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?

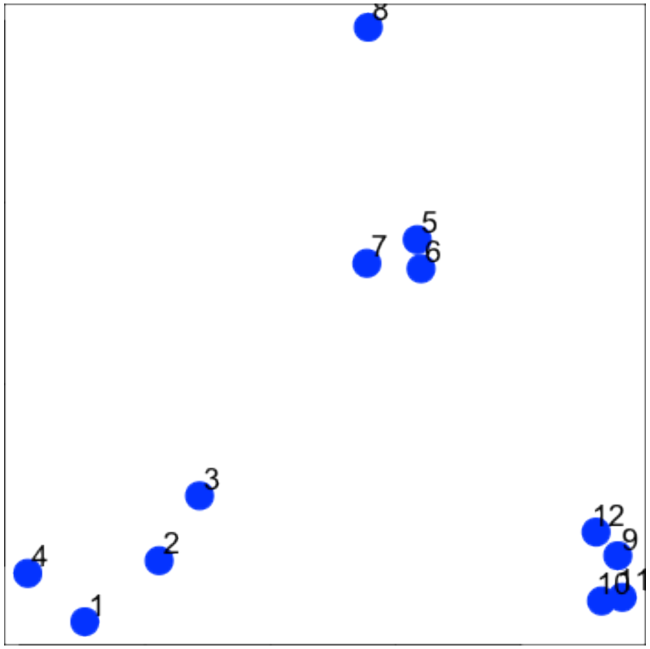
- Most important step
  - Garbage in -> garbage out
- Distance or similarity
  - Continuous - euclidean distance
  - Continous - correlation similarity
  - Binary - manhattan distance
- Pick a distance/similarity that makes sense for your problem

K-means clustering

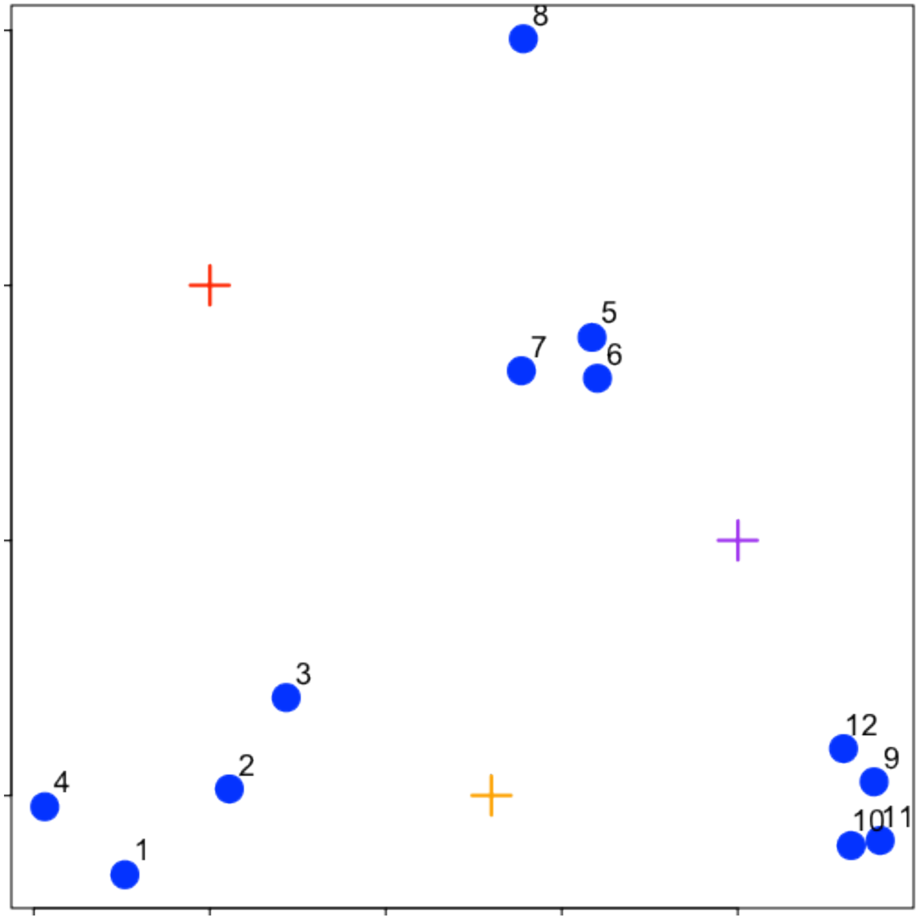
- A partioning approach
    - Fix a number of clusters
    - Get "centroids" of each cluster
    - Assign things to closest centroid
    - Reclaculate centroids
- Requires
    - A defined distance metric
    - A number of clusters
    - An initial guess as to cluster centroids
- Produces
    - Final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



