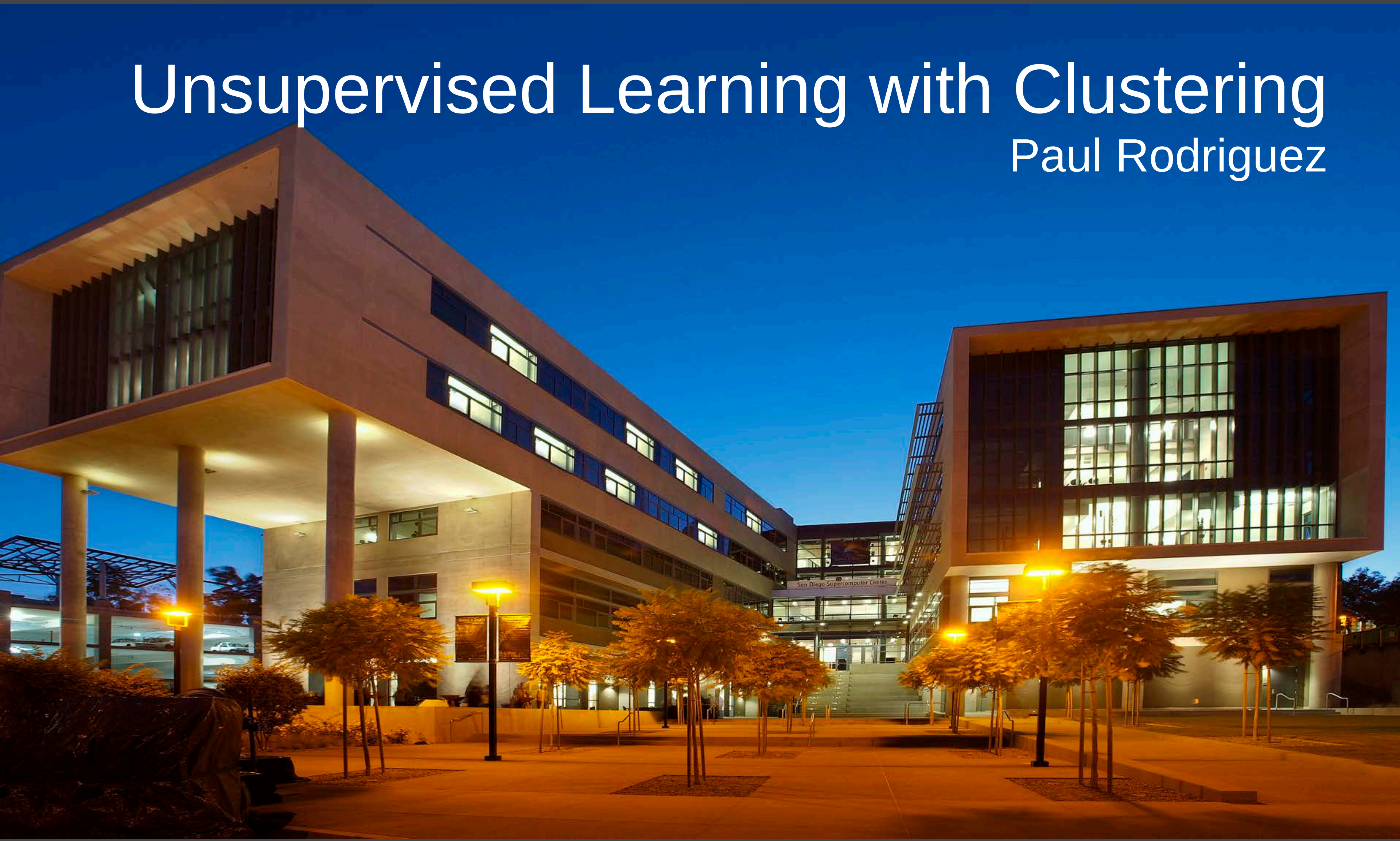
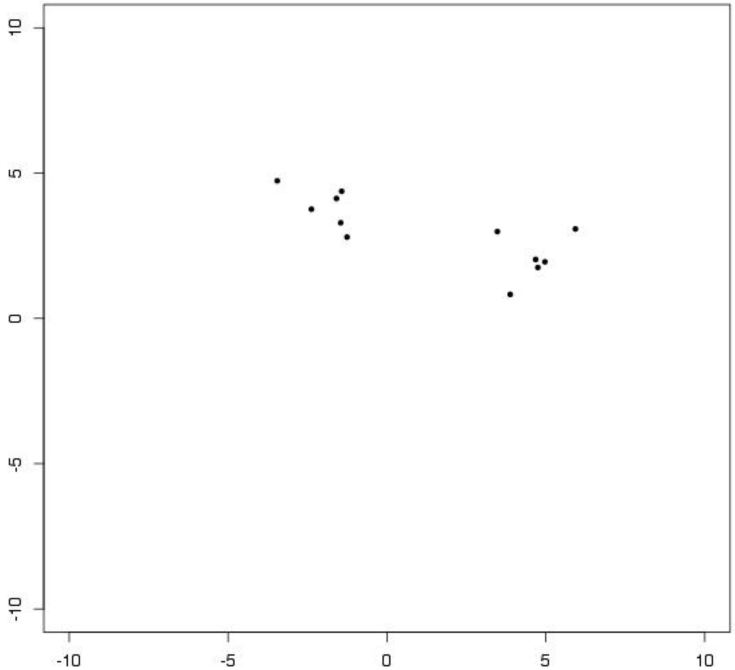
Unsupervised Learning with Clustering

Paul Rodriguez



Clustering Idea

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



X_2

X_1

Essential R commands:

