

# Lab 7: PCA

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## Data Import, Q1

```
url <- "https://tinyurl.com/UK-foods"
x <- read.csv(url)
dim(x)
```

```
[1] 17  5
```

Using the dim function, we see there are 17 rows and 5 columns.

## Checking Data, Q2

```
# Preview first 6 rows
#head(x)

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

#dim(x)

# Solution 2
x <- read.csv(url, row.names=1)
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

```
dim(x)
```

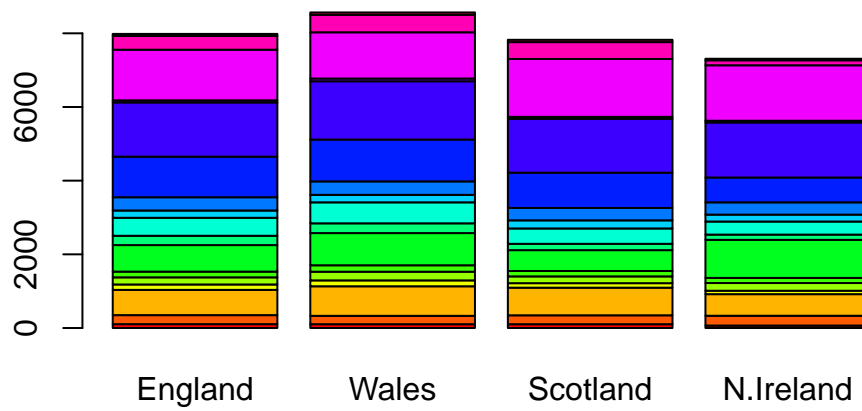
```
[1] 17  4
```

```
#x
```

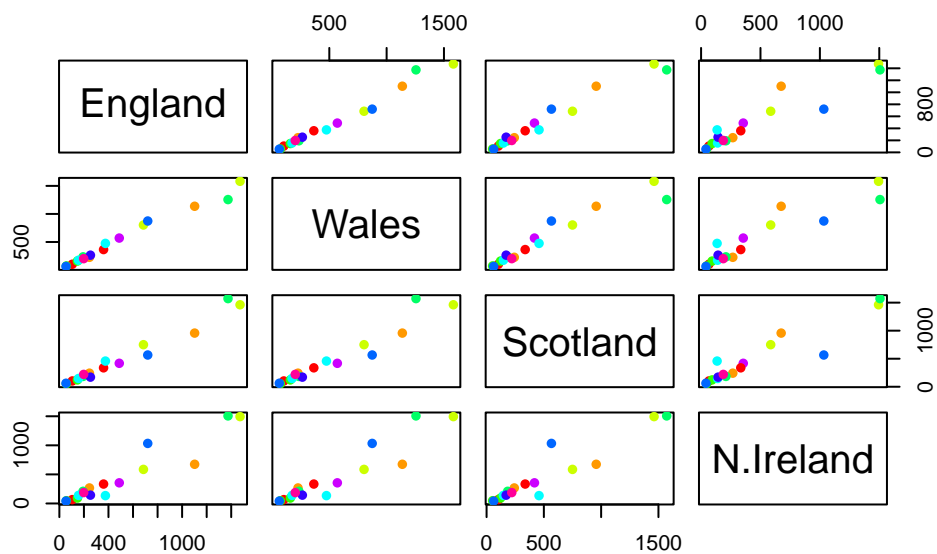
The second approach is more robust and efficient since it solves the problem in 1 line of code. Additionally, running the first solution multiple times will continuously make the data frame dimensions smaller as it sets the first column as the row names.

## Spotting major differences and trends, Q3/Q5/Q6

