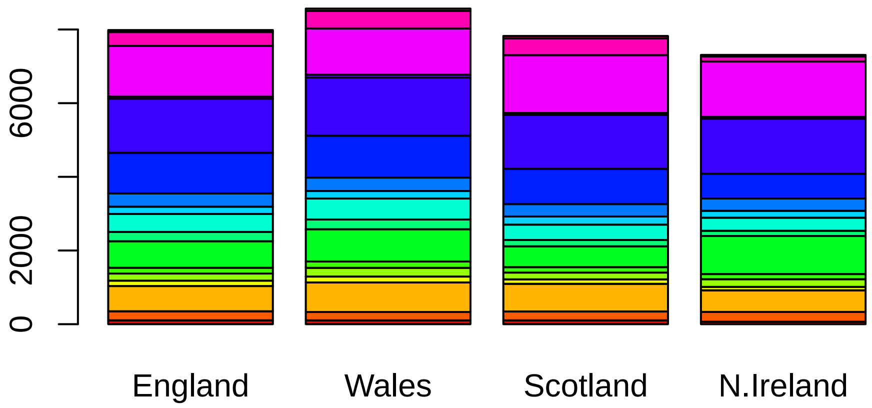
```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url, row.names=1)
x
```

```
                    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
```

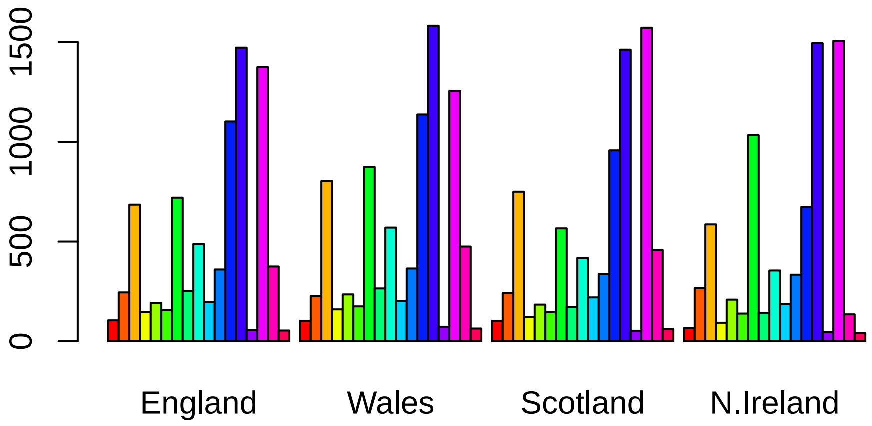
```
dim(x)
```

```
[1] 17  4
```

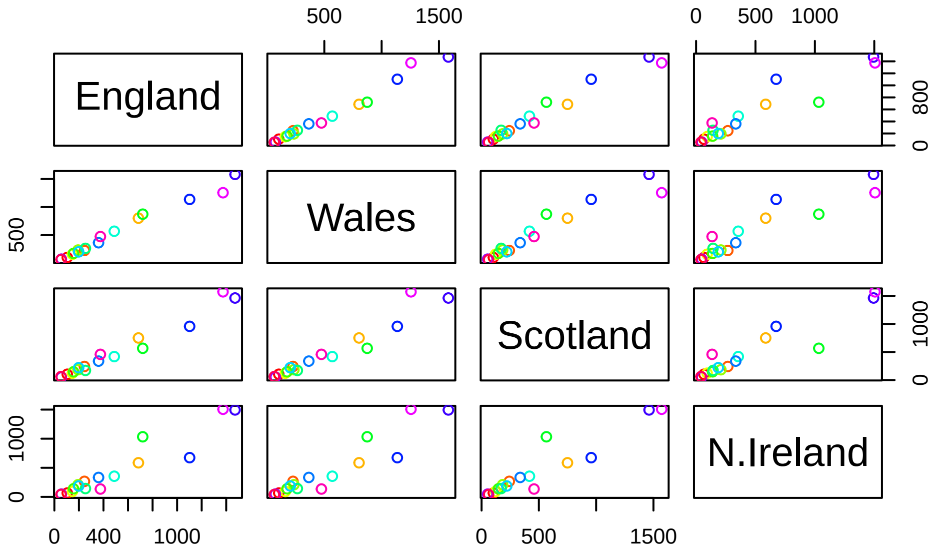
```r
cols <- rainbow(nrow(x))
barplot( as.matrix(x), col=cols )
```



