SDSC Summer Institute 2020

ML5 - Unsupervised Learning with Clustering
Paul Rodriguez
08/05/20
Location: Breakout Room
Gitter (session support): Breakout Room
Gitter (general system support): Help Desk

K-means cluster idea

Group points into clusters by some measure of distance

Assign points to 1 cluster only

Use clusters as a summary of data

Distance Measures

For numeric data

Euclidean distance (or sum squared differences)

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For numeric data

Euclidean distance (or sum squared differences)

For categorical data

‘Gower’ metric uses ‘same’ or ‘different’ counts

Lots of others…

Kmeans Clustering

Objective: minimize within-cluster distances

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Start with K initial cluster centers

spread out initial guesses

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Loop:

Assign each data point to nearest cluster center

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- Calculate mean of cluster for new center

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- Stop when assignments don't change

converges (but not to global min)

Kmeans Clustering

Objective: minimize within-cluster distances

Start with K initial cluster centers

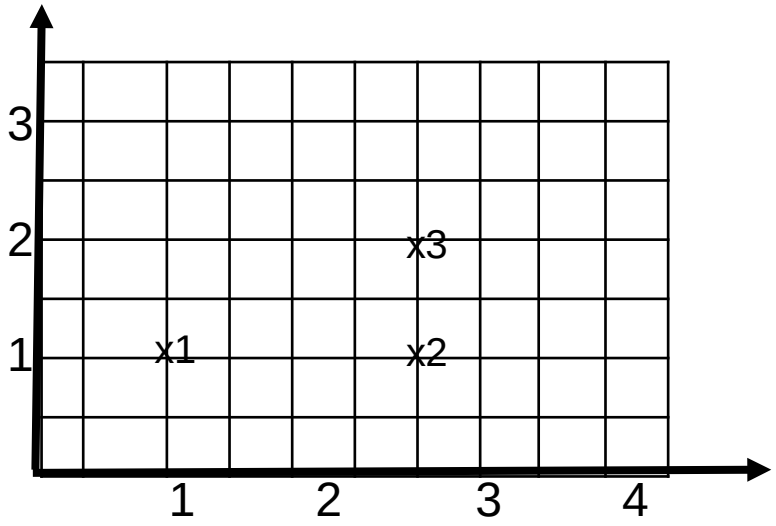
Loop:

- Assign each data point to nearest cluster center
- Calculate mean of cluster for new center
- Stop when assignments don't change

Kmeans works in a variety of situations, but choosing K is sometimes difficult

A quick simple example:

For these points
x1=(1,1)
x2=(3,1)
x3=(3,1.99)



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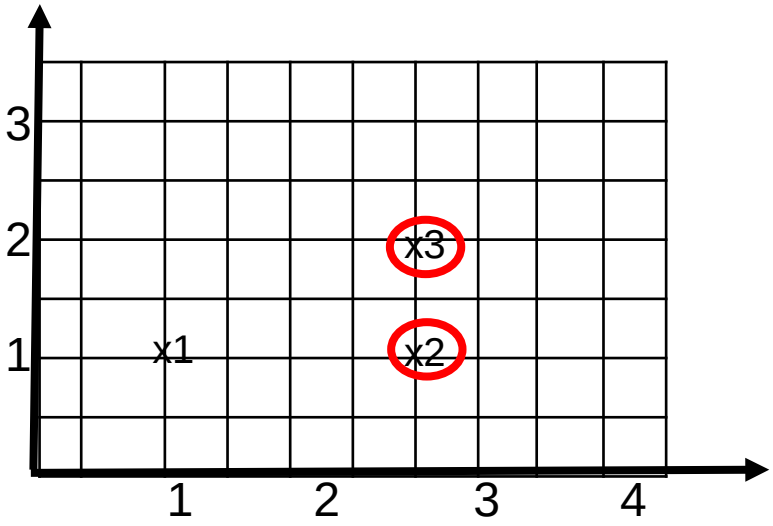

Use K=2, set initial centers as:

$\mu_1 = x_2$ and $\mu_2 = x_3$

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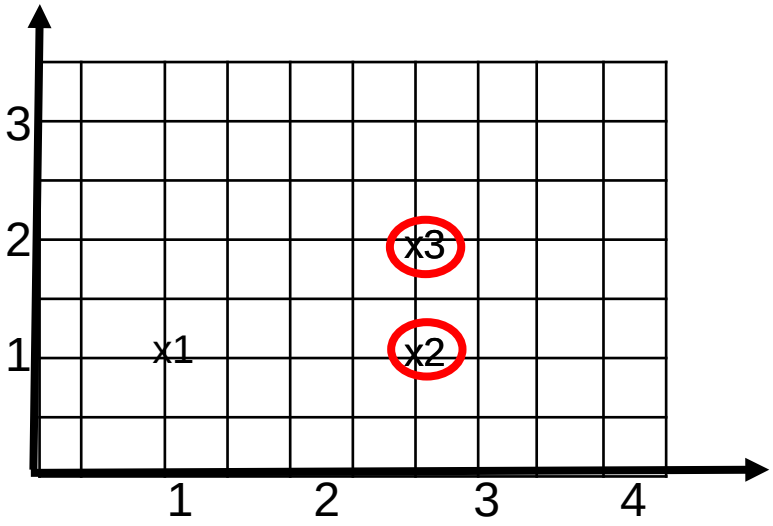

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Loop 1:

get distance of all points to all clusters means, a NxK distance matrix

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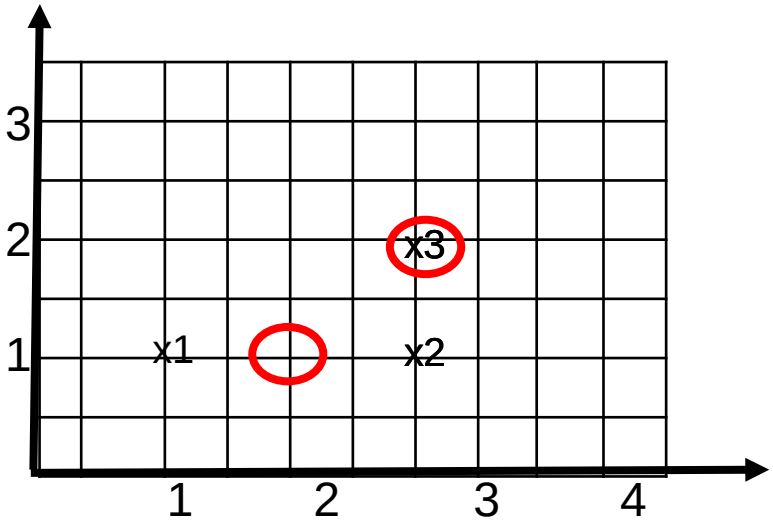

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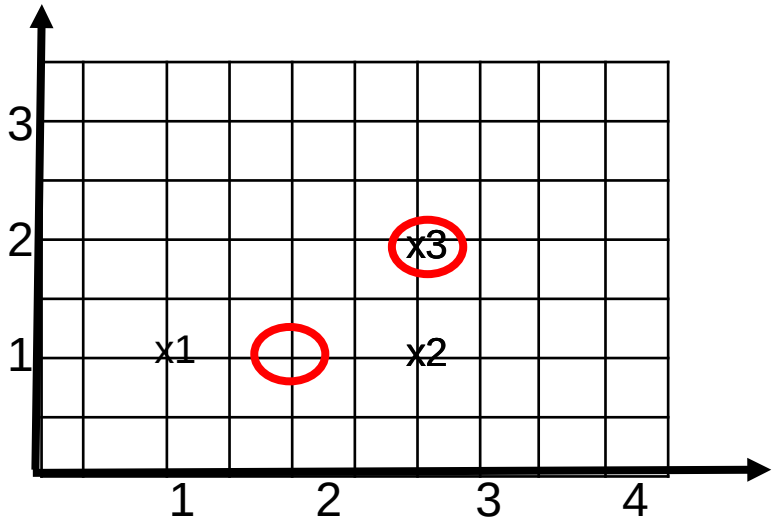

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After calculating new center, what happens to x2 assignment in next loop?

