

K-means Clustering

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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 \longrightarrow garbage out
- ▶ Distance or similarity
 - ▶ Continuous - euclidean distance
 - ▶ Continuous - correlation similarity
 - ▶ Binary - manhattan distance
- ▶ Pick a distance/similarity that makes sense for your problem

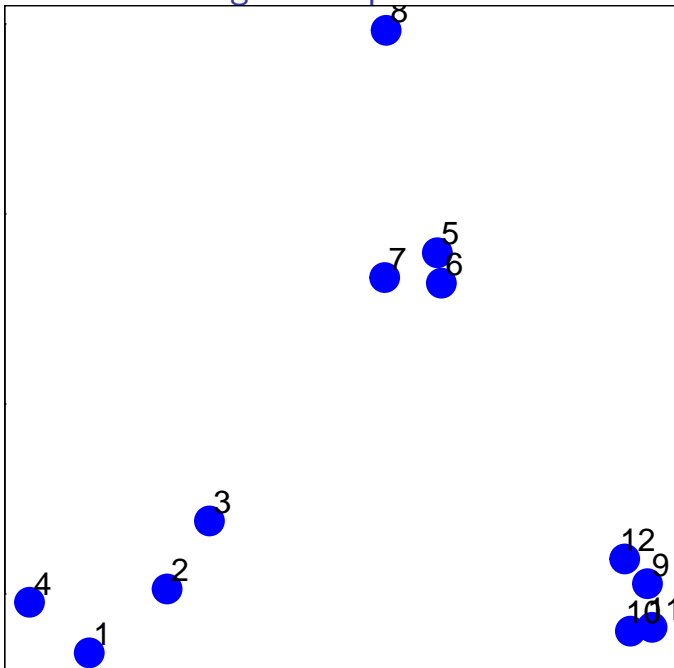
K-means clustering

- ▶ 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

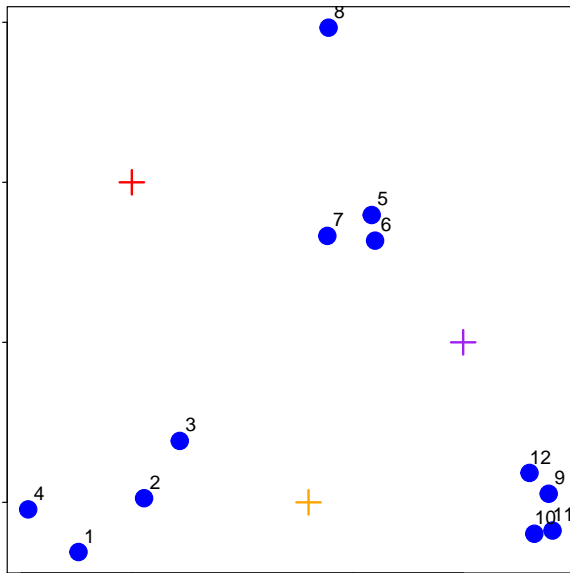
K-means clustering - example

```
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))
```

