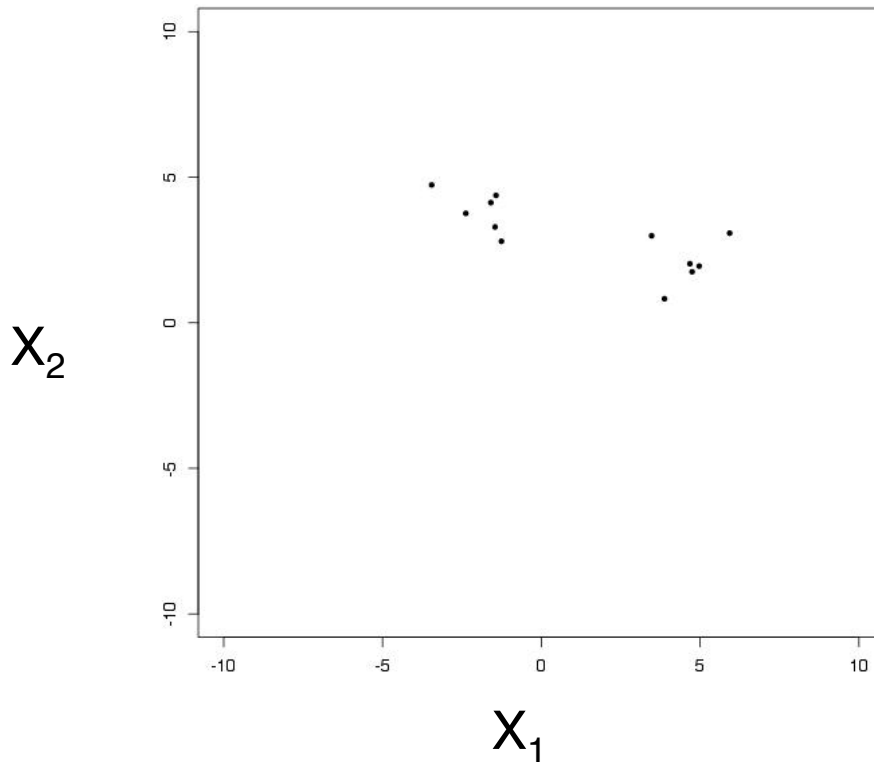# Unsupervised Learning with Clustering

Paul Rodriguez

Clustering Idea

- **Given a set of data can we find a natural grouping?**

Essential R commands:
D   =rnorm(12,0,1) #generate 12
                                        #random normal
X1   =matrix(D,6,2) #put into 6x2 matrix
X1[,1]=X1[,1]+4;   #shift center
X1[,2]=X1[,2]+2;

#repeat for another set of points

#bind data points and plot
plot(rbind(X1,X2),
                xlim=c(-10,10),ylim=c(-10,10));

Why Clustering

- **A good grouping implies some structure**
- **In other words, given a good grouping,**
  we can then:
  - Interpret and label clusters
  - Identify important features
  - Characterize new points by the closest cluster (or nearest neighbors)
  - Use the cluster assignments as a compression or summary of the data
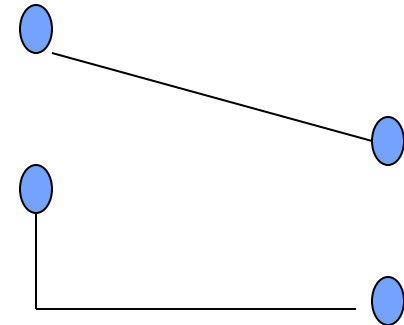
Clustering Objective

- **Objective: find subsets that are similar within cluster and dissimilar between clusters**

- **Similarity defined by distance measures**

  - Euclidean distance

  - Manhattan distance
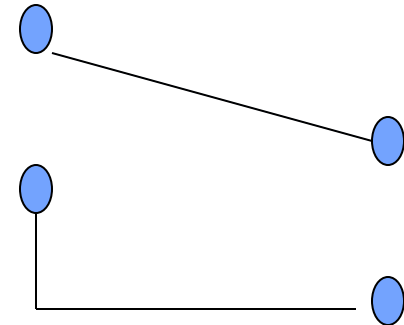
Clustering Objective

- **Objective: find subsets that are similar within cluster and dissimilar between clusters**

- **Similarity defined by distance measures**

  - Euclidean distance   =
      $sqrt[(a1 - b1)^2 + (a2 - b2)^2 + ...)]$
  - Manhattan distance
      $[|a1 - b1| + |a2 - b2| + ...)]$

Kmeans Clustering

- **A simple, effective, and standard method**

    Start with K initial cluster centers

    Loop:

    Assign each data point to nearest cluster center

    Calculate mean of cluster for new center

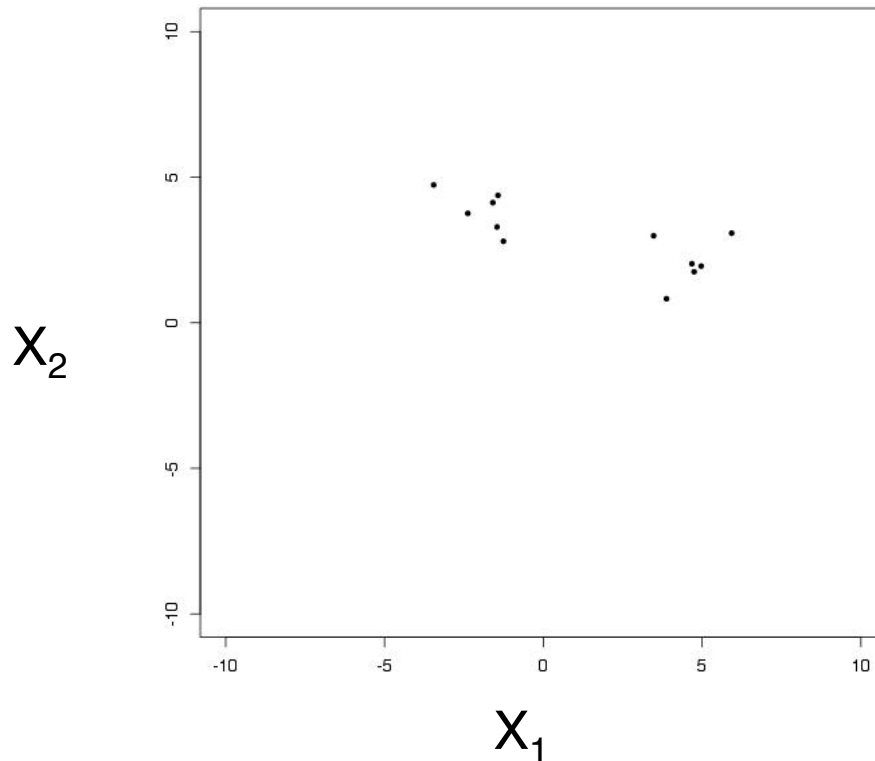   Stop when assignments don't change

- **Issues:**

    How to choose K?

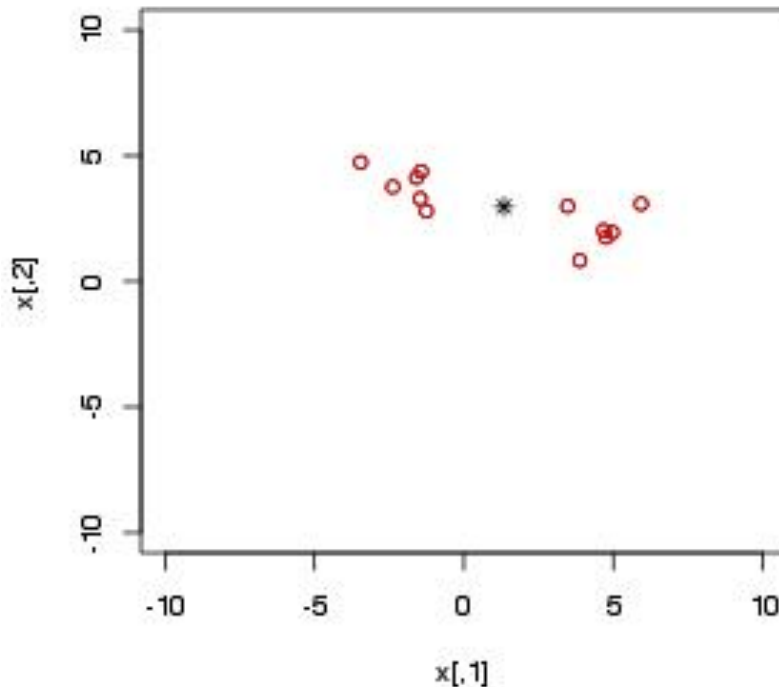   How to choose initial centers?