```
# Q3
barplot(as.matrix(x), beside=F, col=rainbow(nrow(x)))
```



```
# Q5
pairs(x, col=rainbow(10), pch=16)
```



Q3: Changing the optional argument 'beside' to false results in the desired plot.

Q5: If a point lies on the diagonal of a given pairwise plot, it means that the variable the point represents is very correlated between the two countries (equal consumption).

Q6: The main differences between N. Ireland and other UK countries is that seems that they have equal or less consumption on average for almost every category of food. The one outlier is fresh potatoes, which N. Ireland consumes far more than the other 3 countries on average.

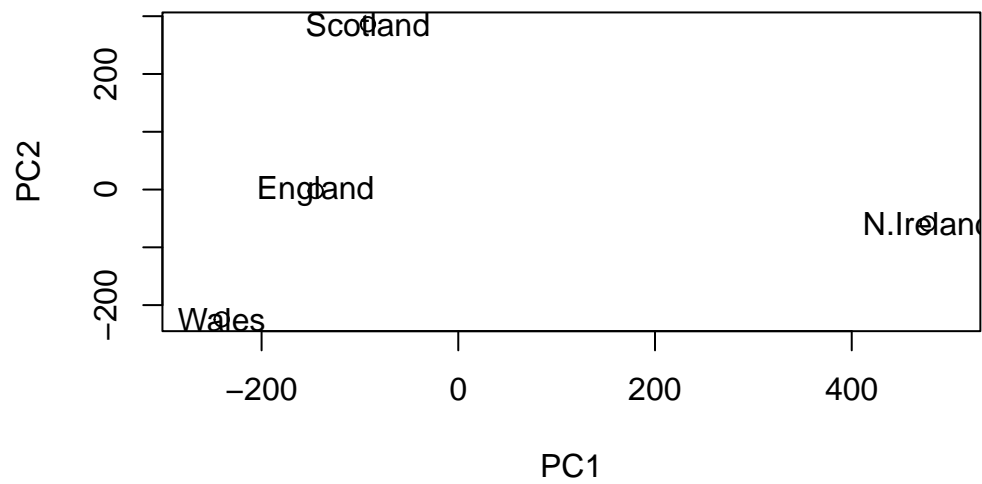
## PCA, Q7/Q8/Q9

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

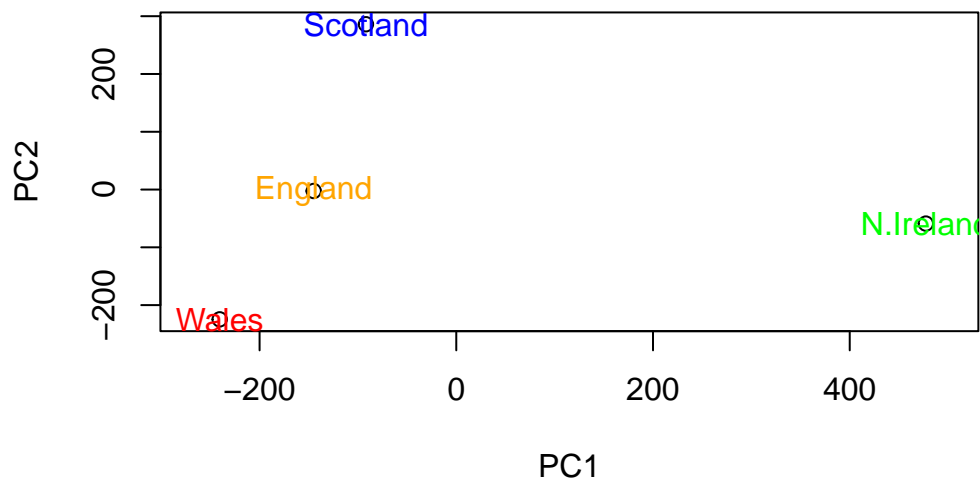
Importance of components:

	PC1	PC2	PC3	PC4
Standard deviation	324.1502	212.7478	73.87622	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

