



K-means Clustering

Roger D. Peng, Associate Professor of Biostatistics
Johns Hopkins Bloomberg School of Public Health

Can we find things that are close together?

- How do we define close?
- How do we group things?
- How do we visualize the grouping?
- How do we interpret the grouping?

How do we define close?

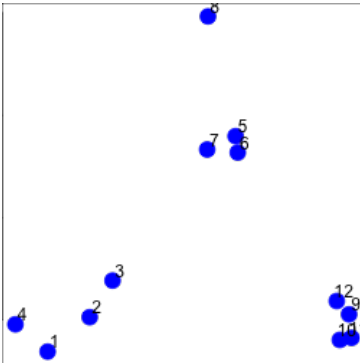
- Most important step
 - Garbage in \rightarrow garbage out
- Distance or similarity
 - Continuous - euclidean distance
 - Continuous - correlation similarity
 - Binary - manhattan distance
- Pick a distance/similarity that makes sense for your problem

K-means clustering

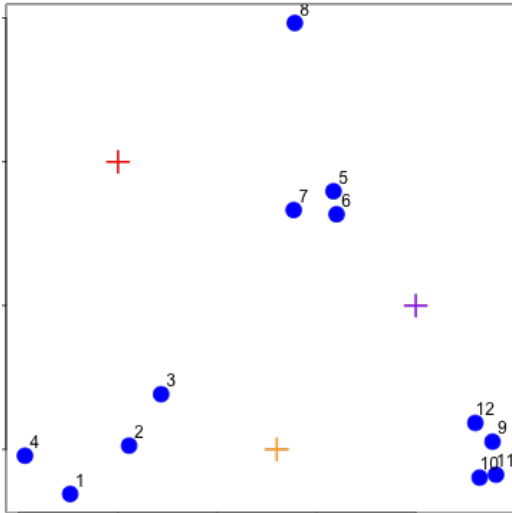
- A partitioning approach
 - Fix a number of clusters
 - Get "centroids" of each cluster
 - Assign things to closest centroid
 - Reclaculate centroids
- Requires
 - A defined distance metric
 - A number of clusters
 - An initial guess as to cluster centroids
- Produces
 - Final estimate of cluster centroids
 - An assignment of each point to clusters

K-means clustering - example

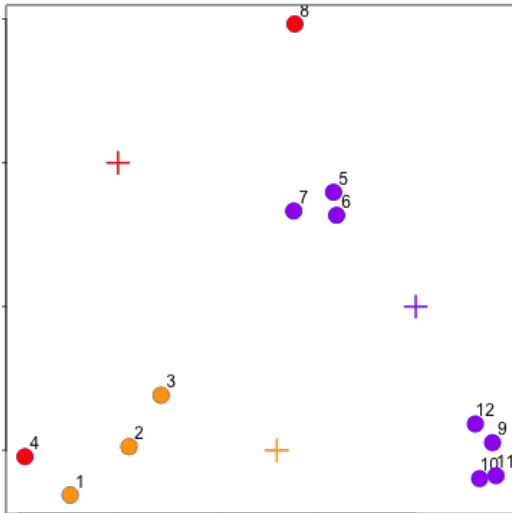
```
set.seed(1234)
par(mar = c(0, 0, 0, 0))
x <- rnorm(12, mean = rep(1:3, each = 4), sd = 0.2)
y <- rnorm(12, mean = rep(c(1, 2, 1), each = 4), sd = 0.2)
plot(x, y, col = "blue", pch = 19, cex = 2)
text(x + 0.05, y + 0.05, labels = as.character(1:12))
```



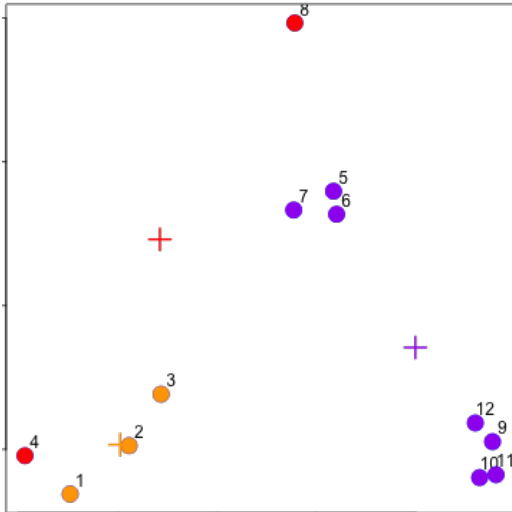
K-means clustering - starting centroids



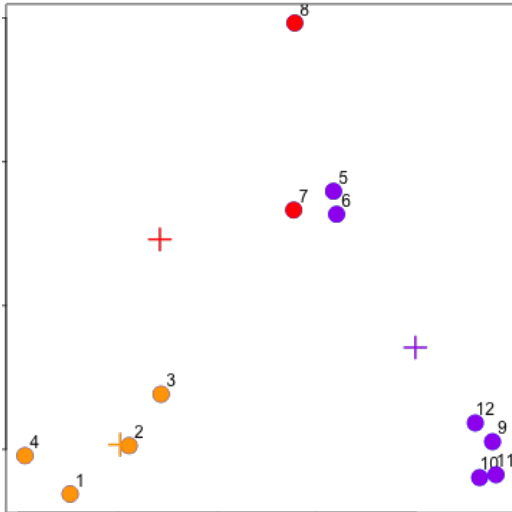
K-means clustering - assign to closest centroid



