Lab8 PCA

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PCA of UK food data

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

dim(x)
```

```
## [1] 17  4
```

Check data, preview the first six rows

```
head(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
```

Fix the rownames:

```
#rownames(x) <- x[,1]
#x <- x[,-1]
#head(x)

#fixed the above by specifiying the row names while reading the csv

#recheck the dimensions
dim(x)
```

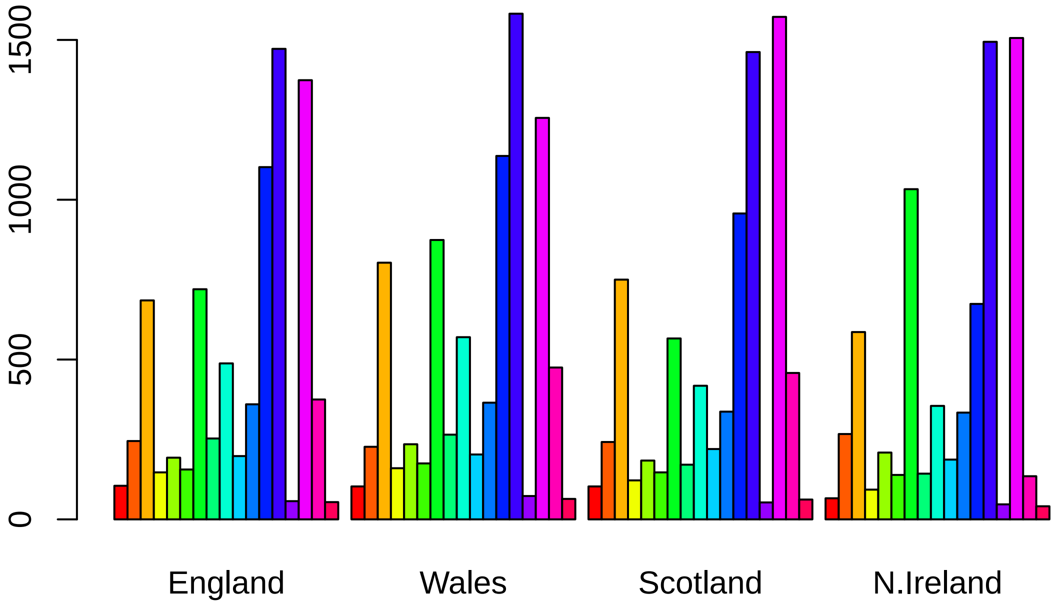
```
## [1] 17  4
```

> Q2. Which approach to solving the 'row-names problem' mentioned above do you prefer and why? Is one approach more robust than another under certain circumstances?

I would prefer the second approach, which is to assign the row names when first reading the file, because if you run x <- x[,-1] multiple times it will keep removing columns which will mess with our data.

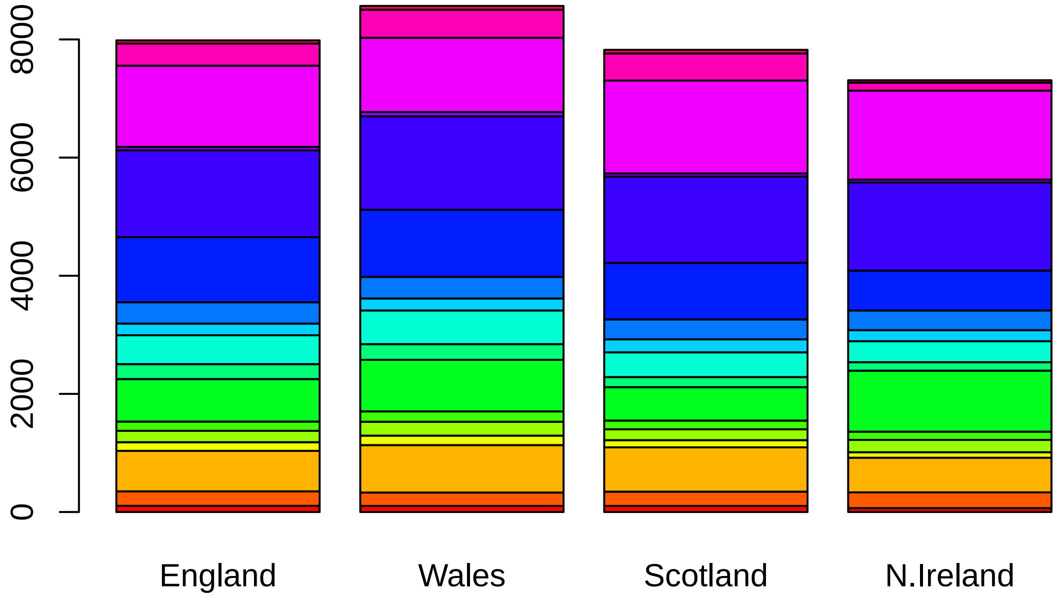
Plot the results:

```
barplot(as.matrix(x), beside=T, col=rainbow(nrow(x)))
```



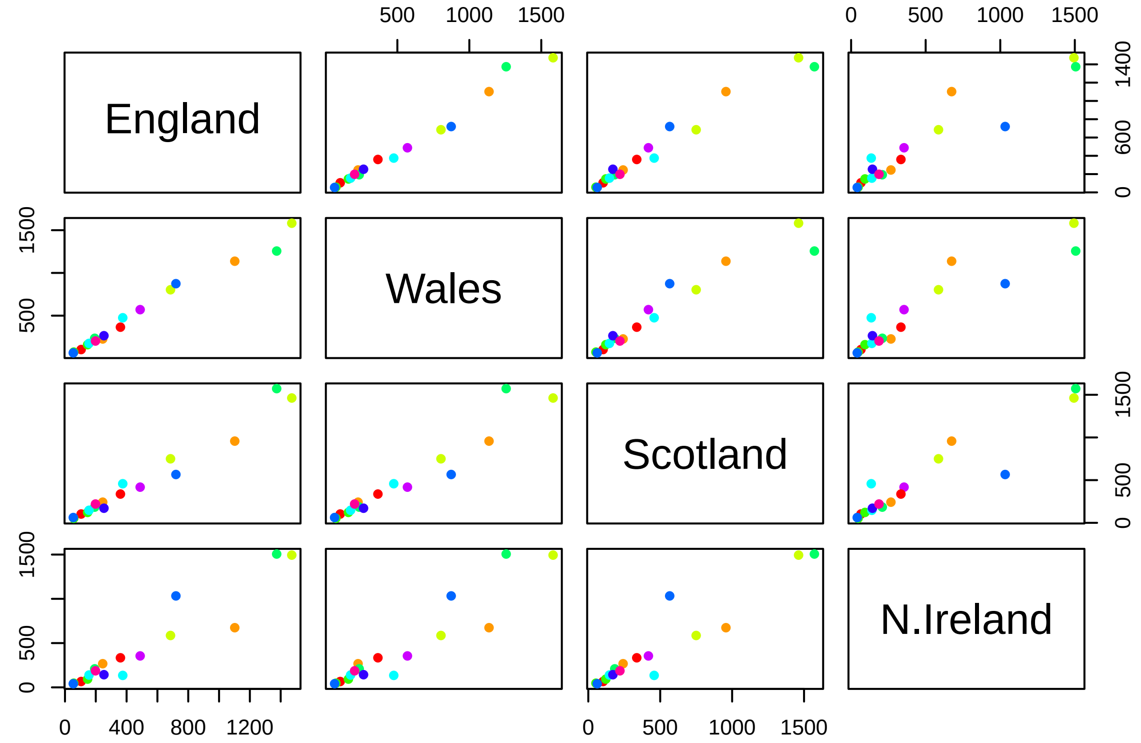
One can set the `beside` parameter to false in order to not display the results side by side.

```
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



Q5: Generating all pairwise plots may help somewhat. Can you make sense of the following code and resulting figure? What does it mean if a given point lies on the diagonal for a given plot?

```
pairs(x, col=rainbow(10), pch=16)
```



If a point aligns along the diagonal, it means that that value is similar for the two countries.

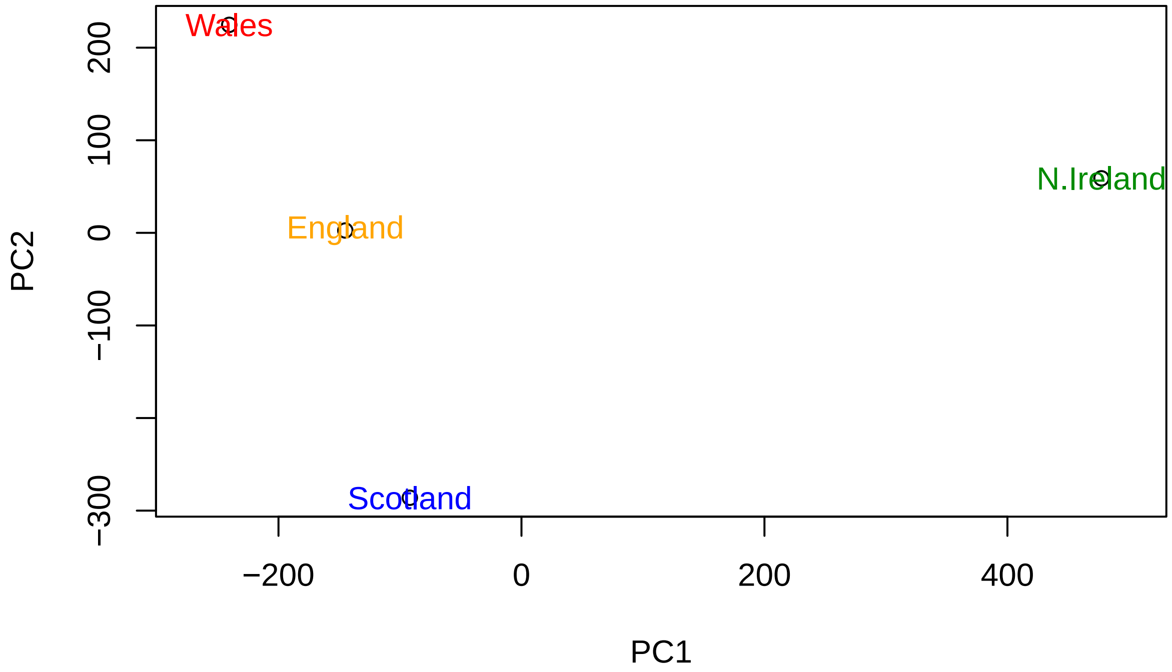
We use PCA to make sense of the data

```
# Use the prcomp() PCA function
pca <- prcomp( t(x) )
summary(pca)
```

```
## Importance of components:
##                              PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 4.189e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

Generate a plot of PC1 vs PC2

