Statistics 452: Statistical Learning and Prediction

Chapter 10, part 2: Cluster Analysis

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Clustering

- Clustering is a set of techniques for finding *subgroups*, or clusters, in a data set.
- A good set of clusters is a partition of the data such that observations are *similar* within clusters and *dissimilar* between clusters.
- Example: Suppose we have n observations of p features for cancer patients.
  - We can cluster to look for cancer sub-types.
  - However, these clusters will be highly dependent on how we measure similarity/dissimilarity.
  - Plus, we don't *know* that clusters correspond to cancer sub-types.

Clustering as Dimension Reduction

- We can view clustering as an exploratory method to understand possible structure in our data.
- Similar in spirit to PCA, but a different mechanism
  - PCA finds a low-dimensional representation of observations explaining a good proportion of the variance
  - Clustering looks to find homogeneous sub-groups.

Clustering Methods

- There are many.
- We focus on K-means/medoids and hierarchical clustering, and assume all features are quantitative.
- In K-means we partition into a pre-specified number of clusters.
- In hierarchical clustering we successively group observations.
  - Represent the nested partitions as a tree-like structure called a *dendrogram*.

K-means Clustering

- Choose the desired number of clusters, K. The K-means clustering algorithm will assign each observation to *exactly one* of the K clusters.
- Let C_k be the set of indices for observations assigned to cluster k, $k = 1, \ldots, K$.
- K-means clustering chooses clusters to solve

$$\min_{C_1,\ldots,C_K} \sum_{k=1}^{K} W(C_k),$$

where $W(C_k)$ is a measure of the amount by which observations within cluster C_k differ from one another.

K-means Clustering: Choice of $W(C_k)$

- For quantitative variables, the standard choice for $W(C_k)$ is the squared Euclidean distance,

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

where $|C_k|$ denotes the number of observations in cluster k.
- It turns out that

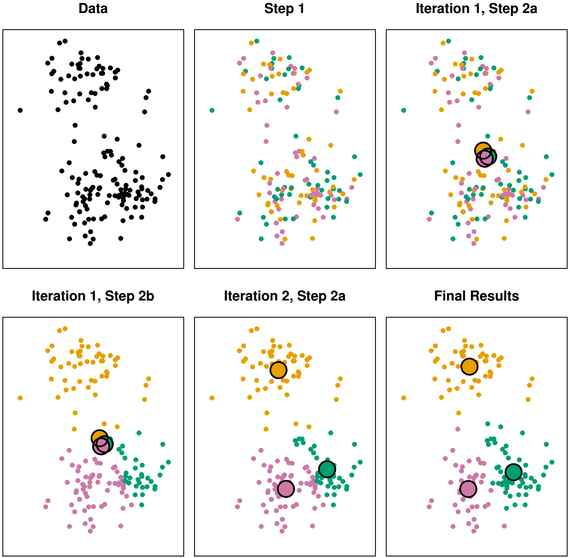
$$\frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{x}_{kj})^2$$

where the *cluster centroid* $\bar{x}_{kj} = \frac{1}{|C_k|} \sum_{i \in C_k} x_{ij}$.
- We can see where the name "K-means" comes from.

K-means Clustering Algorithm

1. Randomly assign a number, from $1, \ldots, K$ to each of the observations. They serve as the initial cluster assignments for the observations.
2. Iterate the following steps until the cluster assignments stop changing:
   (a) For each of the K clusters, compute the cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster for continuous variables.
   (b) Assign each observation to the cluster whose centroid is closest in terms of Euclidean distance.

K-means Clustering Algorithm, Simulated Data Example



- Text, Figure 10.6. Progress of the K-means algorithm with $K = 3$.

- See the video demo at http://www.youtube.com/watch?v=zaKjh2N8jN4.

K-means Clustering and Local Minima

- The algorithm is guaranteed to decrease the value of $\sum_k W(C_k)$ until no further improvement is possible, resulting in a *local* minimum.
- However, the local min depends on the random initialization. Hence, in practice we re-run the algorithm several times and keep the solution that achieves the lowest overall criterion value.

K-means Clustering with Different Initialization

Text, Fig 10.7. K-means clustering performed six times on the same data with $K = 3$ different random initializations. Above each plot is the value of the objective function. Three different local optimums were found. The overall minimum, found four times, is 235.8. Note: Cluster labels different in 3 of 4.

