Machine Learning 1

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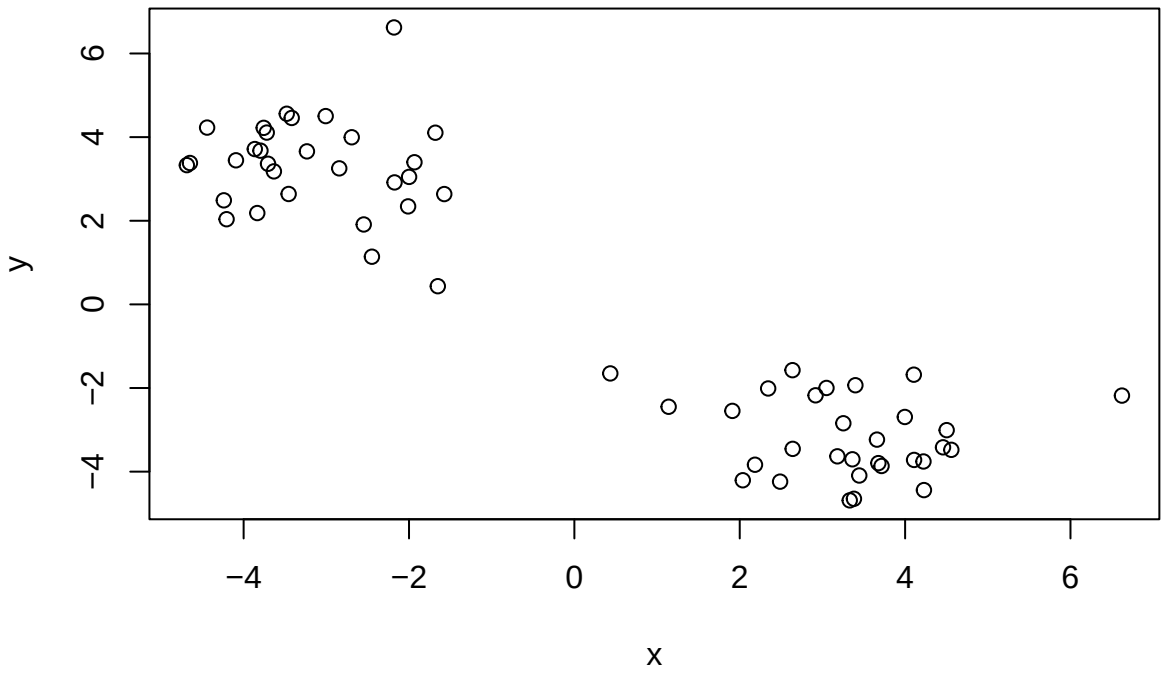
First up kmeans()

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  3.299632 -3.165428
## 2 -3.165428  3.299632
##
## Clustering vector:
##  [1] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
## [39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##
## Within cluster sum of squares by cluster:
## [1] 66.14739 66.14739
##  (between_SS / total_SS =  90.5 %)
##
## 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] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 1 1 1 1
## [39] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```

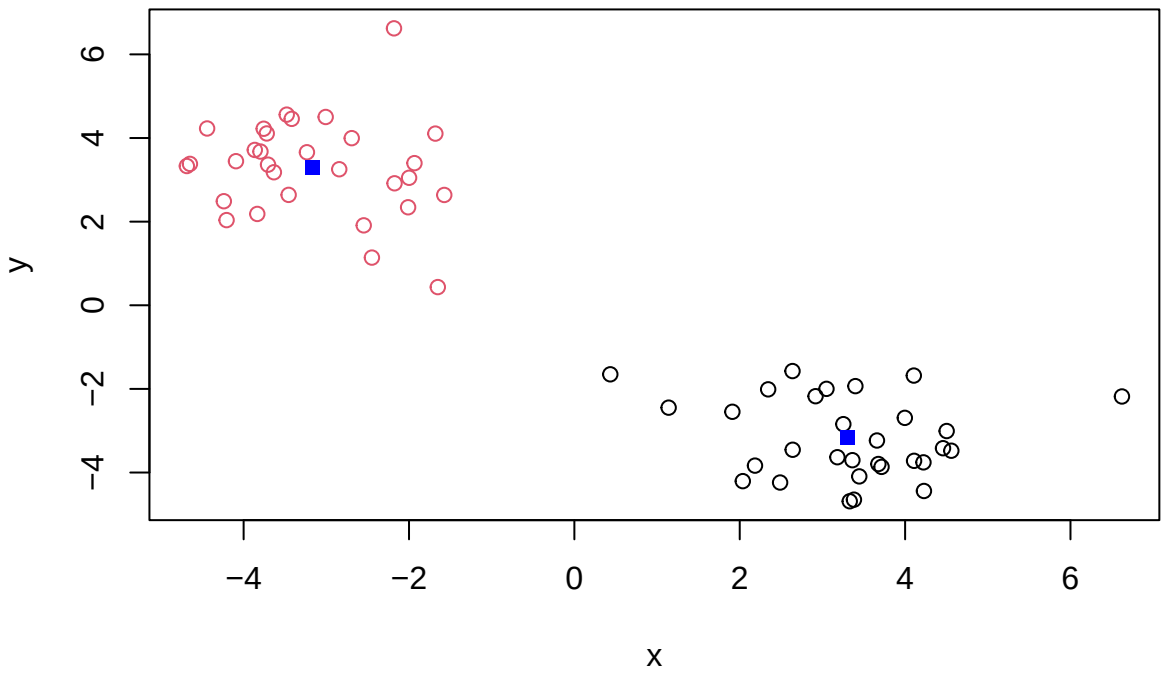
Q. What about cluster centers

```
k$centers
```

```
##          x         y
## 1  3.299632 -3.165428
## 2 -3.165428  3.299632
```