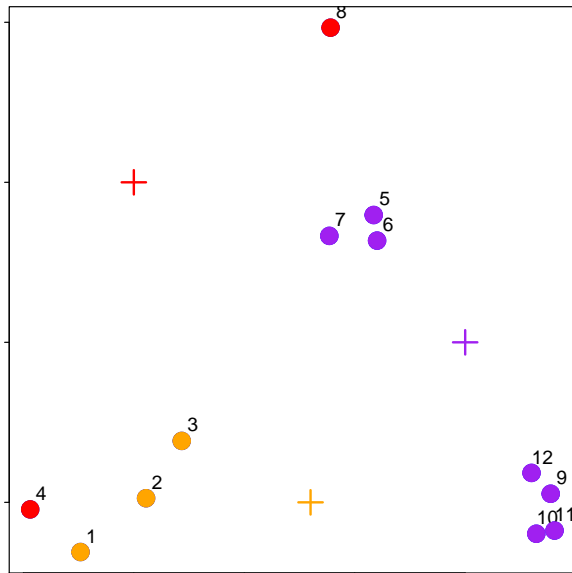
K-means clustering - example



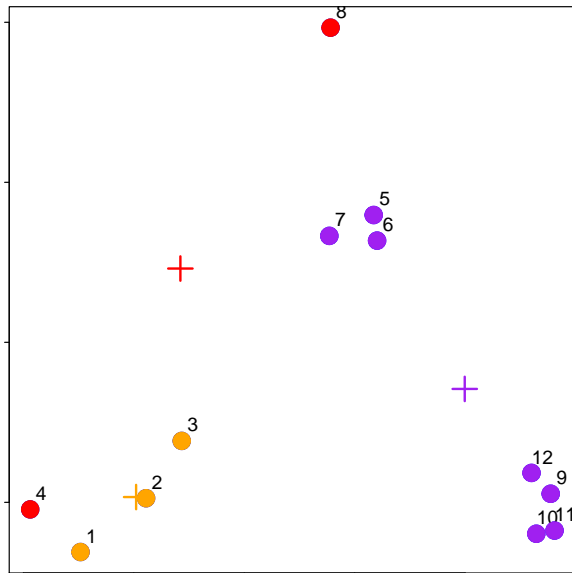
K-means clustering - starting centroids



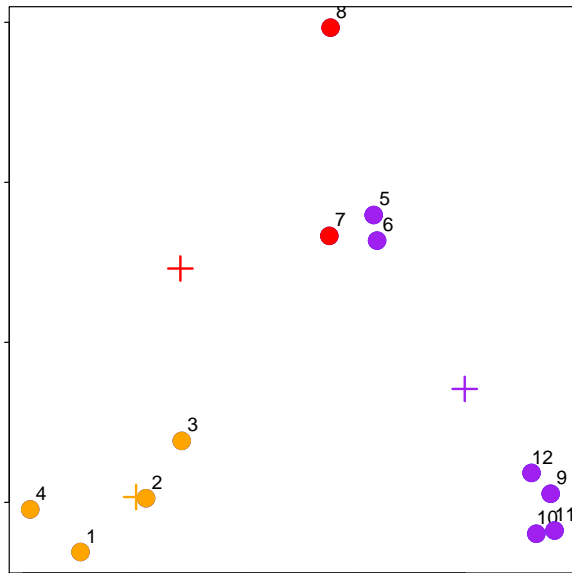
K-means clustering - assign to closest centroid



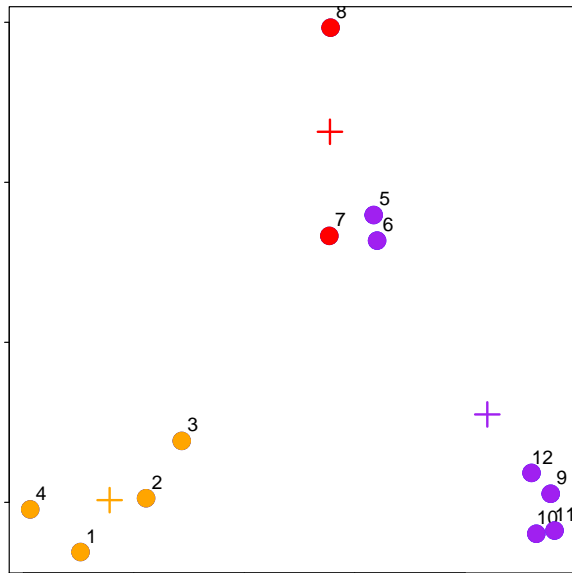
K-means clustering - recalculate centroids



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)
```

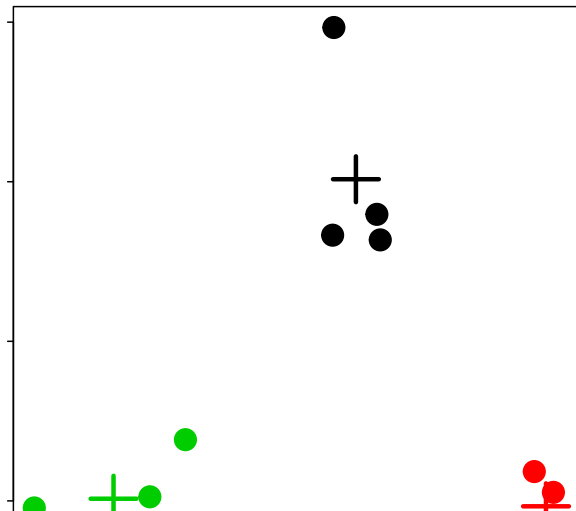
```
## [1] "cluster"      "centers"      "totss"        "withinss"
## [5] "tot.withinss" "betweenss"    "size"         "iter"
## [9] "ifault"
```

```
kmeansObj$cluster
```

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

kmeans()

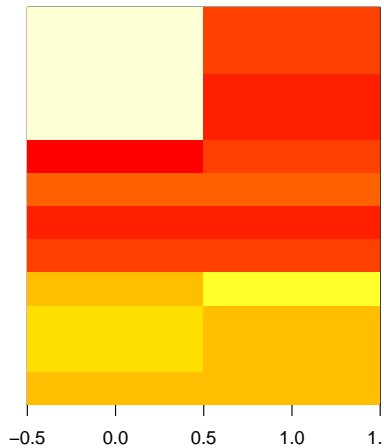
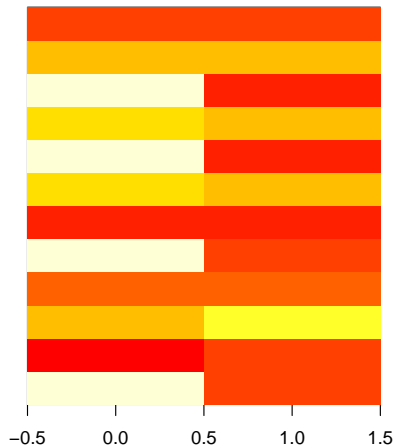
```
par(mar=rep(0.2,4))  
plot(x,y,col=kmeansObj$cluster,pch=19,cex=2)  
points(kmeansObj$centers,col=1:3,pch=3,cex=3,lwd=3)
```



Heatmaps

```
set.seed(1234)
dataMatrix <- as.matrix(dataFrame)[sample(1:12),]
kmeansObj <- 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")
```

Heatmaps



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