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



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



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

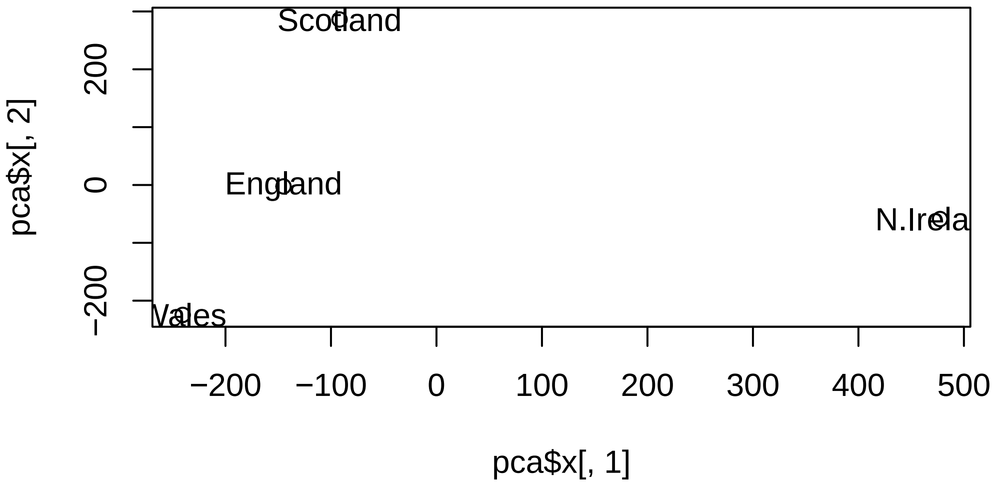
```
pca <- prcomp( t(x) )
```

```
attributes(pca)
```

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

$class
[1] "prcomp"
```

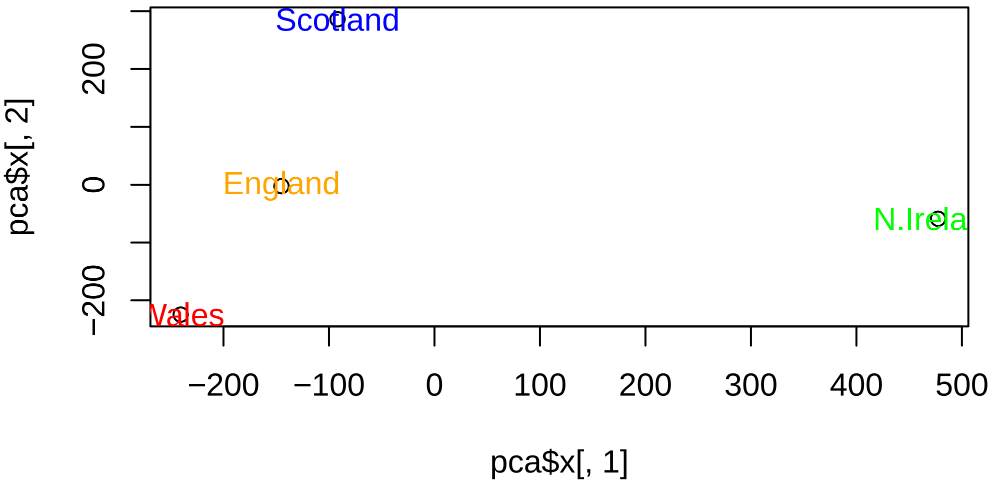
To make our new PCA plot (a.k.a PCA score plot) we access `pca$x`

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



Now to add some colors

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



We can use the square of pca$sdev (standard deviation), to calculate the amount of variation in the original data each PC accounts for