    Will it always stop?

Kmeans Example

- **For K=1, using Euclidean distance, where will the cluster center be?**

X_2

X_1

Kmeans Example

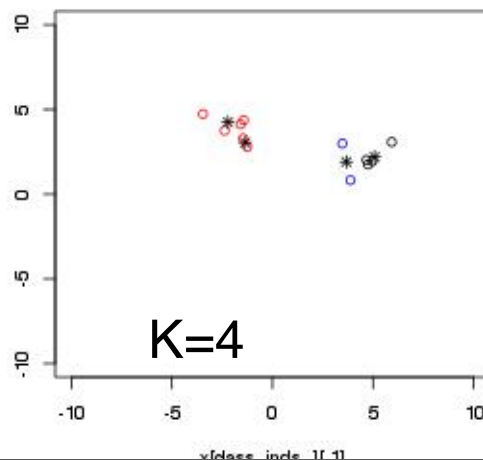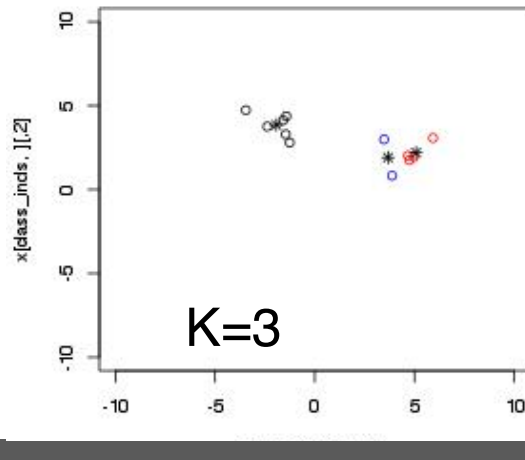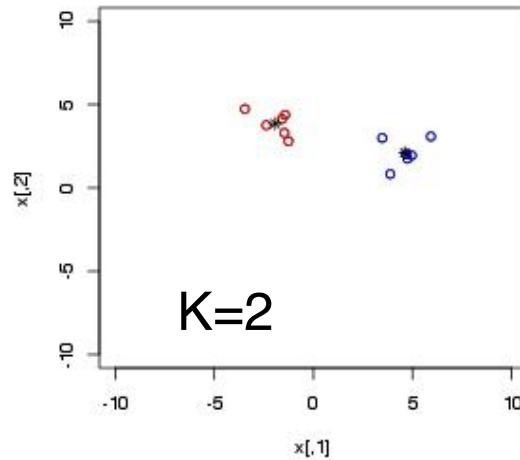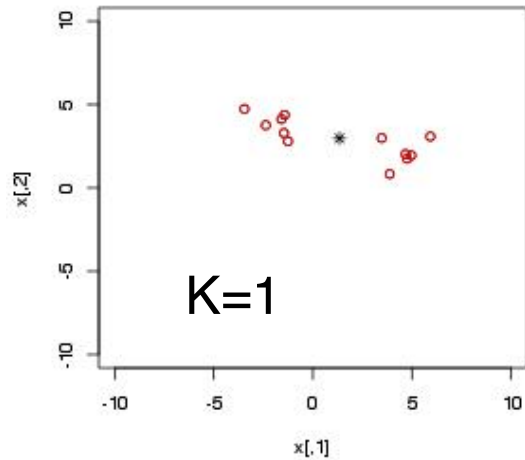- **For K=1, the overall mean minimizes Sum Squared Error (SSE), aka Euclidean distance**

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

#choose 1 data point as initial K centers
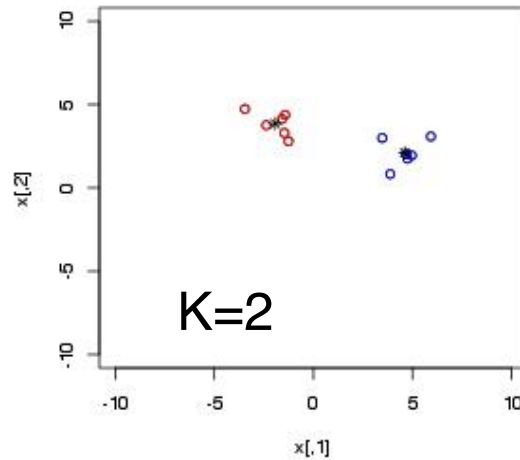#10 is max loop iterations
#1 is number of initial sets to try

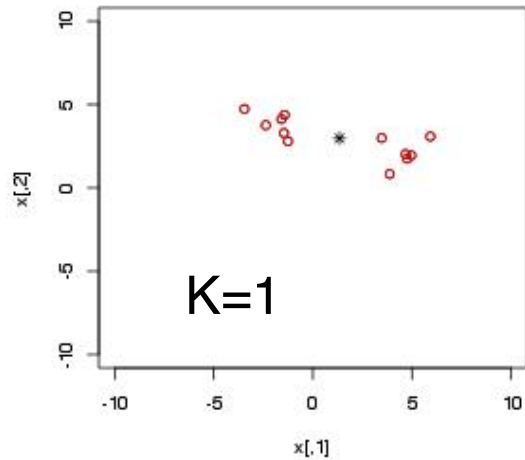#Kresult is an R object with subfields
Kresult$cluster   #cluster assignments
Kresults$tot.withinss # tot within SSE

Kmeans Example

Essential R commands:
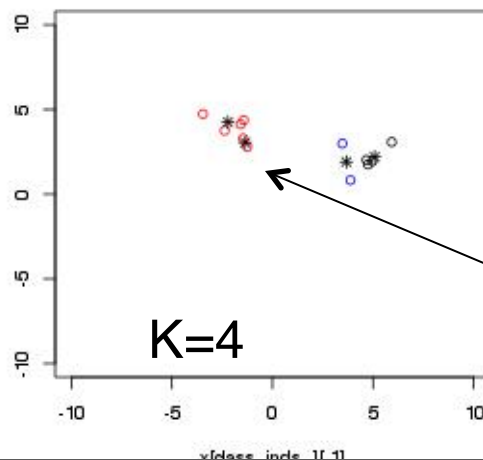inds=which(Kresult$cluster==K)

plot(X[inds,],col2use="red");

. . .

Kmeans Example

K=1

K=2

K=3
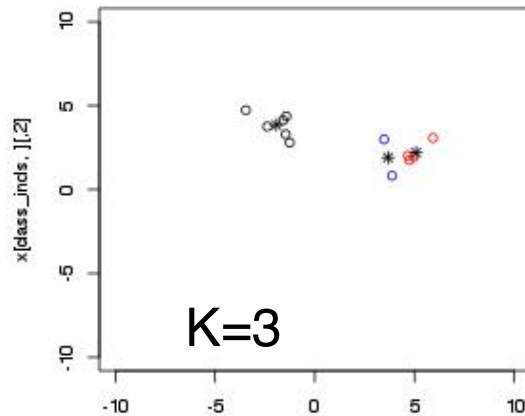
K=4

Essential R commands:
inds=which(Kresult$cluster==K)

plot(X[inds,],col2use="red");

...