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

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



Now for hclust()

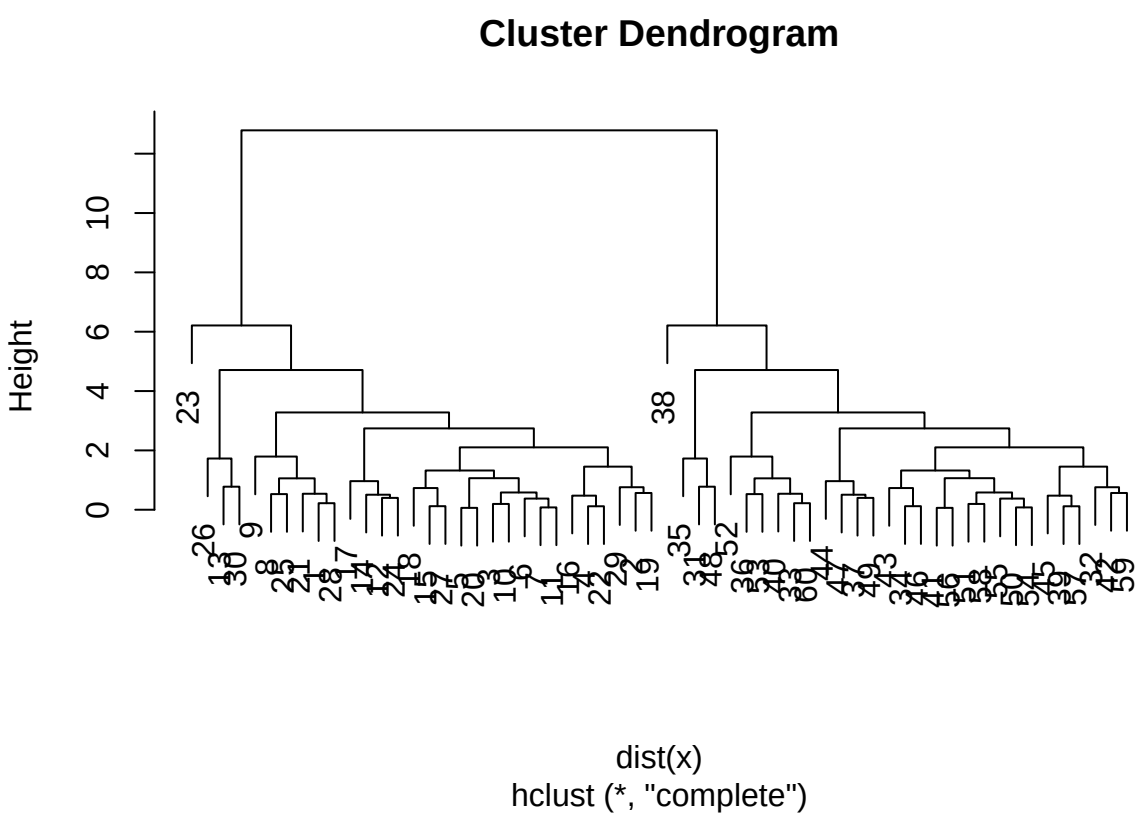
We will cluster the same data `x` with the `hclust()`. In this case `hclust()` requires a distance matrix as output.

```
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 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 2 2 2 2 2 2 2 2 2 2 2
```

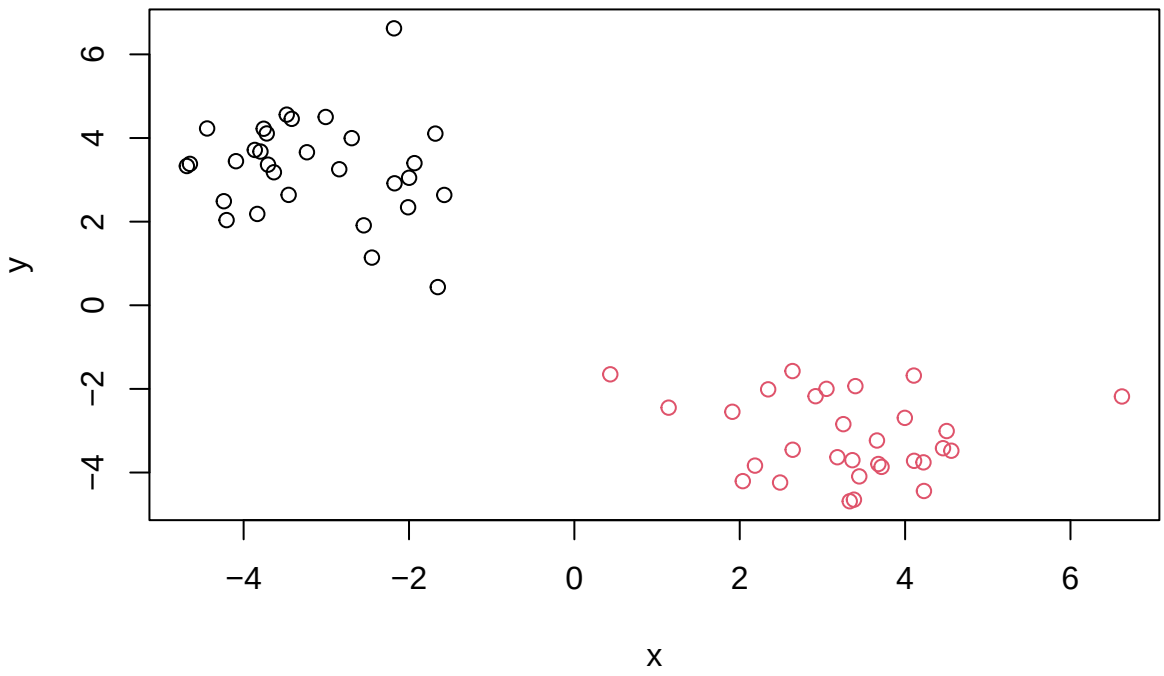
It is often helpful to use the `k=` argument to cutree rather than the `h=` heihgt of cutting with `cutree()`. This will cut the tree to yield the number of clusters you want.

```
cutree(hc, k=4)
```

```
##  [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 1 1 1 1 1 1 1 3 3 3 3 3 3 3 4
## [39] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
```