```
# Q7: 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))
```



```
# Q8: Customize plot
column_colors <- c("orange", "red", "blue", "green")
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 = column_colors)
```



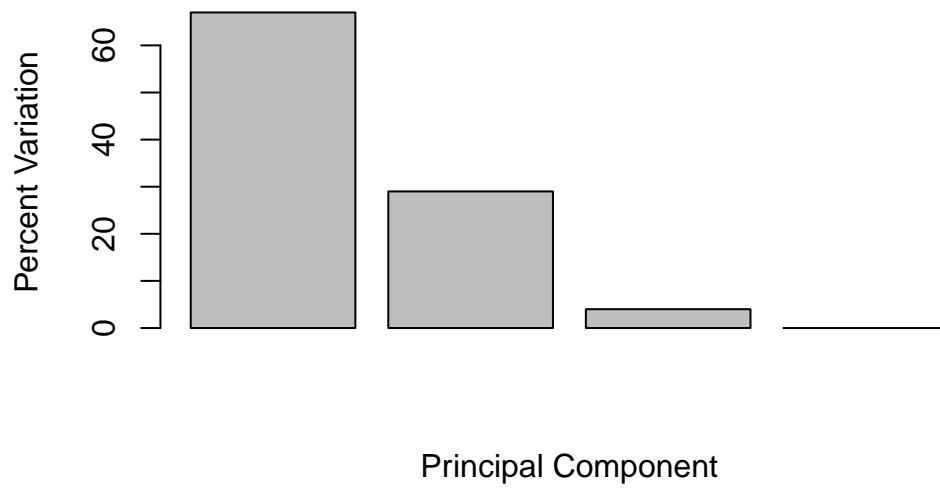
```
v <- round( pca$sdev^2/sum(pca$sdev^2) * 100 )
v
```

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

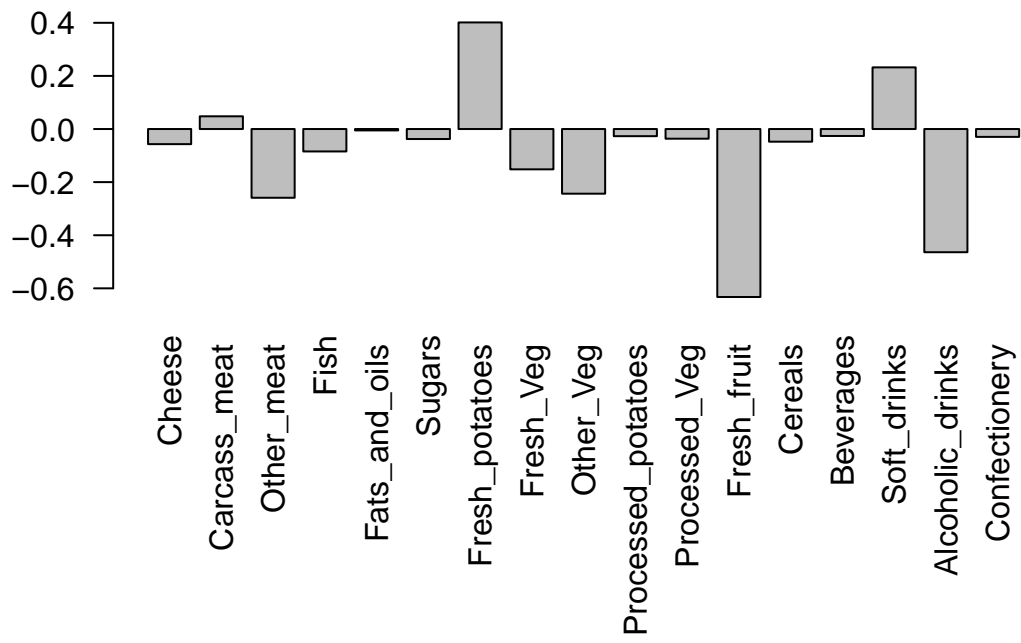
```
z <- summary(pca)
z$importance
```

	PC1	PC2	PC3	PC4
Standard deviation	324.15019	212.74780	73.87622	3.175833e-14
Proportion of Variance	0.67444	0.29052	0.03503	0.000000e+00
Cumulative Proportion	0.67444	0.96497	1.00000	1.000000e+00

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

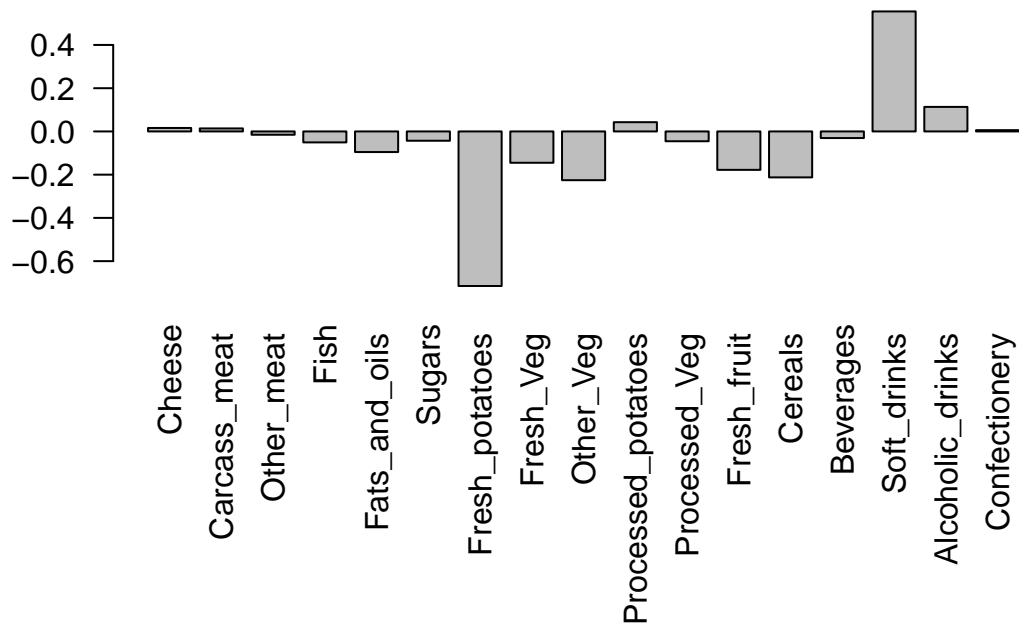


```
# Lets focus on PC1 as it accounts for > 90% of variance  
par(mar=c(10, 3, 0.35, 0))  
barplot( pca$rotation[,1], las=2 )
```