As K increases individual points get a cluster

Choosing K for Kmeans

SSE

Total Within Cluster SSE

K=1 to 10
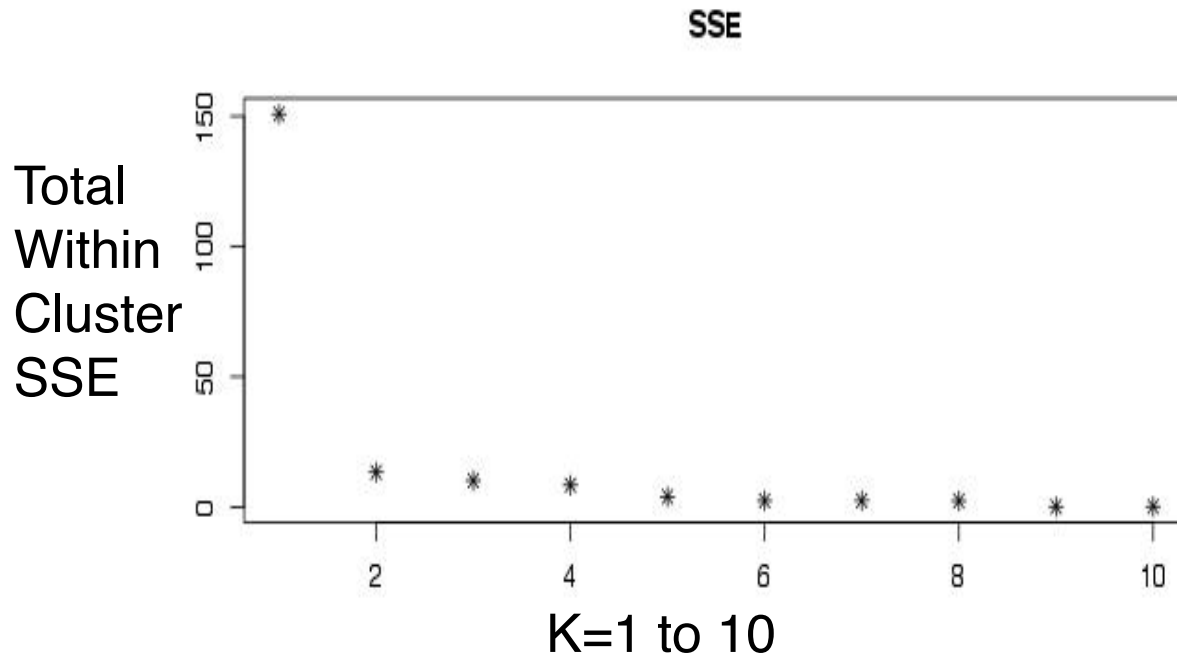
Essential R commands:

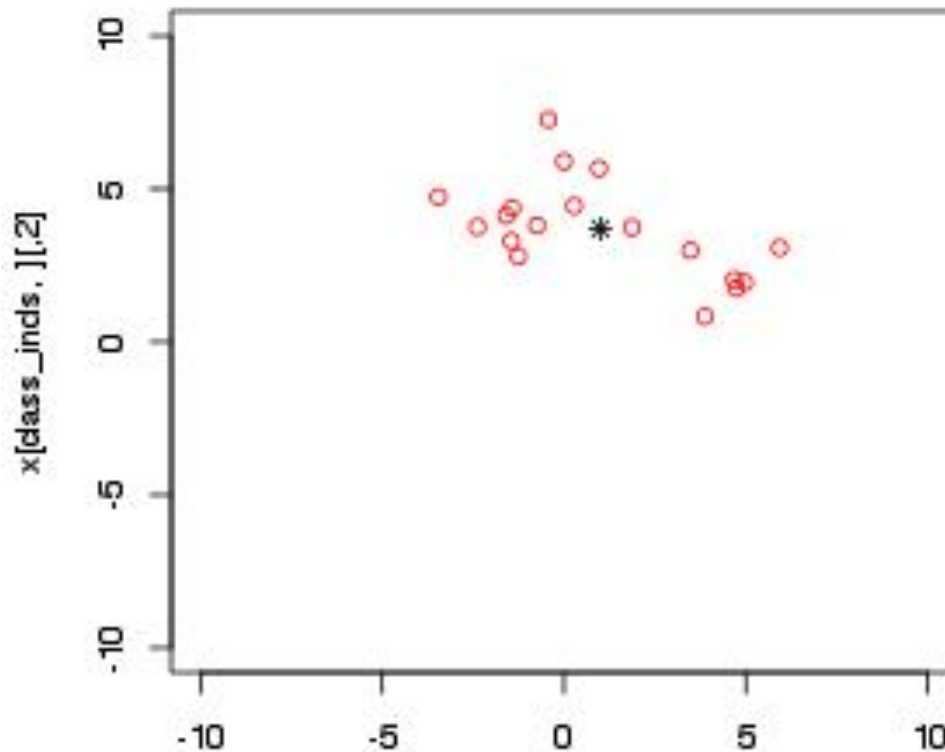for (num_k in 1:10) {
Kres=kmeans(X,num_k,10,1);
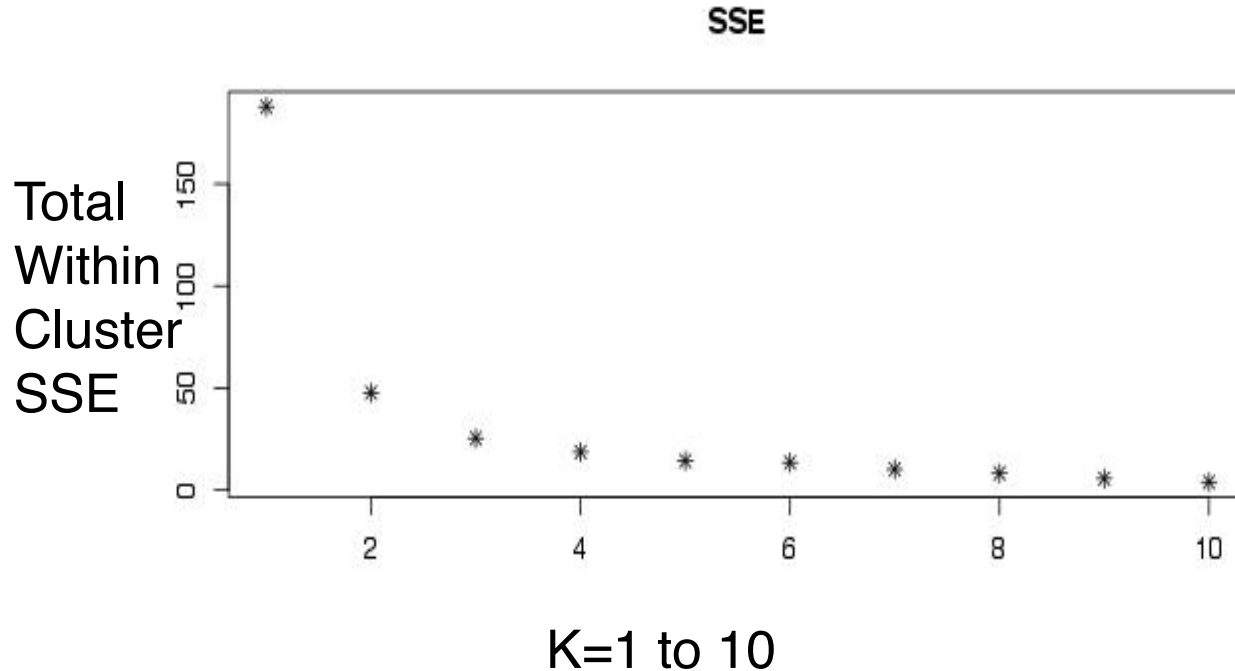
Save and then plot
Kres$tot.withinss

…

- Not much improvement after K=2 ("elbow")

Kmeans Example – more points

How many clusters should there be?

Choosing K for Kmeans

SSE

Total Within Cluster SSE

K=1 to 10

- Smooth decrease at K $\geq$ 2, harder to choose
- In general, smoother decrease => less structure

Kmeans Guidelines

- **Choosing K:**
  - "Elbow" in total-within-cluster SSE as K=1…N
  - Cross-validation: hold out points, compare fit as K=1…N
- **Choosing initial starting points:**
  - take K random data points, do several Kmeans, take best fit
- **Stopping:**
  - may converge to sub-optimal clusters
  - may get stuck or have slow convergence (point assignments bounce around), 10 iterations is often good

Kmeans Example: uniform dist.