Now plot our data with the hclust() results.

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



Principal Component Analysis (PCA)

PCA of UK food data

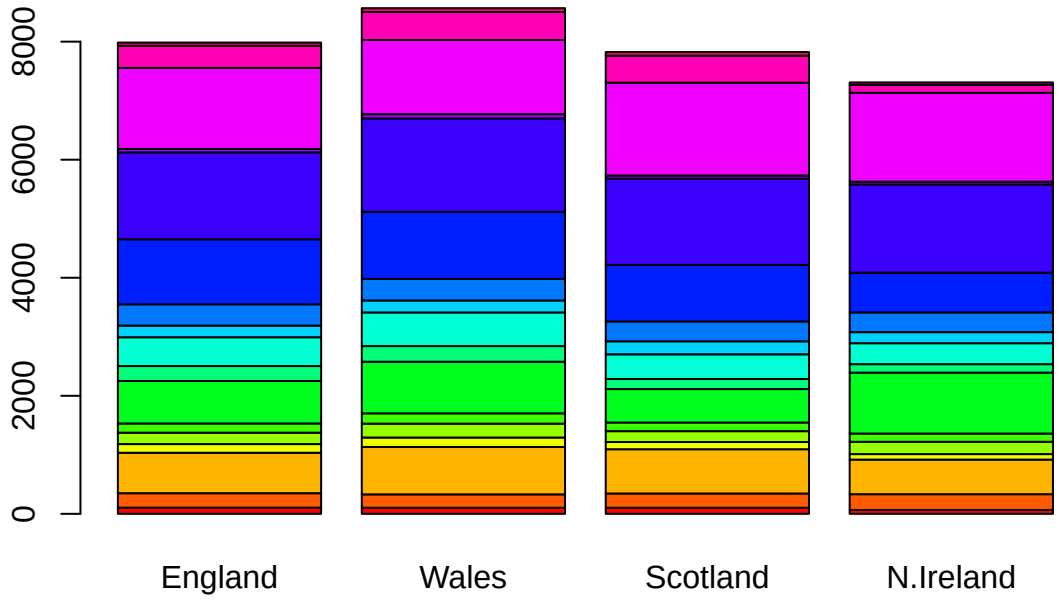
Read data from website and try a few visualizations.

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

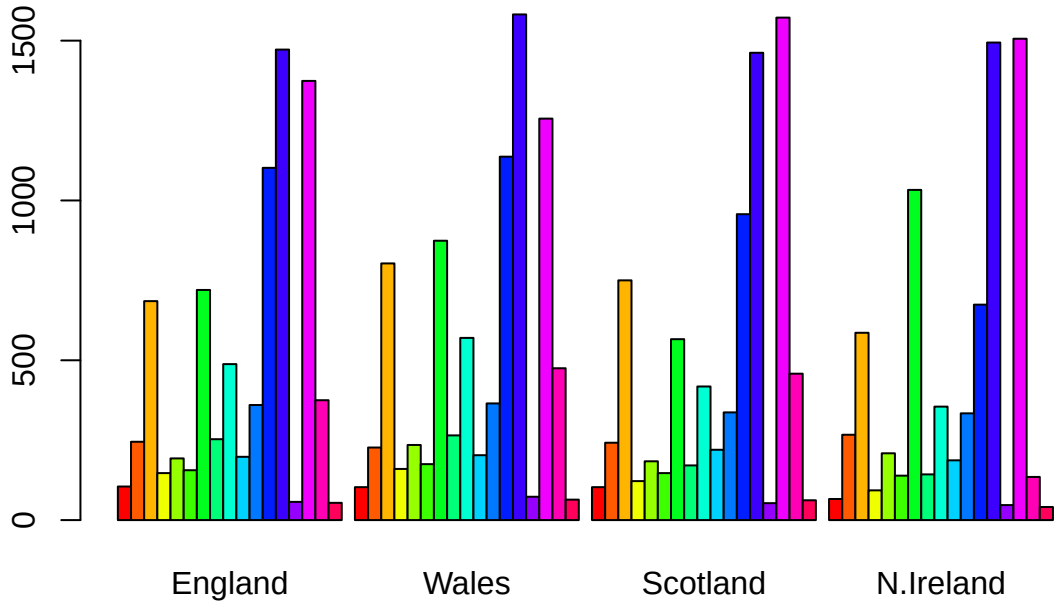
```
##                     England Wales Scotland N.Ireland
## Cheese                  105   103      103        66
## Carcass_meat            245   227      242       267
## Other_meat              685   803      750       586
## Fish                    147   160      122        93
## Fats_and_oils           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
```