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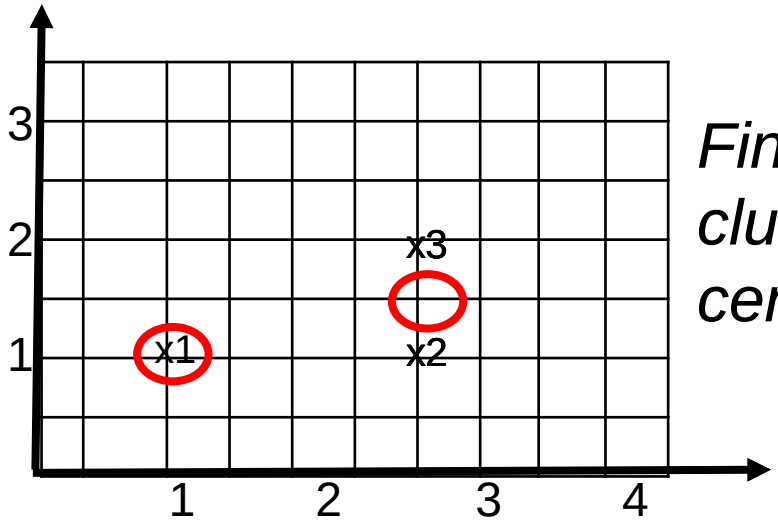

Final cluster centers

Use K=2, set initial centers as:

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assign x_1, x_2 to cluster 1

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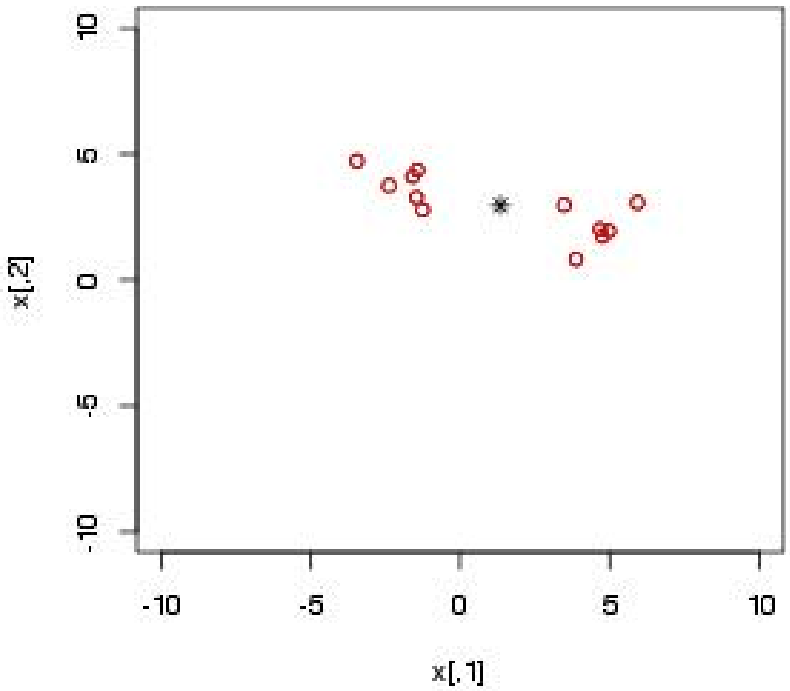
After calculating new center, what happens to x2 assignment in next loop?

Kmeans Examples

Kmeans Example

- **For K=1 where is the cluster center?**

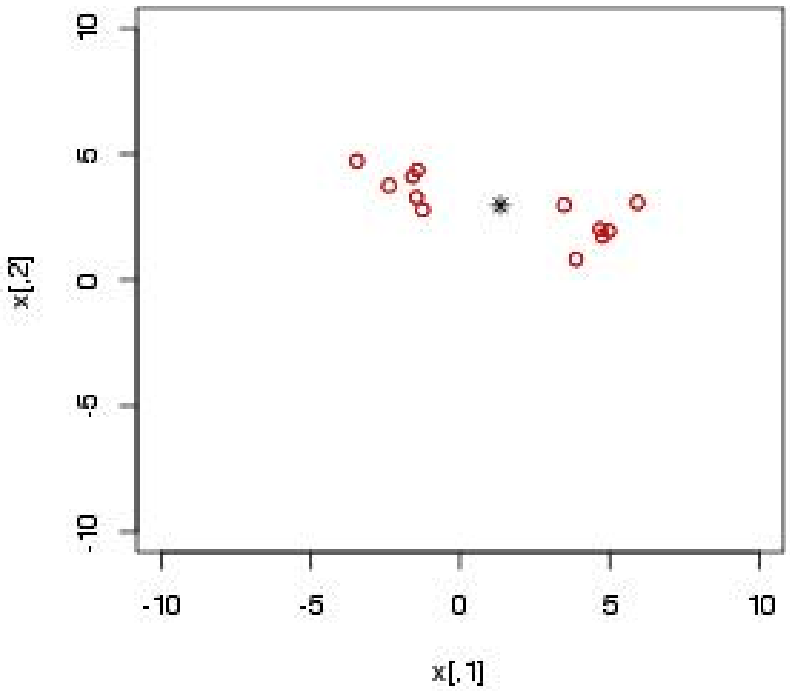


Essential R commands:
Kresult = kmeans(X,1,10,1)