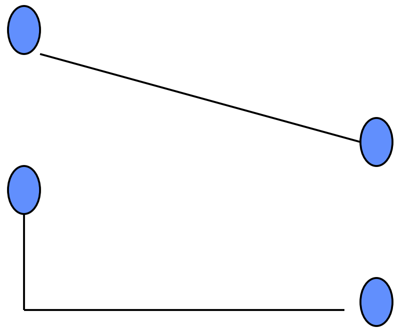
```
D     =rnorm(12,0,1) #generate 12
                     #random normal
X1    =matrix(D,6,2) #put into 6x2 matrix
X1[,1]=X1[,1]+4;     #shift center
X1[,2]=X1[,2]+2;

#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
  - Use the cluster assignments as a summary of the data

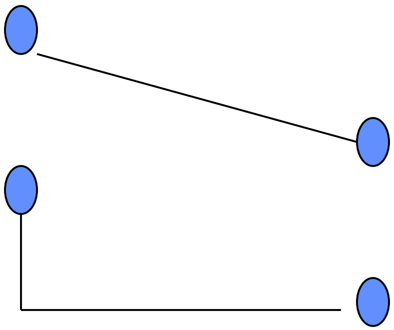
Clustering Objective

- **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**



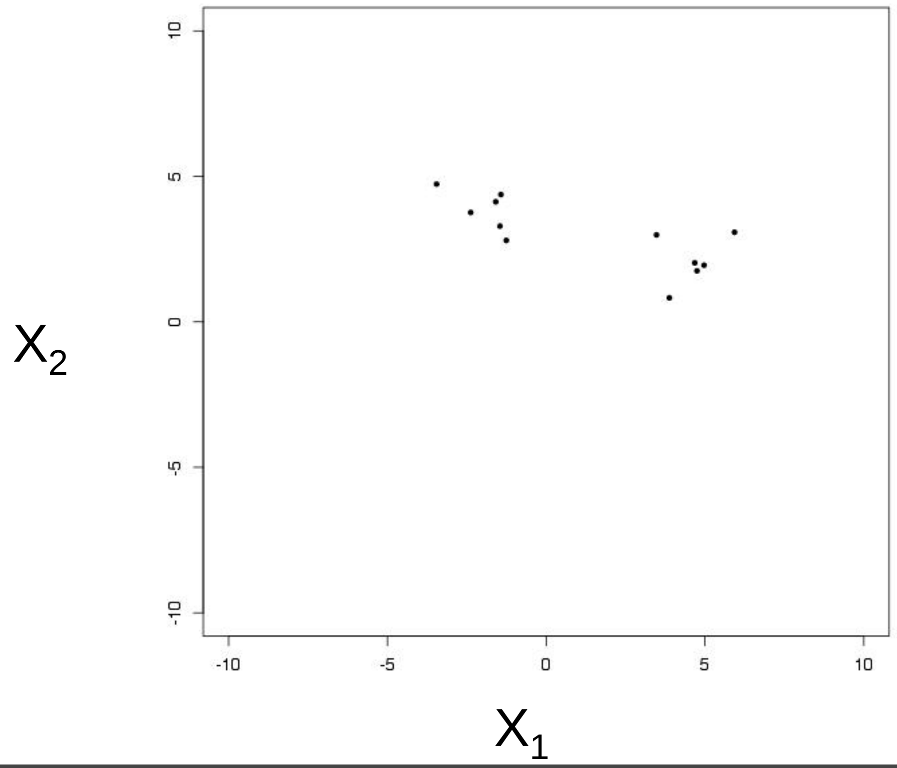
  - Euclidean distance =
    sqrt[(a1 - b1)^2+ (a2 – b2)^2+...)]
  - Manhattan distance
    [|a1 - b1|+ |a2 – b2|+...)]

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?

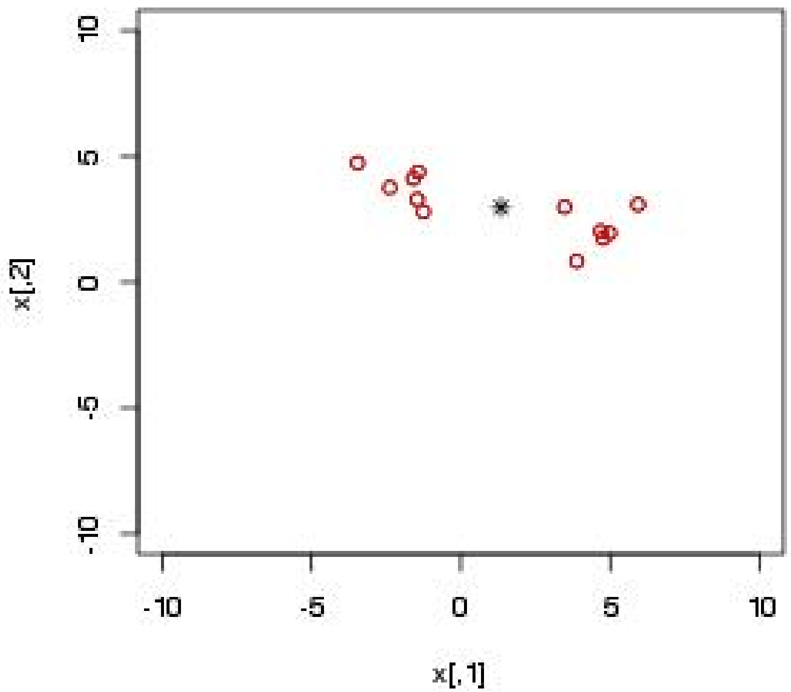
Kmeans Example

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



Kmeans Example

For K=1, the overall mean minimizes Sum Squared Error (SSE), aka Euclidean dist. squared