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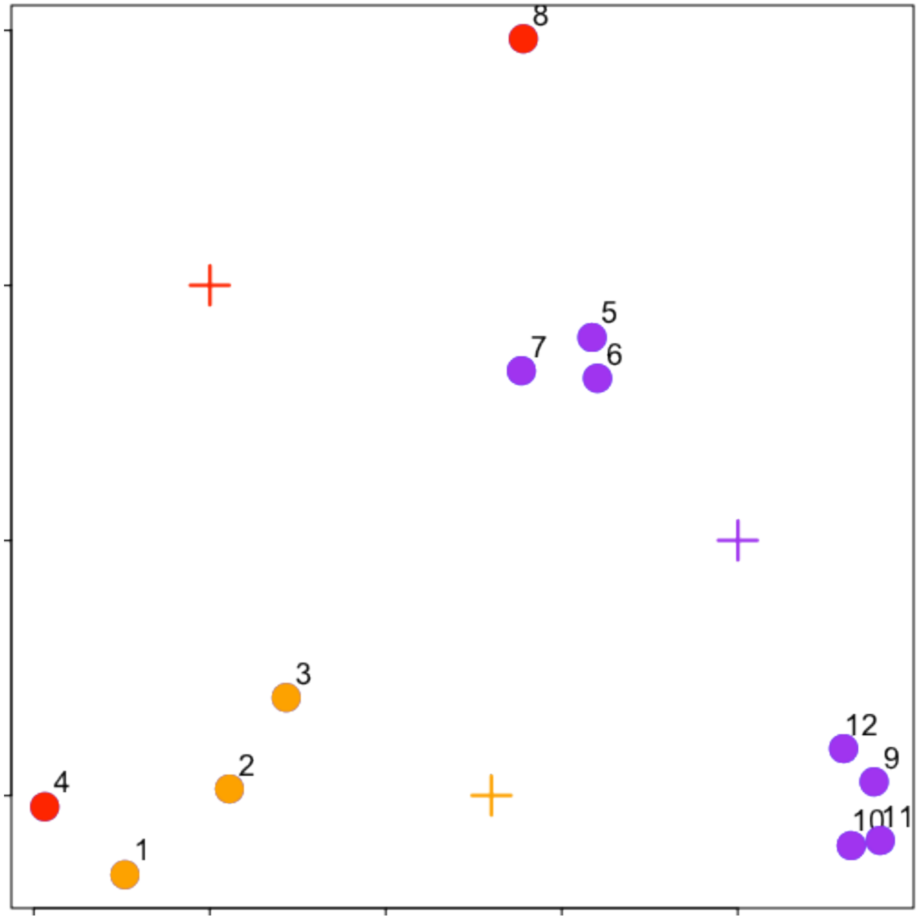