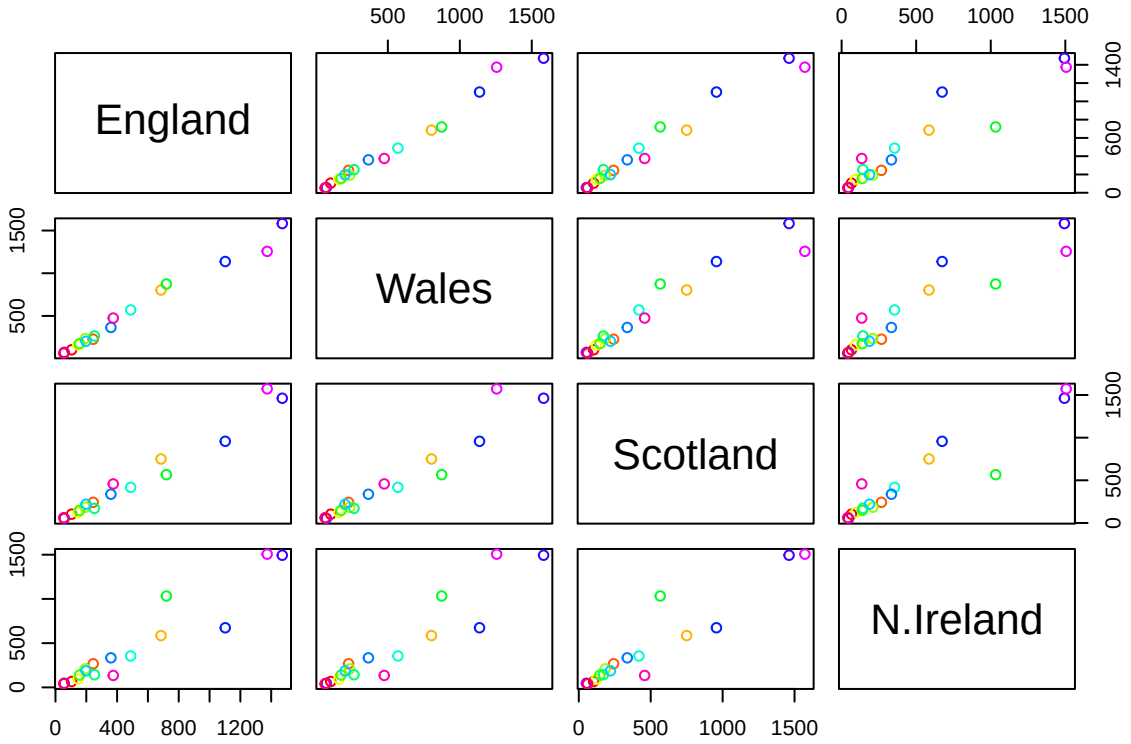
```
cols <- rainbow(nrow(x))
barplot( as.matrix(x), col=cols )
```




```
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 in this case

```
t(x)
```

```
##           Cheese Carcass_meat  Other_meat  Fish Fats_and_oils  Sugars
## England      105           245         685  147            193    156
## Wales        103           227         803  160            235    175
## Scotland     103           242         750  122            184    147
## N.Ireland     66           267         586   93            209    139
##           Fresh_potatoes  Fresh_Veg  Other_Veg  Processed_potatoes
## England              720        253        488                 198
## Wales                874        265        570                 203
## Scotland             566        171        418                 220
## N.Ireland           1033        143        355                 187
##           Processed_Veg  Fresh_fruit  Cereals  Beverages Soft_drinks
## England             360         1102     1472         57         1374
## Wales               365         1137     1582         73         1256
## Scotland            337          957     1462         53         1572
## N.Ireland           334          674     1494         47         1506
##           Alcoholic_drinks  Confectionery
## England                375             54
## Wales                  475             64
## Scotland               458             62
## N.Ireland              135             41
```

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

There is a nice summary of how well PCA accounts for the original dataset variance

```
summary(pca)
```

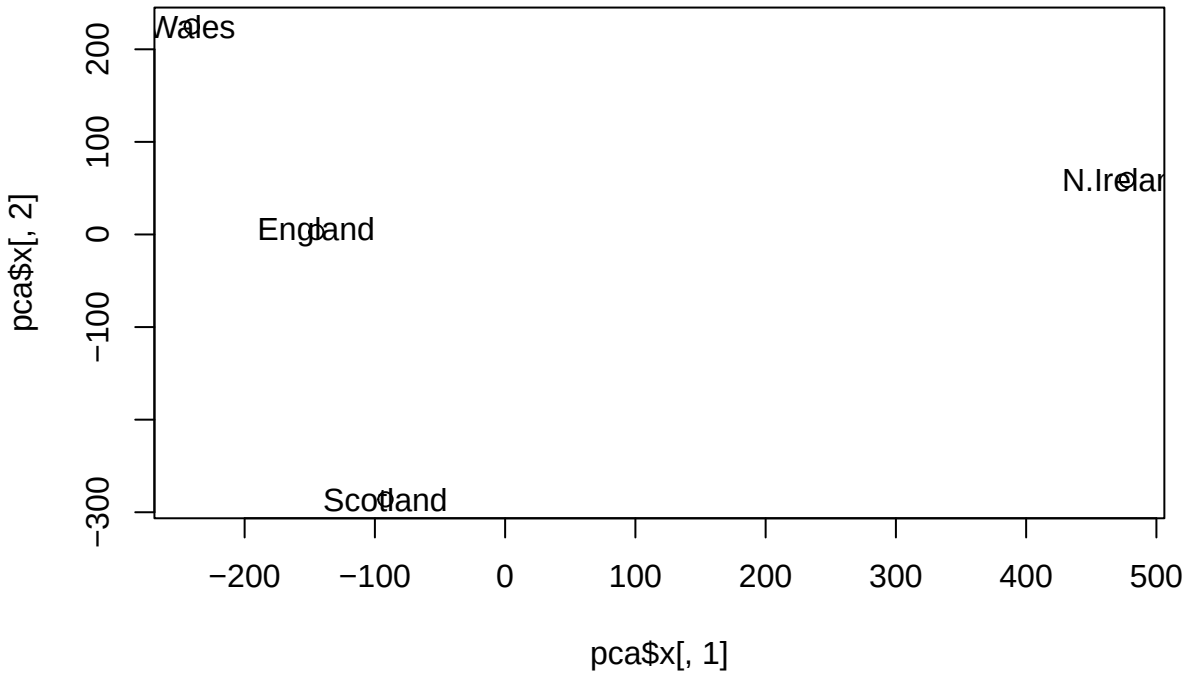
```
## Importance of components:
##                             PC1      PC2      PC3       PC4
## Standard deviation     324.1502 212.7478 73.87622 5.552e-14
## Proportion of Variance   0.6744   0.2905  0.03503 0.000e+00
## Cumulative Proportion    0.6744   0.9650  1.00000 1.000e+00
```