```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

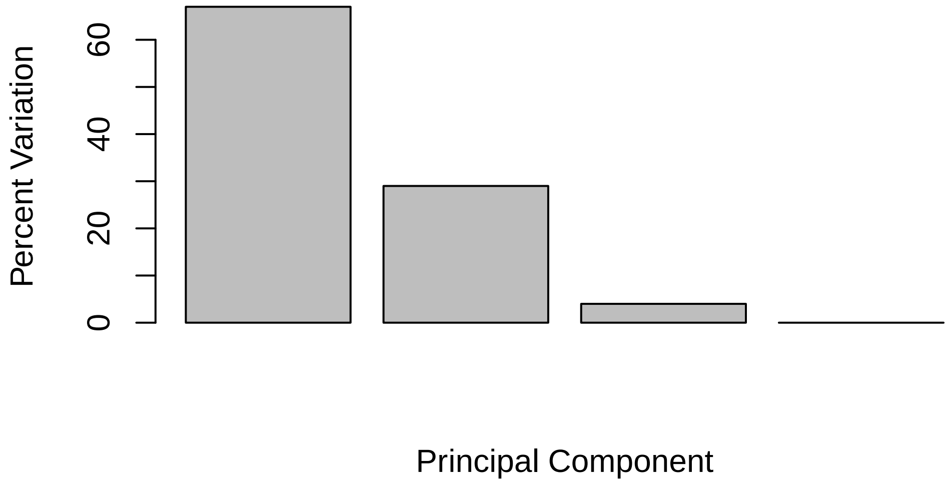
```
[1] 67 29  4  0
```

```
z <- summary(pca)
z$importance
```

```
                             PC1       PC2      PC3          PC4
Standard deviation     324.15019 212.74780 73.87622 2.921348e-14
Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

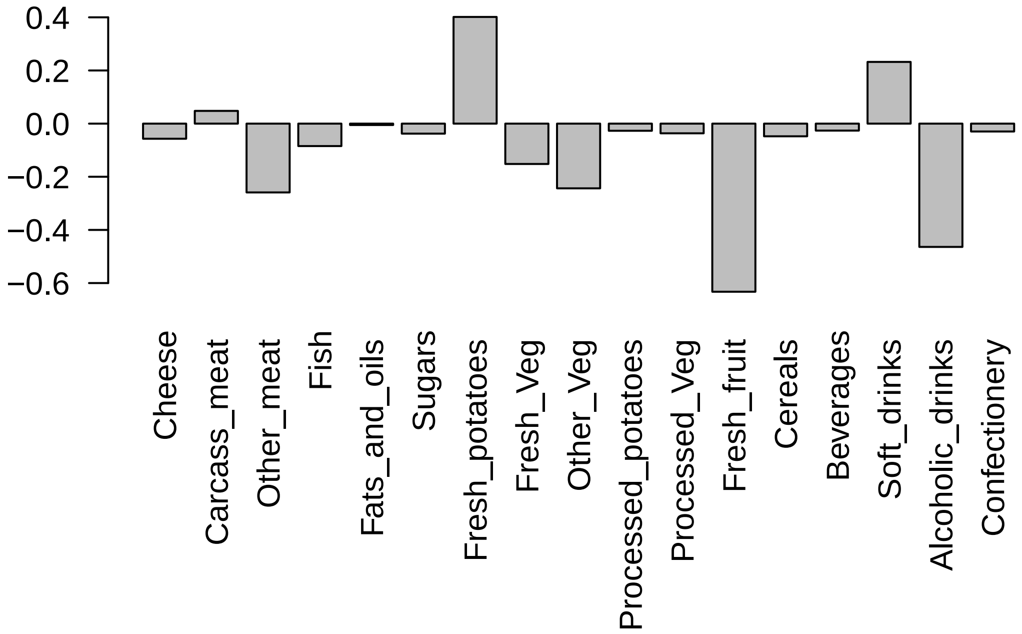
Let's turn this into a bar plot

```
barplot(v, xlab="Principal Component", ylab="Percent Variation")
```



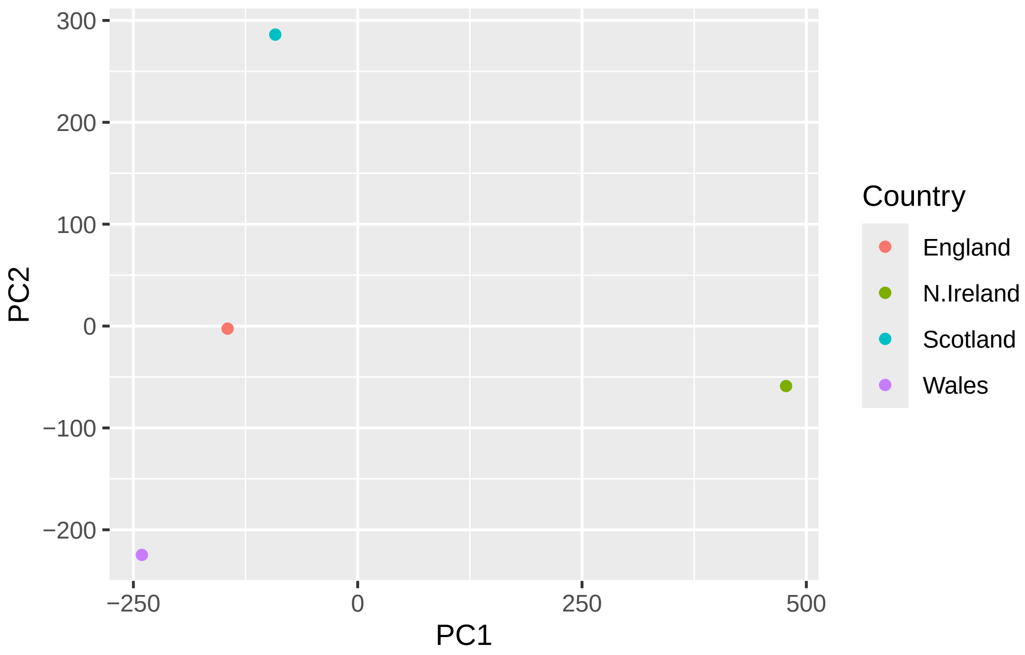
We can also consider the influence of each orginal variable