#K=1
#10 is max loop iterations
#1 is number of initial sets to try

Kmeans Example

- **For K=1 where is the cluster center?** ***At the overall mean***



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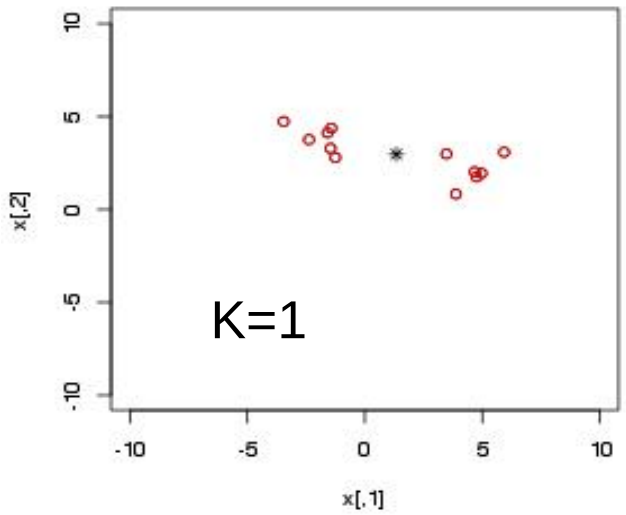
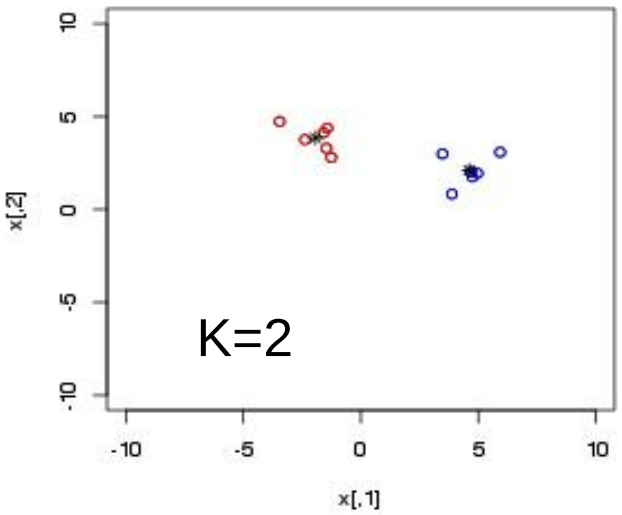
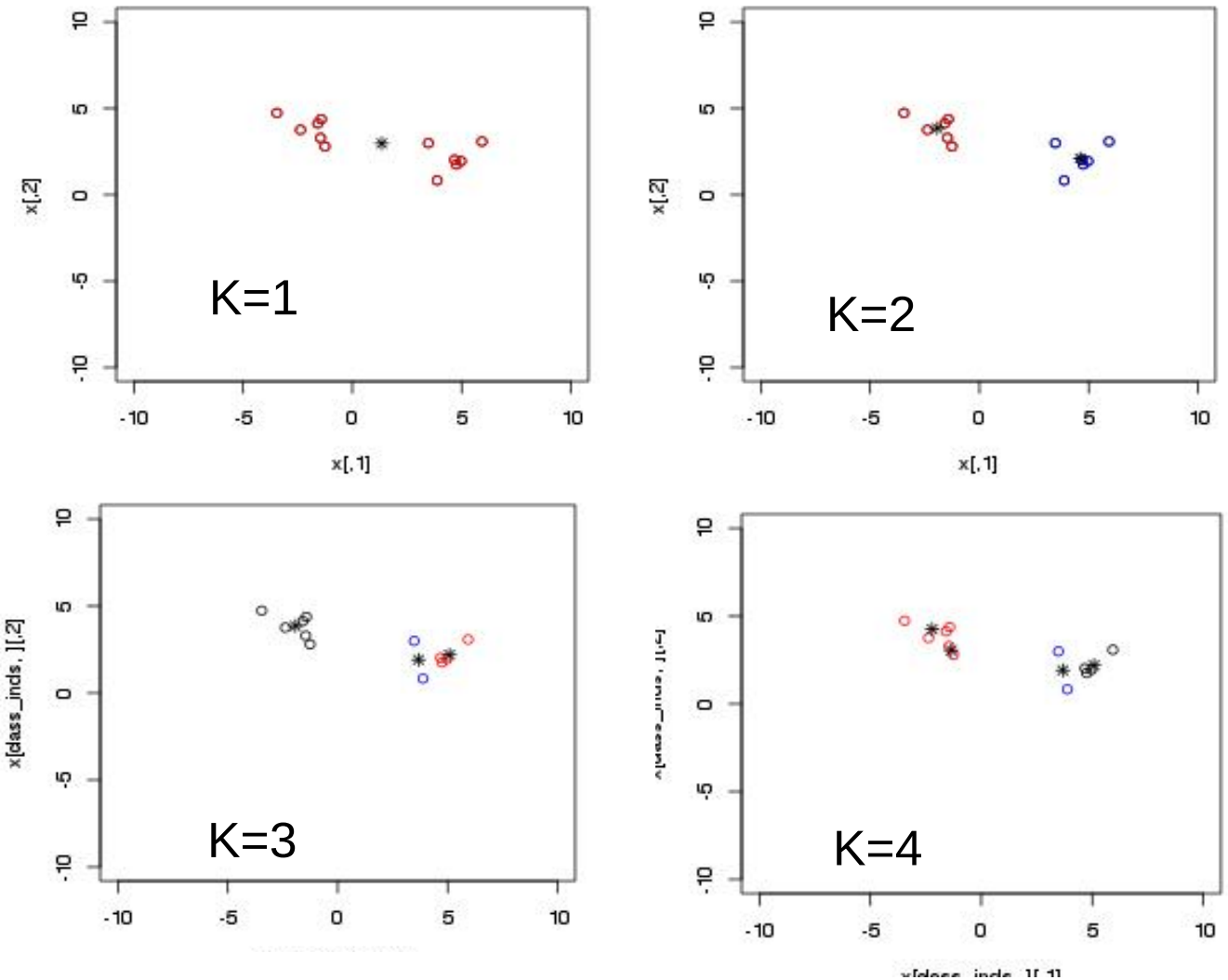