```
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`

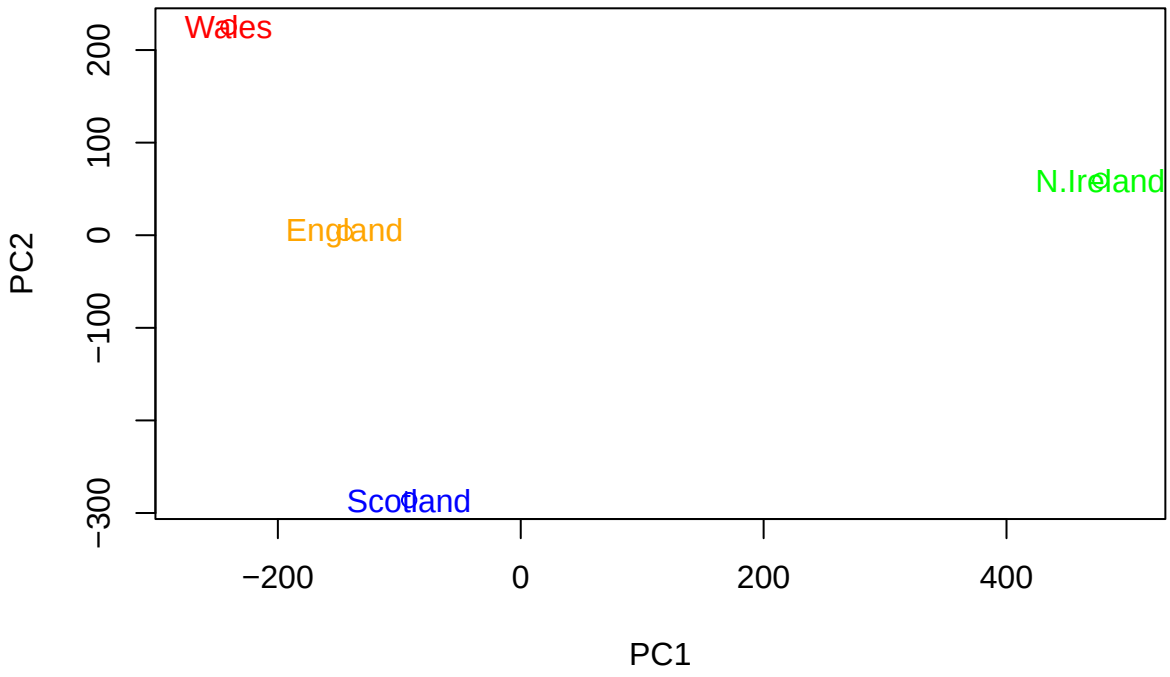
```
plot(pca$x[,1], pca$x[,2])
text(pca$x[,1], pca$x[,2], colnames(x))
```



We really only needed PC1 to see the variance in this dataset.

color up the plot

```
country_cols <- c("orange", "red", "blue", "green")
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500),col=country_cols)
text(pca$x[,1], pca$x[,2], colnames(x), col=country_cols)
```



We can find how much variation from the original plot each PC accounts for through this formula...