```
# PCA2
par(mar=c(10, 3, 0.35, 0))
barplot( pca$rotation[,2], las=2 )
```





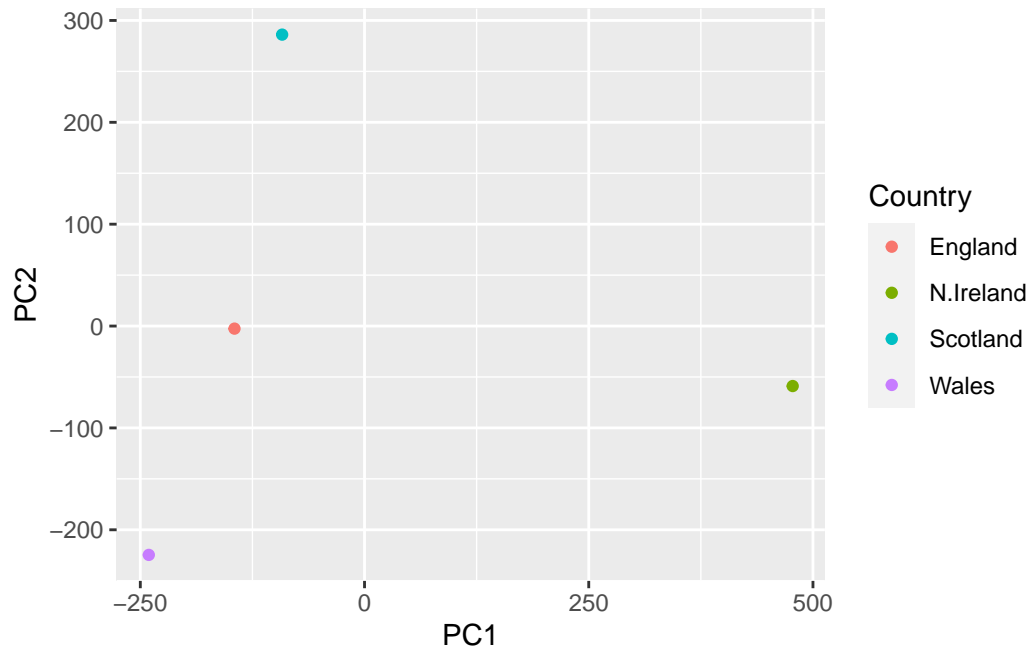
Q9: Fresh potatoes and soft drinks are prominent features on the loading plot. PC2 tells us that fresh potatoes push countries down while soft drinks push countries up.

## ggplot

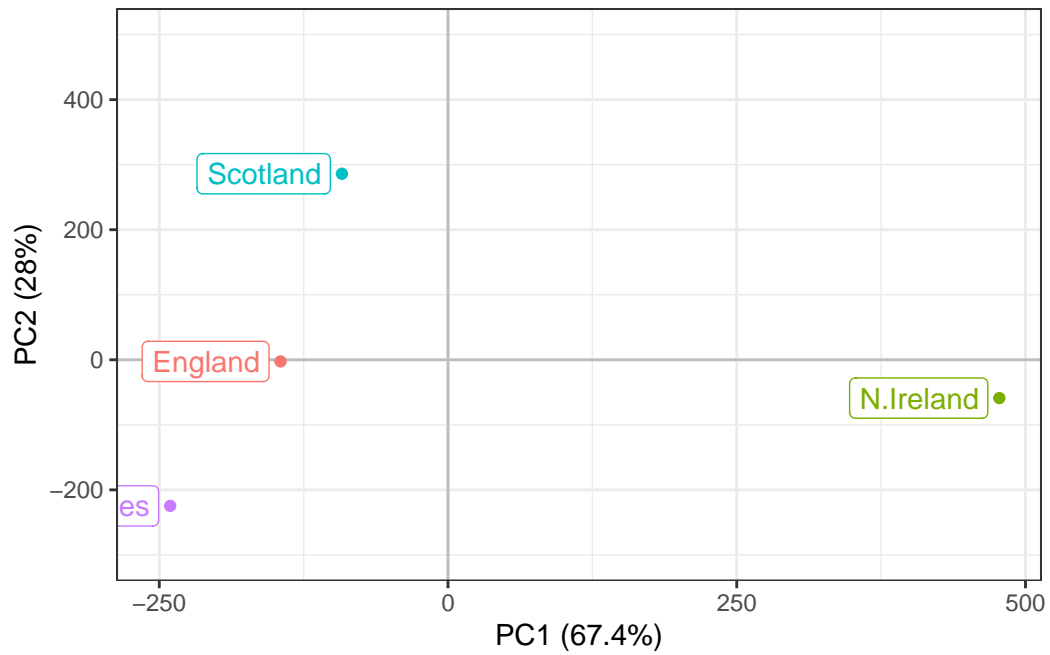
```
library(ggplot2)