Kmeans Example



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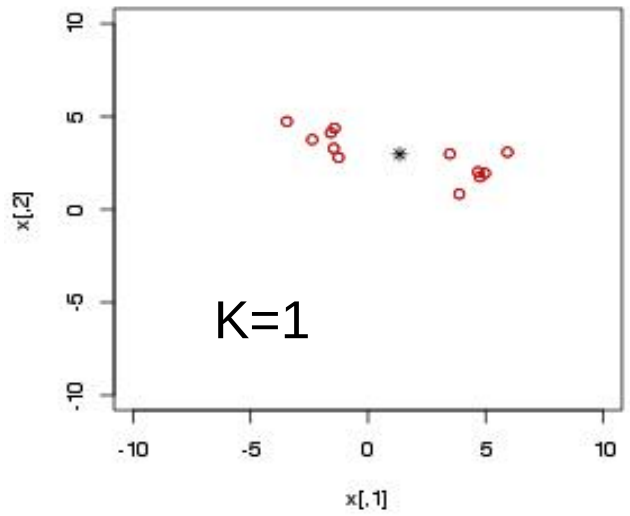
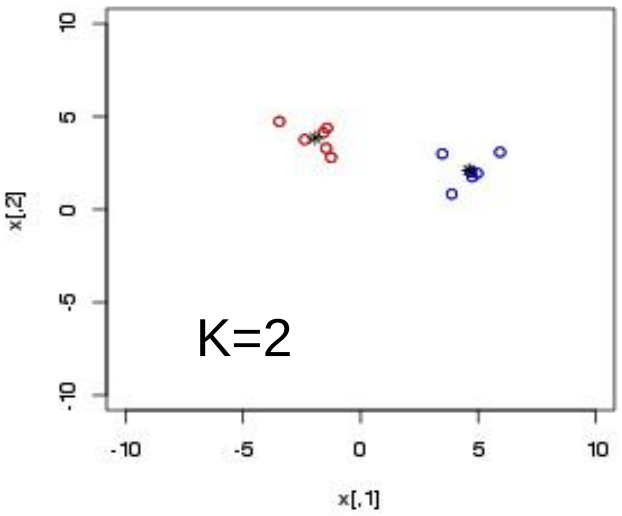
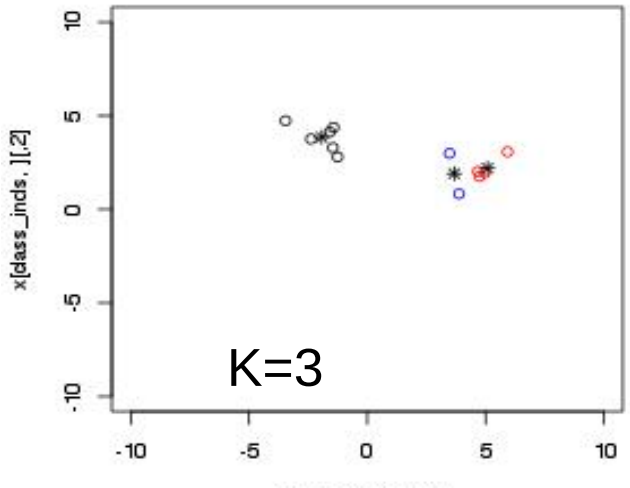
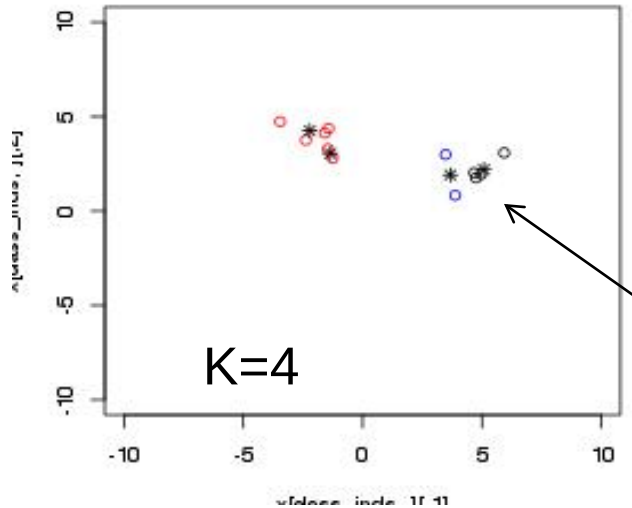




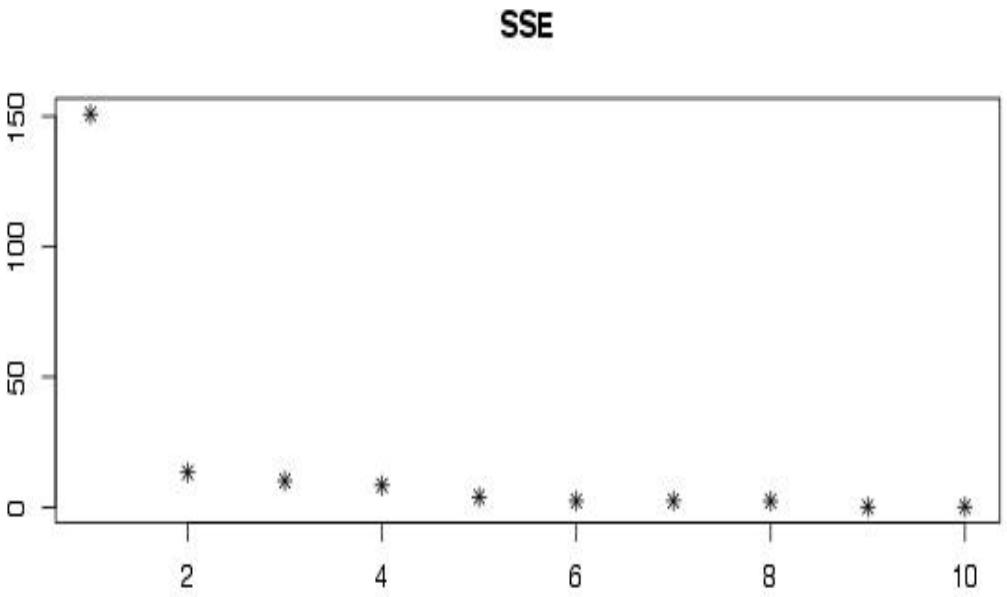




As K increases individual points get a cluster

Choosing K for Kmeans

Total Within Cluster SSE



K=1 to 10

Essential R commands:

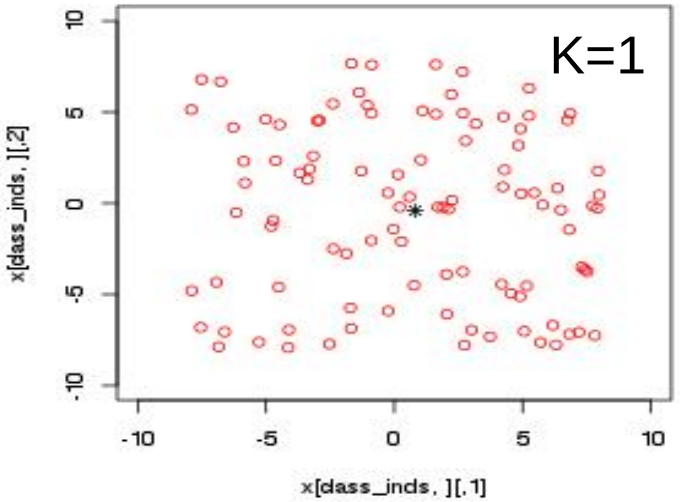
```
for (num_k in 1:10) {
Kres=kmeans(X,num_k,10,1);
```