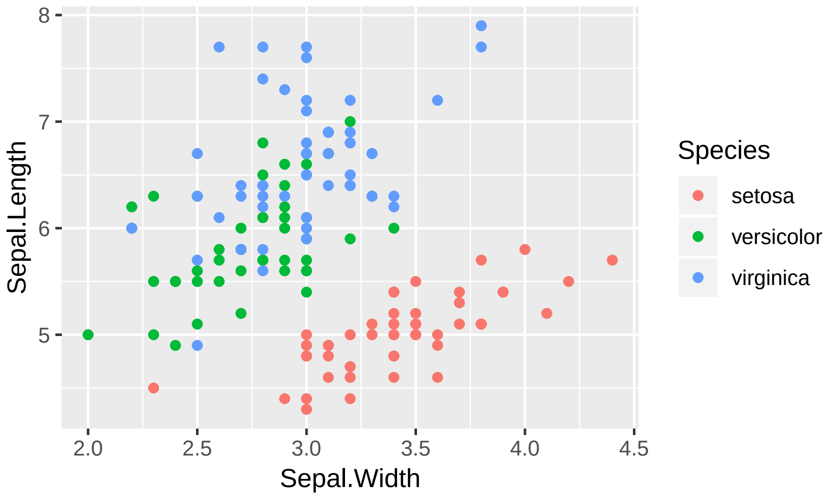
K Means Clustering of the Iris Data

- We know there are three species of iris. Ignore the species labels and do the clustering.

```
library(ggplot2)
data(iris) # help(iris)
head(iris) # plot sepal length vs width with labels
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         0.2  setosa
## 5          5.0         3.6          1.4         0.2  setosa
## 6          5.4         3.9          1.7         0.4  setosa
```

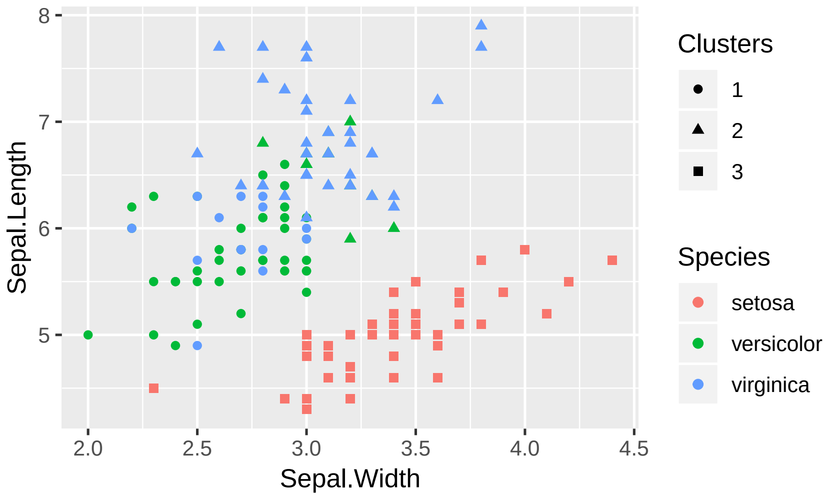
```r
ggplot(iris,aes(x=Sepal.Width,y=Sepal.Length,color=Species)) +
  geom_point()
```



```r
library(dplyr)
set.seed(1)
irisX <- iris %>% select(-Species) %>% scale()
kout3 <- kmeans(irisX,centers=3,nstart=10)
iris <- data.frame(iris,Clusters=factor(kout3$cluster))
with(iris,table(Species,Clusters))
```

```
##             Clusters
## Species       1  2  3
##   setosa      0  0 50
##   versicolor 39 11  0
##   virginica  14 36  0
```