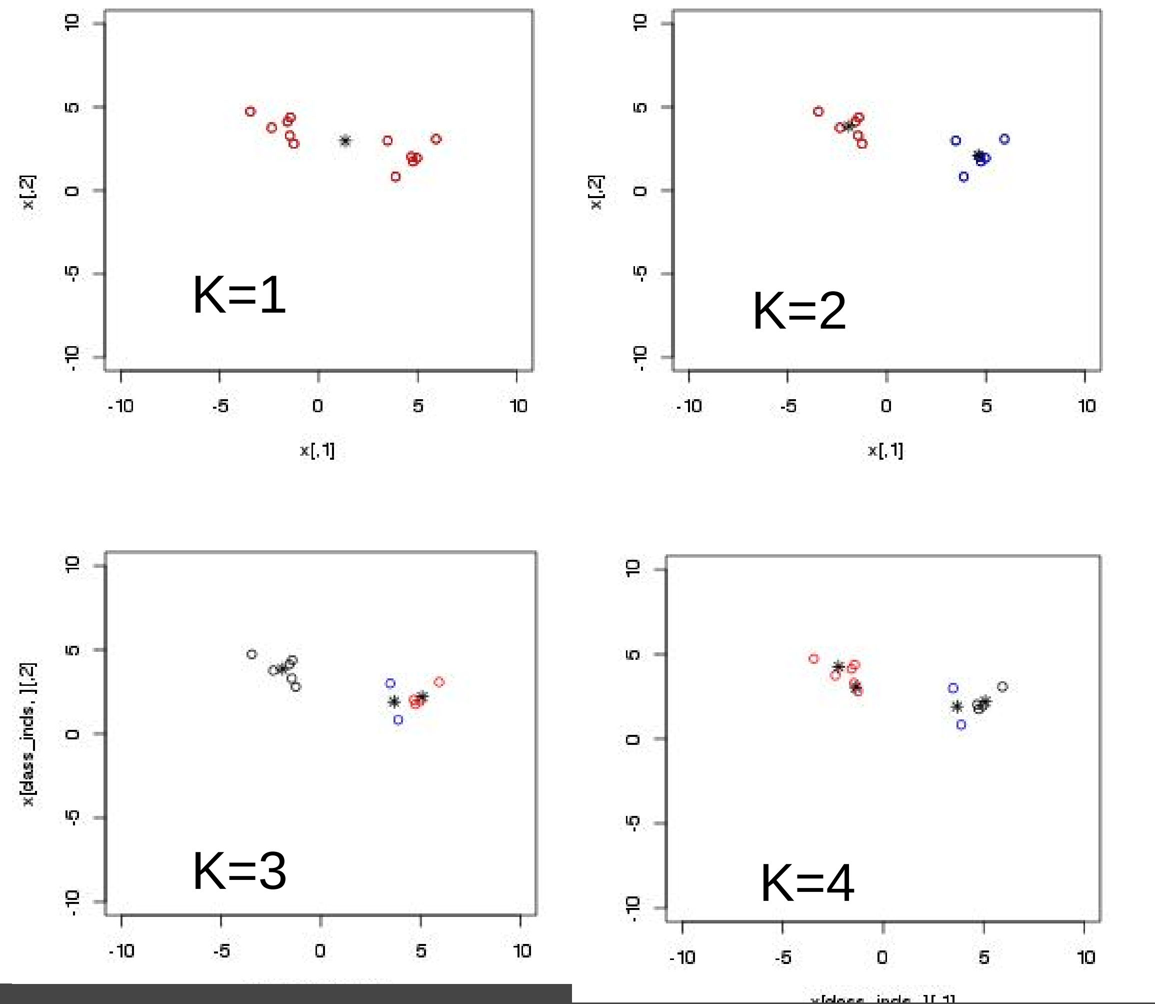


Essential R commands:
Kresult = kmeans(X,1,10,1)

#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

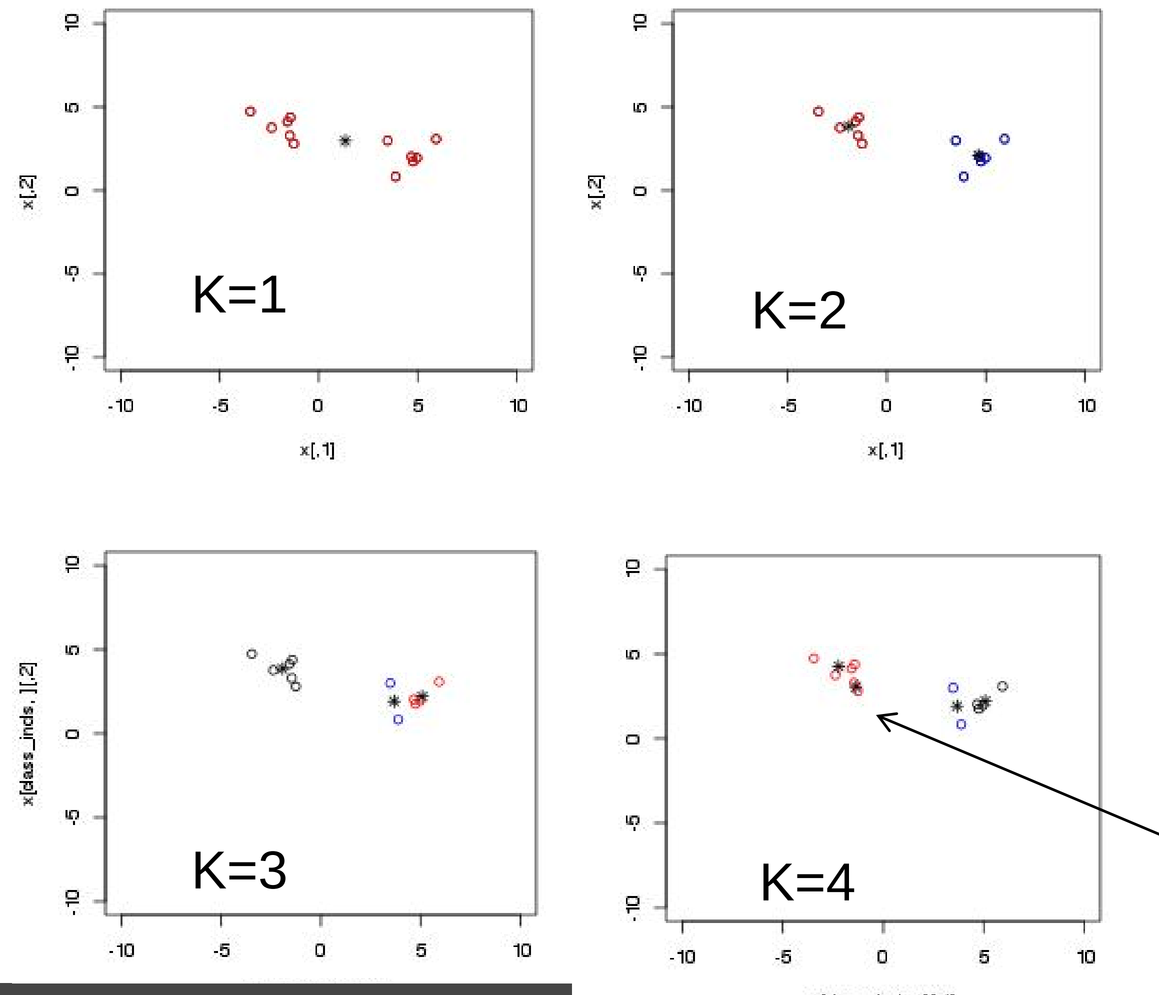


Essential R commands:
inds=which(Kresult$cluster==K)

plot(X[inds,],col2use=“red”);

…

Kmeans Example



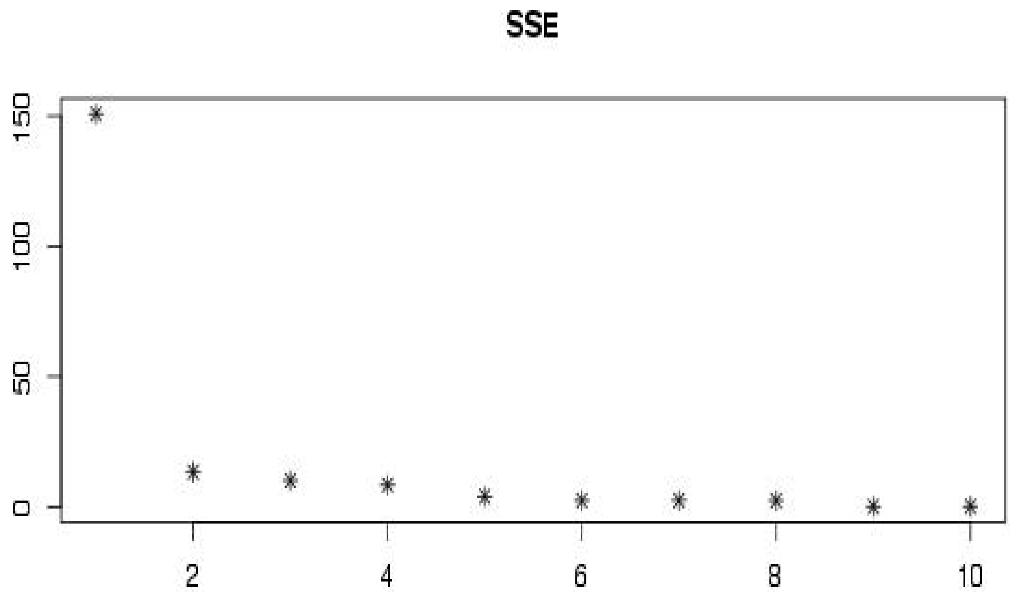
Essential R commands:
inds=which(Kresult$cluster==K)

plot(X[inds,],col2use=“red”);

…

As K increases individual points get a cluster

Choosing K for Kmeans



Total Within Cluster SSE

K=1 to 10

Essential R commands:

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

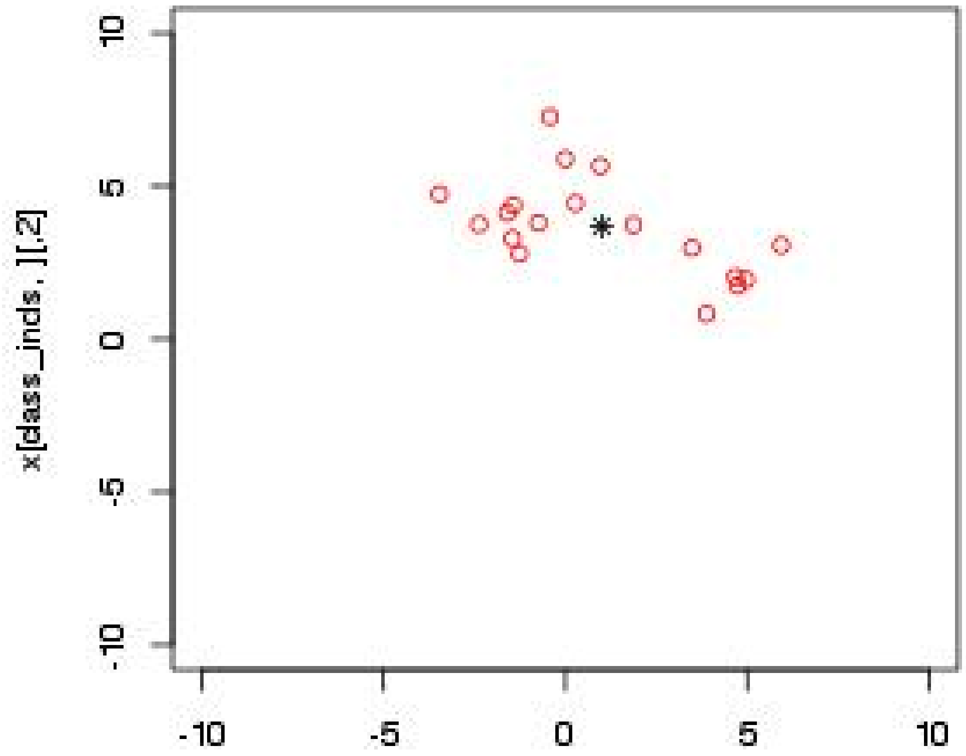
Save and then plot
Kres$tot.withinss

…

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

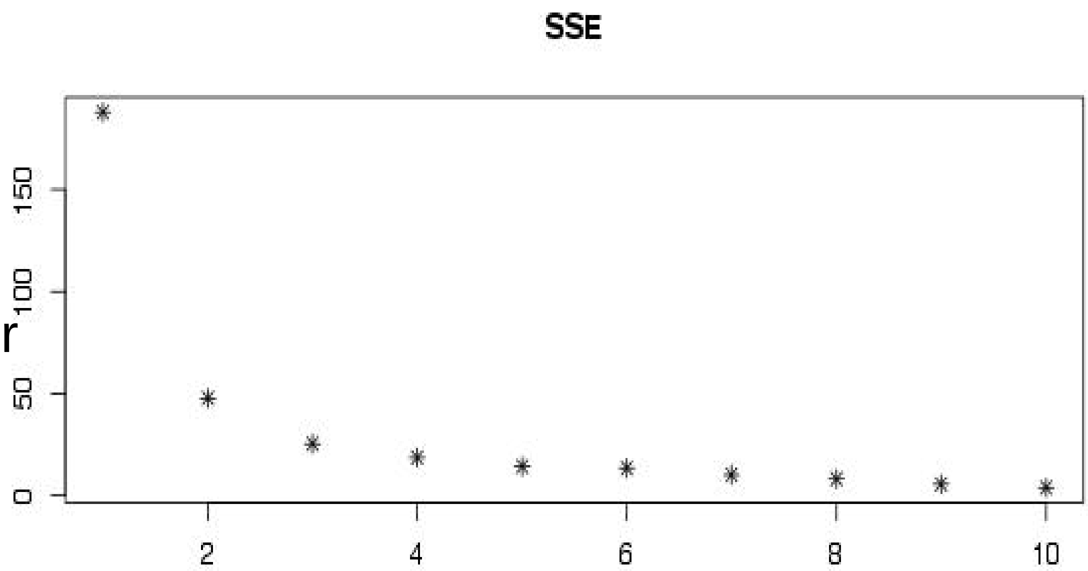
Kmeans Example – more points

How many clusters should there be?



Choosing K for Kmeans

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