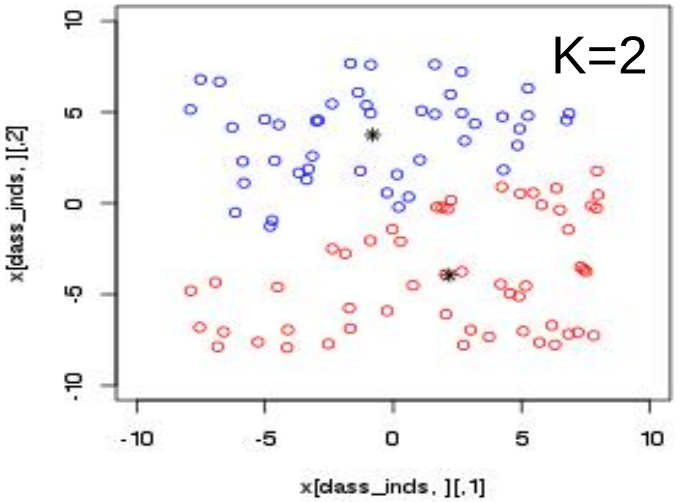
Save and then plot
Kres$tot.withinss

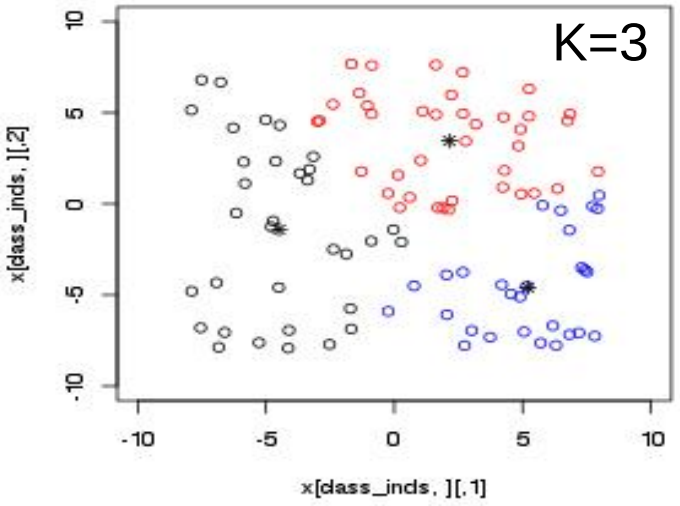
…

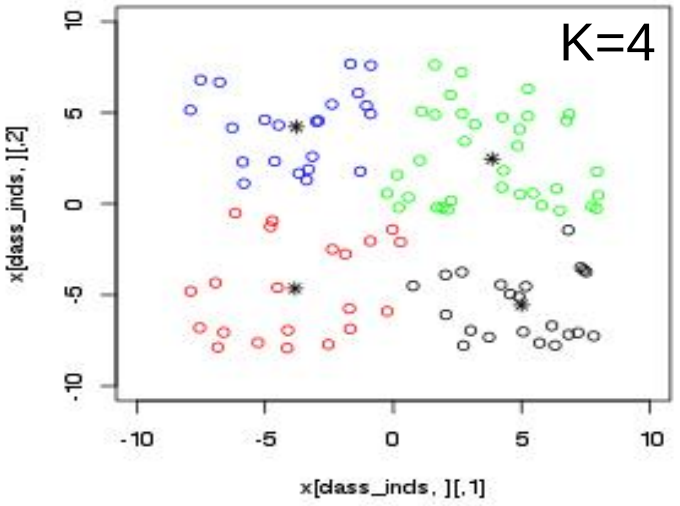
- Not much improvement after K=2 (“elbow”)

Kmeans Example: uniform dist.