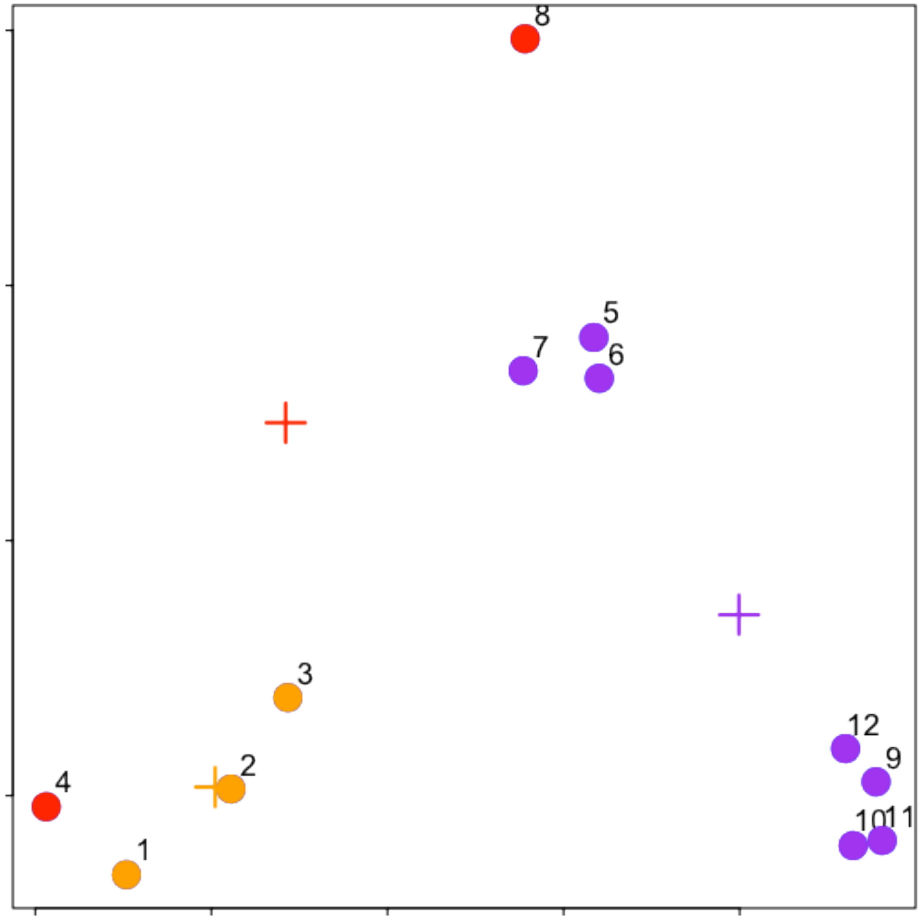
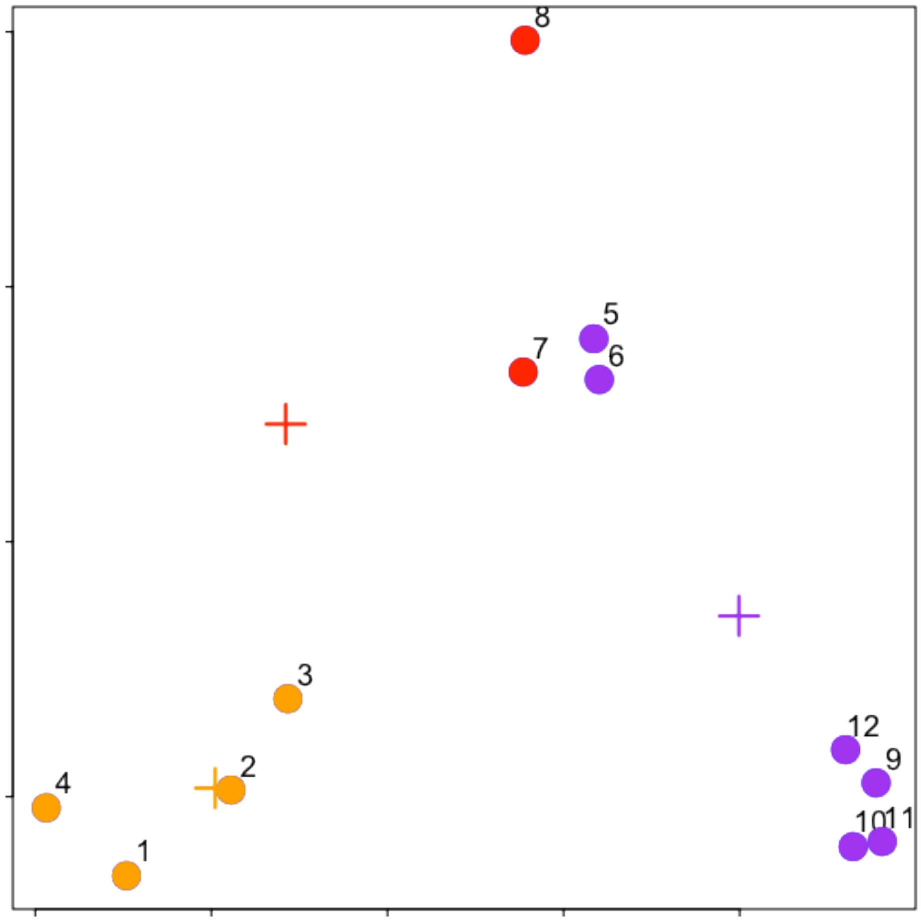
K-means clustering - assign to closest centroid