```
# Plot PC1 vs PC2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500))
text(pca$x[,1], pca$x[,2], colnames(x), col=c("ORANGE", "RED", "BLUE", "GREEN4"))
```



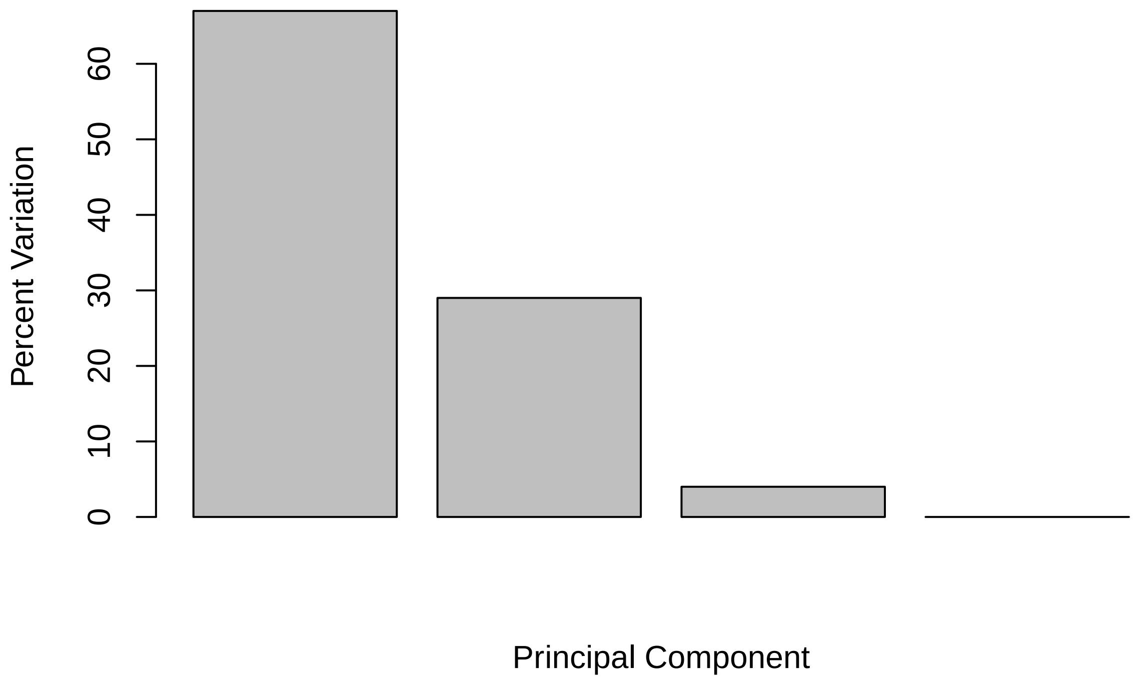
Calculate the variation within the original data that each PC accounts for (rounded up)

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

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

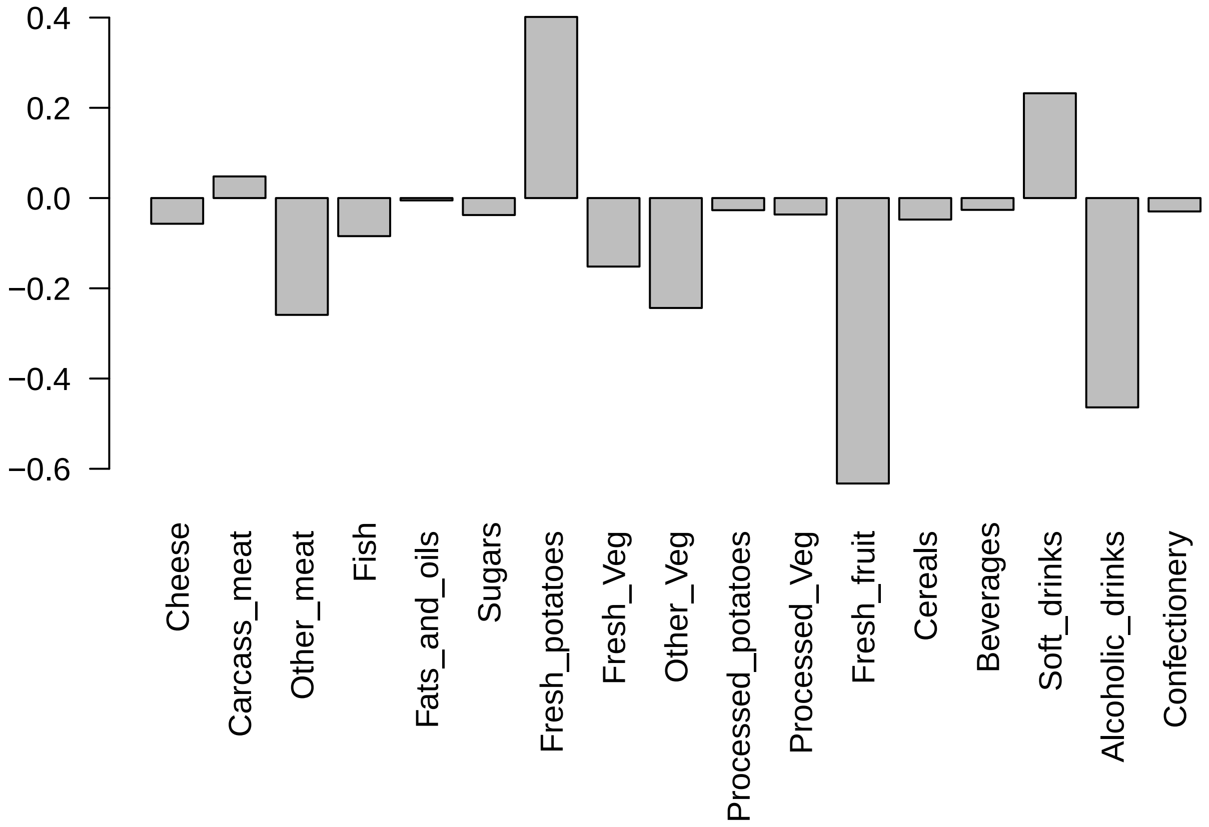
Summarizing plot of the variances (visually representation of above info)

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



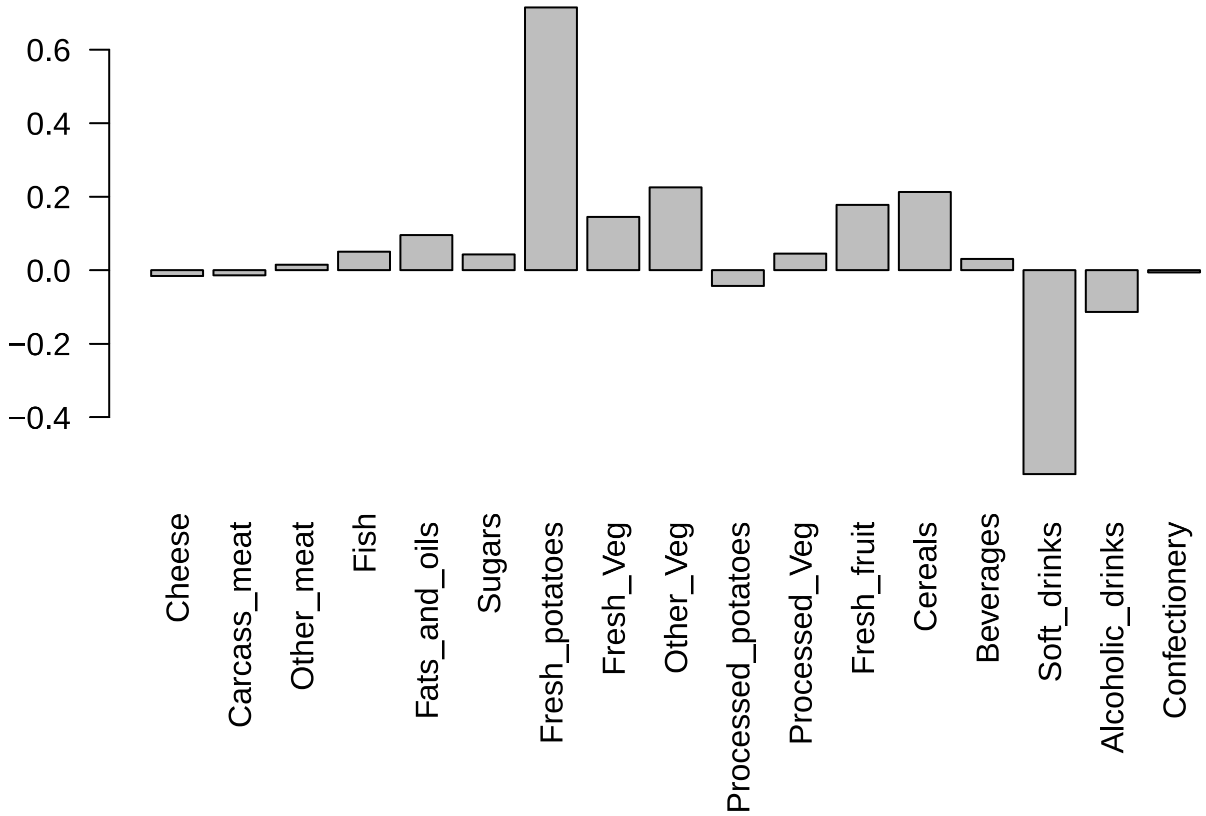
Finding and representing loading scores:

```
## Lets focus on PC1 as it accounts for > 90% of variance
par(mar=c(10, 3, 0.35, 0))

#Barplot for PC1
barplot( pca$rotation[,1], las=2 )
```



Q9: Generate a similar 'loadings plot' for PC2. What two food groups feature prominantely and what does PC2 maninly tell us about?

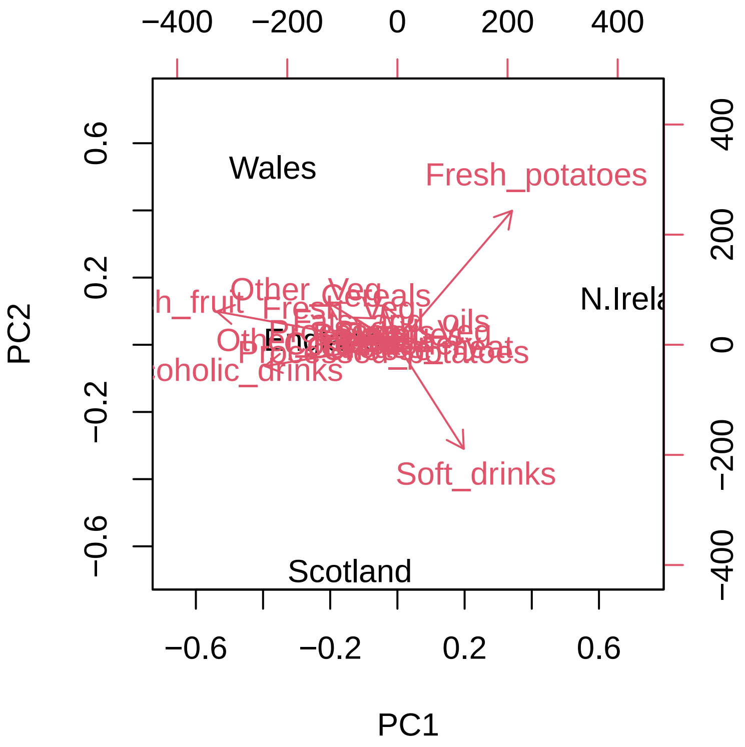
```
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```



The two prominent food groups are potatoes and soft drinks.

