# 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?

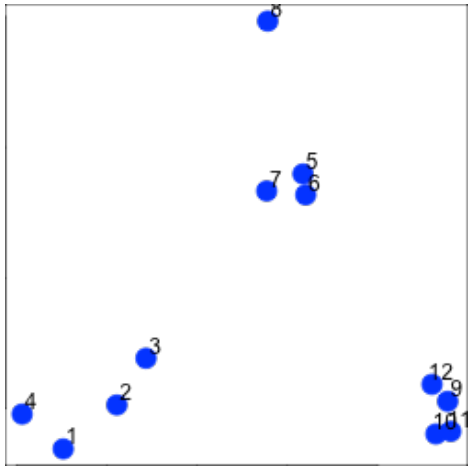
- Most important step
  - Garbage in ⟶ garbage out
- Distance or similarity
  - Continuous - euclidean distance
  - Continous - correlation similarity
  - Binary - manhattan distance
- Pick a distance/similarity that makes sense for your problem

# K-means clustering

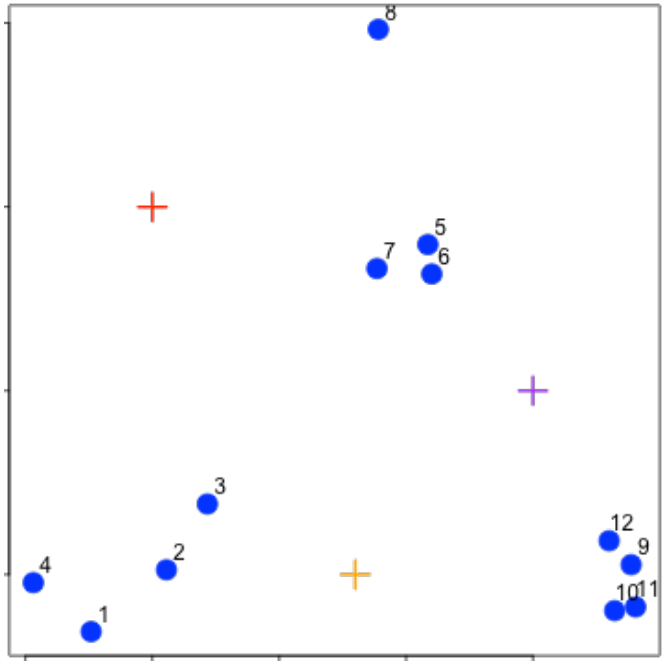
- A partioning approach
  - Fix a number of clusters
  - Get "centroids" of each cluster
  - Assign things to closest centroid
  - Reclaculate centroids
- Requires
  - A defined distance metric
  - A number of clusters
  - An initial guess as to cluster centroids
- Produces
  - Final estimate of cluster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

# K-means clustering - example

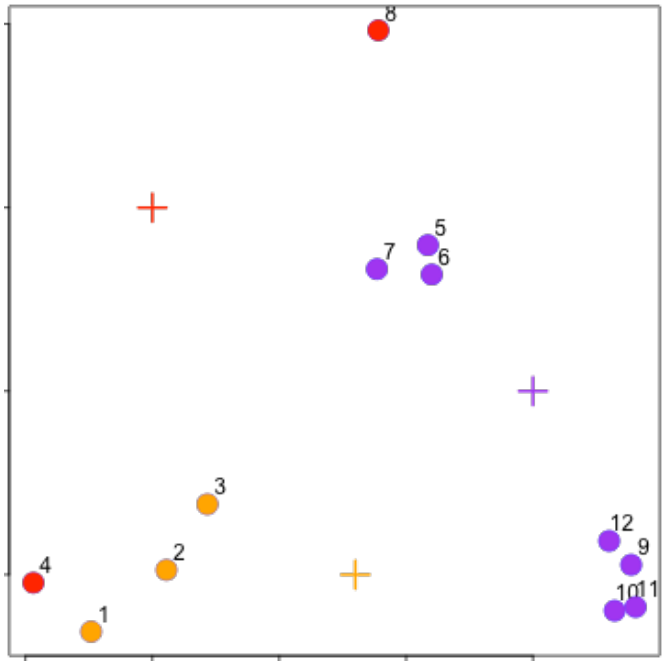
```
set.seed(1234)
par(mar = c(0, 0, 0, 0))
x <- rnorm(12, mean = rep(1:3, each = 4), sd = 0.2)
y <- rnorm(12, mean = rep(c(1, 2, 1), each = 4), sd = 0.2)
plot(x, y, col = "blue", pch = 19, cex = 2)
text(x + 0.05, y + 0.05, labels = as.character(1:12))
```