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()
```

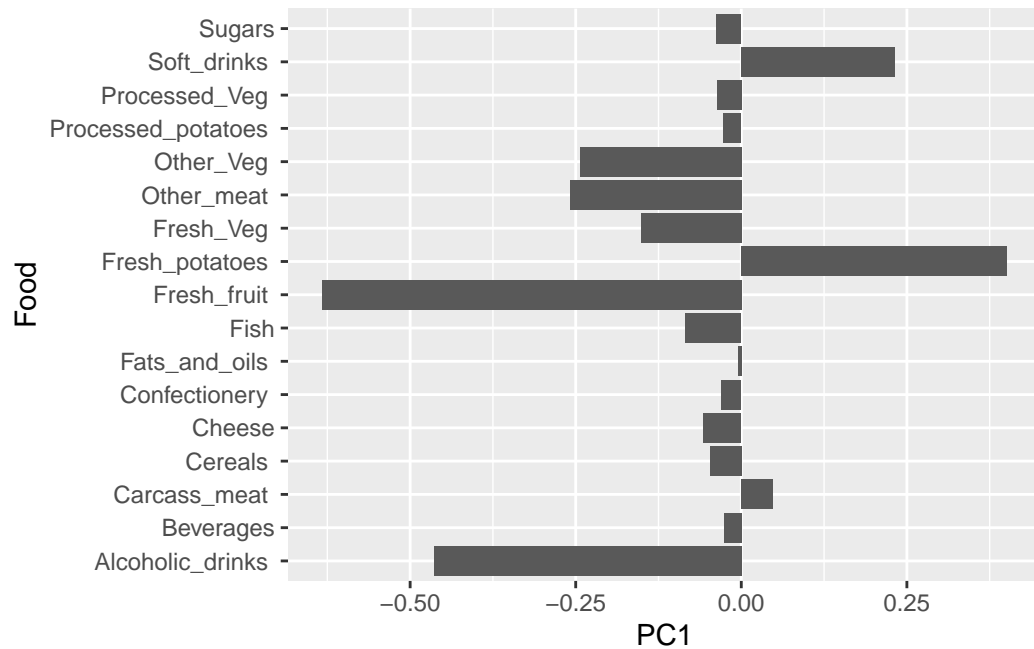


```
ggplot(df_lab) +  
  aes(PC1, PC2, col=Country, label=Country) +  
  geom_hline(yintercept = 0, col="gray") +  
  geom_vline(xintercept = 0, col="gray") +  
  geom_point(show.legend = FALSE) +  
  geom_label(hjust=1, nudge_x = -10, show.legend = FALSE) +  
  expand_limits(y = c(-300,500)) +  
  xlab("PC1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

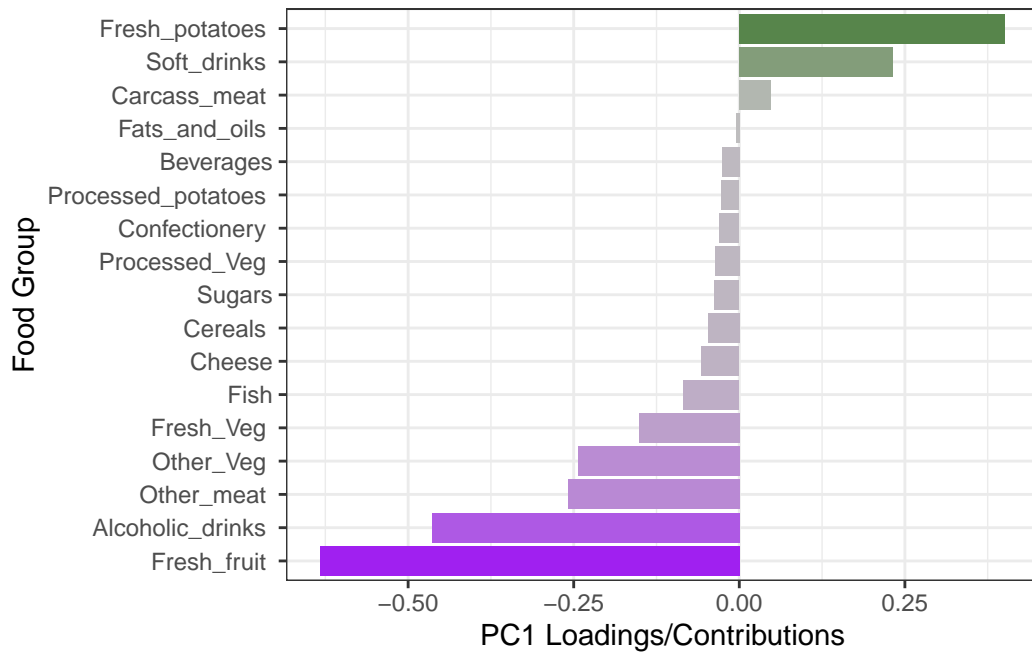


```
ld <- as.data.frame(pca$rotation)
ld_lab <- tibble::rownames_to_column(ld, "Food")

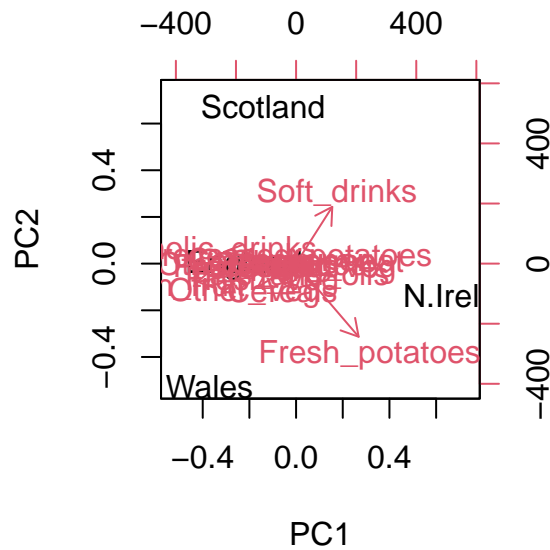
ggplot(ld_lab) +
  aes(PC1, Food) +
  geom_col()
```



```
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()
```



```
biplot(pca)
```