Choosing K - uniform

Total Within Cluster SSE

K=1 to 10
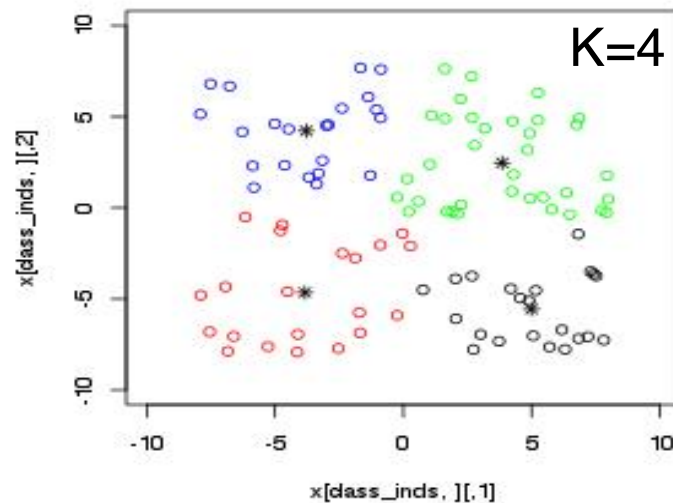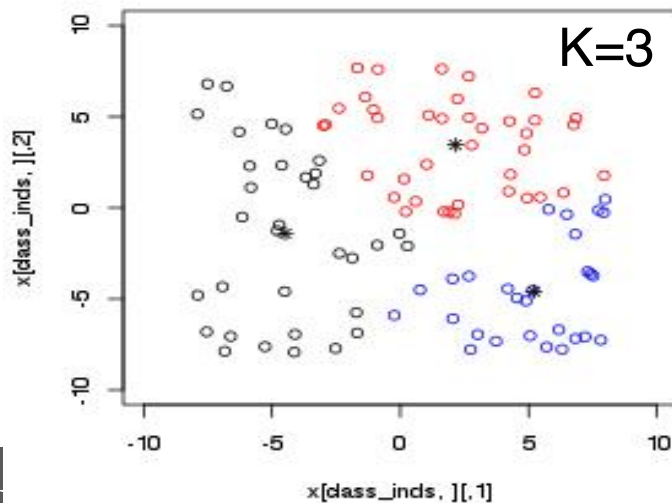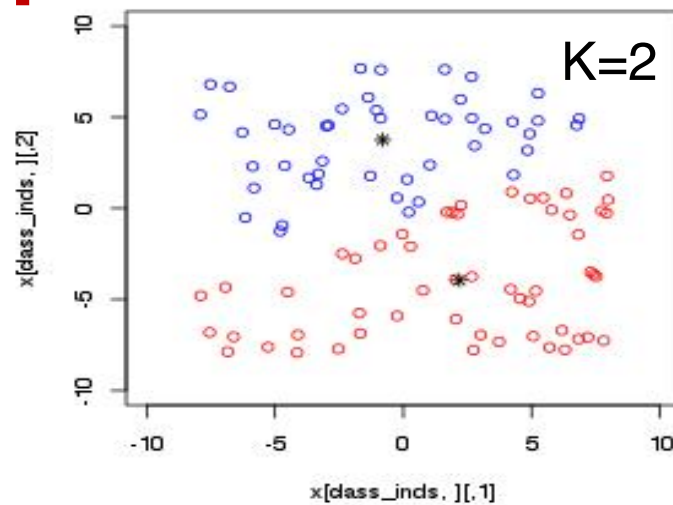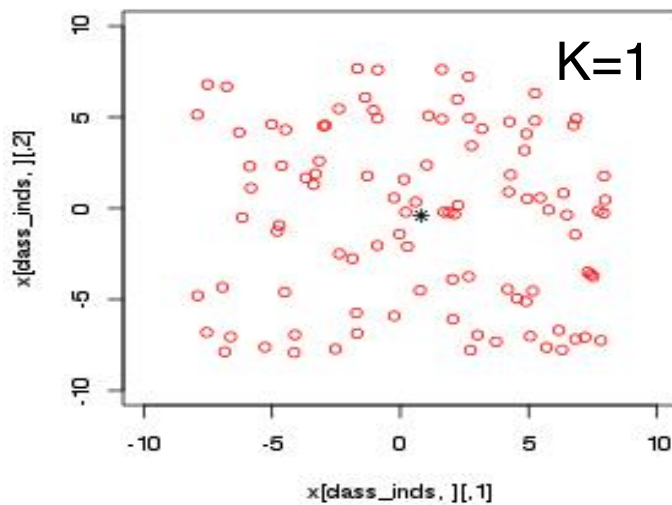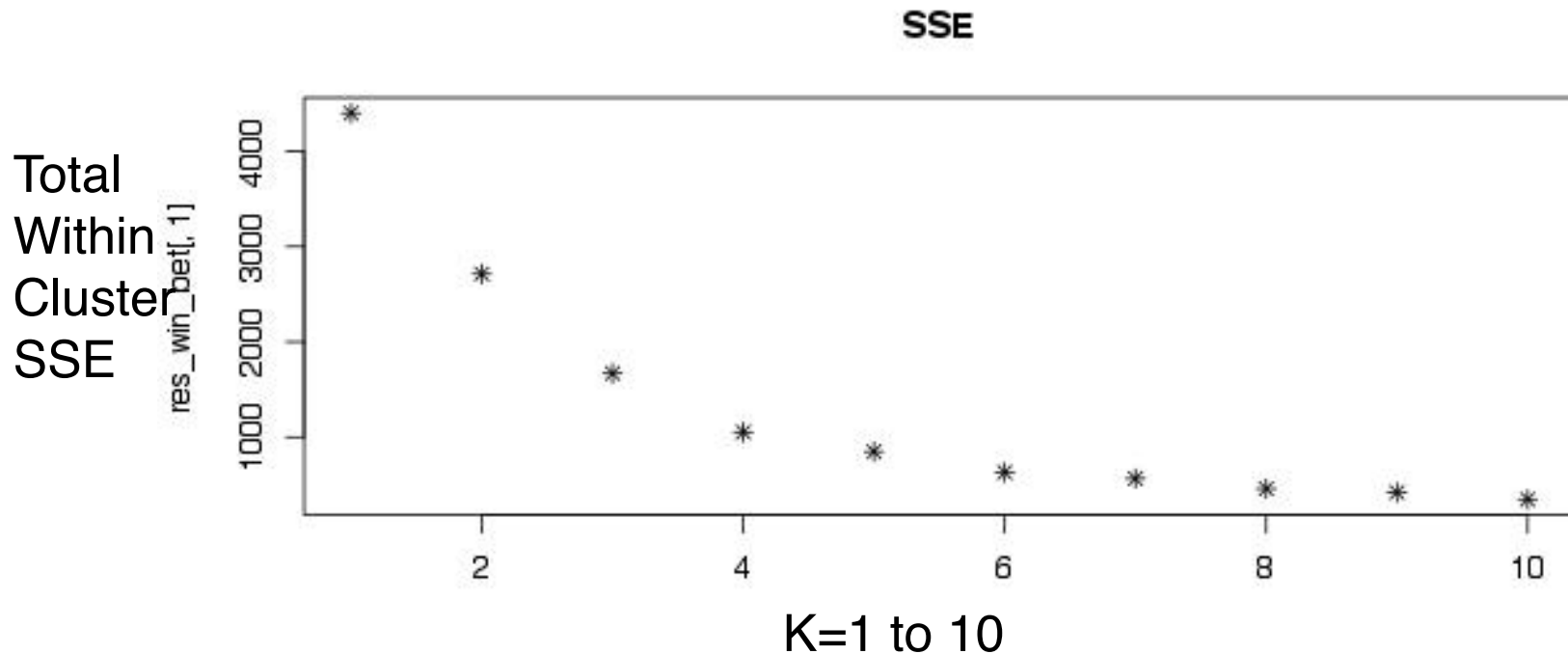
- Smooth decrease across K => less structure