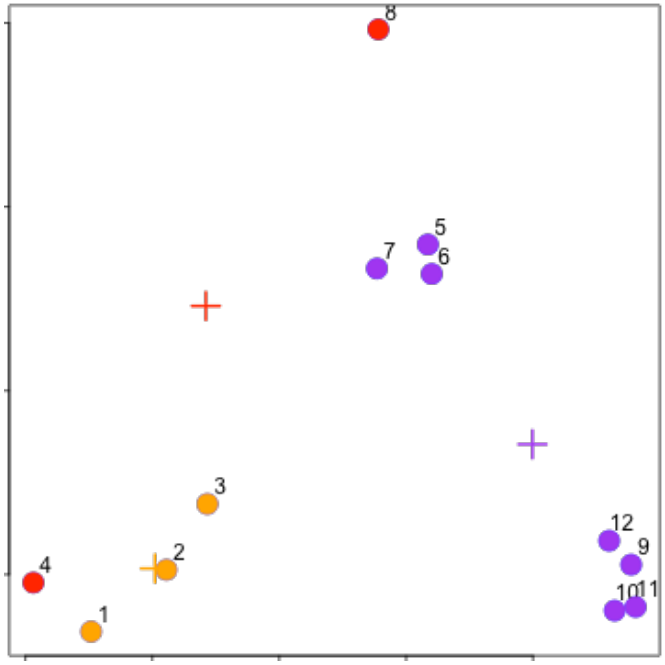
# K-means clustering - starting centroids



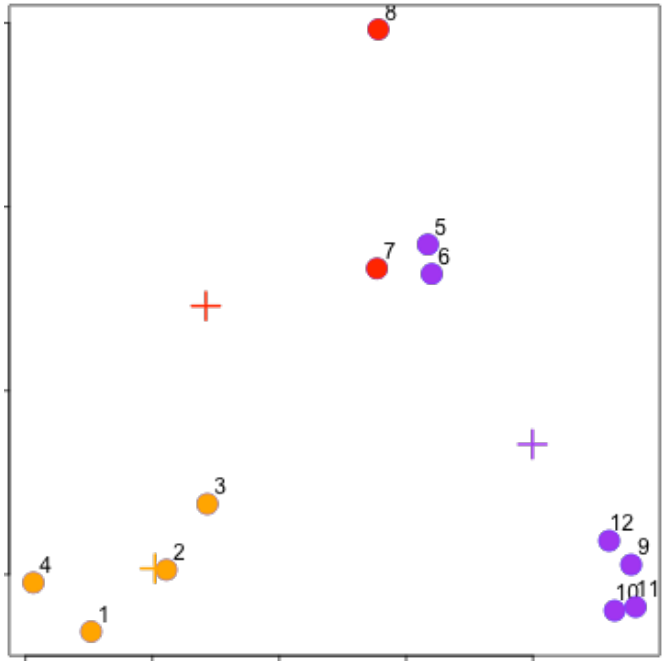
# K-means clustering - assign to closest centroid