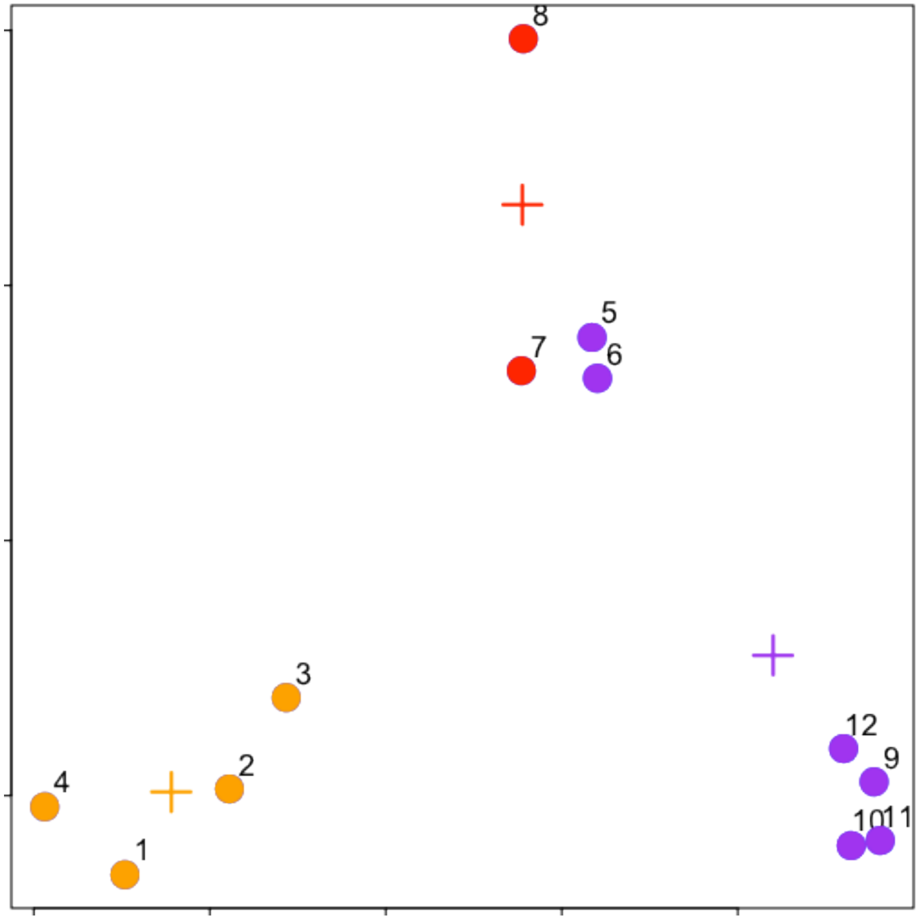
K-means clustering - recalculate centroids