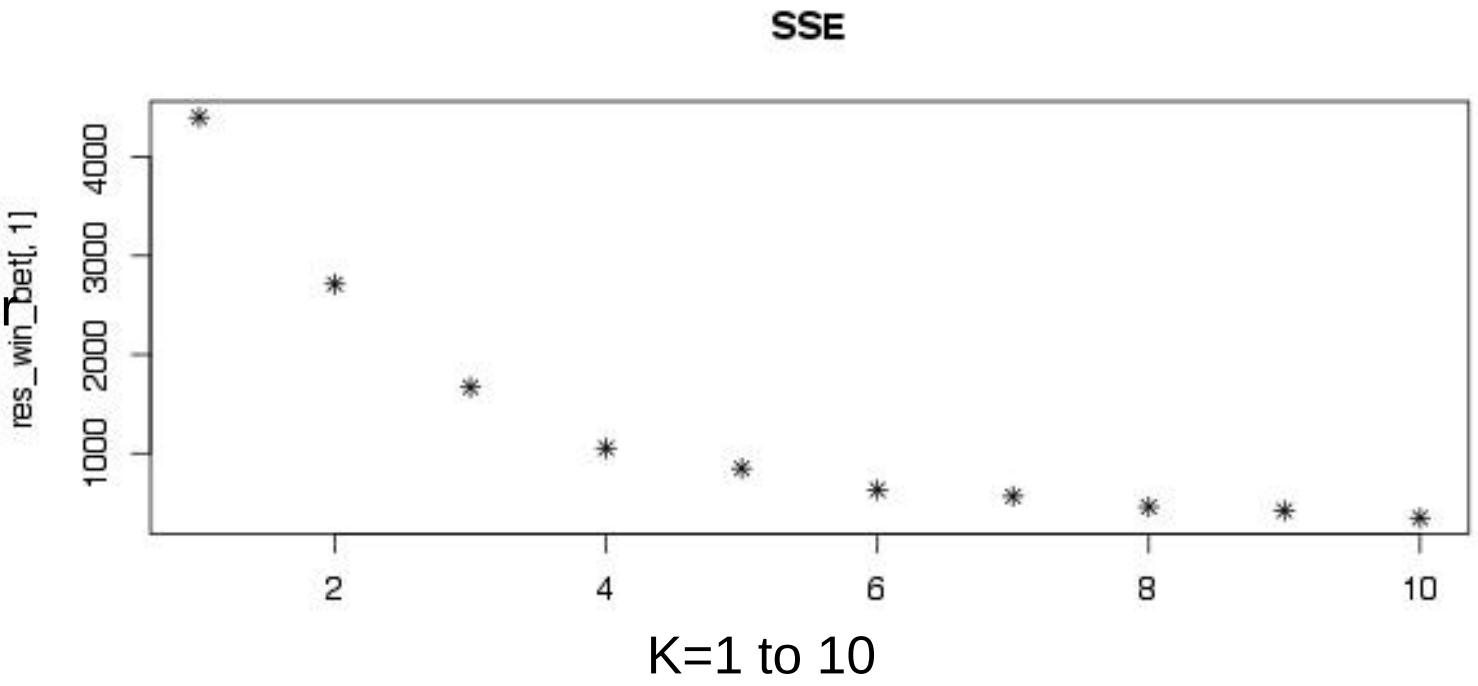






Choosing K - uniform

Total Within Cluster SSE



K=1 to 10

- Smooth decrease across K => less structure

Choosing K methods

- **“Elbow” of Sum Squared Error Within Clusters**

Choosing K methods

- **“Elbow” of Sum Squared Error Within Clusters**

- **“Silhouette”: mean SSE within a cluster vs to next best cluster**

  take maximum value over K=1…Kmax

Choosing K methods

- **“Elbow” of Sum Squared Error Within Clusters**

- **“Silhouette”: mean SSE within a cluster vs to next best cluster**

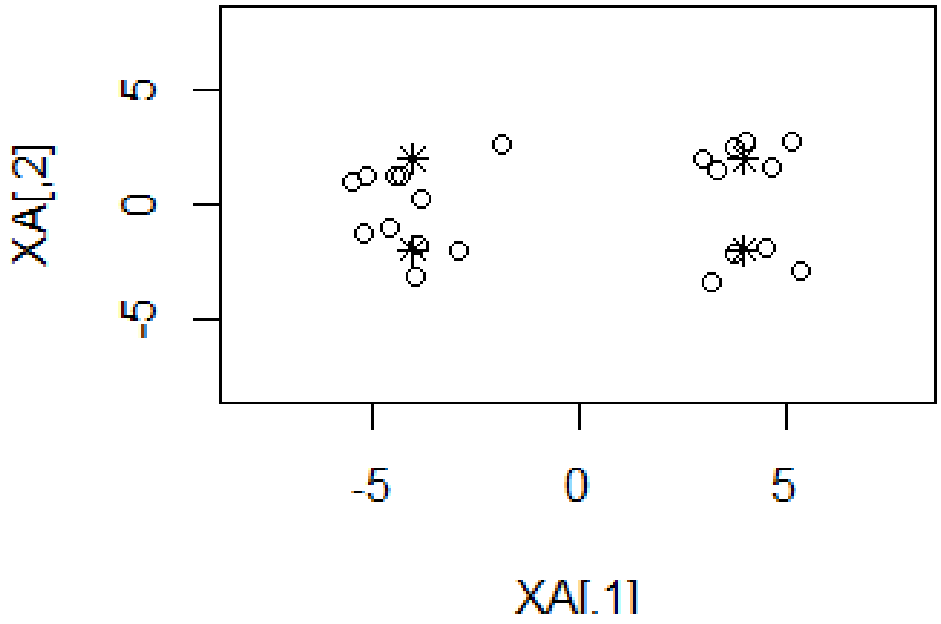
  take maximum value over K=1…Kmax

- **“Gap” value of SSE-within-cluster of data vs uniform distribution**

  take maximum value over K=1 …Kmax

Choosing K methods

- **Example, 4 clusters normal distribution, small sample**

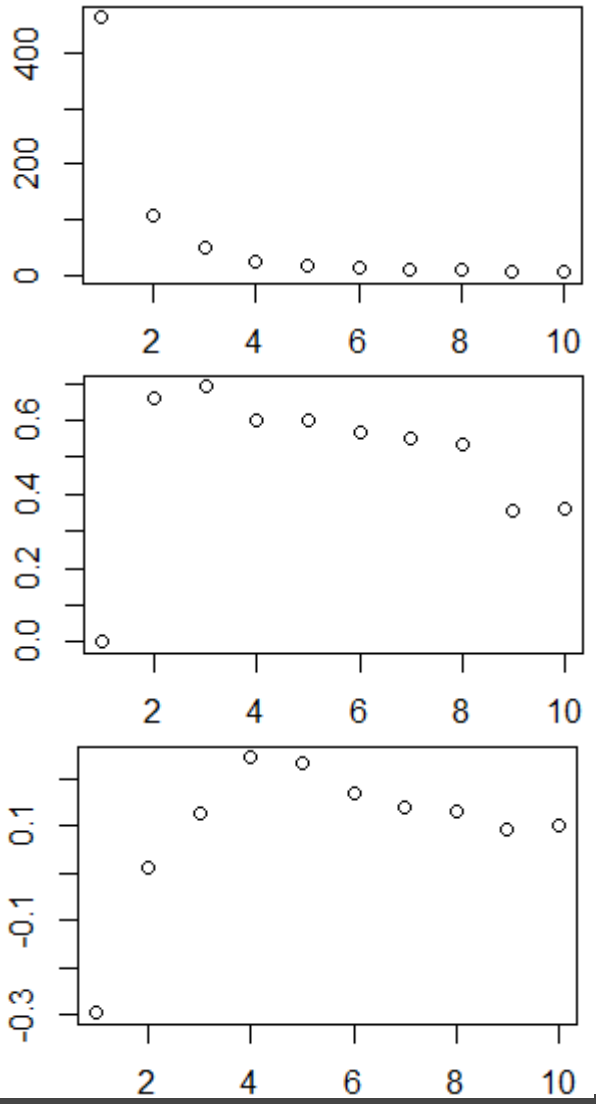


Choosing K methods

SSE within cluster (elbow)

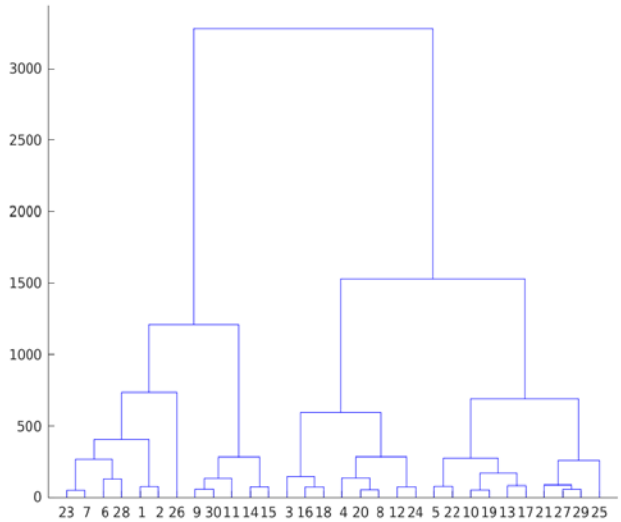
Silhouette within vs next best

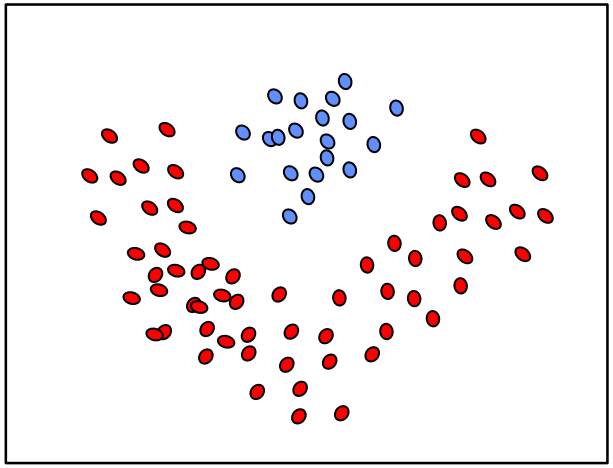
Gap SSE within cluster vs uniform data baseline



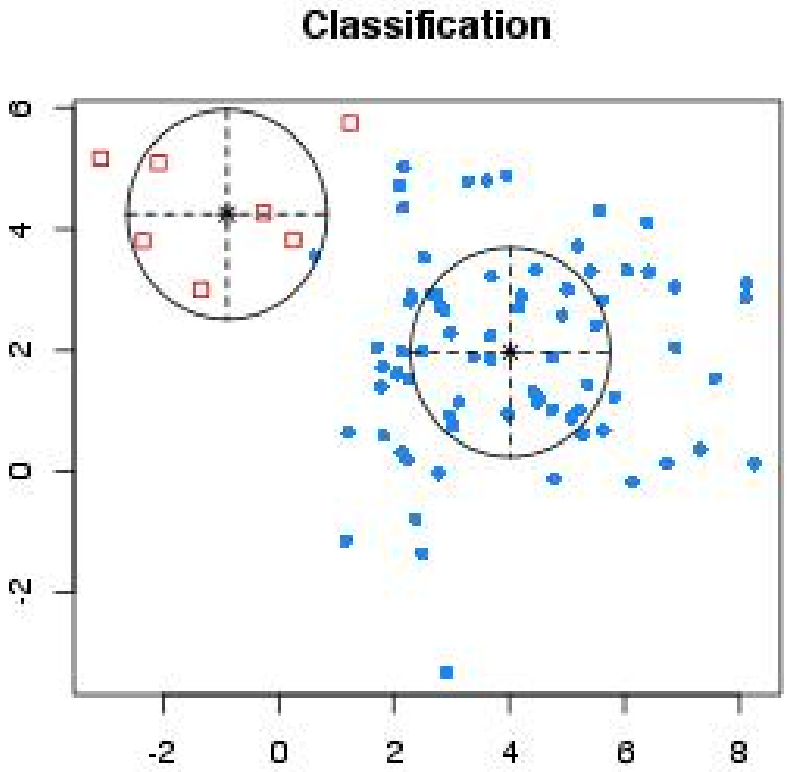
Many other clustering variations -

- **Hierarchical clustering – start with N clusters and merge points into large clusters (good to get whole tree)**
- **Density based clustering - build and link neighborhoods (good for spatial data)**