Kmeans Clustering Issues

- **Scale:**
  - Dimensions with large numbers may dominate distance metrics (so can be good to normalize or scale data)

- **Outliers:**
  - Outliers can pull cluster mean

    (K-mediods uses median instead of mean)

Soft Clustering Methods

- **Fuzzy Clustering**
  - Kmeans with weighted assignments to all clusters
  - Weights depend on relative distance
  - Find min weighted SSE
- **Expectation-Maximization:**
  - Initialize a mixture of multivariate Gaussian distributions
  - Find means, variances, and mixture weights that maximize probability of data

Kmeans with unequal cluster variance and/or size
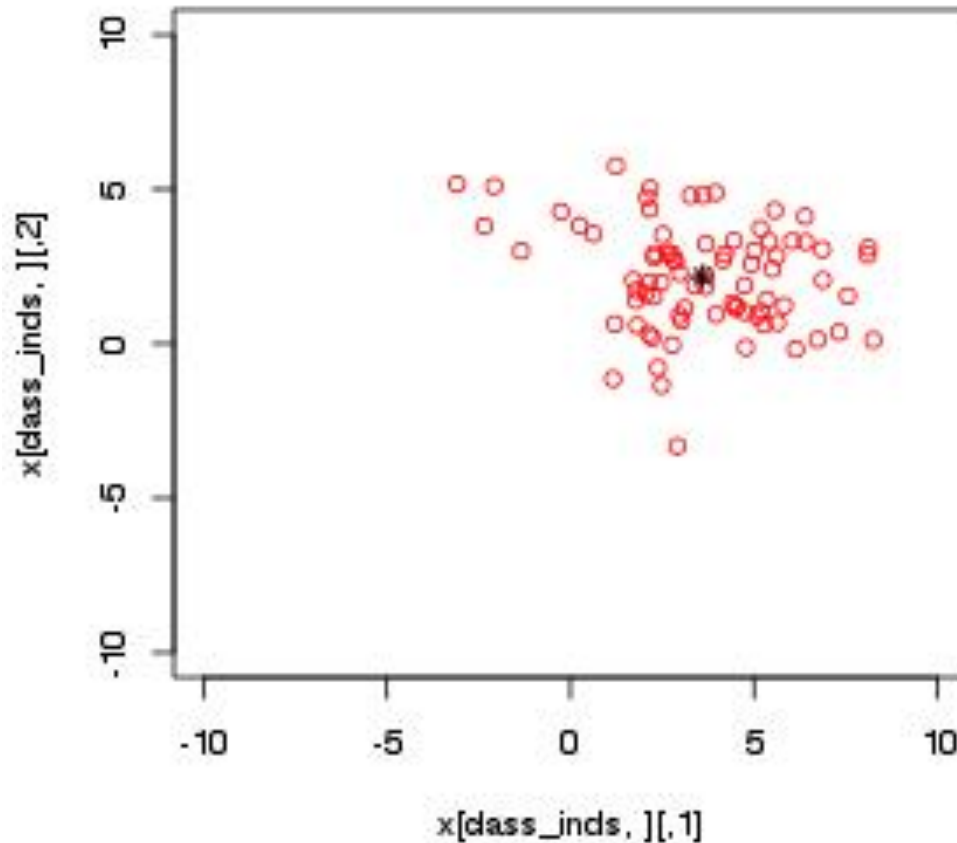
Can you guess K?

Kmeans – unequal cluster variance
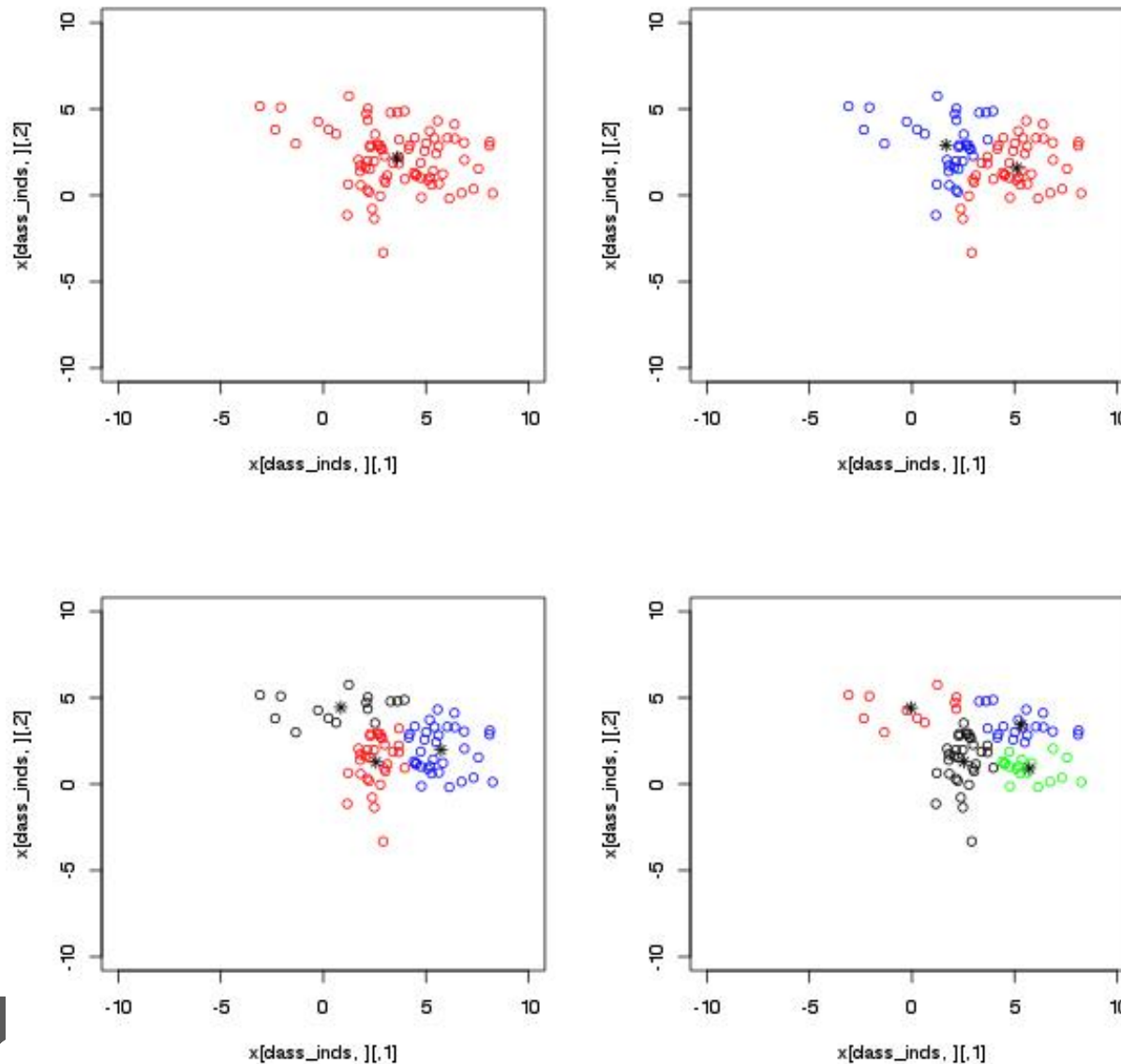
Choosing K – unequal distributions