K-means clustering - reassign values



K-means clustering - update centroids



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kmeans()

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

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

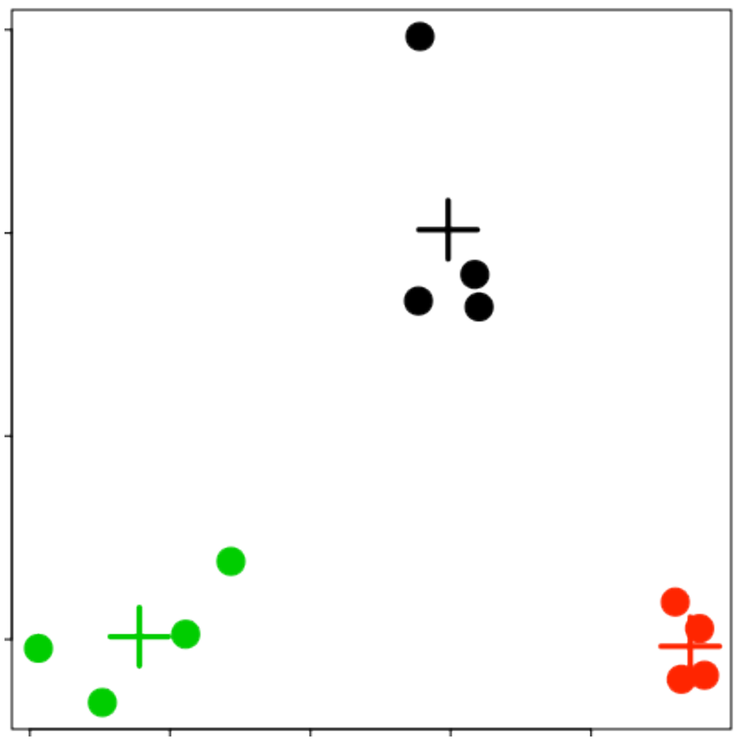
```
[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss" "betweenss"
[7] "size"
```

```
kmeansObj$cluster
```

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

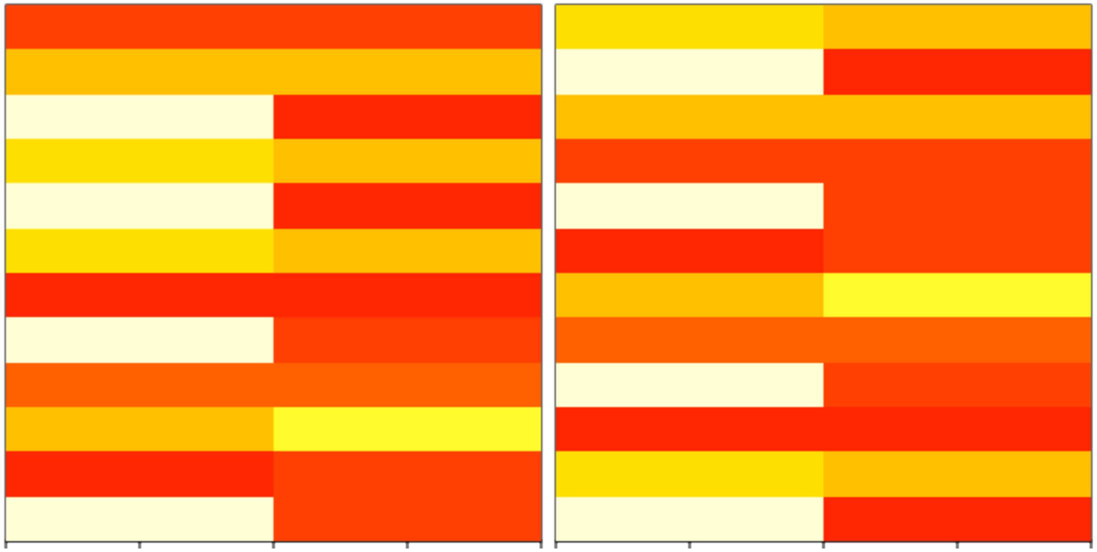
kmeans()

```
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=rep(0.2,4))
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
- Rafa's Distances and Clustering Video
- Elements of statistical learning