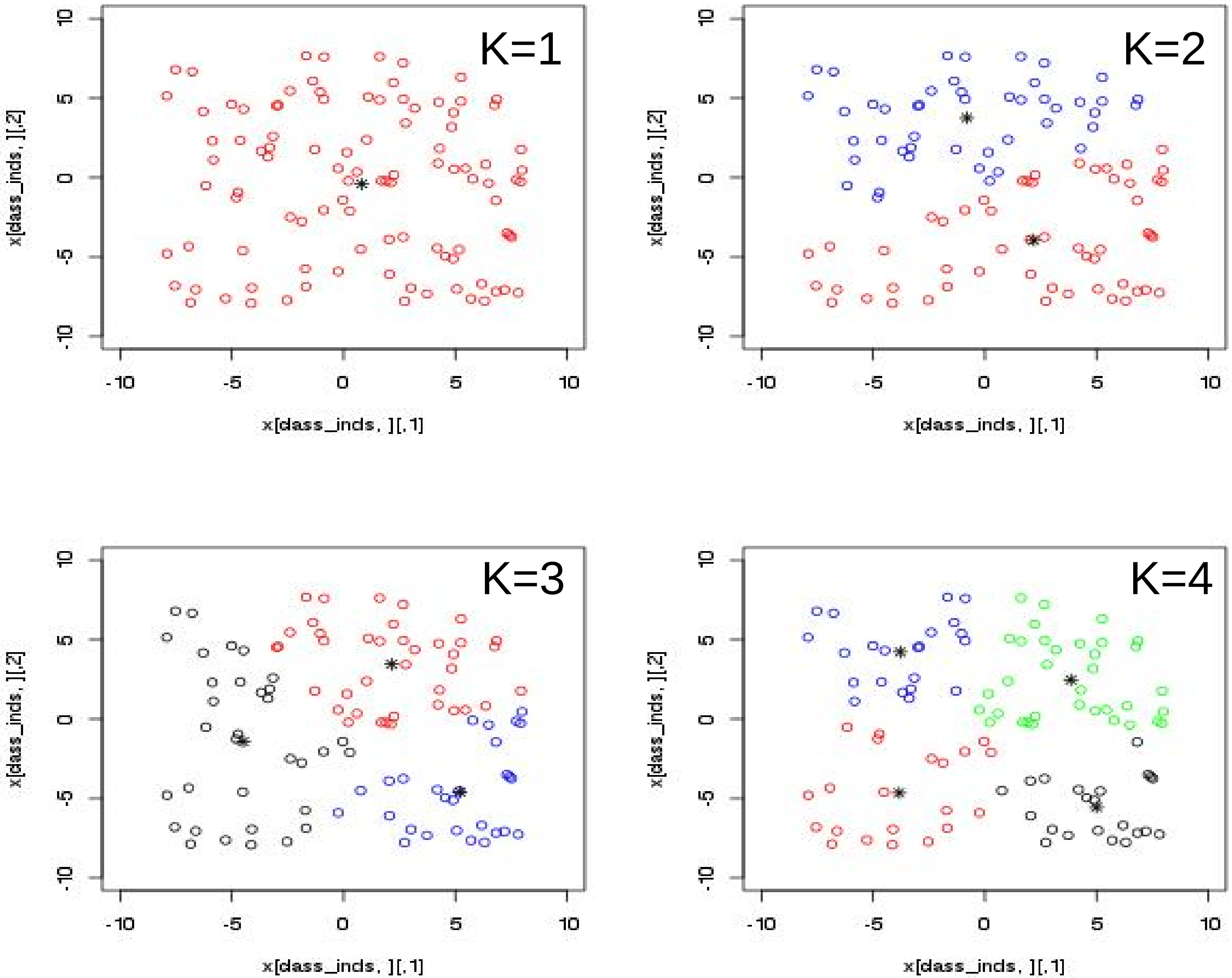
- **Initial starting points and convergence:**

  Kmeans++ algorithm selects good initial clusters that also helps convergence

  10 iterations often good

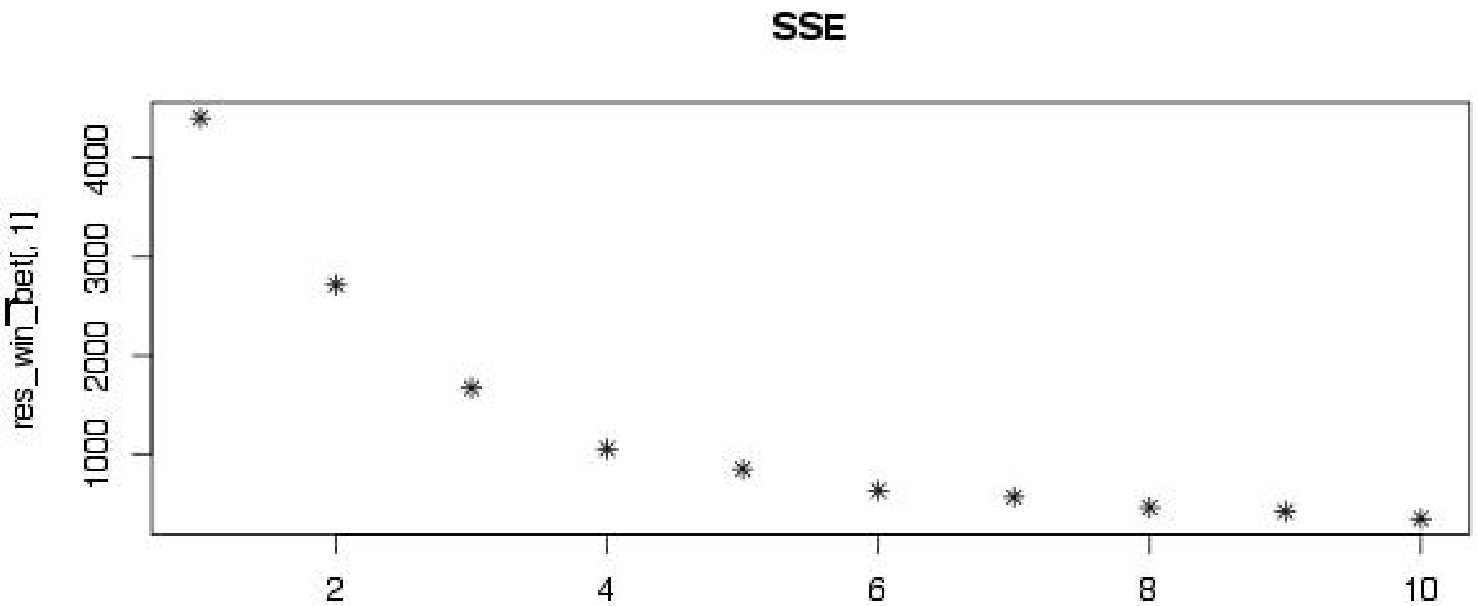
  Can also run several times and choose best result

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)

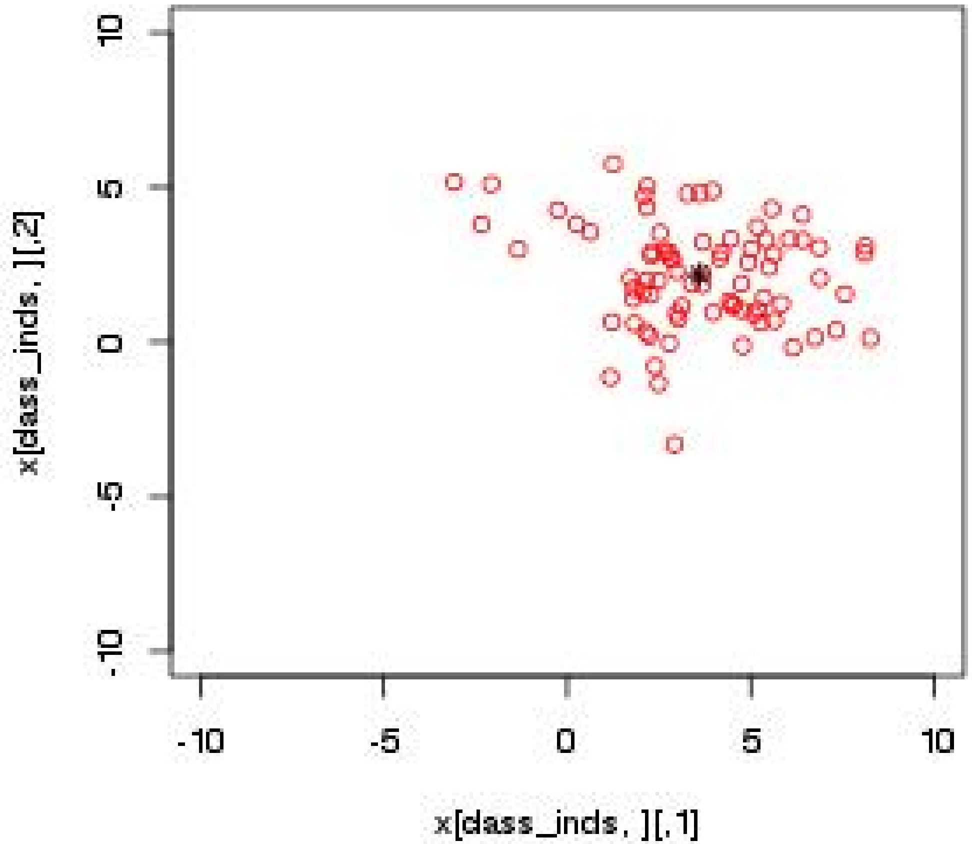
- **Outliers:**
  - Outliers can pull cluster mean

    (K-mediods uses median instead of mean)

Soft Clustering Methods

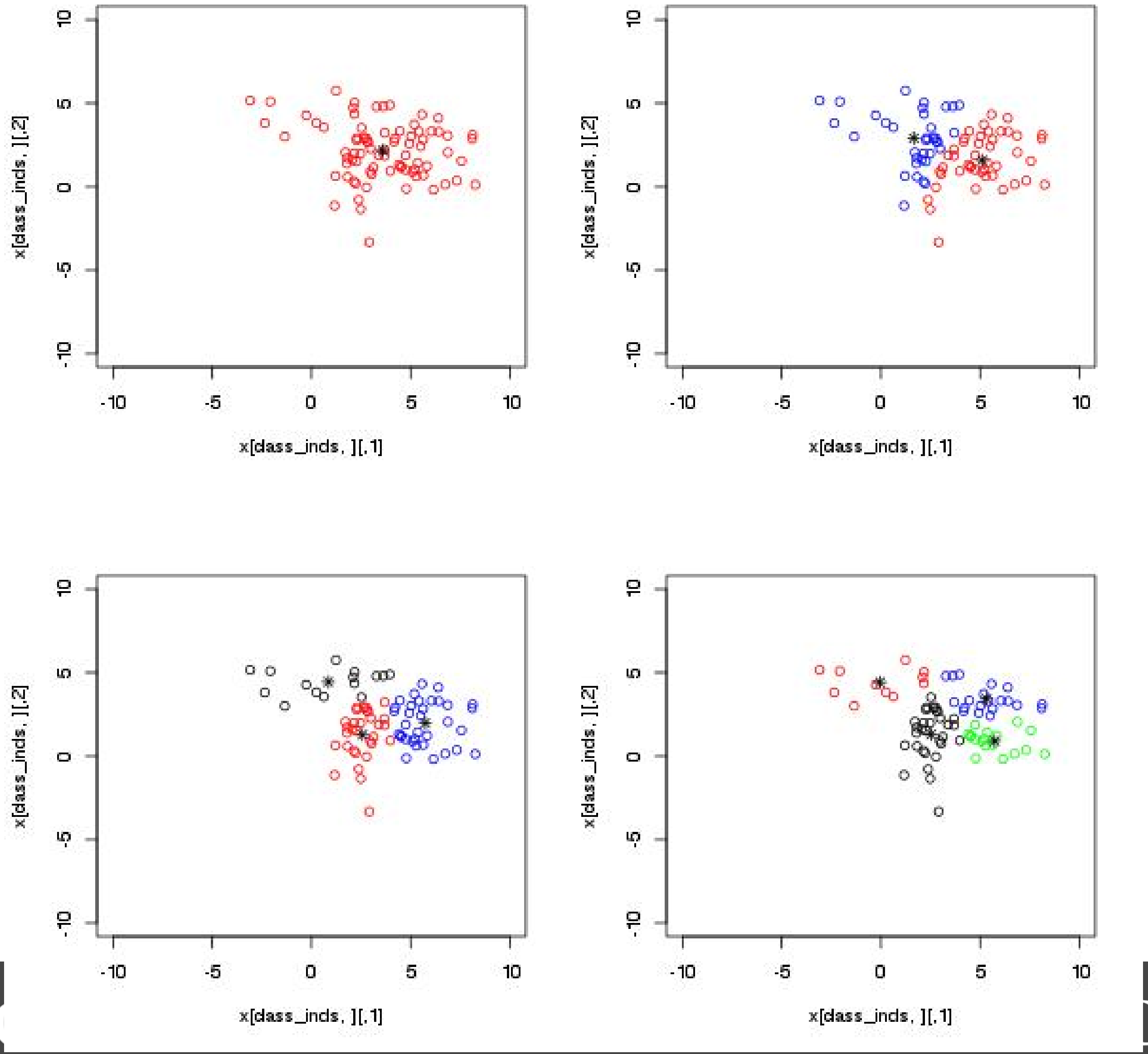
- **Fuzzy Clustering**
  - Kmeans with weighted assignments to all clusters
  - Weights depend on relative distance
  - Find min weighted SSE
- **Expectation-Maximization:**
  - Initialize a mixture of multivariate Gaussian distributions
  - Find means, variances, and mixture weights that maximize probability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