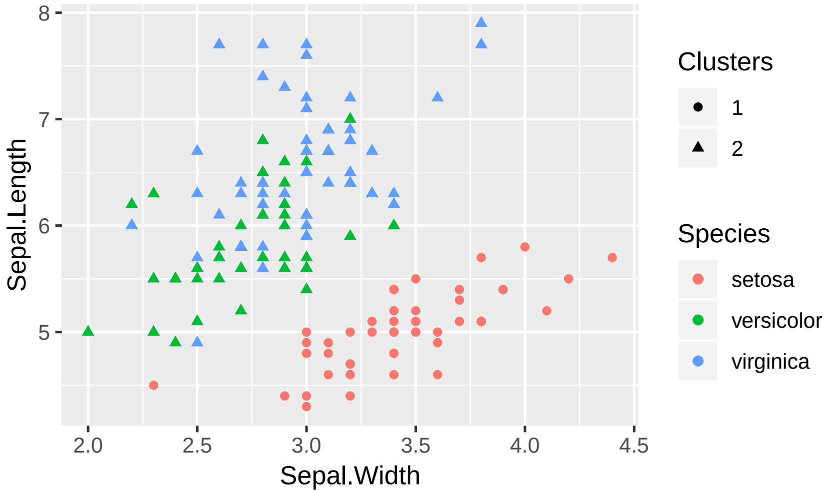
```r
ggplot(iris,
       aes(x=Sepal.Width,y=Sepal.Length,color=Species,shape=Clusters)) +
  geom_point()
```



```r
kout2 <- kmeans(irisX,centers=2,nstart=10)
iris$Clusters <- factor(kout2$cluster)
with(iris,table(Species,Clusters))
```

```
##             Clusters
## Species       1  2
##   setosa     50  0
##   versicolor  0 50
##   virginica   0 50
```

```r
ggplot(iris,
       aes(x=Sepal.Width,y=Sepal.Length,color=Species,shape=Clusters)) +
  geom_point()
```



Scaling Variables

- Whether or not to scale variables depends on the context, but usually we will.

Choosing K

- Like PCA, there is no "best" method for choosing K.
- Cross-validation is not an option because there is no outcome.
- For small p, can visualize the clusters, but this becomes difficult as p grows.
- The silhouette plot is a graphical approach.
  - Discussed after the PAM algorithm below.

Sensitivity to Outliers

- Means and Euclidean distances are sensitive to outliers and K-means depends on both
  - Means are cluster centroids.
  - Criterion to minimize is a sum of squared Euclidean distances.

K-Medoids Clustering

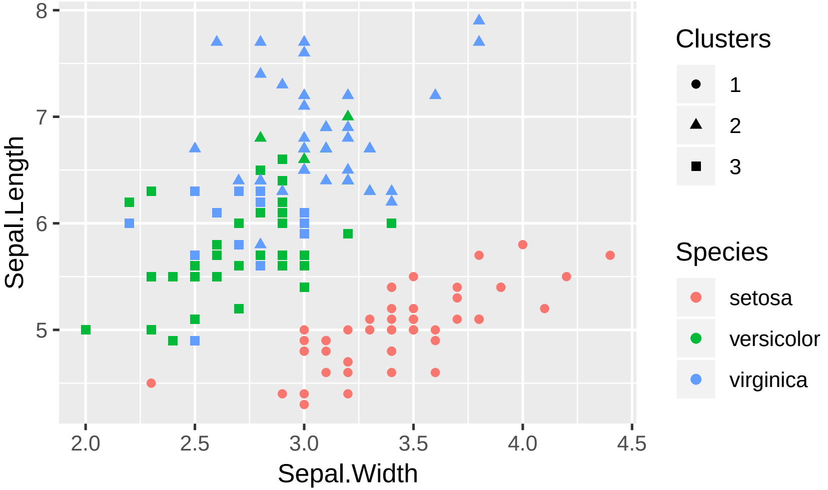
- An alternative to K-means is K-medoids clustering.
- Cluster centres are medoids, which are observations chosen to represent each cluster.
- There is flexibility in choosing the dissimilarity measure
  - Can choose a more robust measure, such as ℓ_1 (so-called Manhattan) distance.
- An implementation of K-medoids is the PAM (partitioning around medoids) algorithm.

PAM on the Iris Data

```
library(cluster)
pout3 <- pam(irisX,k=3)
iris$Clusters <- factor(pout3$cluster)
with(iris,table(Species,Clusters))
```

```
##             Clusters
## Species       1  2  3
##   setosa     50  0  0
##   versicolor  0  9 41
##   virginica   0 36 14
```