```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,1], las=2 )
```



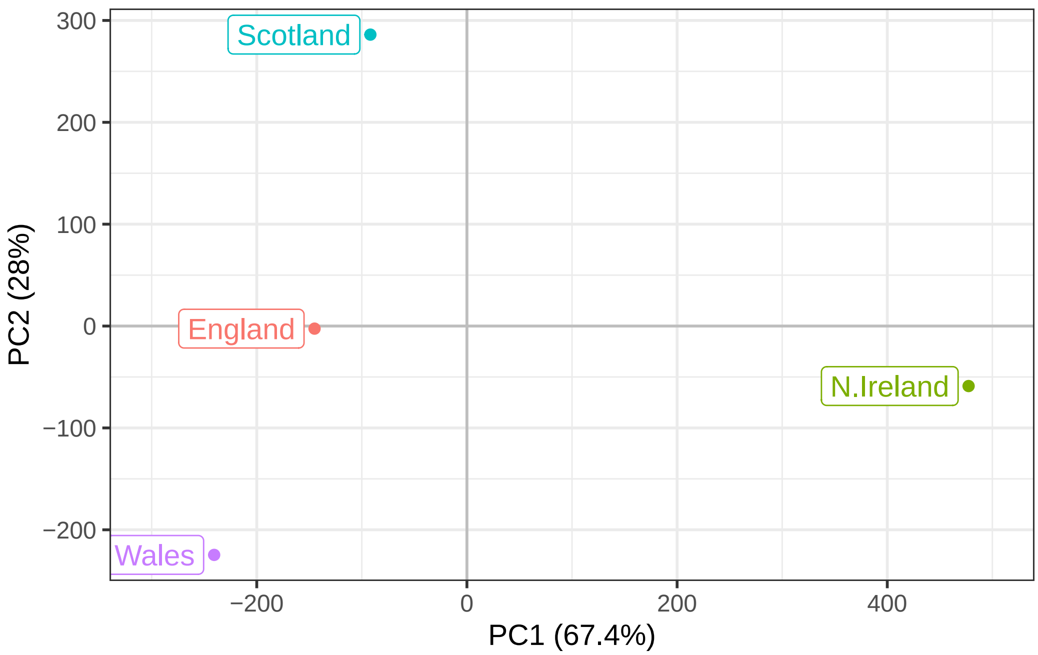
Now to use ggplot for these figures

```
library(ggplot2)

df <- as.data.frame(pca$x)
df_lab <- tibble::rownames_to_column(df, "Country")

# Our first basic plot
ggplot(df_lab) +
  aes(PC1, PC2, col=Country) +
  geom_point()
```



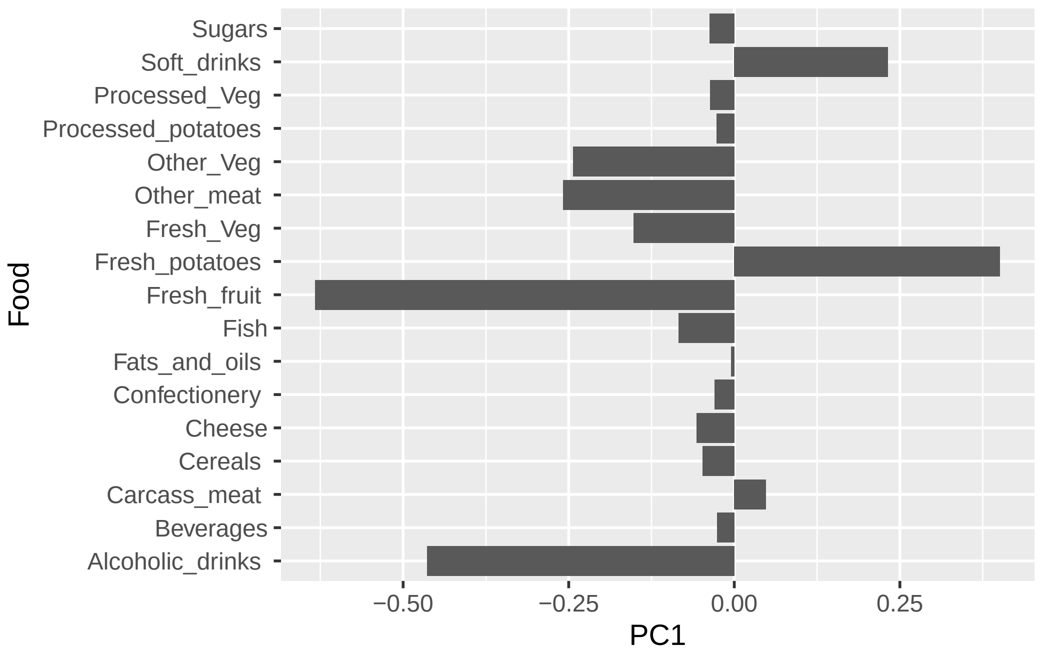
We can also make the plot look much nicer by adding aesthetics and organization