SSE

Total Within Cluster SSE

K=1 to 10
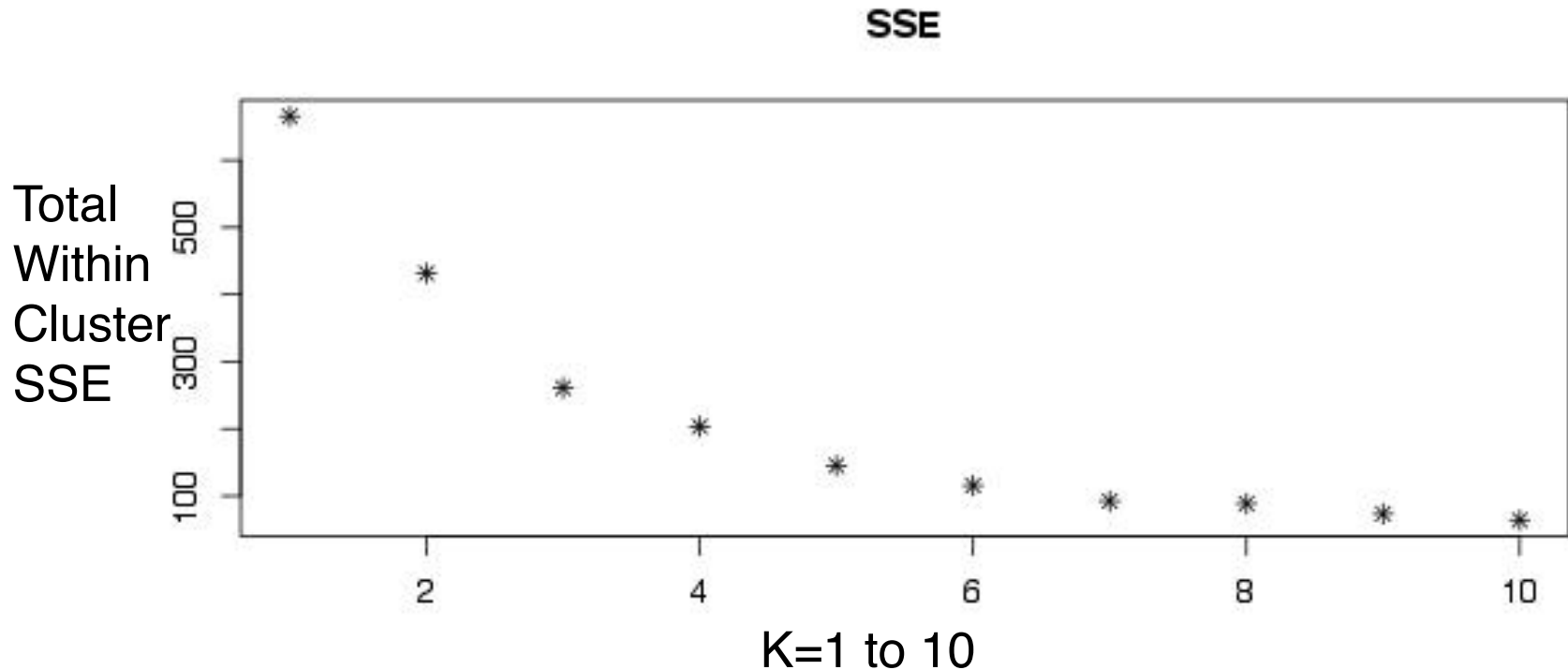
- Smooth decrease across K => less structure

EM clustering

Classification
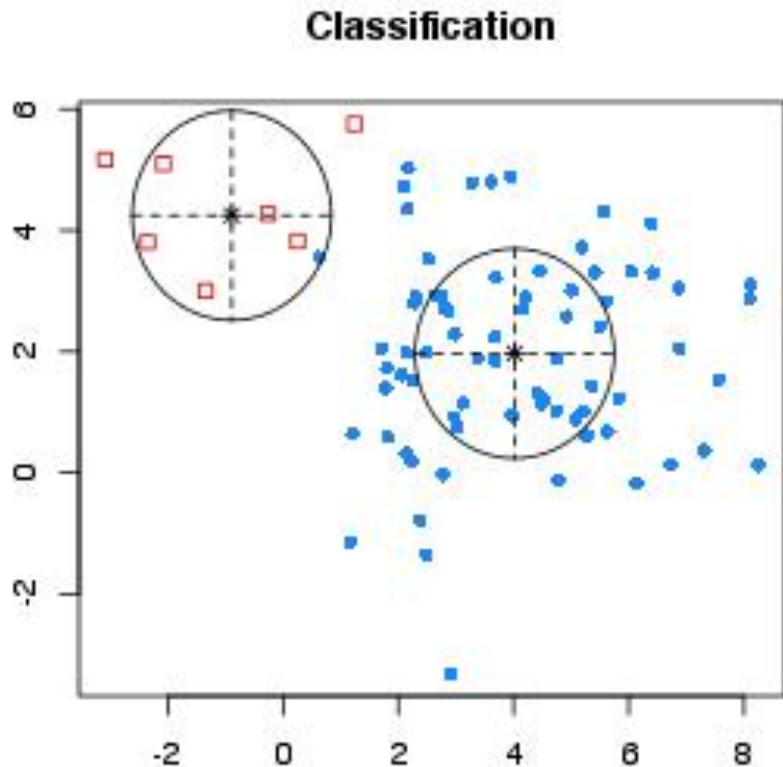
- Selects K=2
  (either by Information Criterion=
  min of SSE+ K*logN,
  Or by cross-validation)

- Handles unequal variance
  and/or size

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

Kmeans computations

- **Distance of each point to each cluster center**
  - For N points, D dimensions: each loop requires $N*D*K$ operations

- **Update Cluster centers**
  - only track points that change, get change in cluster center

- **But for EM errors to each cluster center update a probability function**

Kmeans vs EM performance

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

15 min

Wall
Time
(secs)   10 min

EM: 1000 pts

Kmeans:1000 pts

1K   4K   8K

Number of Dimensions (i.e. columns in data matrix)
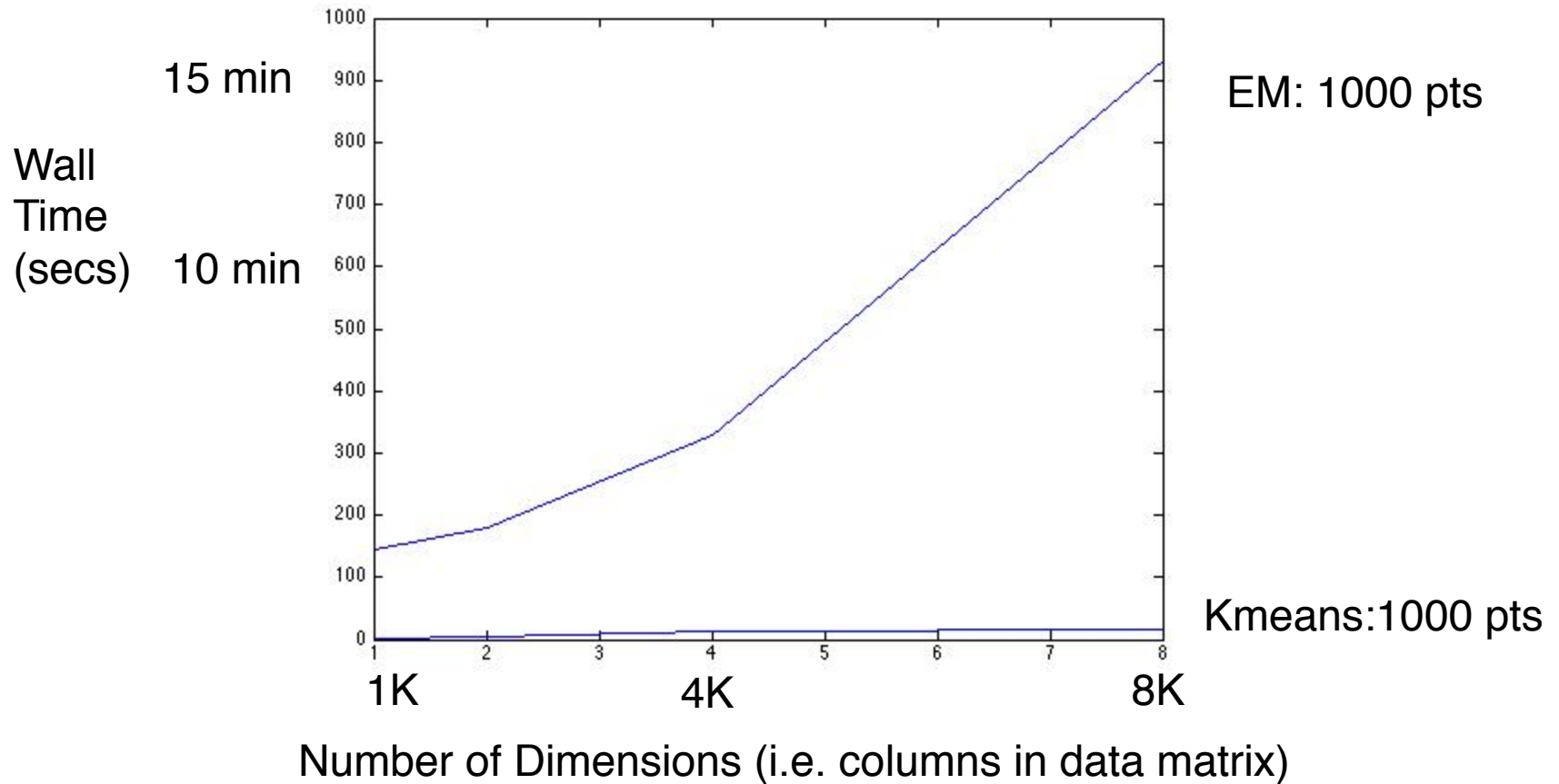
Other distance measures

