Clustering

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Libraries

Reading in Data

```
setwd("~/harvard-summer-biostats")
df <- read_csv("data/wide_illinois.csv") #read in data
```

```
## Parsed with column specification:
## cols(
##   .default = col_double(),
##   well_id = col_character(),
##   site = col_character(),
##   disposal_area = col_character(),
##   type = col_character(),
##   gradient = col_character()
## )
```

```
## See spec(...) for full column specifications.
```

```
df1 <- na.omit(df) #get rid of na's
```

Hierarchical Methods

If we want to look for cereal groups via hierarchical clustering, we need to construct a distance matrix. Distances are constructed with the *dist* function, and we need to choose whether we compute them on scaled or unscaled variables (standardize or not).

```
df.dist <- dist(df1[, -c(1:5)])
```

Now we look at how hierarchical clustering is applied. The relevant function is *hclust*.

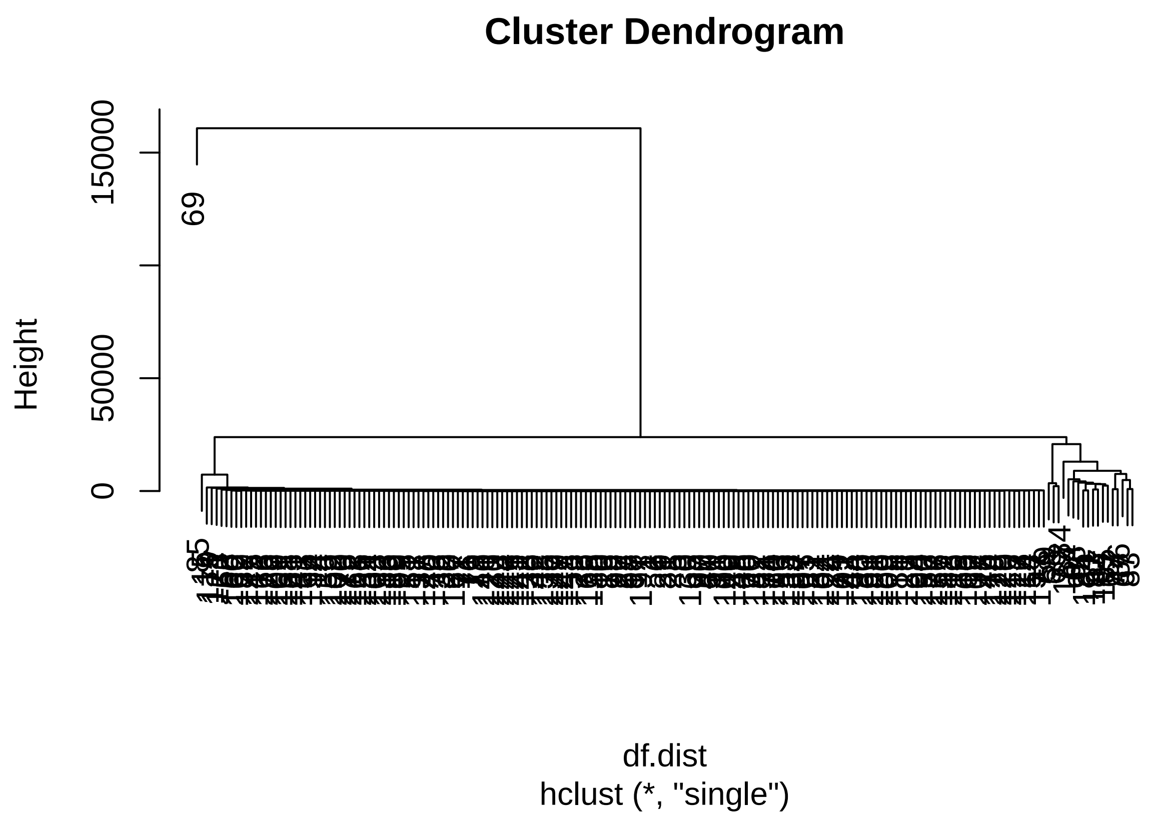
```
hcsingle <- hclust(df.dist, method = "single")
list(hcsingle) # reminds you of properties of the solution, if desired
```

```
## [[1]]
##
## Call:
```

```
## hclust(d = df.dist, method = "single")
##
## Cluster method   : single
## Distance         : euclidean
## Number of objects: 191
```

This creates the solution, and we can look at the dendrogram as:

```
plot(hcsingle)
```



The options for hclust in terms of linkages are provided in the help under options for method. The following options are listed: “ward.D”, “ward.D2”, “single”, “complete”, “average”, “mcquitty”, “median” or “centroid”.