```
ggplot(df_lab) +
  aes(PC1, PC2, col=Country, label=Country) +
  geom_hline(yintercept = 0, col="gray") +
  geom_vline(xintercept = 0, col="gray") +
  geom_point(show.legend = FALSE) +
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +
  expand_limits(x = c(-300,500)) +
  xlab("PC1 (67.4%)") +
  ylab("PC2 (28%)") +
  theme_bw()
```



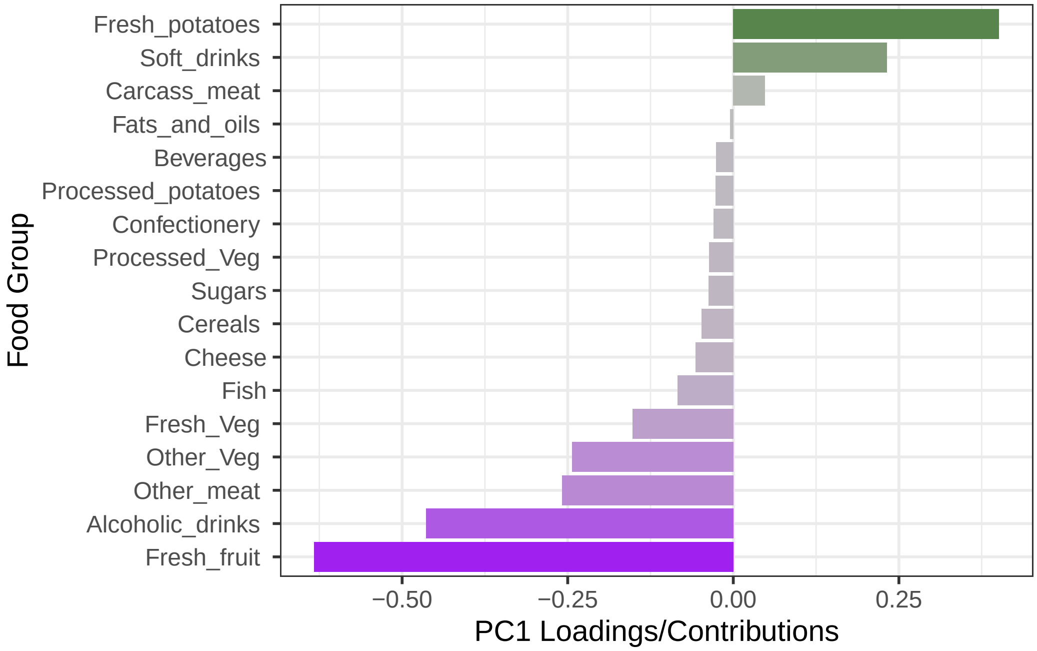
Now customise the plot with layers

```
ld <- as.data.frame(pca$rotation)
ld_lab <- tibble::rownames_to_column(ld, "Food")

ggplot(ld_lab) +
  aes(PC1, Food) +
  geom_col()
```



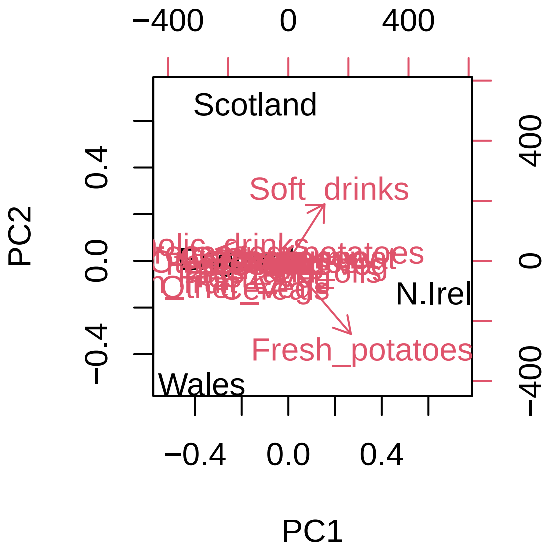
Now let's reorder the y-axis by PC1 loadings and add a color scale

```
ggplot(ld_lab) +
  aes(PC1, reorder(Food, PC1), bg=PC1) +
  geom_col() +
  xlab("PC1 Loadings/Contributions") +
  ylab("Food Group") +
  scale_fill_gradient2(low="purple", mid="gray", high="darkgreen", guide=NULL) +
  theme_bw()
```



We can also utilize a biplot to view the data