## PCA of RNA-seq Data, Q10

```
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

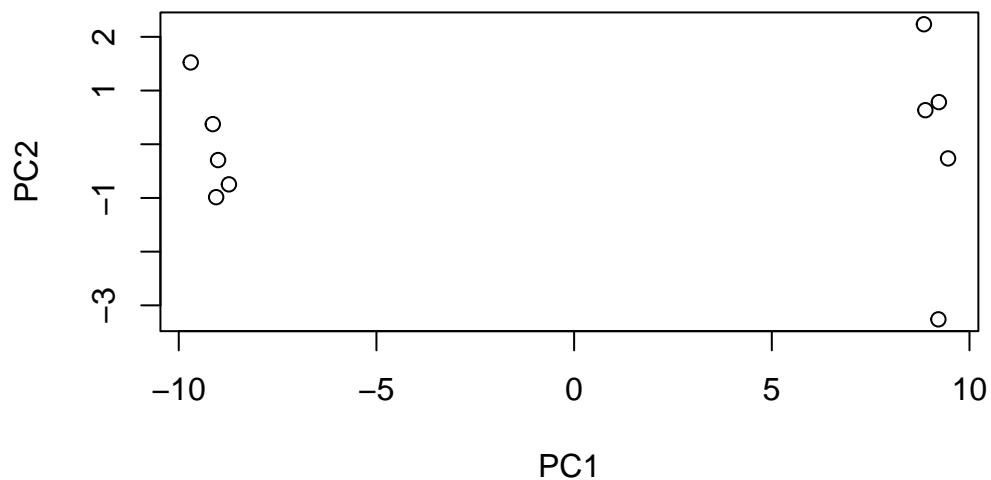
```
dim(rna.data)
```

```
[1] 100  10
```

Q10: There are 100 genes and 10 samples in the data.

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

# Simple unpolished 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	3.457e-15
Proportion of Variance	0.00385	0.00364	0.000e+00
Cumulative Proportion	0.99636	1.00000	1.000e+00

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

## Quick scree plot



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

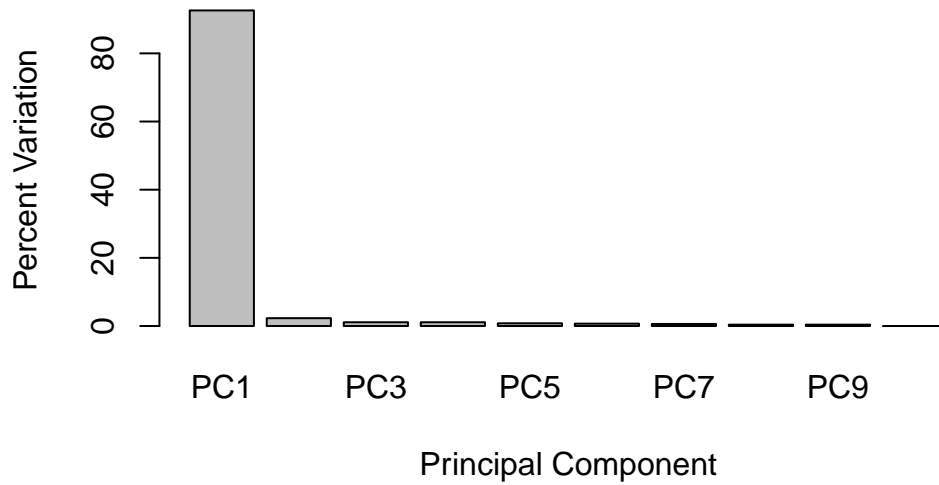
# Percent variance is often more informative to look at
pca.var.per <- round(pca.var/sum(pca.var)*100, 1)
pca.var.per
```

```
[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")
```