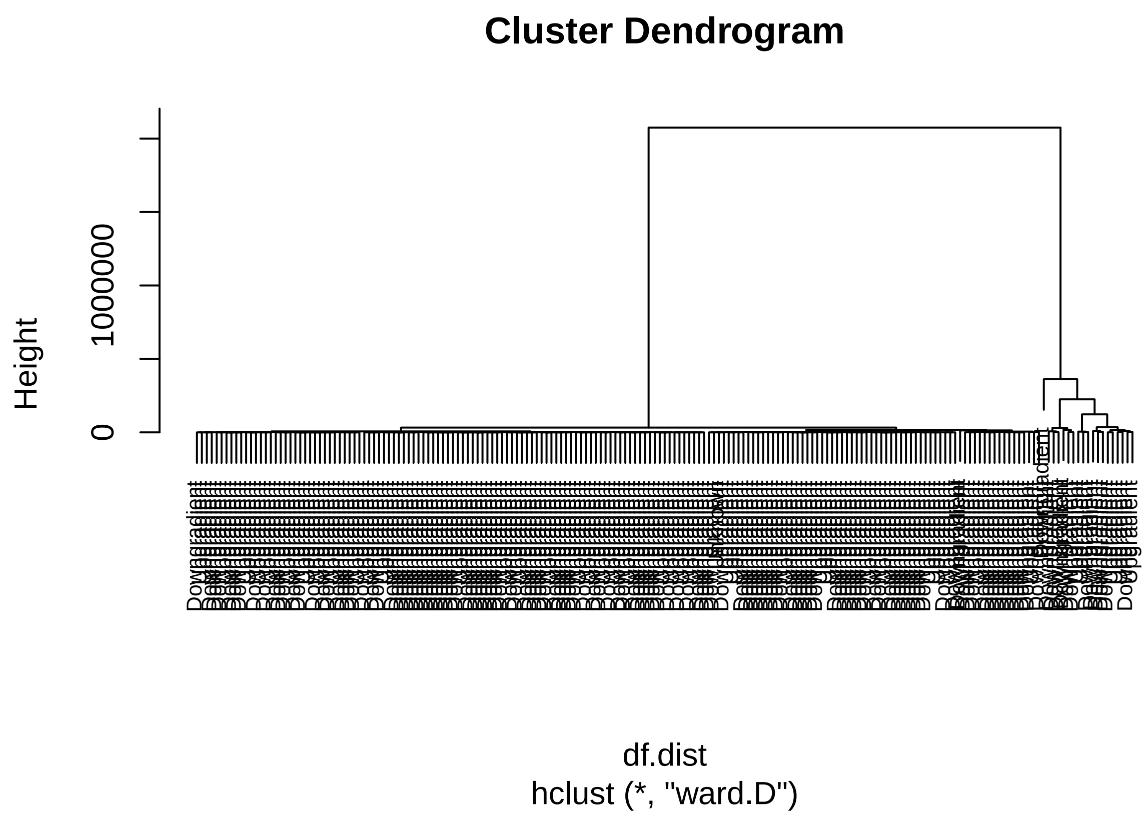
In order to obtain cluster labels, we need to *cut* our dendrograms.

```
singleSol <- (cutree(hcsingle, k = 3)) #cluster labels are numeric, k= # clusters
summary(as.factor(singleSol)) #as factor to get table
```

```
##   1   2   3
## 172  18   1
```

To learn more details about the clusters we found:

```
hcward <- hclust(df.dist, method = "ward.D")
plot(hcward, labels = df1$gradient, cex = 0.7) #cex adjusts size of label
```