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

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

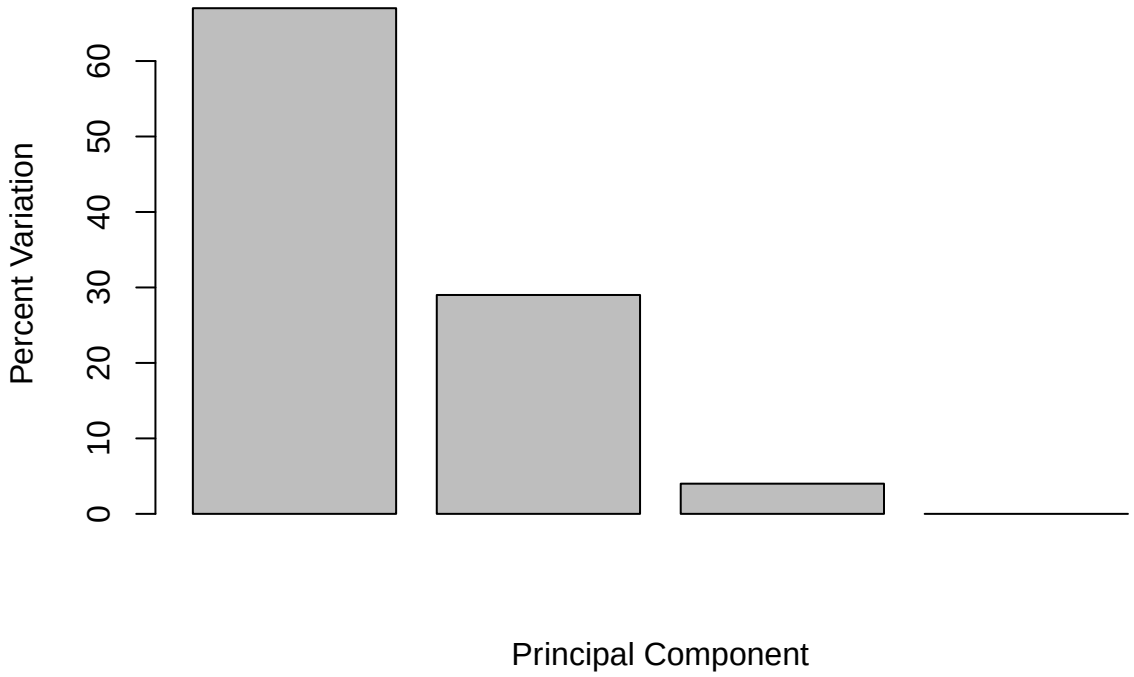
...or by using this function:

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

```
##                             PC1       PC2      PC3           PC4
## Standard deviation     324.15019 212.74780 73.87622 5.551558e-14
## Proportion of Variance   0.67444   0.29052  0.03503 0.000000e+00
## Cumulative Proportion    0.67444   0.96497  1.00000 1.000000e+00
```