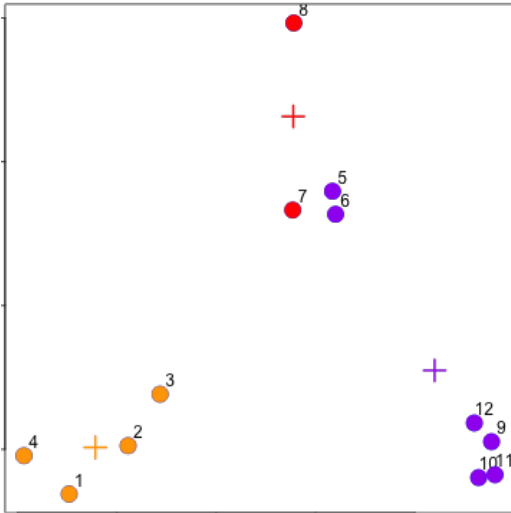
K-means clustering - recalculate centroids



K-means clustering - reassign values



K-means clustering - update centroids



kmeans ()

- Important parameters: *x*, *centers*, *iter.max*, *nstart*

```
dataFrame <- data.frame(x, y)
kmeansObj <- kmeans(dataFrame, centers = 3)
names(kmeansObj)
```

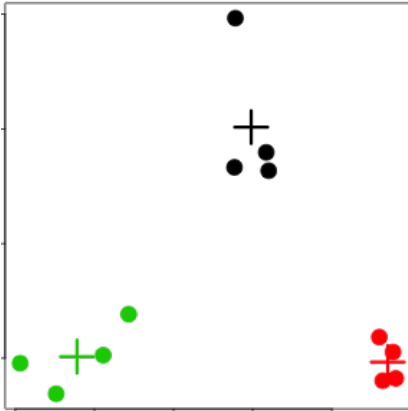
```
## [1] "cluster"      "centers"      "totss"       "withinss"
## [5] "tot.withinss" "betweenss"   "size"        "iter"
## [9] "ifault"
```

```
kmeansObj$cluster
```

```
## [1] 3 3 3 3 1 1 1 1 2 2 2 2
```

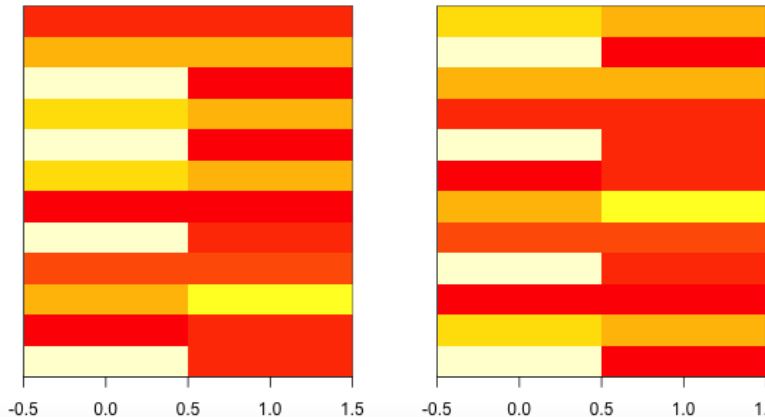
kmeans ()

```
par(mar = rep(0.2, 4))  
plot(x, y, col = kmeansObj$cluster, pch = 19, cex = 2)  
points(kmeansObj$centers, col = 1:3, pch = 3, cex = 3, lwd = 3)
```



Heatmaps

```
set.seed(1234)
dataMatrix <- as.matrix(dataFrame)[sample(1:12), ]
kmeansObj2 <- kmeans(dataMatrix, centers = 3)
par(mfrow = c(1, 2), mar = c(2, 4, 0.1, 0.1))
image(t(dataMatrix)[, nrow(dataMatrix):1], yaxt = "n")
image(t(dataMatrix)[, order(kmeansObj2$cluster)], yaxt = "n")
```



Notes and further resources

- K-means requires a number of clusters
 - Pick by eye/intuition
 - Pick by cross validation/information theory, etc.
 - [Determining the number of clusters](#)
- K-means is not deterministic
 - Different # of clusters
 - Different number of iterations
- [Rafael Irizarry's Distances and Clustering Video](#)
- [Elements of statistical learning](#)