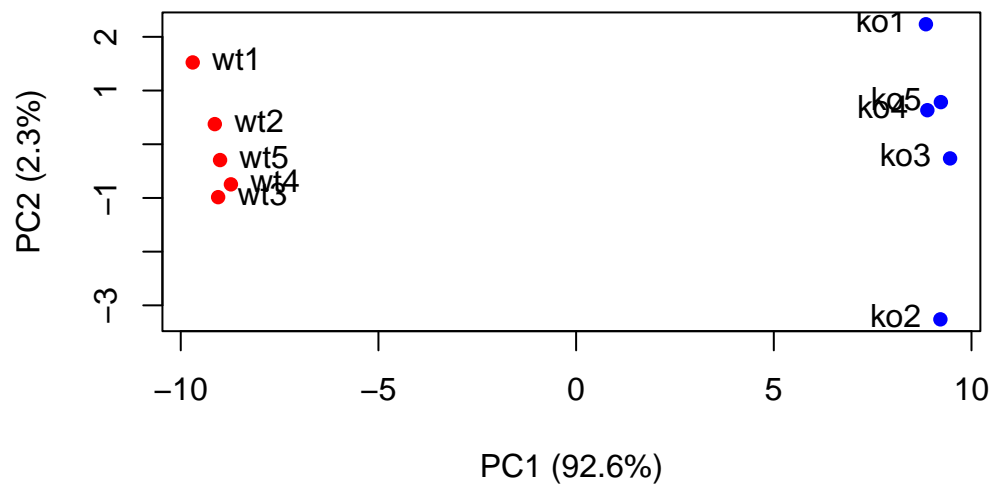
## Scree Plot



```
# 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], "%)"))

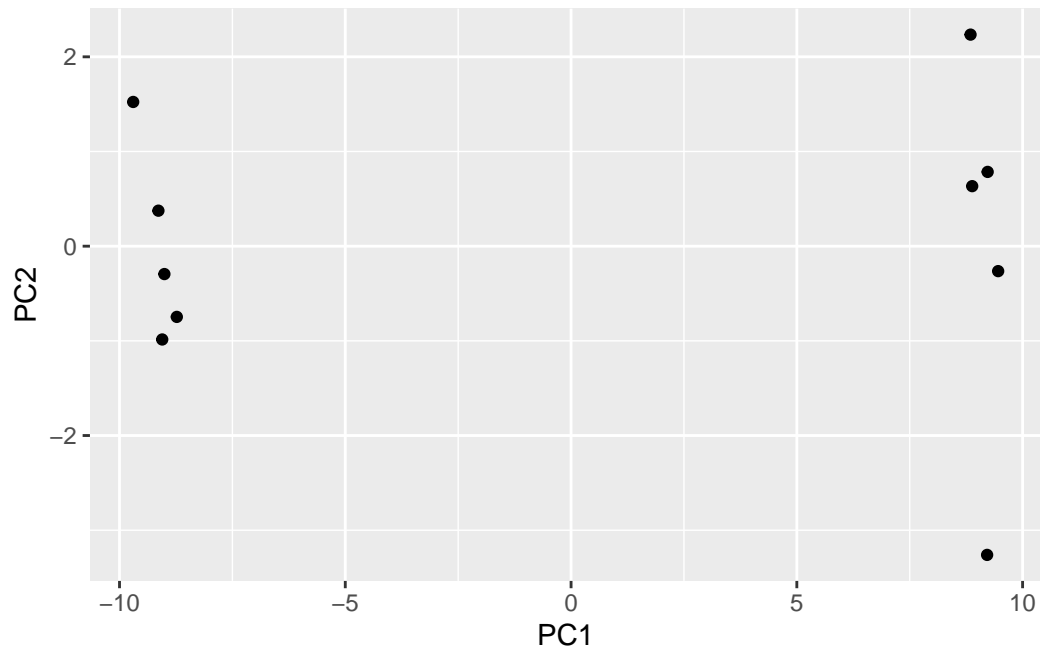
text(pca$x[,1], pca$x[,2], labels = colnames(rna.data), pos=c(rep(4,5), rep(2,5)))
```



```
library(ggplot2)

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

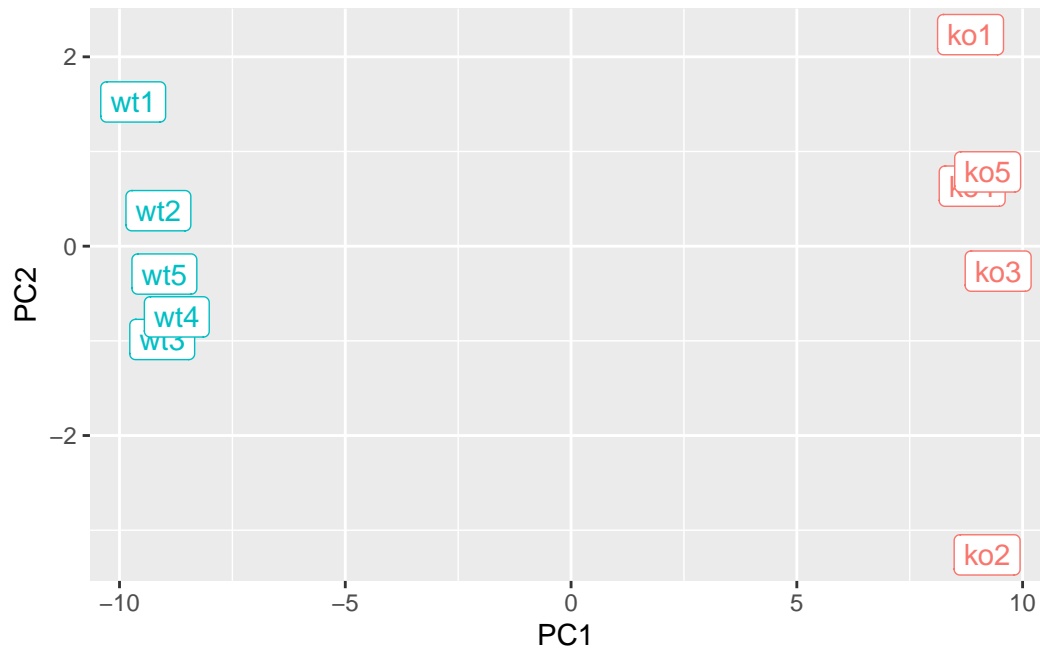
# Our first basic plot
ggplot(df) +
  aes(PC1, PC2) +
  geom_point()
```



```
# 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)

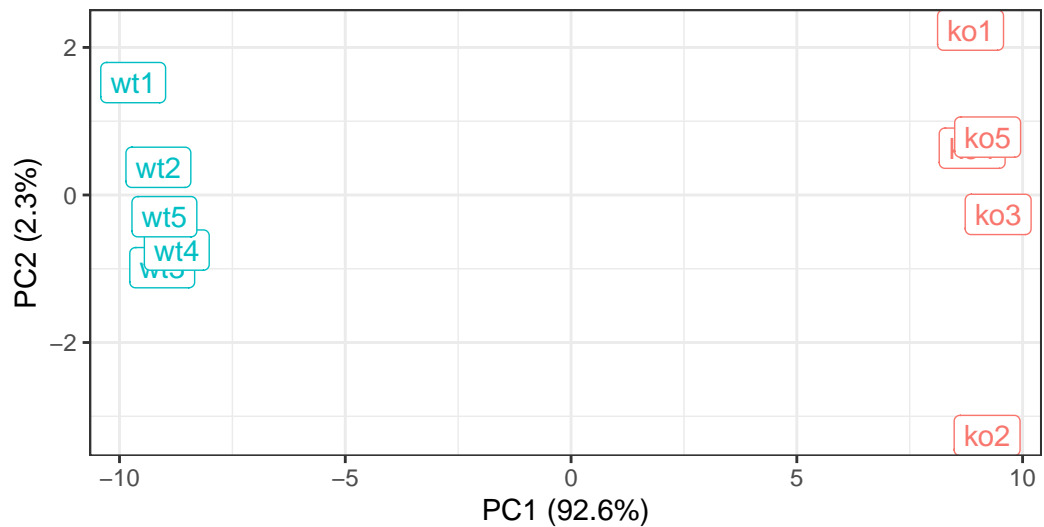
p
```



```
p + labs(title="PCA of RNASeq Data",
  subtitle = "PC1 clearly separates 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 clearly separates wild-type from knock-out samples



Class example data

### Gene Loadings

```
loading_scores <- pca$rotation[,1]

# Find the top 10 measurements (genes) that contribute
# most to PC1 in either direction (+ or -)
gene_scores <- abs(loading_scores)
gene_score_ranked <- sort(gene_scores, decreasing=TRUE)

# show the names of the top 10 genes
top_10_genes <- names(gene_score_ranked[1:10])
top_10_genes
```

```
[1] "gene100" "gene66"  "gene45"  "gene68"  "gene98"  "gene60"  "gene21"
[8] "gene56"  "gene10"  "gene90"
```