EM clustering
(expectation maximization)

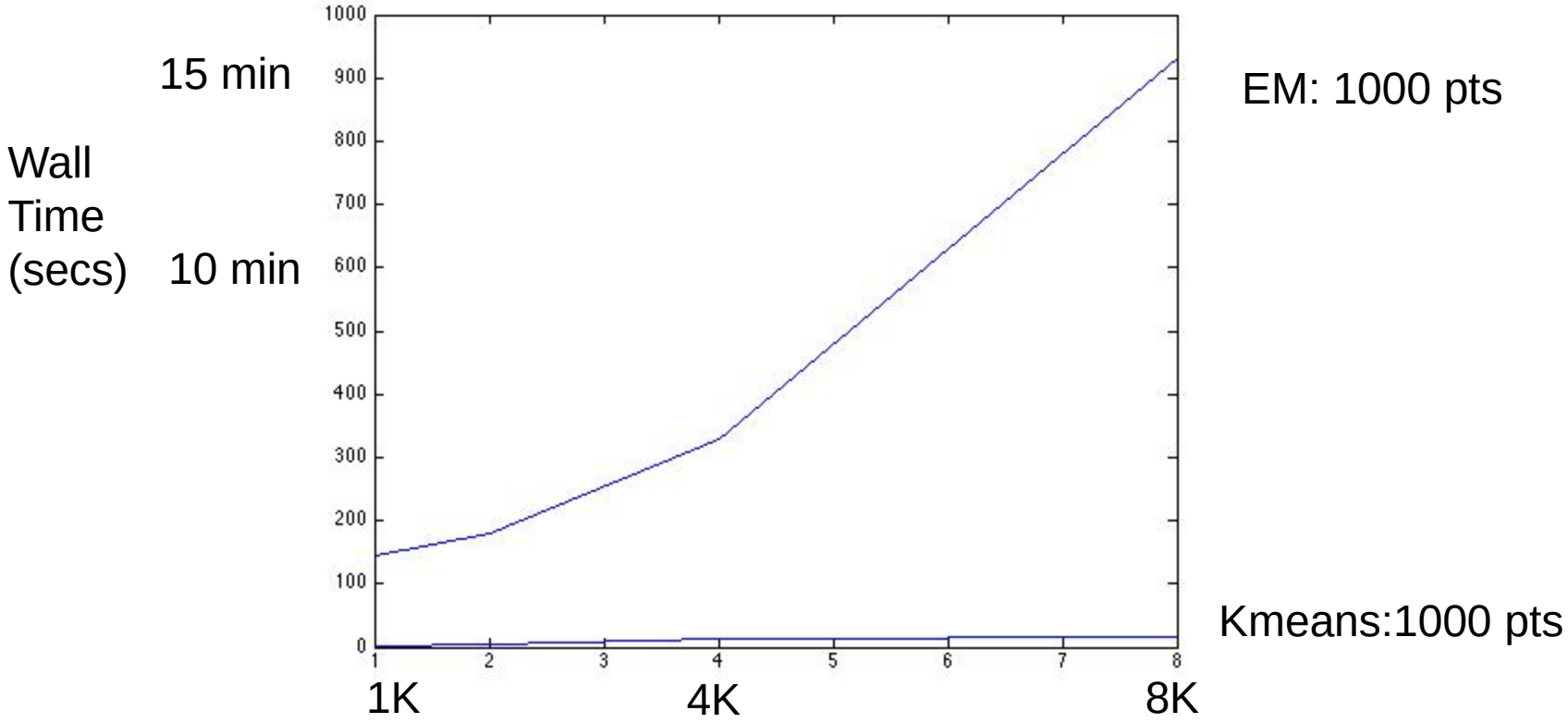


- **A probabilistic model using mixture of Gaussians**
- **Handles unequal variance and/or cluster sizes better than K-means**

R:
library('mclust')
em_fit=Mclust(x);
plot(em_fit);