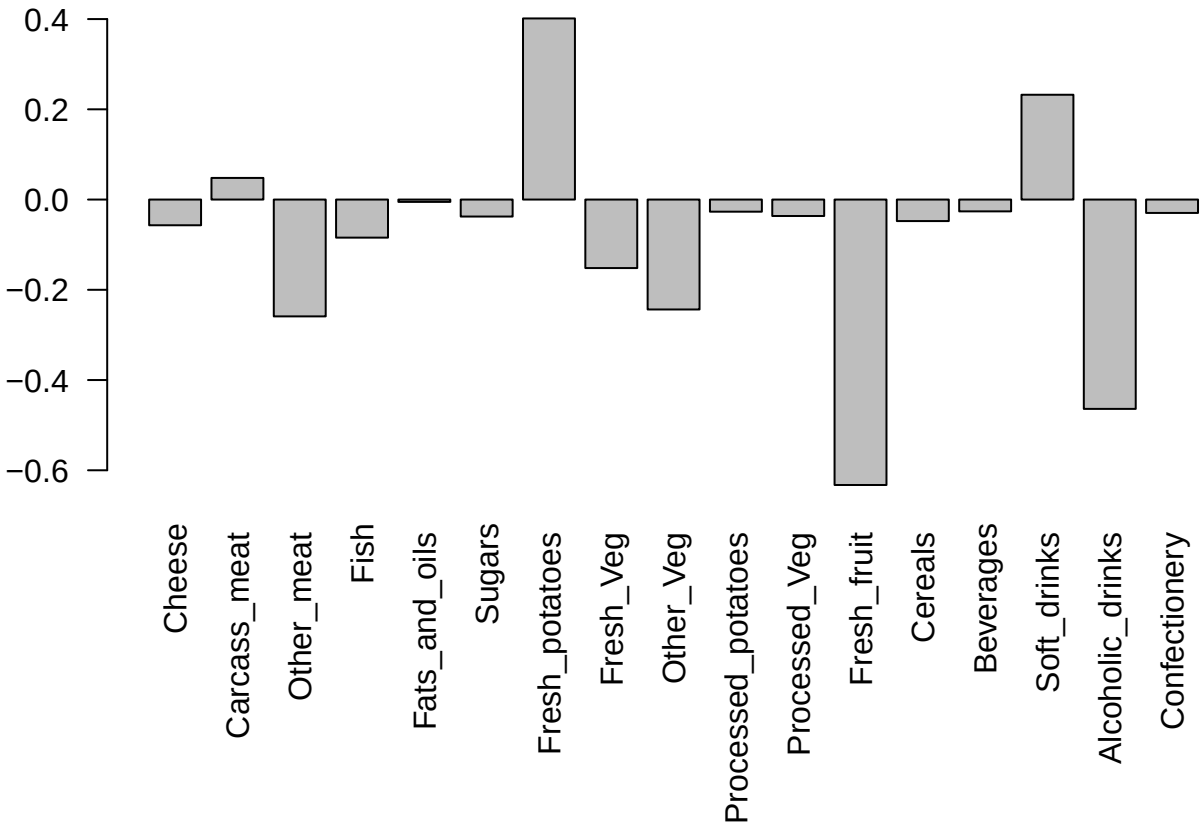
We can visualize this in a barplot

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



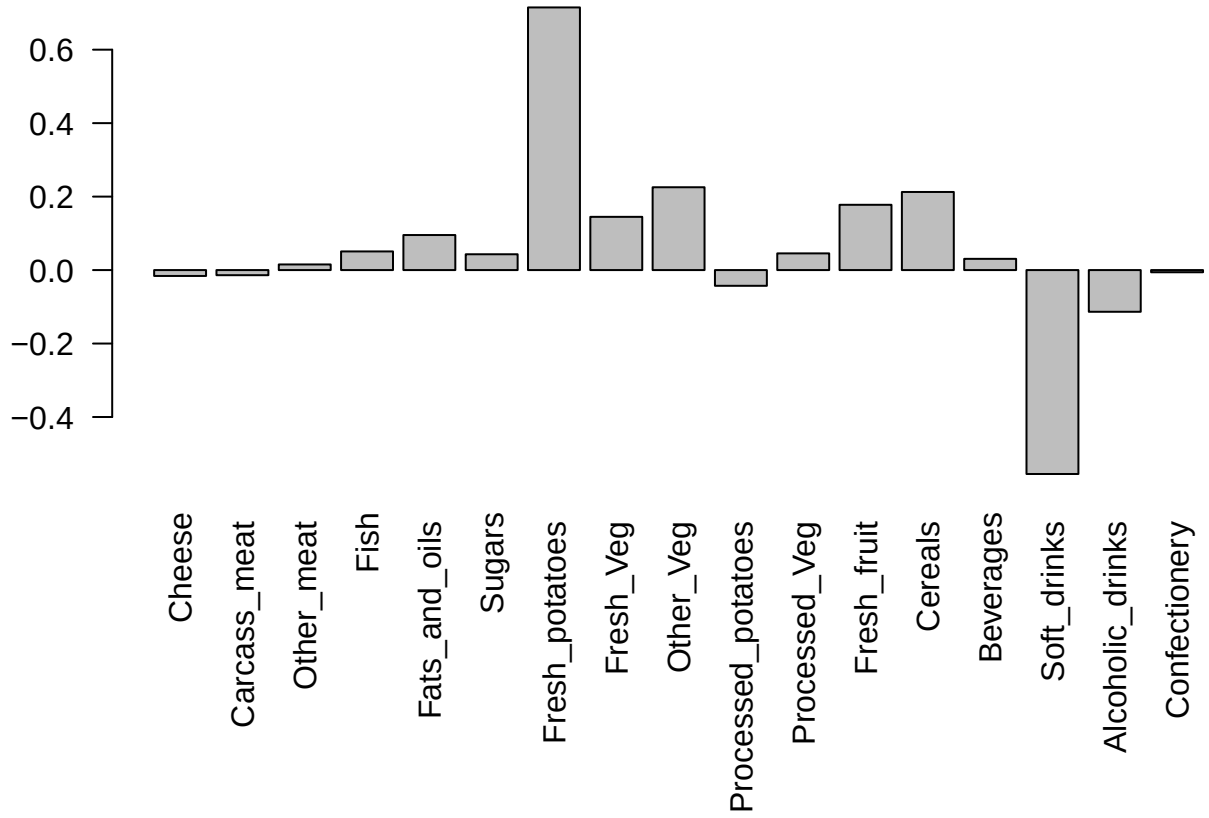
PC1 accounts for most of the variance, so we'll focus on that:

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



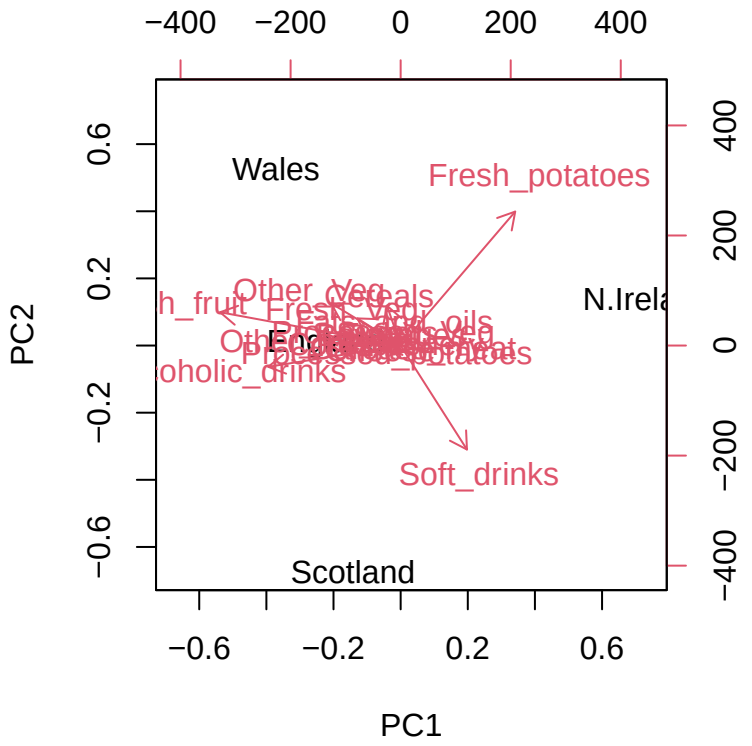
We can also examine PC2, which reflects the second largest source of variance in the data:

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



We can also visualize the PCA results with the `biplot()` function:

```
biplot(pca)
```



This plot hints at the association between the variables positioned farther away from the clustered data, and the country positioned farthest away from the clustered data.