Representing data using a Biplot:

```
biplot(pca)
```



//Part 2// 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
```

Q10: How many genes and samples are in this data set?

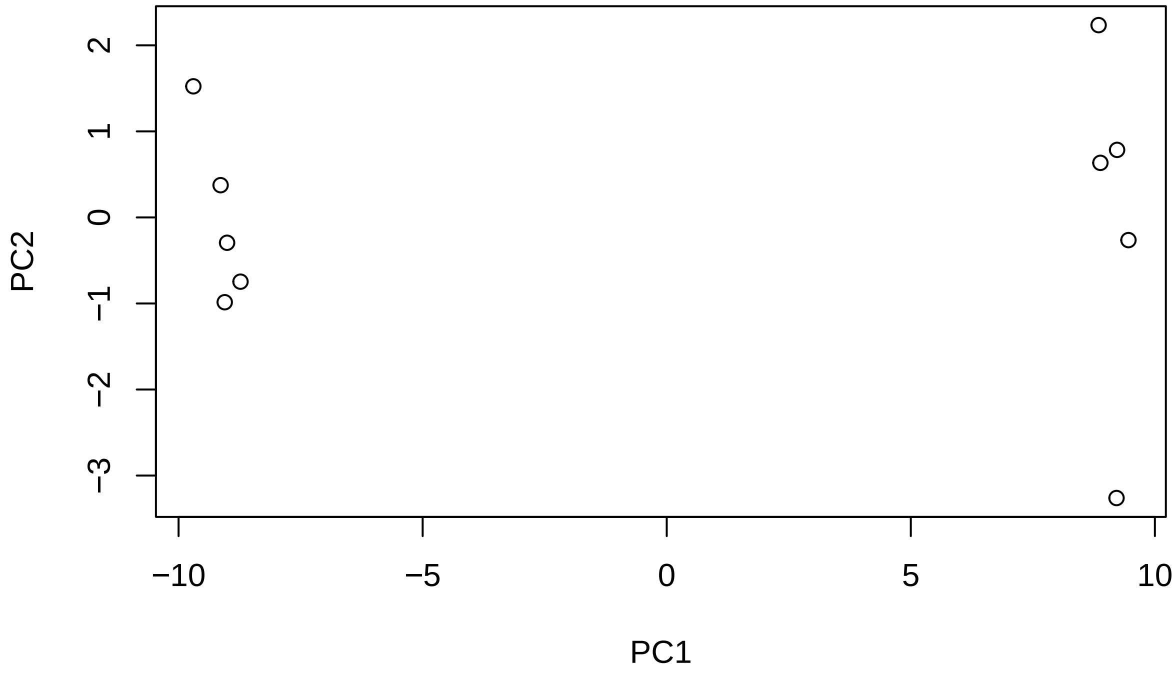
```
dim(rna.data)
```

```
## [1] 100  10
```

We have 100 genes, and 10 samples.

Use PCA to analyze data

```
## Again we have to take the transpose of our data
pca <- prcomp(t(rna.data), scale=TRUE)

## Simple un polished plot of pc1 and pc2
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2")
```

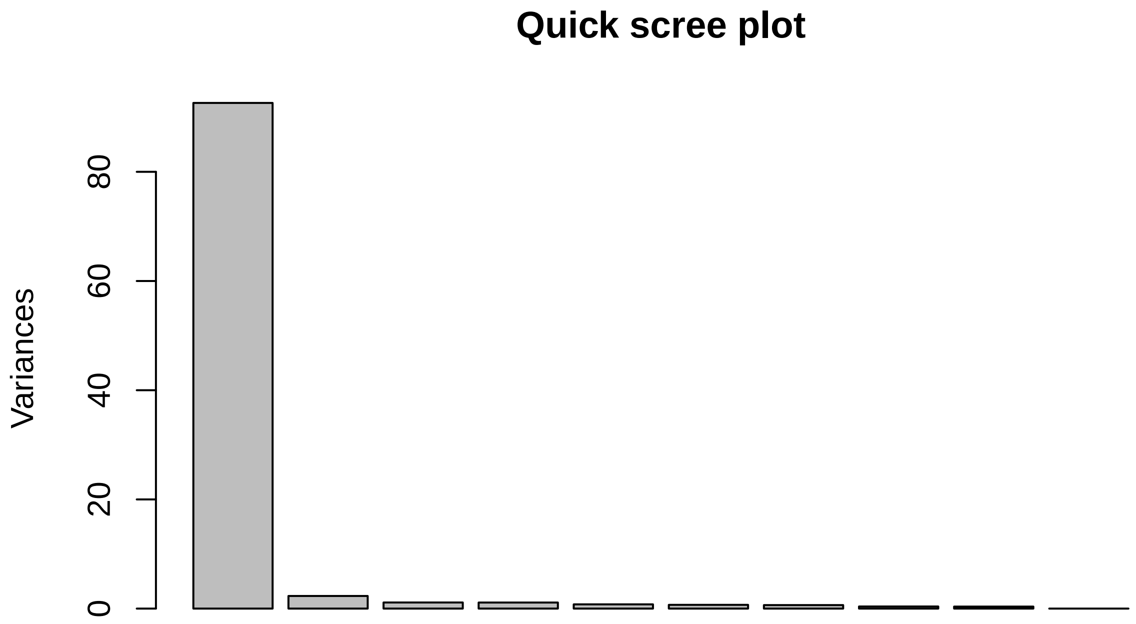