Kmeans with unequal cluster variance and/or size

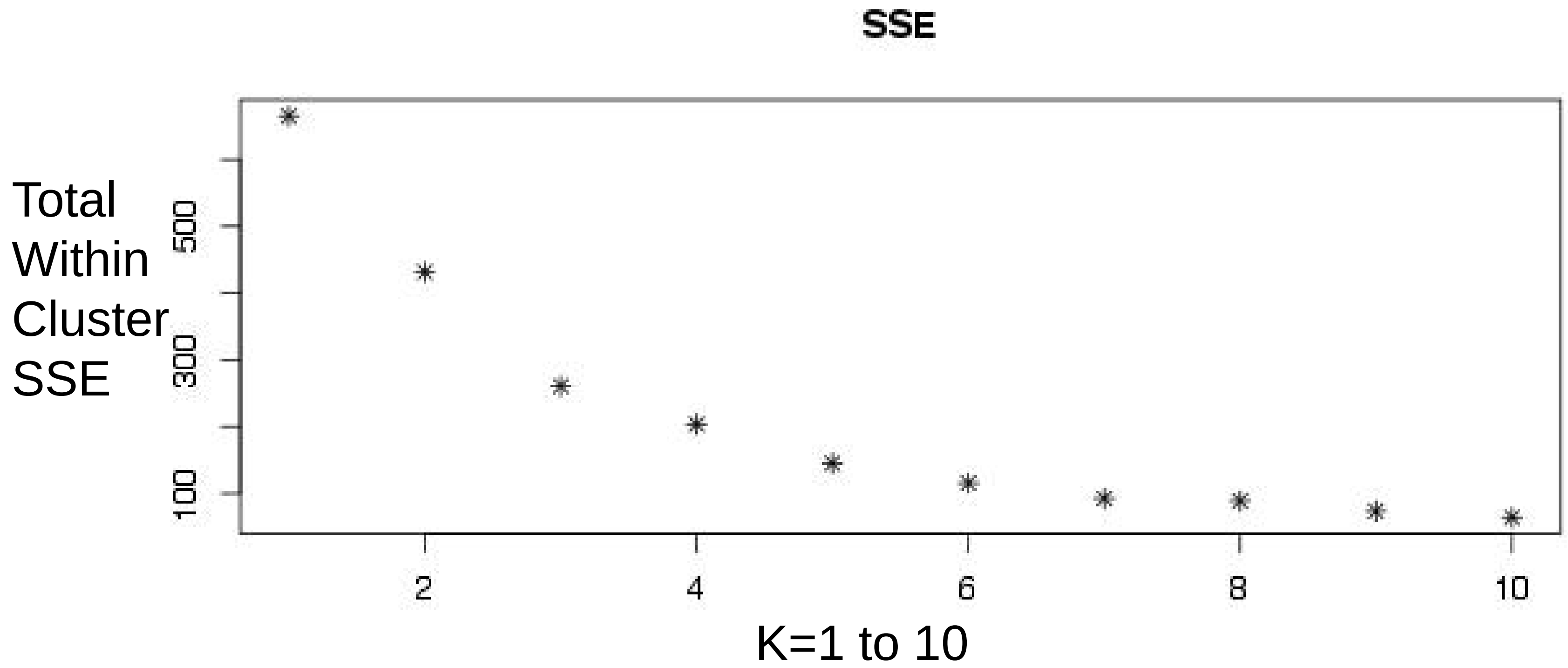


Can you guess K?

Kmeans – unequal cluster variance

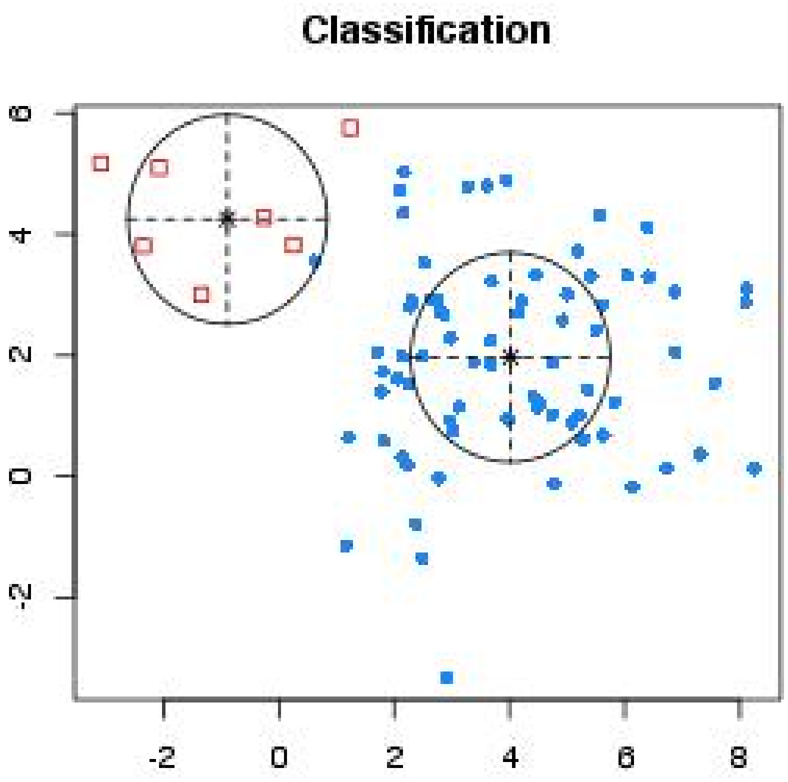


Choosing K – unequal distributions



- Smooth decrease across K => less structure

EM clustering



- 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

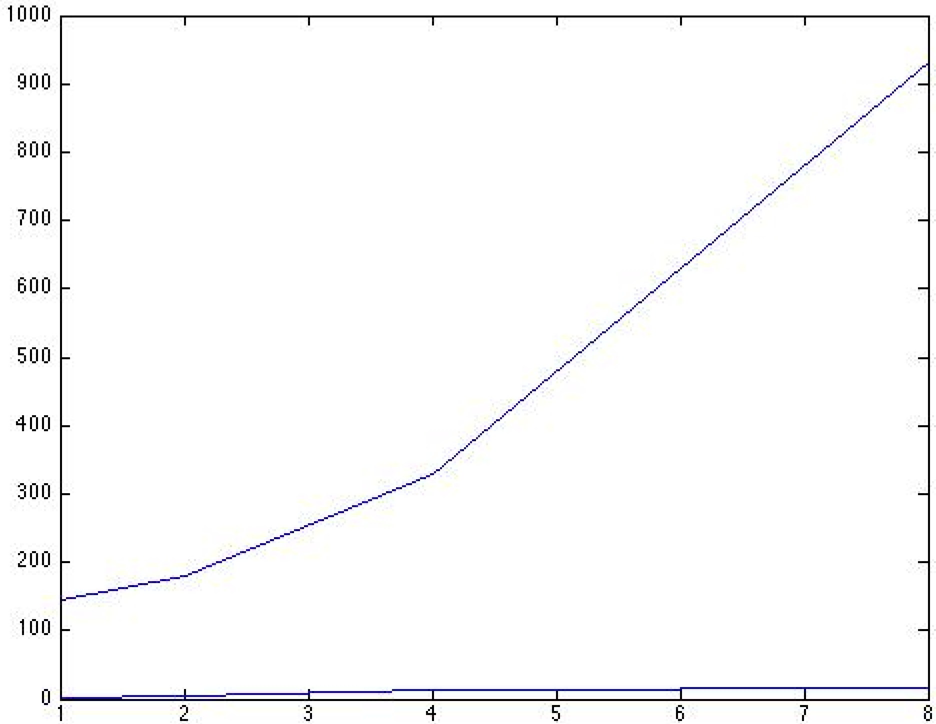
- **Distance of each point to each cluster center**
  - For *N* points, *D* dimensions: each loop requires *N*D*K* operations
- **Update Cluster centers**
  - only track points that change, get change in cluster center
- **But for EM errors to each cluster center update a probability function**

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

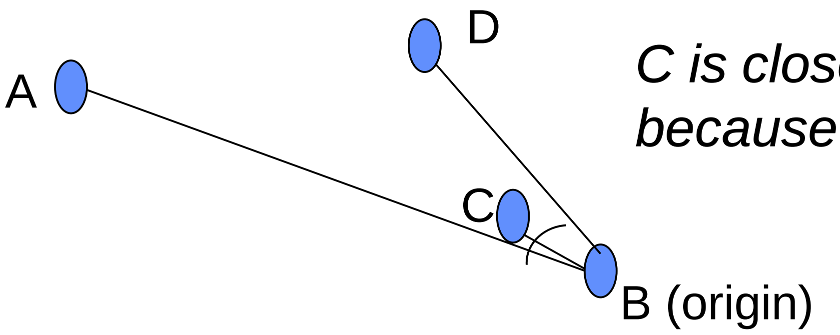
Kmeans:1000 pts

1K 4K 8K

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

Other distance measures