PCA of RNA-Seq data

Read input 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
```

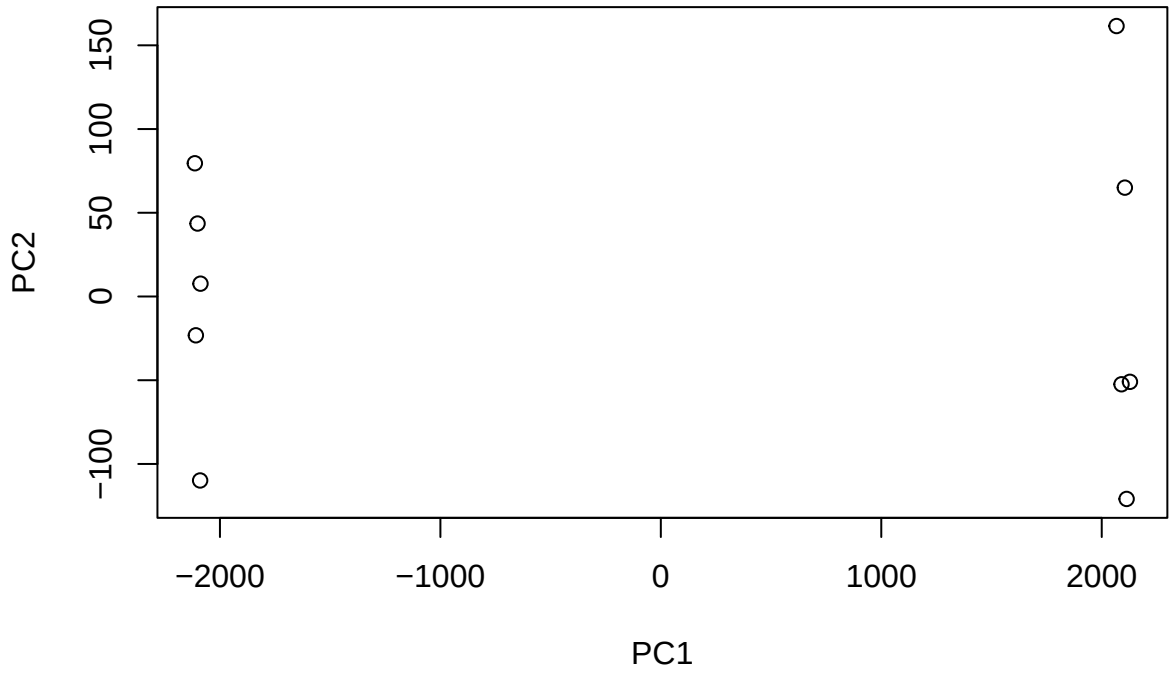
```
pca <- prcomp(t(rna.data))
summary(pca)
```

```
## Importance of components:
##                             PC1     PC2      PC3      PC4      PC5      PC6
## Standard deviation     2214.2633 88.9209 84.33908 77.74094 69.66341 67.78516
```

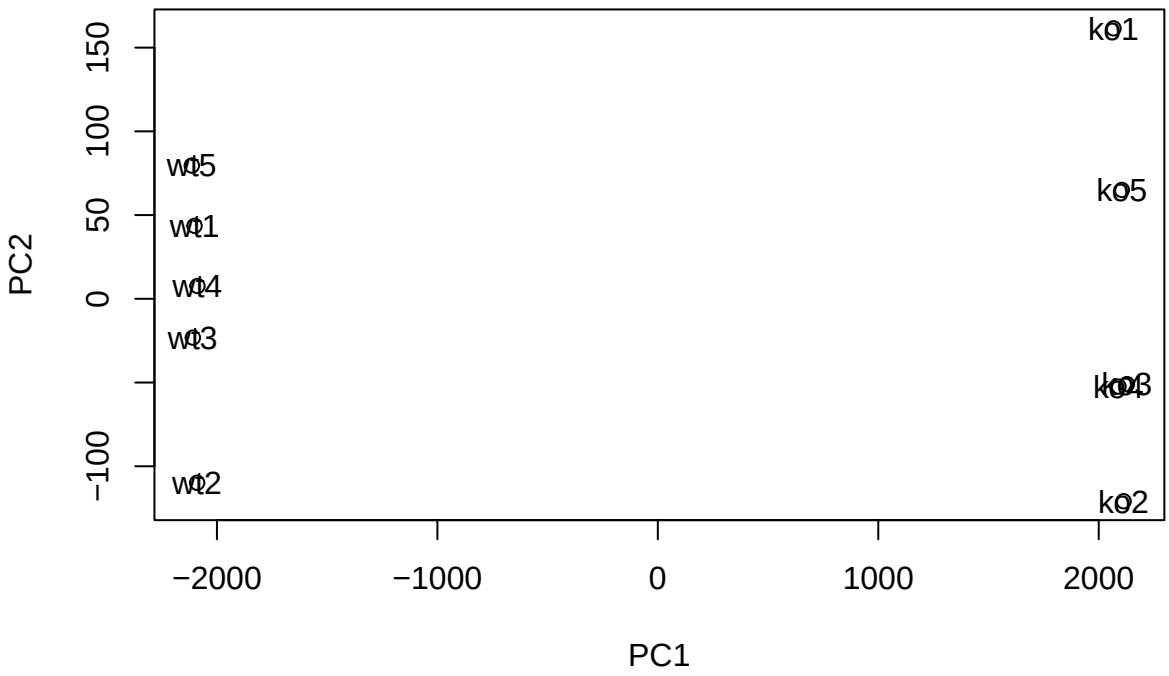
```
## Proportion of Variance    0.9917  0.0016  0.00144  0.00122  0.00098  0.00093
## Cumulative Proportion     0.9917  0.9933  0.99471  0.99593  0.99691  0.99784
##                             PC7      PC8      PC9      PC10
## Standard deviation     65.29428 59.90981 53.20803 2.715e-13
## Proportion of Variance  0.00086  0.00073  0.00057 0.000e+00
## Cumulative Proportion   0.99870  0.99943  1.00000 1.000e+00
```

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))
```


PC2
150
100
50
0
−100
wt5
wt1
wt4
wt3
wt2
ko1
ko5
ko4
ko3
ko2
−2000
−1000
0
1000
2000
PC1