```
summary(pca)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     9.6237 1.5198 1.05787 1.05203 0.88062 0.82545 0.80111
## Proportion of Variance 0.9262 0.0231 0.01119 0.01107 0.00775 0.00681 0.00642
## Cumulative Proportion  0.9262 0.9493 0.96045 0.97152 0.97928 0.98609 0.99251
##                            PC8     PC9      PC10
## Standard deviation     0.62065 0.60342 3.348e-15
## Proportion of Variance 0.00385 0.00364 0.000e+00
## Cumulative Proportion  0.99636 1.00000 1.000e+00
```

Scree barplot to represent variance

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

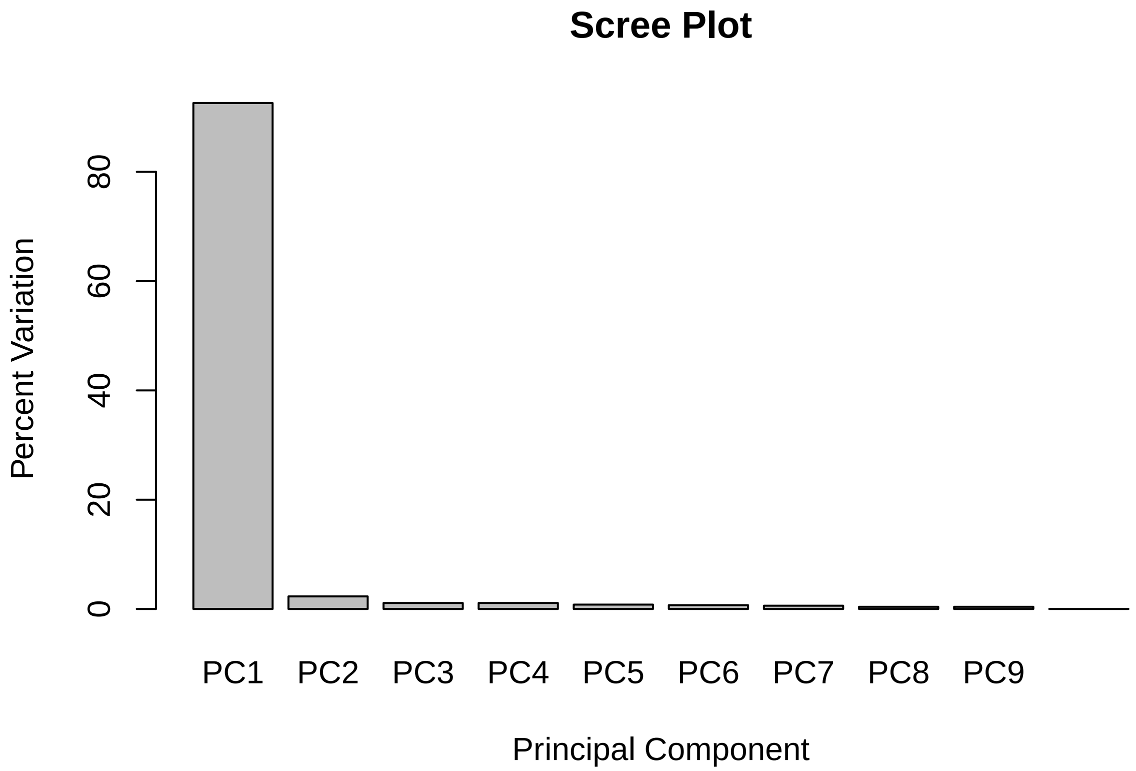


More in-depth Scree plot with our calculated values