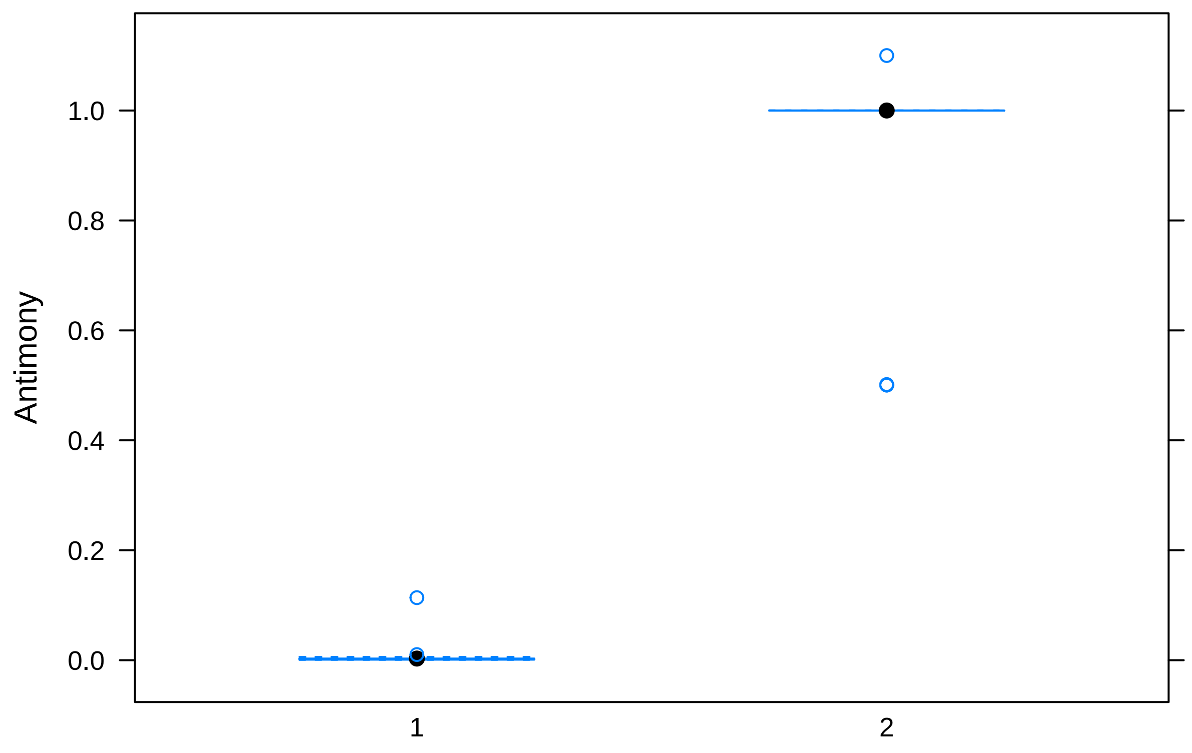
```
wardSol <- (cutree(hcward, k = 2)) #cluster labels are numeric, k= # clusters
summary(as.factor(wardSol)) #as factor to get table
```

```
##   1   2
## 172  19
```

```
favstats(Antimony ~ wardSol, data = df1) #can choose any variable
```

```
##   wardSol       min    Q1 median    Q3       max        mean         sd   n
## 1       1 0.0007625 0.001  0.003 0.003 0.1137778 0.002903086 0.00858458 172
## 2       2 0.5005000 1.000  1.000 1.000 1.1000000 0.926447368 0.19071691  19
##   missing
## 1       0
## 2       0
```

```
bwplot(Antimony ~ as.factor(wardSol), data = df1)
```



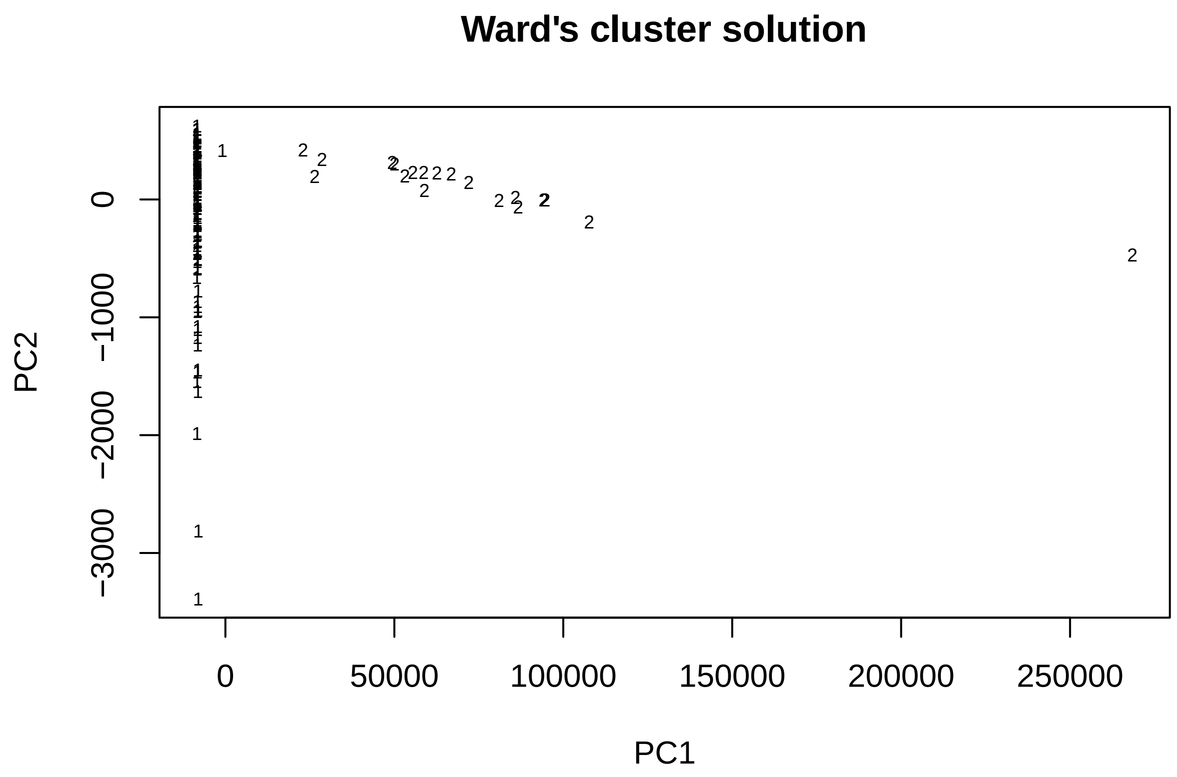
Our cluster sizes are extremely uneven… Our first clsuter has 172 wells and the second has 19.

```
favstats(#chemical here ~ wardSol, data = df1)
bwplot(#chemical here ~ as.factor(wardSol), data = df1)
```