```
biplot(pca)
```



PCA of RNA-Seq data

```
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
```

There is a nice summary of how well PCA is doing

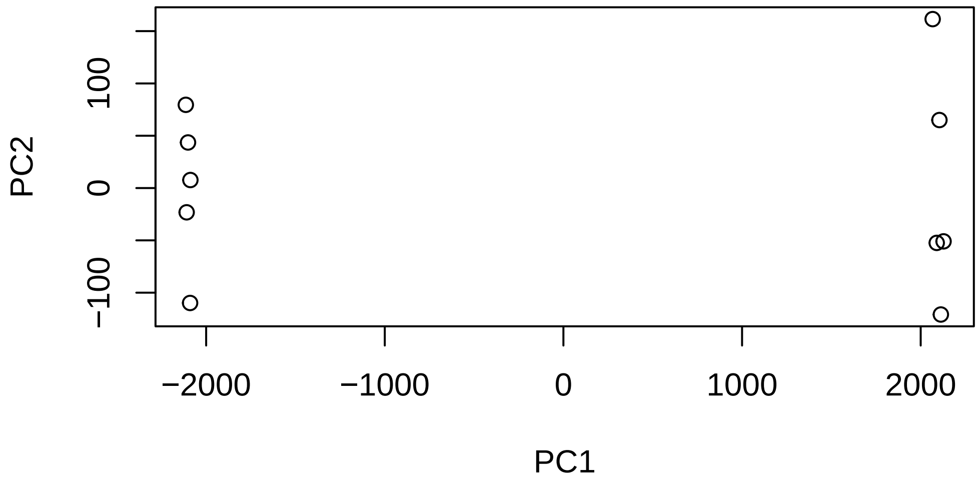
```
pca <- prcomp( t(rna.data) )
summary(pca)
```

```
Importance of components:
```

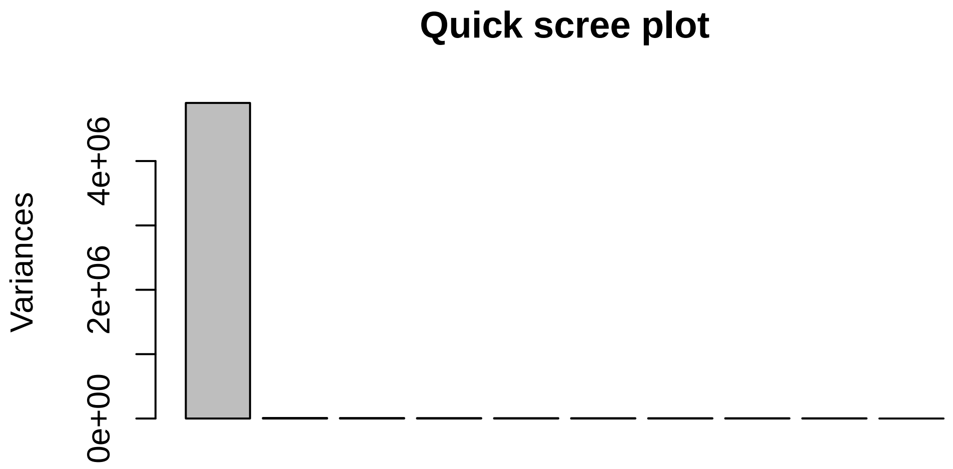
```
                             PC1     PC2      PC3      PC4      PC5      PC6
Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
                            PC7      PC8      PC9      PC10
Standard deviation     65.29428 59.90981 53.20803 2.662e-13
Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

Now to add our PCA plot

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



```
plot(pca, main="Quick scree plot")
```



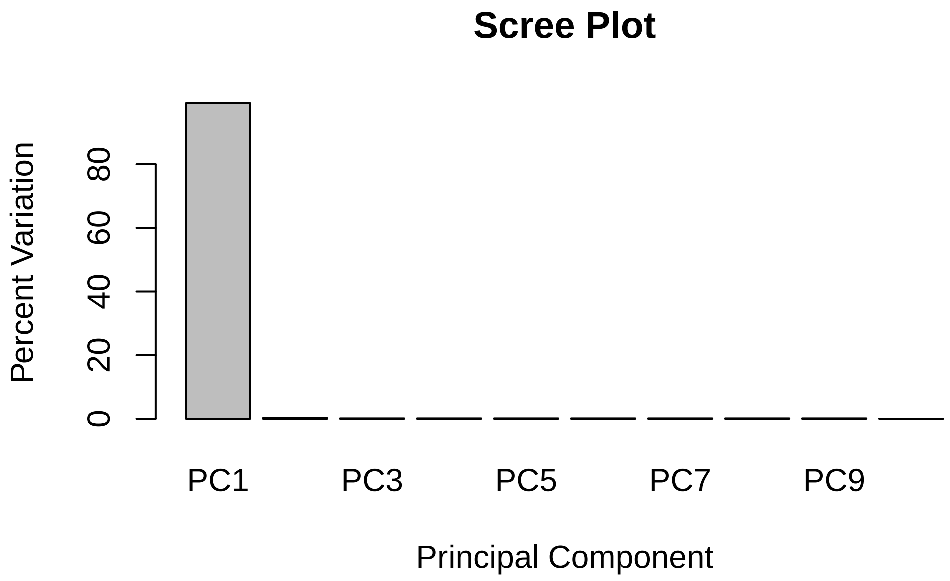
Now to calculate the variation in the original data

```
## 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
```