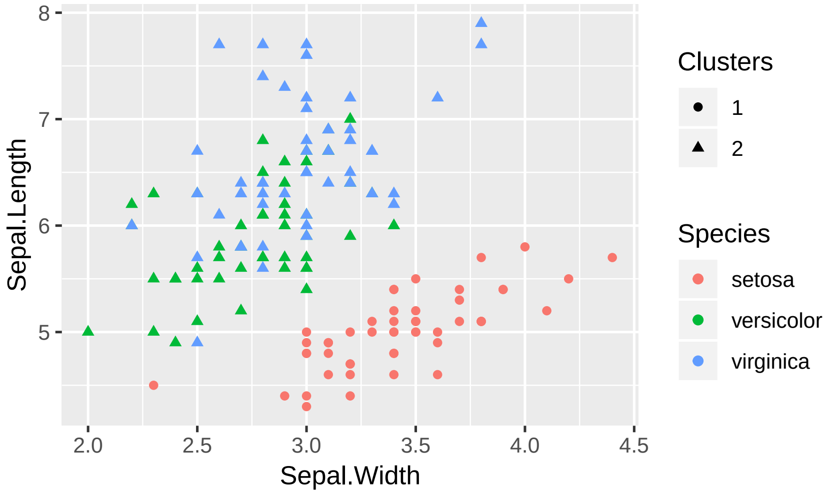
```r
ggplot(iris,
       aes(x=Sepal.Width,y=Sepal.Length,color=Species,shape=Clusters)) +
  geom_point()
```



```r
pout2 <- pam(irisX,k=2)
iris$Clusters <- factor(pout2$cluster)
with(iris,table(Species,Clusters))
```

```
##             Clusters
## Species       1  2
##   setosa     50  0
##   versicolor  0 50
##   virginica   0 50
```

```r
ggplot(iris,
       aes(x=Sepal.Width,y=Sepal.Length,color=Species,shape=Clusters)) +
  geom_point()
```



The Silhouette Plot

- For each observation we compute a measure of cluster certainty, called the silhouette width, that takes values in $[-1, 1]$.
  - Values near 1 indicate certainty that the observation is in the right cluster and
  - Values near -1 indicate that the observation is in the wrong cluster.
- Formula for silhouette width is given in on the next slide.
- If the silhouette values in a cluster are, say, below average, this suggests the cluster can be merged with another.

Silhouette Widths

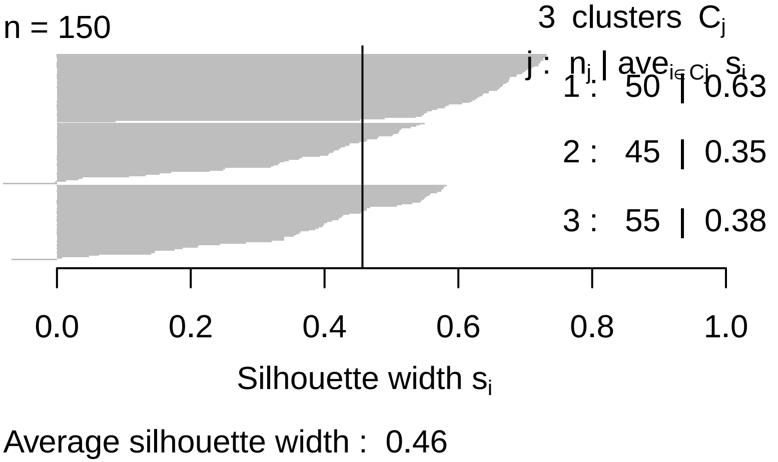
- For observation i in cluster k, the silhouette width $s(i)$ is defined as follows.
- Let $a(i)$ be the average dissimilarity between i and all other observations in **cluster** k.
- For **any other cluster** C (i not in C), let $d(i, C)$ be the average dissimilarity between i and all observations in cluster C.
- Let $b(i) = \min_C d(i, C)$ (minimum over all C such that i not in C).
- Then

$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

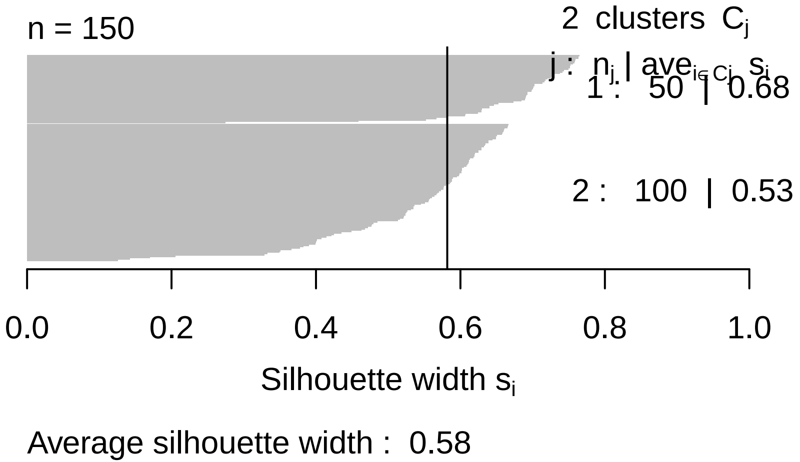
  - Note: $a(i)$ is a *dissimilarity* measure, and should be $\ll b(i)$ if i confidently in cluster k.