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



C is closer to A
because $ABC^{\circ} < ABD^{\circ}$

- Mahalanobis: dimensions rescaled by variance

- Jaccard (over sets A,B): $1- (|A \cap B| / |A \cup B|)$
  (e.g. sets of words in documents)

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)

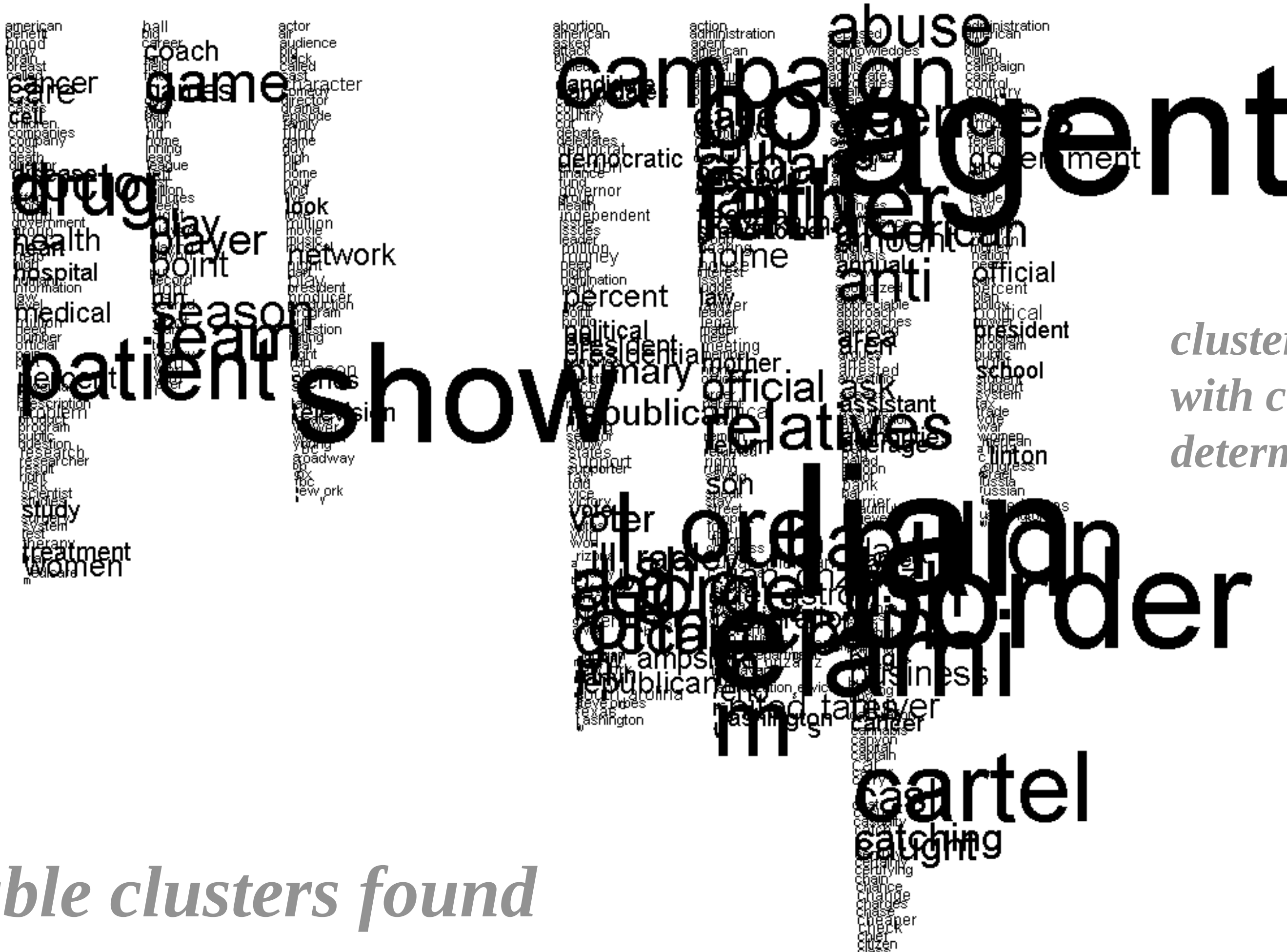
- **Full Data Matrix: 45Kx102K ~ 40Gb**

a and … … … zebra zoo

article 1 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 0 1 0 0 0 1 0 0 0
article 2 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
article 3 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
…
…
…
…
…
article 45K 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 i^{th}-word in j^{th}-article

Kmeans results



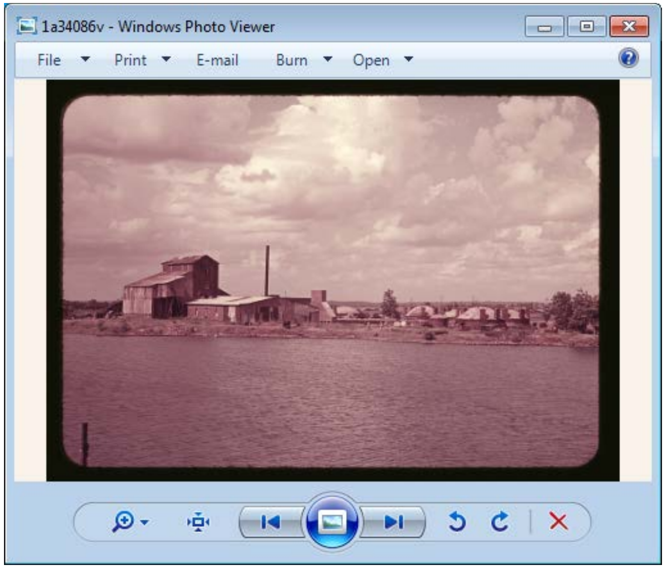
cluster means shown with coordinates determining fontsize

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)
```