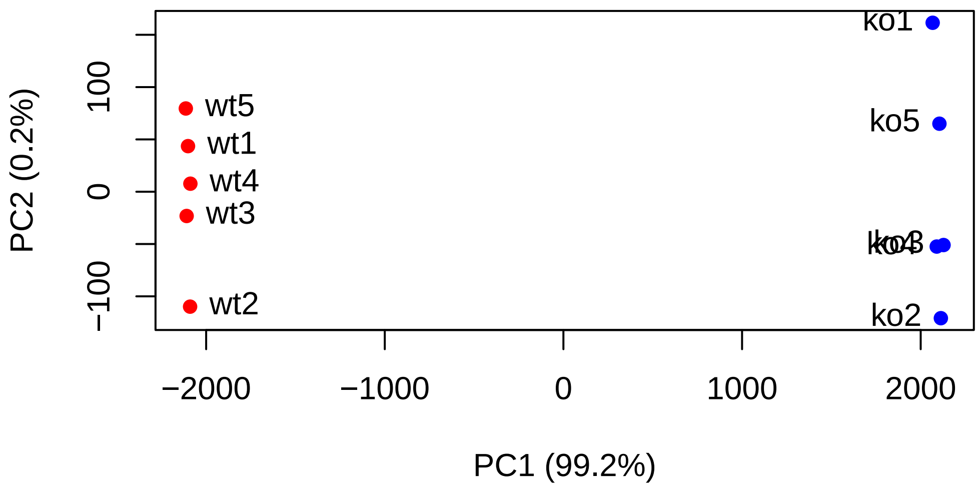
Let’s use this to make a bar plot

```
barplot(pca.var.per, main="Scree Plot",
        names.arg = paste0("PC", 1:10),
        xlab="Principal Component", ylab="Percent Variation")
```



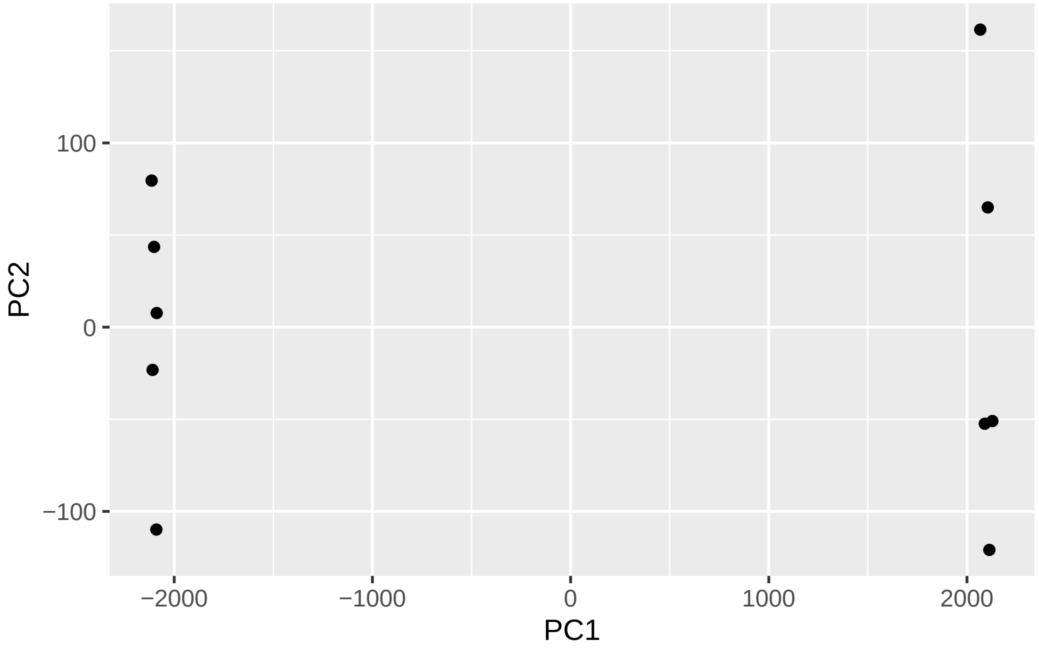
Let us add a vector of colors for our samples

```
## A vector of colors for wt and ko samples
colvec <- colnames(rna.data)
colvec[grep("wt", colvec)] <- "red"
colvec[grep("ko", colvec)] <- "blue"

plot(pca$x[,1], pca$x[,2], col=colvec, pch=16,
     xlab=paste0("PC1 (", pca.var.per[1], "%)"),
     ylab=paste0("PC2 (", pca.var.per[2], "%)"))

text(pca$x[,1], pca$x[,2], labels = colnames(rna.data), pos=c(rep(4,5), rep(2,5)))
```