Kmeans vs EM performance

1 Gordon compute node, normal random matrices
R: system.time(Mclust())

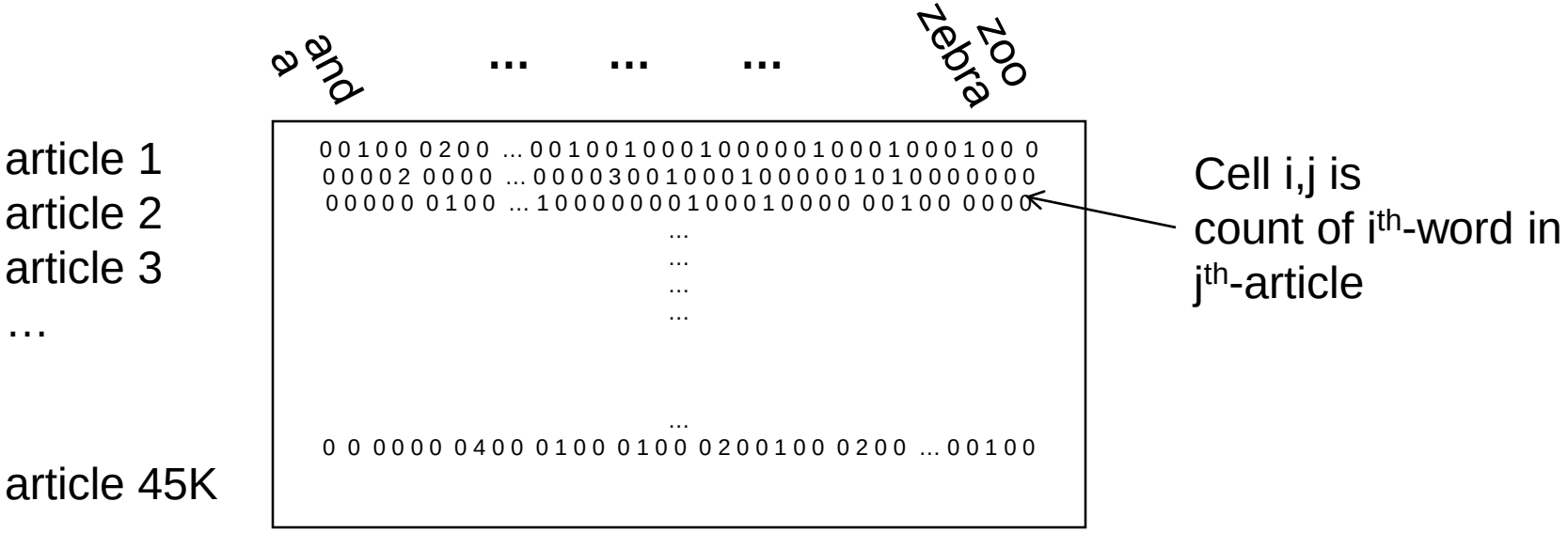


Kmeans big data example

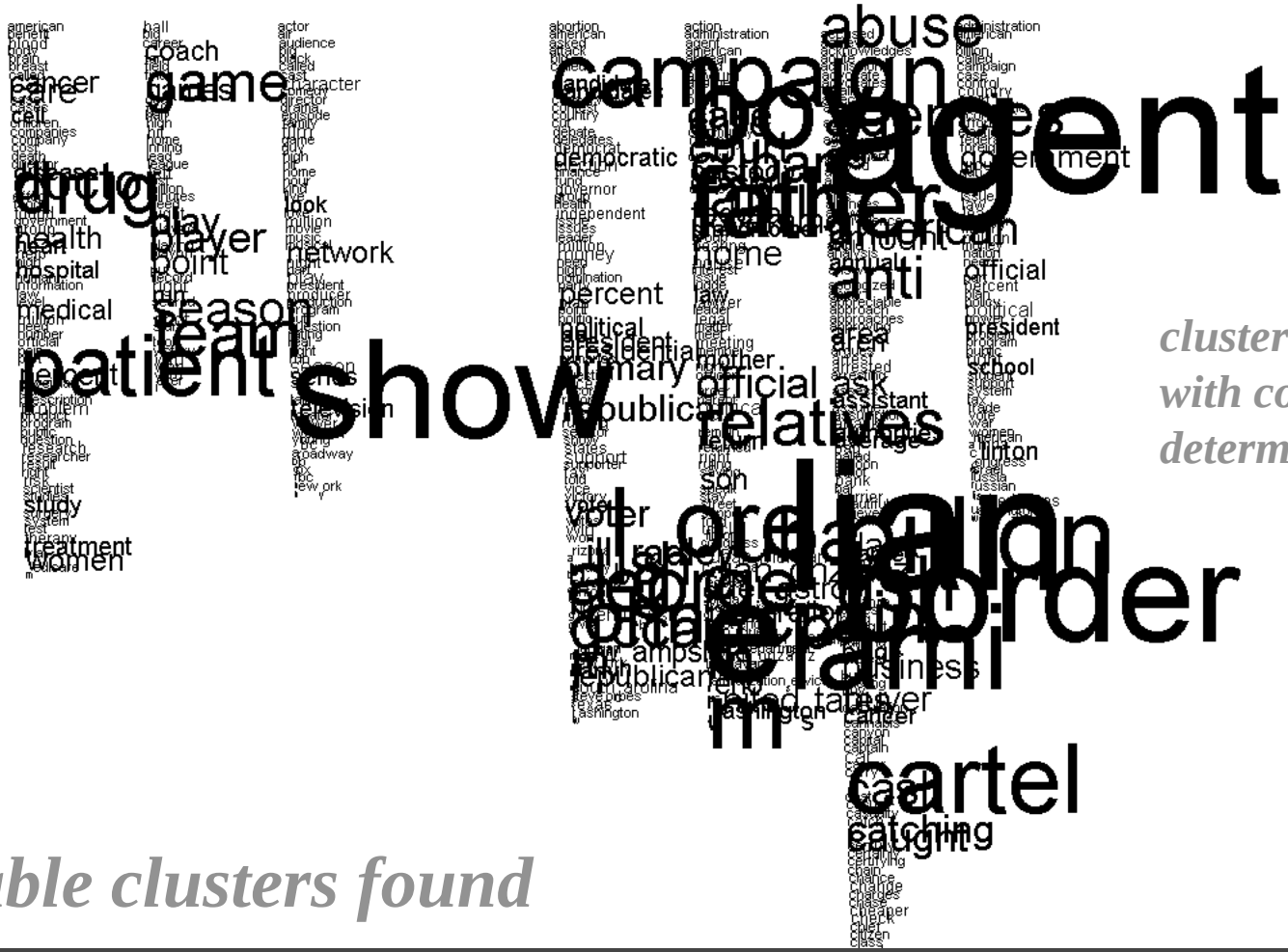
- **45,000 NYTimes articles, 102,000 unique words**

  (UCI Machine Learning repository)

- **Full Data Matrix: 45Kx102K ~ 40Gb**



Kmeans results



cluster means shown with coordinates determining fontsize

7 viable clusters found

Kmeans for image segmentation

R snippet with K=8

```
install.packages('ripa')
library('ripa')

source("http://bioconductor.org/biocLite.R")
biocLite()
biocLite("EBImage")

library('EBImage')
im=readImage('1a34086v.jpg')

library('ripa')
img=rgb2grey(im, coefs=c(0.30, 0.59, 0.11))

imgx1  =as.vector(img)
numk=8
km_imx1=kmeans(imgx1,numk,50,1);
img_km_mat =matrix(km_imx1$cluster,dim(im)[1],dim(im)[2])

display(img_km_mat/numk)
```

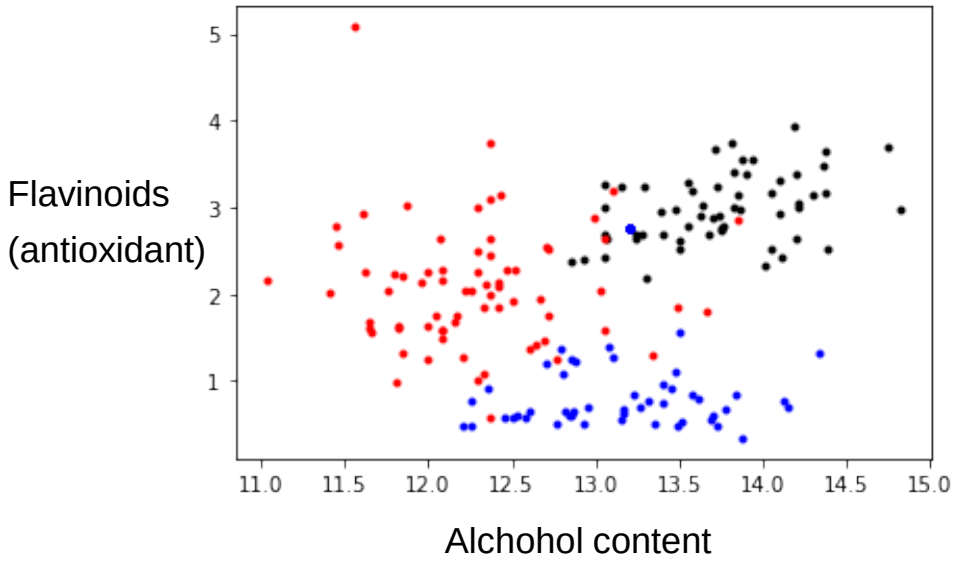
Kmeans with a Winery dataset

(UCI Machine Learning Repository)

178 observations

13 variables of wine characteristics

3 target classes that indicate which winery produced the wine



Black=58 cases
Red=71
Blue=48

Will cluster match classes?

Pause

Principle Components vs Clustering

- PCA, SVD reduces dimensions, Clustering reduces to categorical groups
- In some cases, *k* PCs ⇔ *k* clusters
- It is also useful to visualize clusters in PC space

Summary

- **Having no label doesn’t stop you from finding structure in data**
- **Unsupervised methods are somewhat related**