Silhouette Plots for the Iris Data

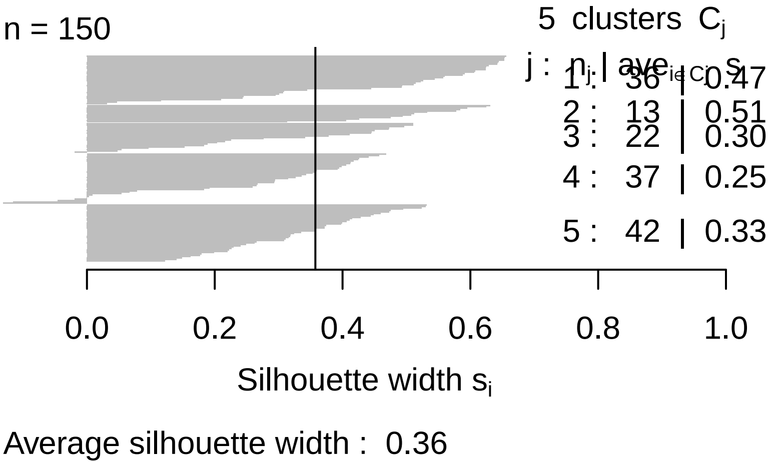
```
sil3 <- silhouette(pout3)
plot(sil3,main=""); abline(v=mean(sil3[,"sil_width"]))
```



```r
sil2 <- silhouette(pout2)
plot(sil2,main=""); abline(v=mean(sil2[,"sil_width"]))
```



```
sil5 <- silhouette(pam(irisX,k=5))
plot(sil5,main=""); abline(v=mean(sil5[,"sil_width"]))
```



- Had to go to about $K = 15$ before silhouettes suggested merging clusters (not shown).

Clustering with categorical data.

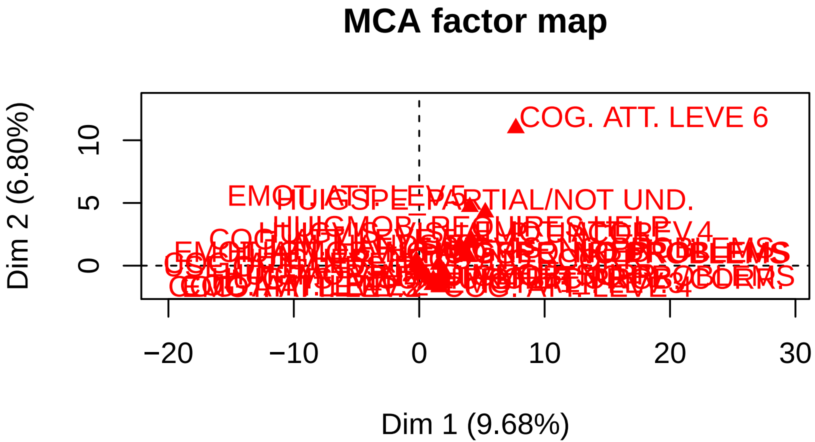
- Use the HUI data

```
hui <- read.csv("HUI.csv.gz",na.strings = "NOT STATED")
hui[hui=="NA"] <- NA
hui <- na.omit(hui)
library(dplyr)
hsub <- select(hui,HUIDCOG,HUIGDEX,HUIDEMO,HUIGHER,HUIGMOB,
               HUIGSPE,HUIGVIS)
names(hsub)
```

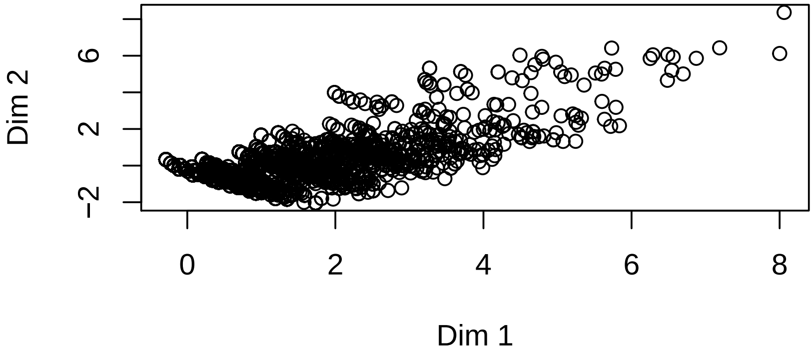
```
## [1] "HUIDCOG" "HUIGDEX" "HUIDEMO" "HUIGHER" "HUIGMOB" "HUIGSPE" "HUIGVIS"
```