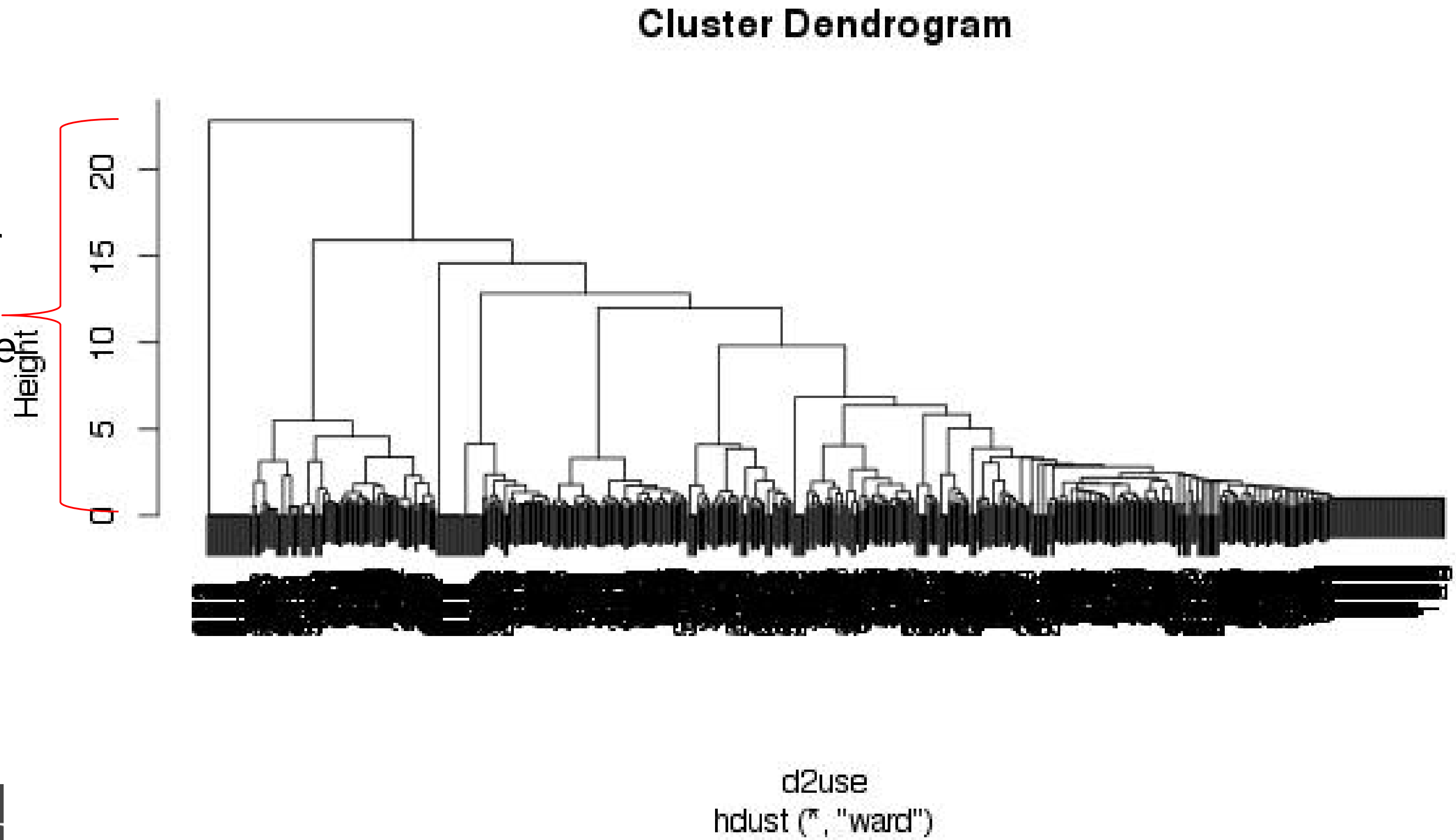


Other Clustering Methods

Hierarchical Clustering

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

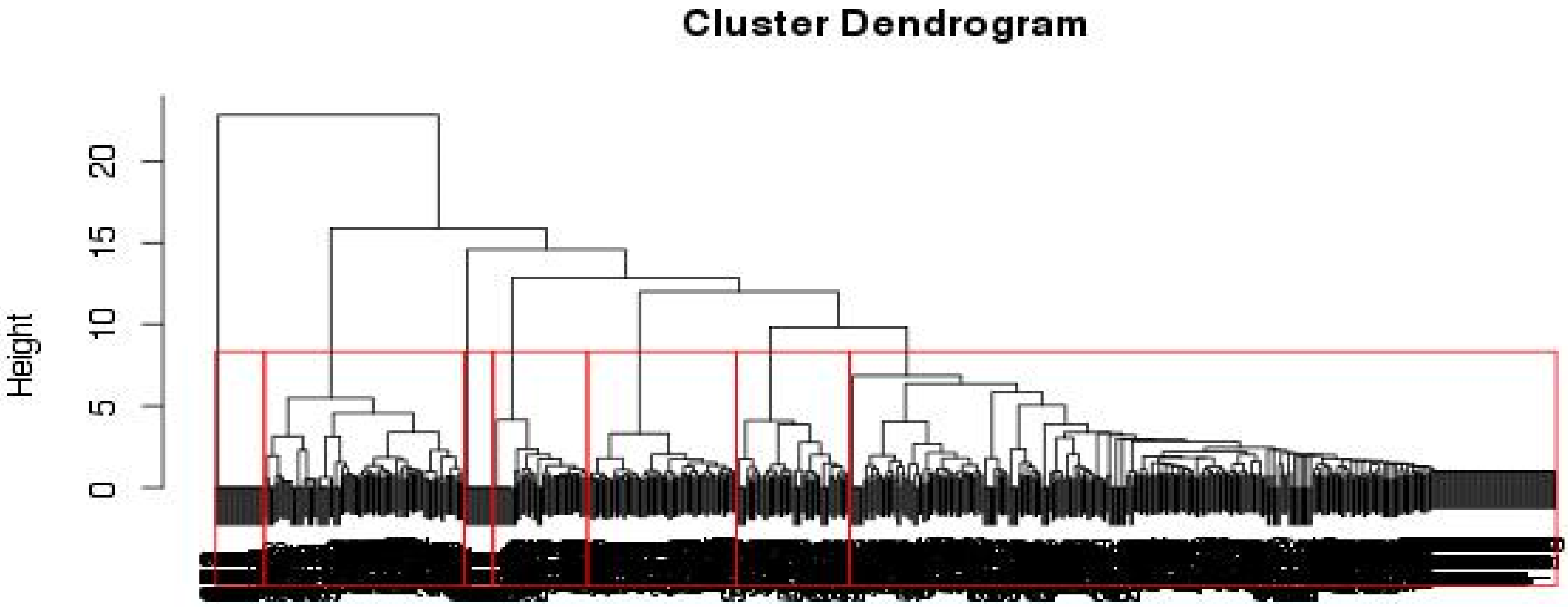
the cluster distance when 2 are combined