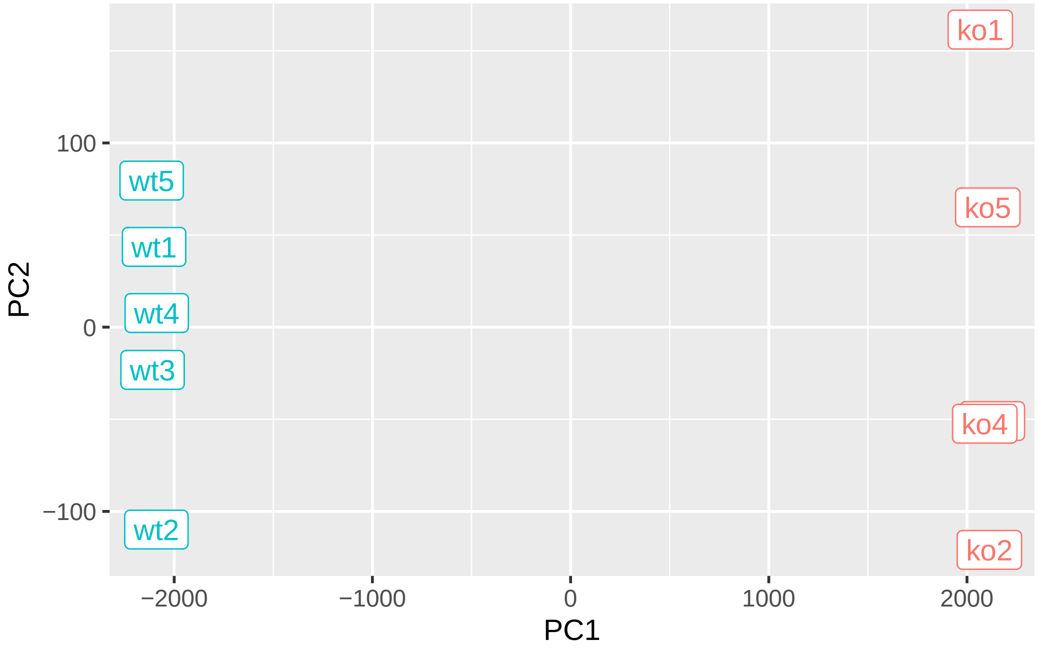
Now to use ggplot

```
library(ggplot2)

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

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



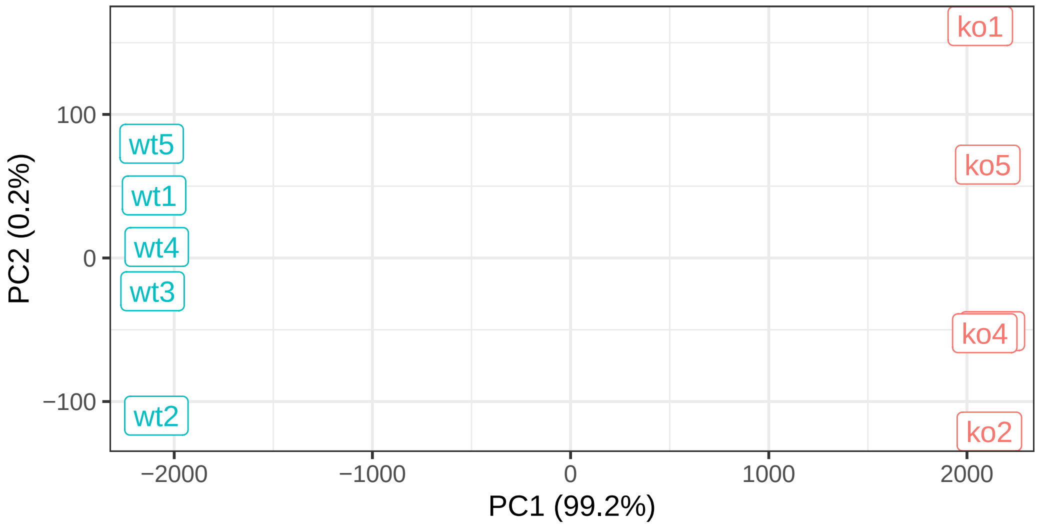
Now to add some condition specific colors and aesthetics

```
# 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 let's polish up the plot

```
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

Class example data