- Cosine: take angle difference (good for sparse vectors)

D

A

*C is closer to A
because ABCº<ABDº*

C

B (origin)
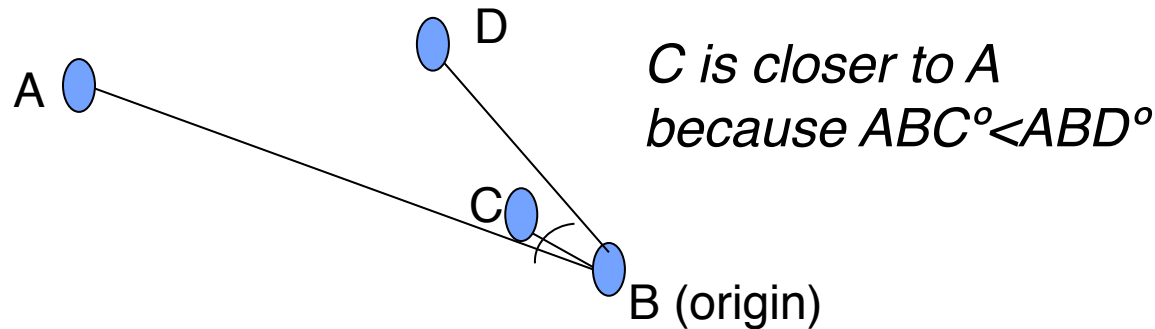
- Mahalanobis: dimensions rescaled by variance

- Jaccard (over sets A,B): 1- (|A∩B| / |AUB|)

Other distance measures

- Hamming distance: count 1 if values different

     e.g. appropriate for binary strings

$$010100110$$
$$000100010$$

↑   ↑

Total difference is 2

Kmeans big data example

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

  (UCI Machine Learning repository)

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

a and ... ... zebra zoo
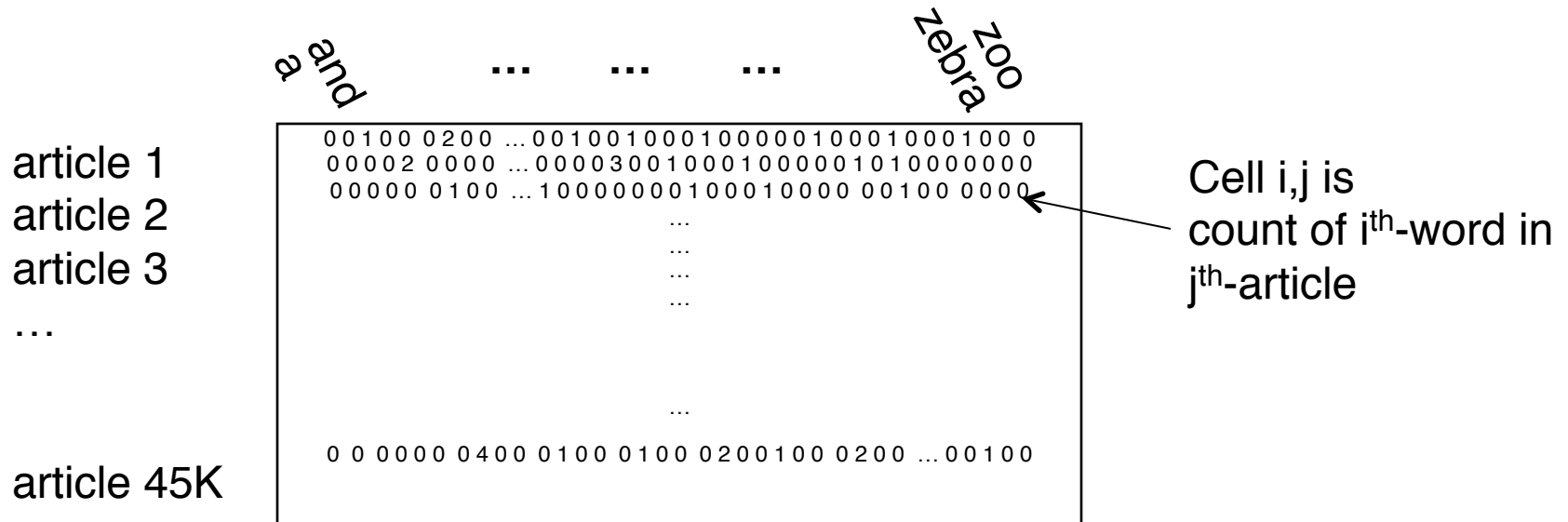
article 1
article 2
article 3
…

article 45K

```
0 0 1 0 0 0 2 0 0 ... 0 0 1 0 0 1 0 0 0 1 0 0 0 0 0 1 0 0 1 0 0 0 1 0 0 0
0 0 0 0 2 0 0 0 0 ... 0 0 0 0 3 0 0 1 0 0 0 1 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0
0 0 0 0 0 0 1 0 0 ... 1 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0
                  ...
                  ...
                  ...
                  ...

                  ...
0 0 0 0 0 0 0 4 0 0 0 1 0 0 0 1 0 0 0 2 0 0 1 0 0 0 2 0 0 ... 0 0 1 0 0
```

Cell i,j is
count of ith-word in
j^{th}-article

Kmeans results

cluster means shown with coordinates determining fontsize

7 viable clusters found

Kmeans for image segmentation

R snippet
get packages
read 1024X718X3 RGB image
convert to matrix 1024*718 X 3
Choose K by trial and error
run Kmeans and display
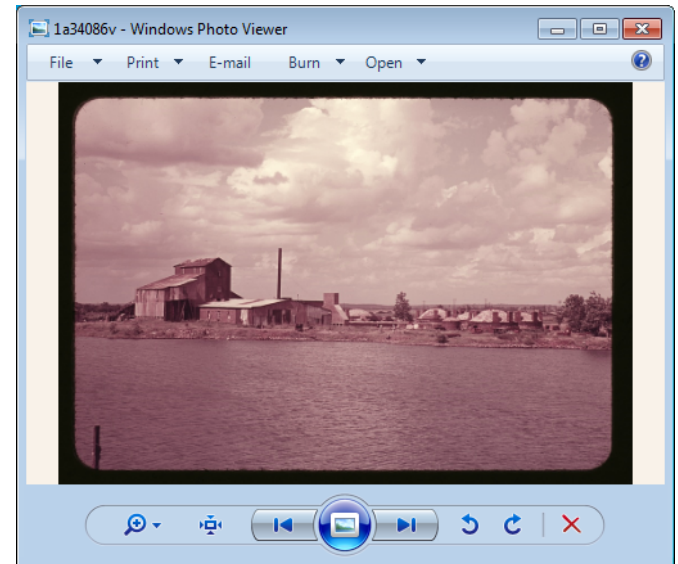
```
install.packages('ripa')
library('ripa')

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)
```