```
## 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
```

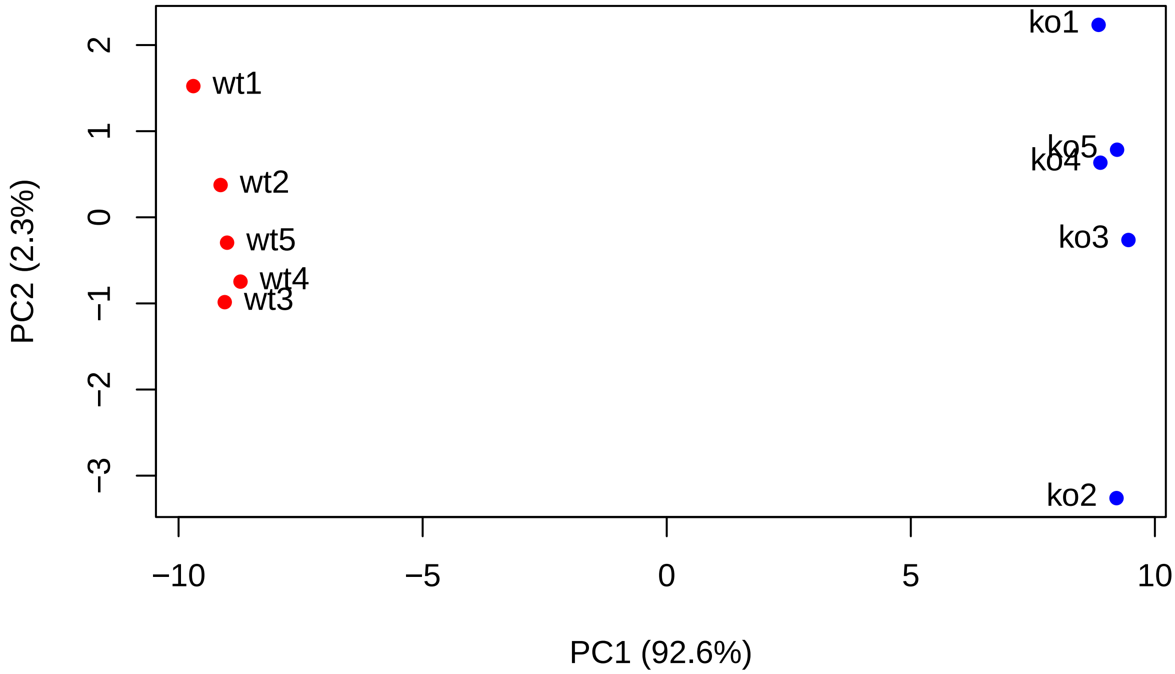
```
##  [1] 92.6  2.3  1.1  1.1  0.8  0.7  0.6  0.4  0.4  0.0
```

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



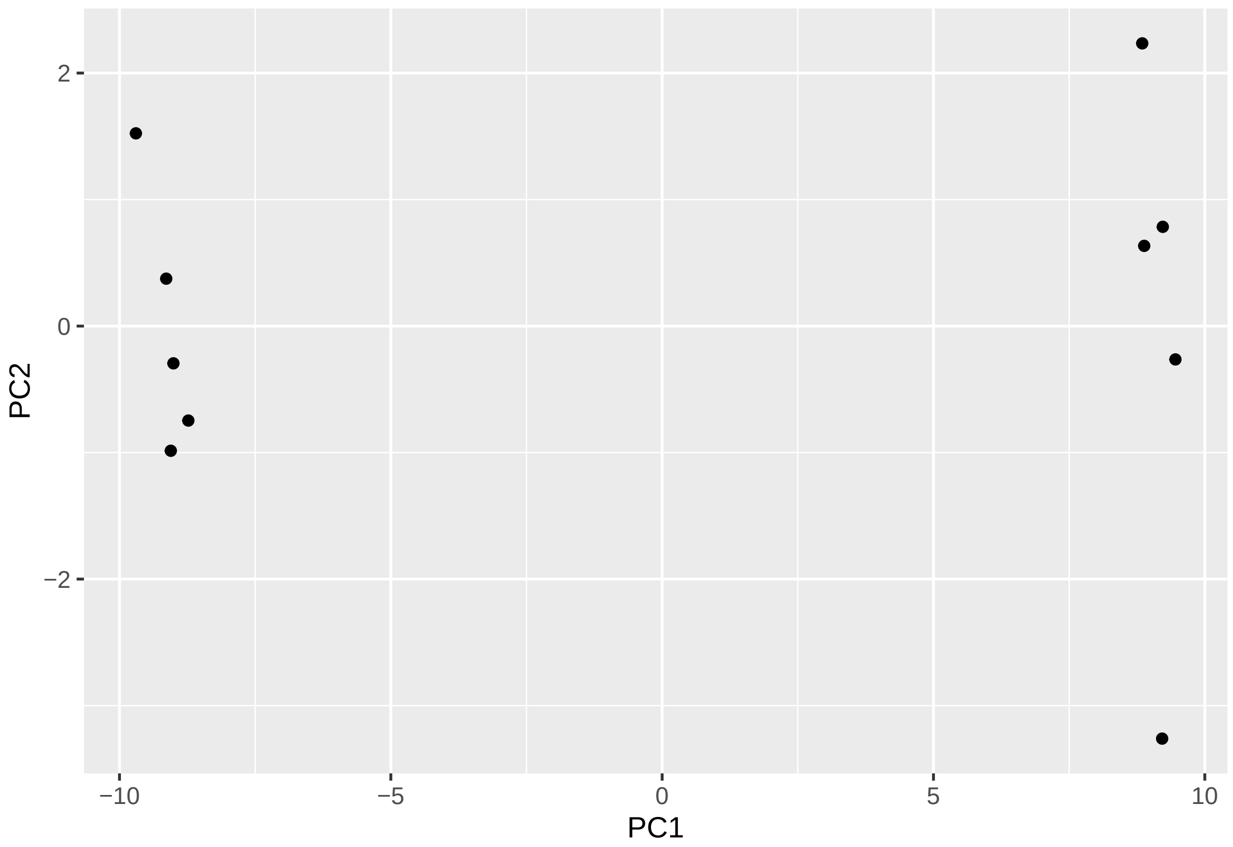
Add details to original PCA plot:

```
## 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)))
```

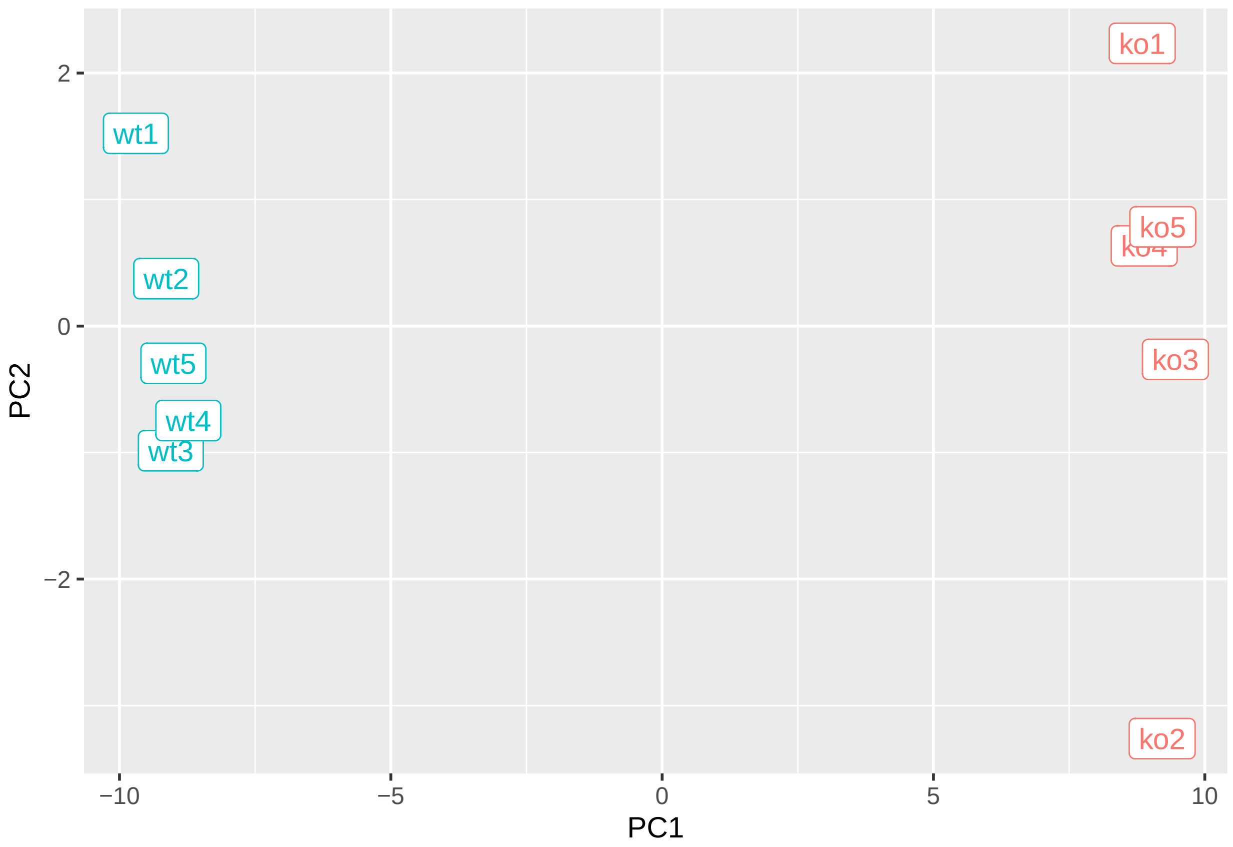


Building a similar plot using ggplot2

```
library(ggplot2)

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

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



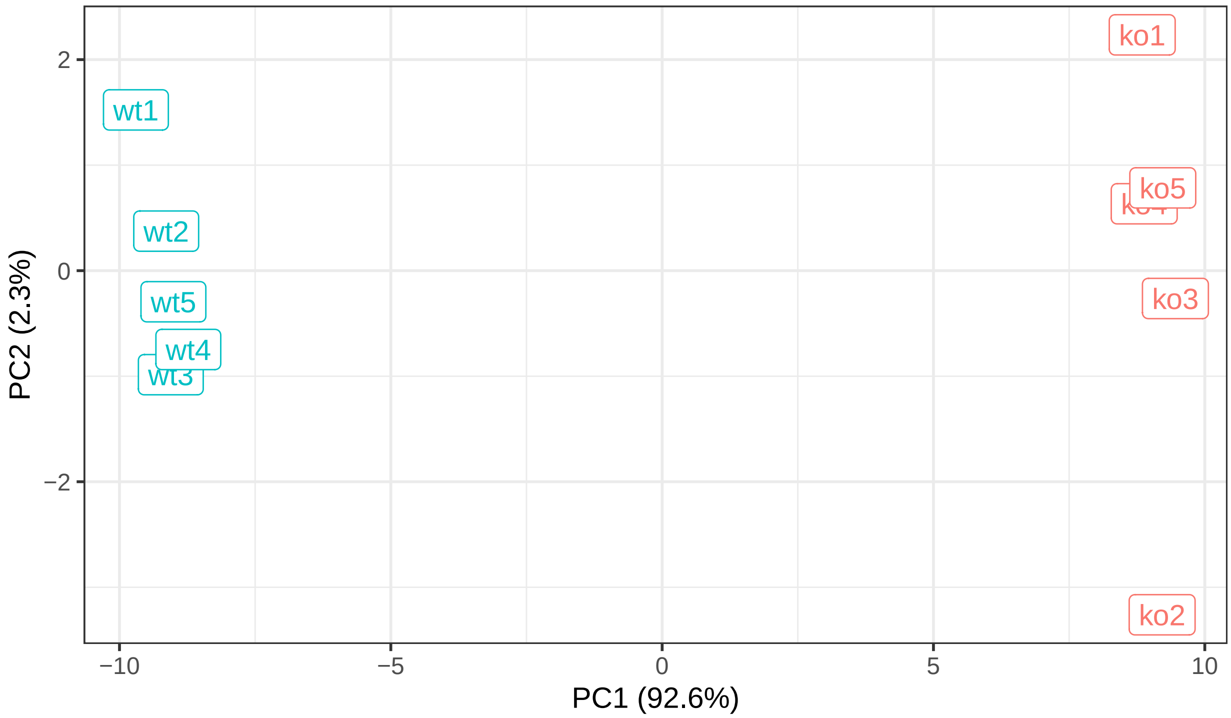
```
# Add a 'wt' and 'ko' "condition" column
df$samples <- colnames(rna.data)
df$condition <- substr(colnames(rna.data),1,2)

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



```
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="BIMM143 example data") +
     theme_bw()
```

PCA of RNASeq Data

PC1 clealy seperates wild−type from knock−out samples



BIMM143 example data