We can view the solution in the PC space (say 2-D) to see how well-separated the clusters are in that space. Because we used an unstandardized distance, we will run the PCA on the covariance matrix.

```
dfPCA <- princomp(df1[, -c(1:5)], cor = FALSE)

plot(dfPCA$scores[, 1:2], type = "n", xlab = "PC1", ylab = "PC2", main = "Ward's cluster solution") #bl
text(dfPCA$scores[, 1:2], labels = wardSol, cex = 0.6) #add the text
```



We may want to go into investigation to see what sort of traits/attributes are shared by the wells in each cluster and seeing if we can find meaning in them.

K-means Methods

For k-means, we don't need to compute the distance matrix ourselves. We feed the function the data set to operate on:

```r
Ksol1 <- kmeans(scale(df1[, -c(1:5)]), centers = 2) #centers is the # of clusters desired
list(Ksol1) #so you can see what it gives you
```

```
## [[1]]
## K-means clustering with 2 clusters of sizes 175, 16
##
## Cluster means:
##     Antimony    Arsenic     Barium  Beryllium      Boron    Cadmium    Calcium
## 1 -0.2940444 -0.2282068 -0.2466646 -0.2848593 -0.2843138 -0.2846909 -0.2584705
## 2  3.2161104  2.4960121  2.6978935  3.1156481  3.1096817  3.1138065  2.8270214
##      Chloride   Chromium     Cobalt    Fluoride       Lead   Lithium    Mercury
## 1  0.03609133 -0.1358476 -0.153635  0.01245822 -0.1283667 -0.257573 -0.2939304
## 2 -0.39474887  1.4858331  1.680383 -0.13626181  1.4040106  2.817204  3.2148635
##   Molybdenum          pH Radium 226+228   Selenium     Sulfate  Thallium
## 1 -0.2312114 -0.05314213    -0.03041831 -0.2863342  0.04864265 -0.292776
## 2  2.5288750  0.58124207     0.33270030  3.1317800 -0.53202903  3.202237
##   Total Dissolved Solids
## 1              0.04257438
## 2             -0.46565729
##
## 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 1 1 1 1 1 1 1 1 1
##  [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 1 2 1 1 2 2 2 1 1 1 1 1
##  [75] 1 1 2 1 1 1 1 1 2 2 1 2 2 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## [112] 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 1 1 1 1 1 1 1 1
## [149] 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 1 1 1 1 1 2 2 2
## [186] 1 2 1 1 1 1
##
## Within cluster sum of squares by cluster:
## [1] 1210.3005  792.9099
##  (between_SS / total_SS =  49.8 %)
##
## Available components:
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

The list option provides us with lots of information. We can pull out the cluster means as:

```
Ksol1$centers
```

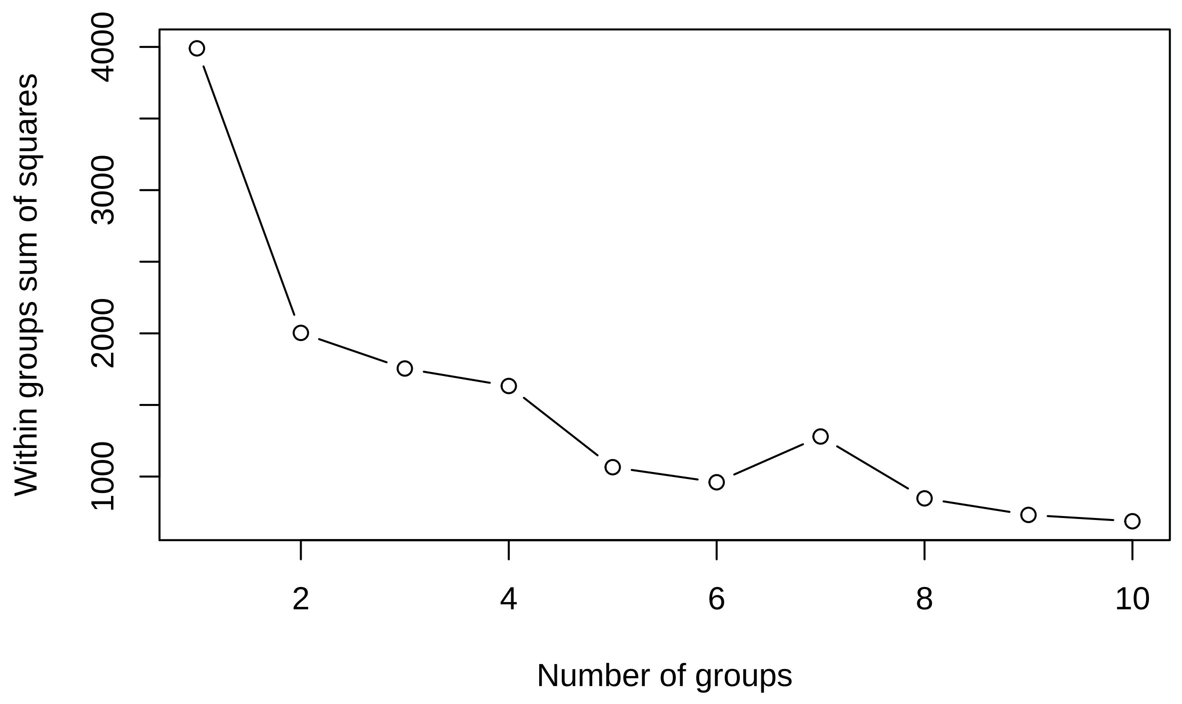
```
##     Antimony    Arsenic     Barium  Beryllium      Boron    Cadmium    Calcium
## 1 -0.2940444 -0.2282068 -0.2466646 -0.2848593 -0.2843138 -0.2846909 -0.2584705
## 2  3.2161104  2.4960121  2.6978935  3.1156481  3.1096817  3.1138065  2.8270214
##      Chloride   Chromium    Cobalt    Fluoride       Lead    Lithium    Mercury
## 1  0.03609133 -0.1358476 -0.153635  0.01245822 -0.1283667 -0.257573 -0.2939304
## 2 -0.39474887  1.4858331  1.680383 -0.13626181  1.4040106  2.817204  3.2148635
##   Molybdenum          pH Radium 226+228   Selenium     Sulfate  Thallium
## 1 -0.2312114 -0.05314213    -0.03041831 -0.2863342  0.04864265 -0.292776
## 2  2.5288750  0.58124207     0.33270030  3.1317800 -0.53202903  3.202237
##   Total Dissolved Solids
## 1             0.04257438
## 2            -0.46565729
```

In order to determine if we have chosen a "good" value of the number of clusters, we can look at the within cluster sum of squares for this solution and a few other options for k, the number of clusters. This runs the solution from 1 to 10 clusters and pulls the within group sum of squares from each.

```
n <- nrow(df1) #number of observations

wss <- rep(0, 10) #creates 10 copies of 0 to create an empty vector
for(i in 1:10){
  wss[i] <- sum(kmeans(scale(df1[, -c(1:5)]), centers = i)$withinss)
}

plot(1:10, wss, type = "b", xlab = "Number of groups", ylab = "Within groups sum of squares")
```



We look for elbows in the plot - here there are elbows at 2 and 6 (ish?), maybe these values will be good to use?

With two clusters, we should see if there is any relationship with sites…

```
tally(Ksol1$cluster ~ type, data = df1, format = "count")
```

```
##               type
## Ksol1$cluster   L   M  SI
##             1  32   5 138
##             2  16   0   0
```

There does seem to be something of interest here… The first cluster has a varied mix between all types with the majority in SI, while wells in cluster 2 seem to only consist of L.

We can compare clustering solutions with similar tables. How do the K-means and Ward's solutions overlap?

```
tally(Ksol1$cluster ~ wardSol, data = df1, format = "count")
```

```
##               wardSol
## Ksol1$cluster   1   2
##             1 172   3
##             2   0  16
```

They seem to match up fairly well!