Extract PCs from MCA

```r
library(FactoMineR)
res.mca <- MCA(hsub,row.w = hui$WTS_M)#huiPCs <- res.mca$ind$coord
```



```r
plot(huiPCs[,1:2])
```

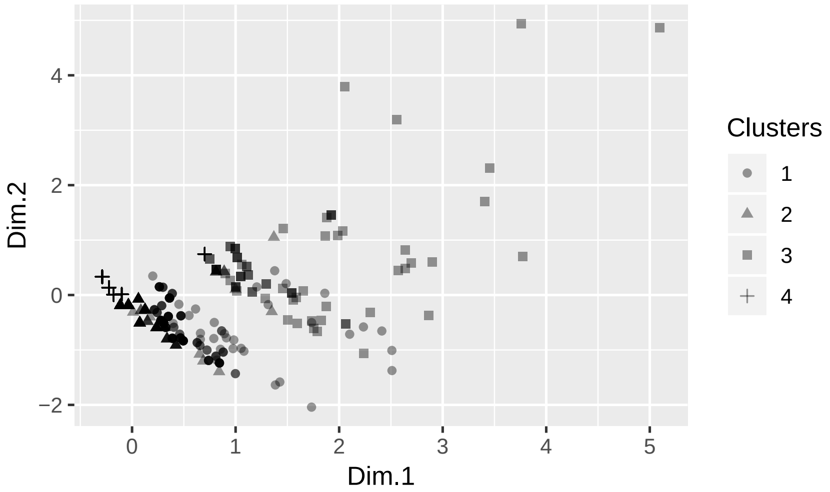


Cluster on PCs

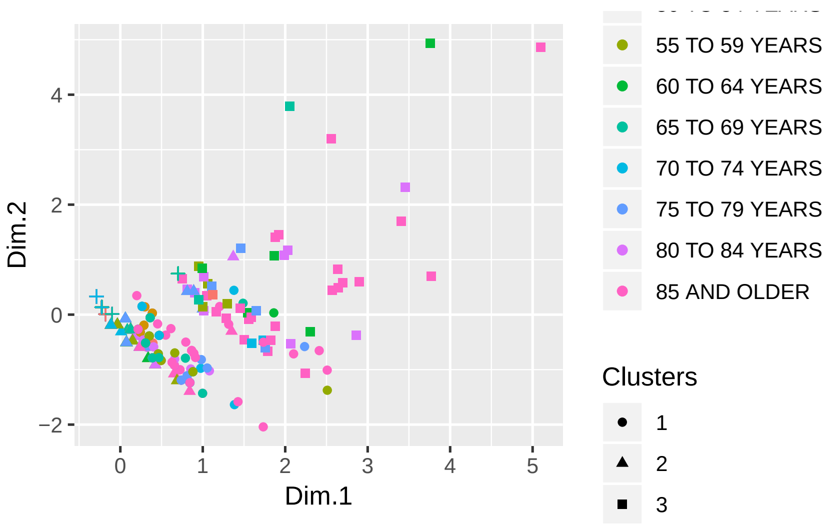
- Will work with a small subset (first 1000 people) to keep computation and overplotting down.

```
n <- 1000
hk <- kmeans(huiPCs,centers=4,nstart=10)
# plot for a small sample of the dataset
huiPCs <- data.frame(huiPCs[1:n,])
huiPCs$Clusters <- factor(hk$cluster[1:n])
huiPCs$age <- hui$DHHGAGE[1:n]
huiPCs$sex <- hui$DHH_SEX[1:n]
```

```
library(ggplot2)
ggplot(huiPCs,
       aes(x=Dim.1,y=Dim.2,shape=Clusters)) +
  geom_point(alpha=.4)
```



```r
ggplot(huiPCs,
       aes(x=Dim.1,y=Dim.2,color=age,shape=Clusters)) +
  geom_point()
```



```r
ggplot(huiPCs,
       aes(x=Dim.1,y=Dim.2,color=sex,shape=Clusters)) +
  geom_point()
```