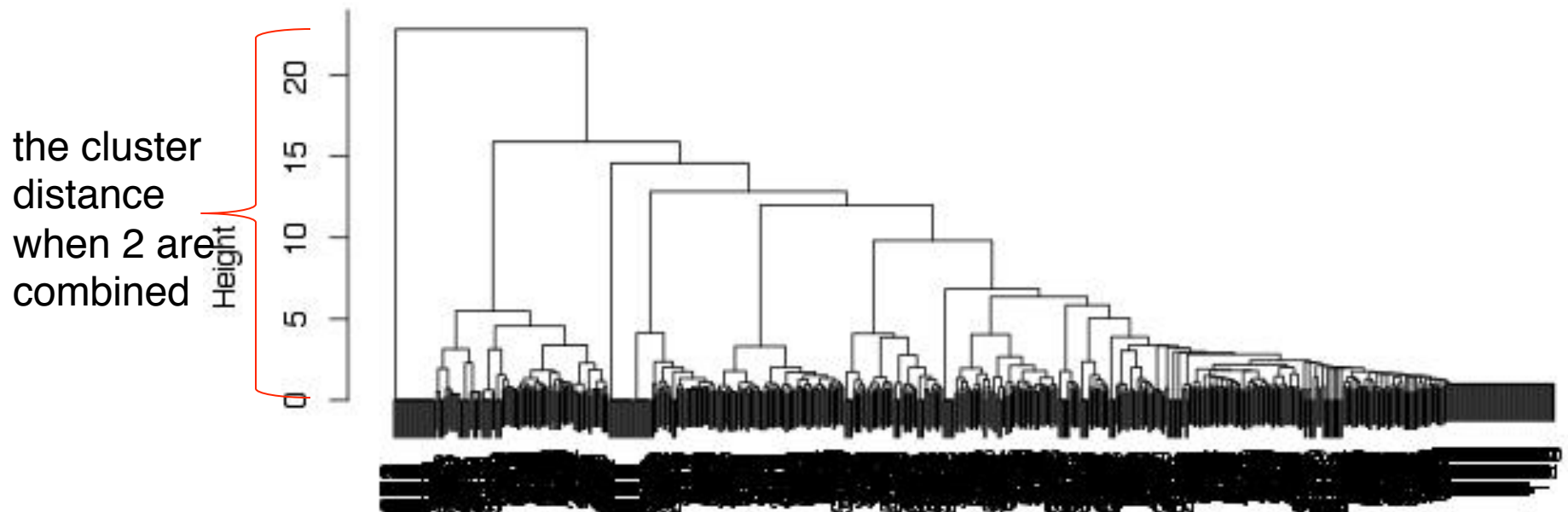# Other Clustering Methods

Hierarchical Clustering

- **hclust with "Ward" distance gives spherical clusters**

Cluster Dendrogram

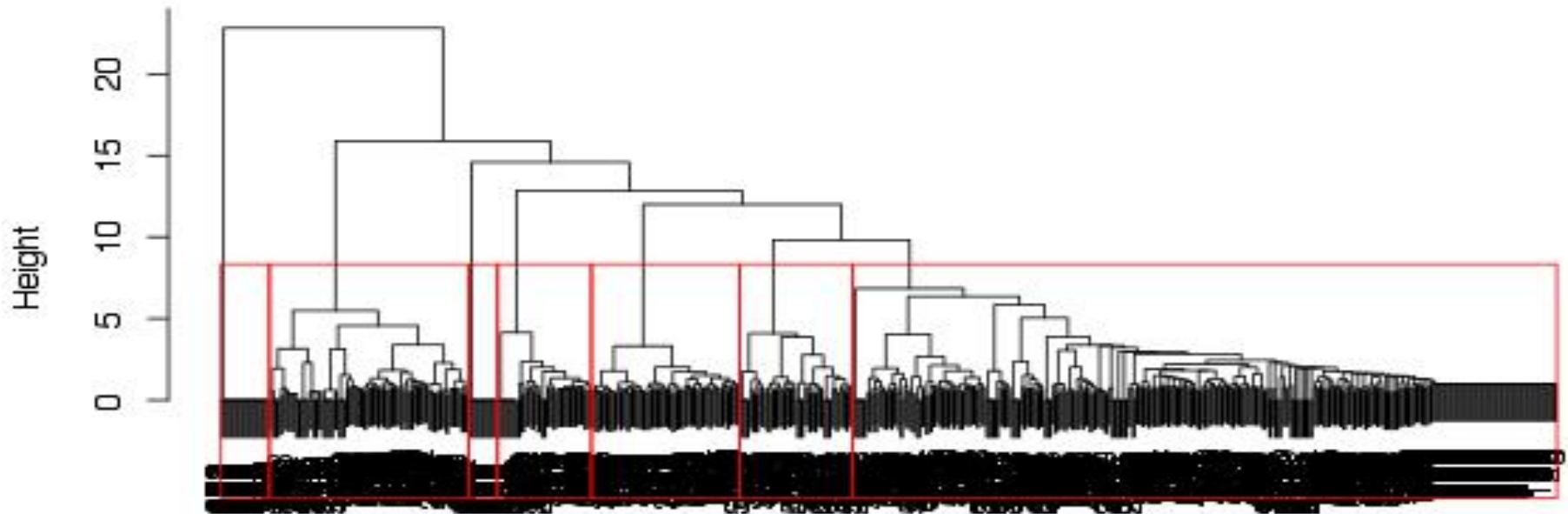the cluster distance when 2 are combined

d2use
hclust (*, "ward")

Hierarchical Clustering

- **Where height change looks big, cut off tree**

```
groups <- cutree(fit, k=7)
rect.hclust(fit, k=7, border="red")
```
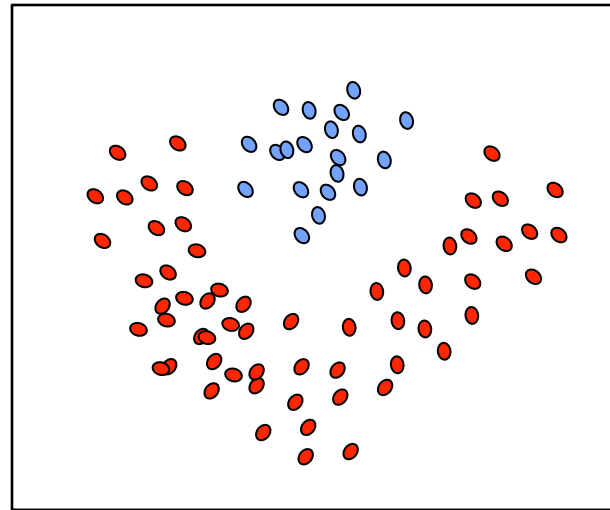

Cluster Dendrogram

Other Clustering

- **Density based clustering**

  build neighborhoods around seed points
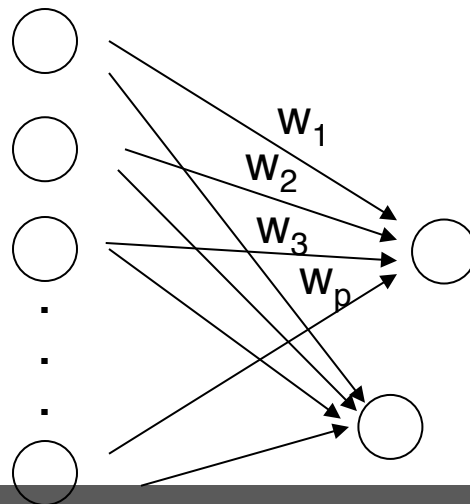
  link neighborhoods

  Results in arbitrary cluster shapes, good for image and spatial clustering

Other Clustering

- **Neural Network Based (e.g.)**

  initialize weights to coordinate values for a seed point

  set input nodes to coordinate values for data points

  get best match to seed for each data point and adjust weights toward the data point

w_1
w_2
w_3
w_p

Target node(s), starts as a seed point and ends up as a cluster mean