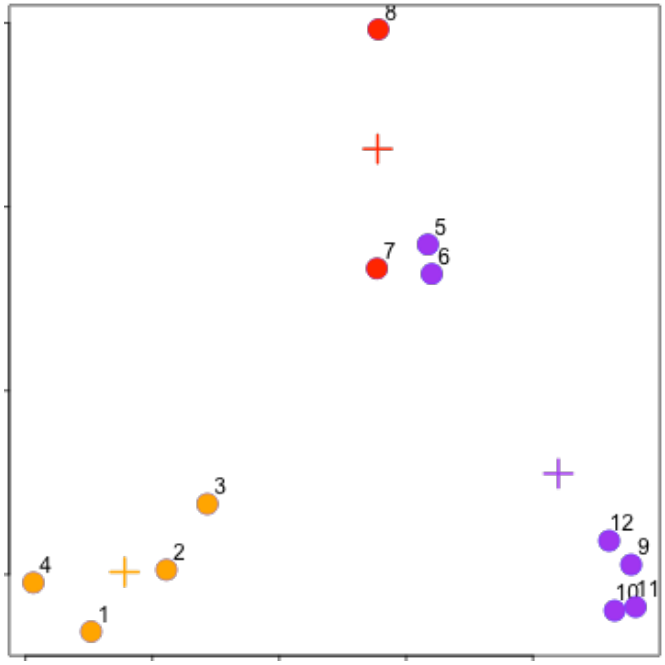
# K-means clustering - recalculate centroids



# 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)
```

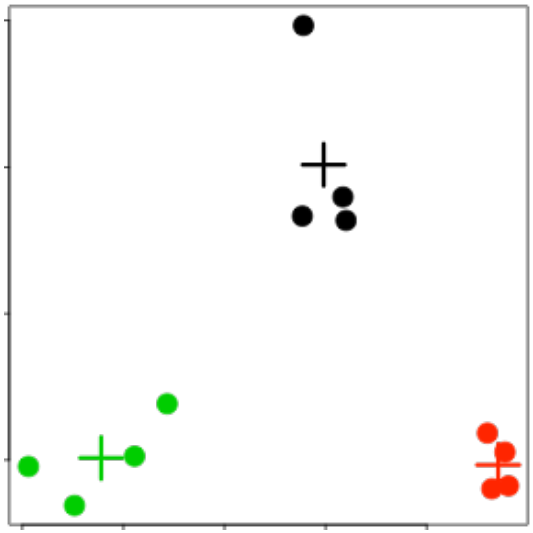
```
## [1] "cluster"      "centers"      "totss"        "withinss"
## [5] "tot.withinss" "betweenss"    "size"         "iter"
## [9] "ifault"
```

```
kmeansObj$cluster
```

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

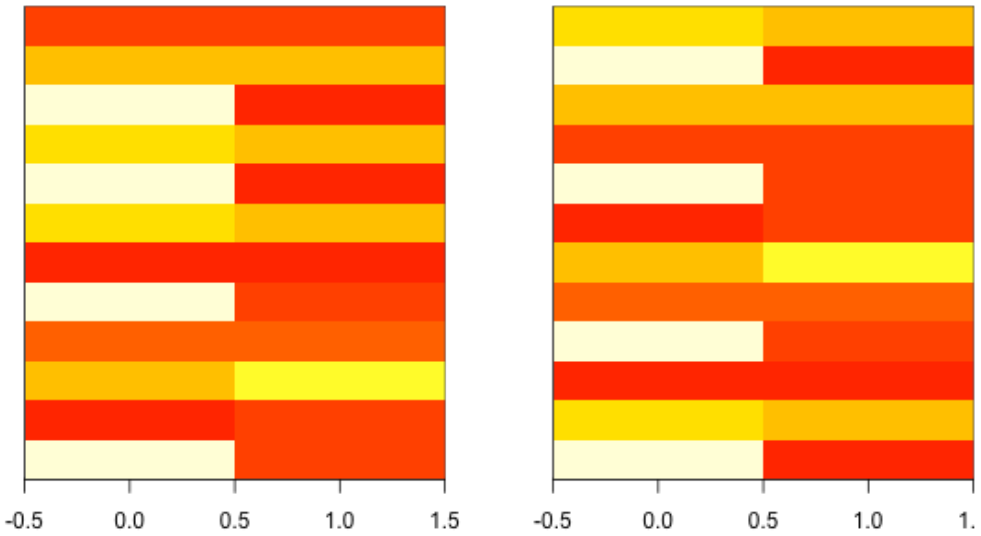
# kmeans()

```
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(kmeansObj$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