Hierarchical Clustering

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

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



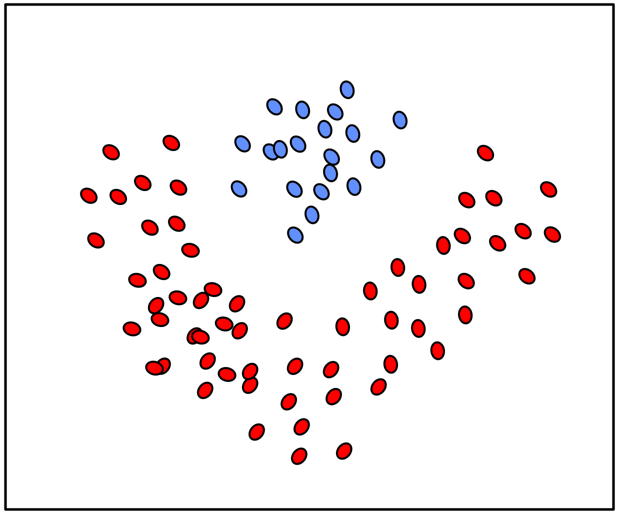
Other Clustering

- **Density based clustering**

  build neighborhoods around seed points

  link neighborhoods

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



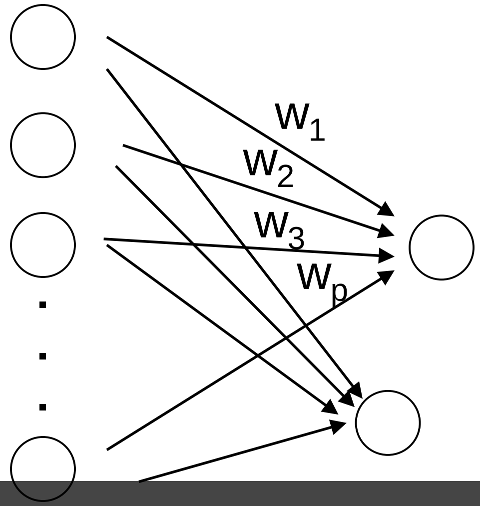
Other Clustering

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

  initialize weights to coordinate values for a seed point

  set input nodes to data points

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

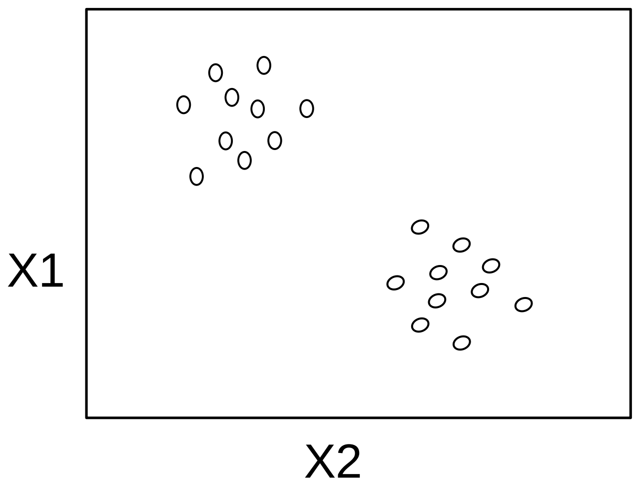


Target node(s), starts as a seed point and ends up as a cluster mean

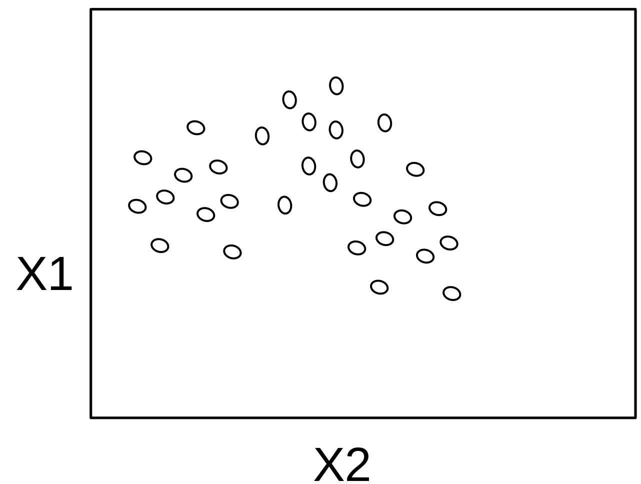
Pause

Imagine these 2 dimensional input spaces:
Which of these is easy or hard to cluster? (no class labels)

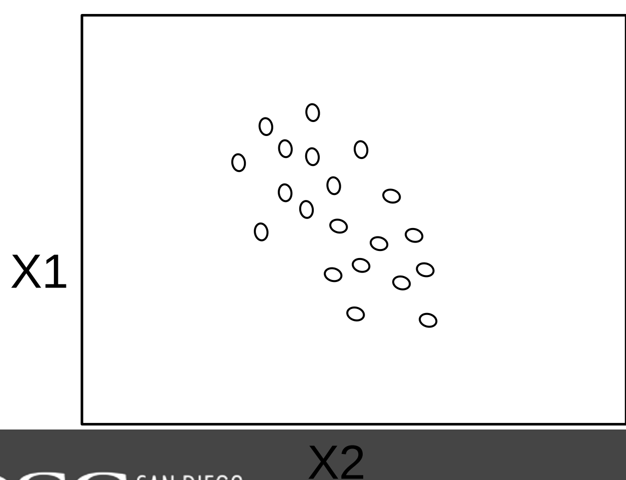
A



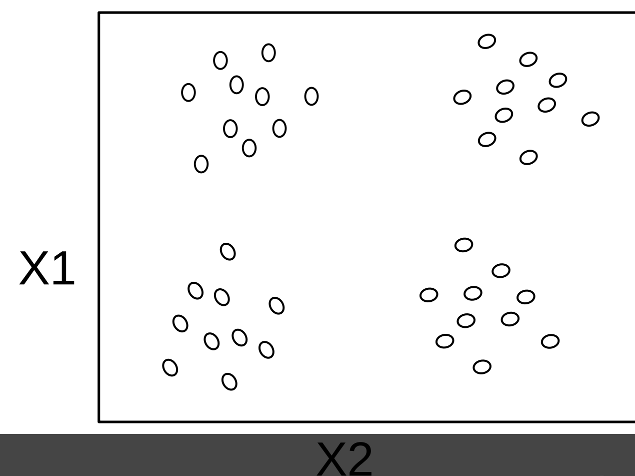
C



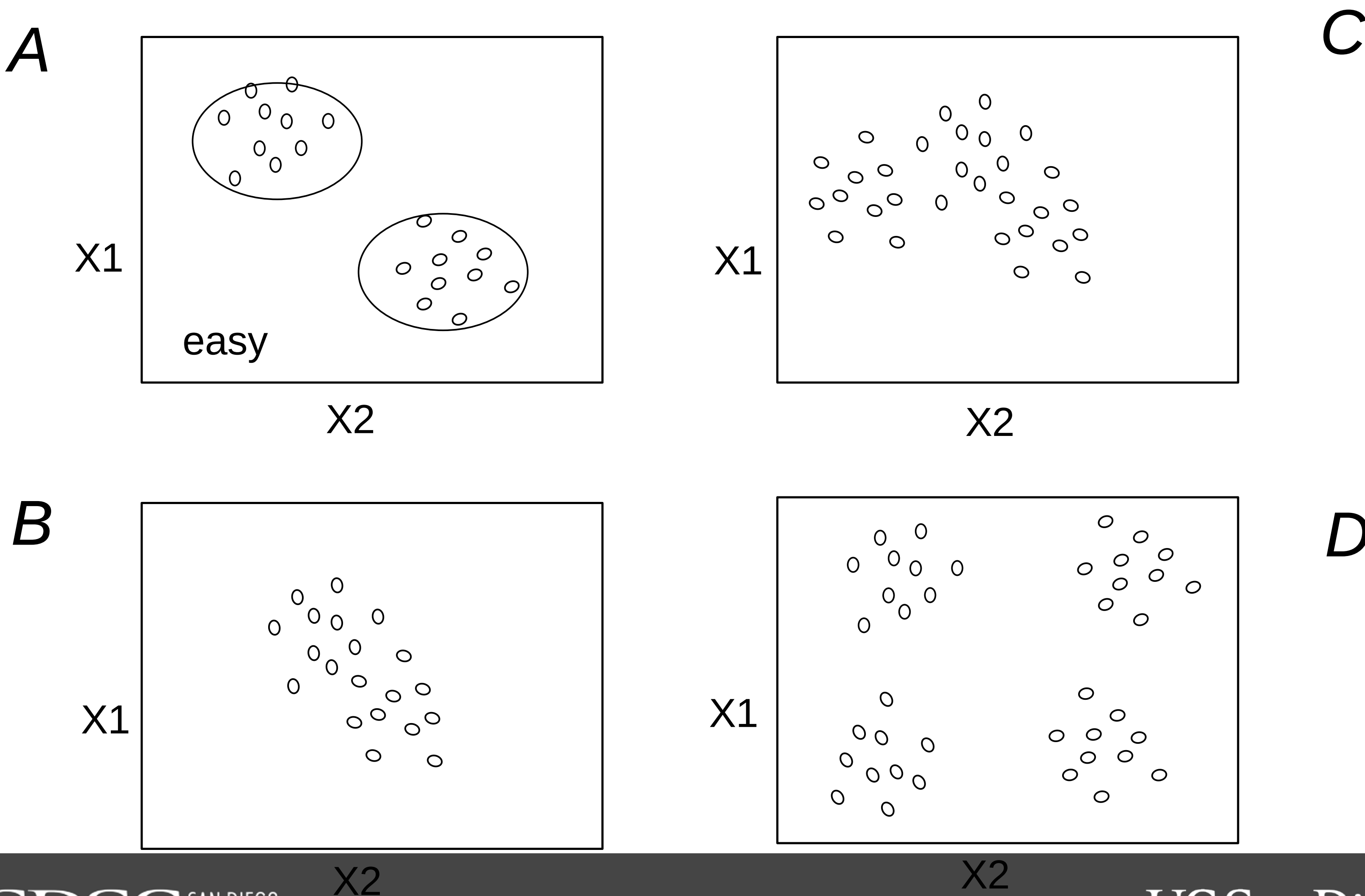
B



D



Potential clusters



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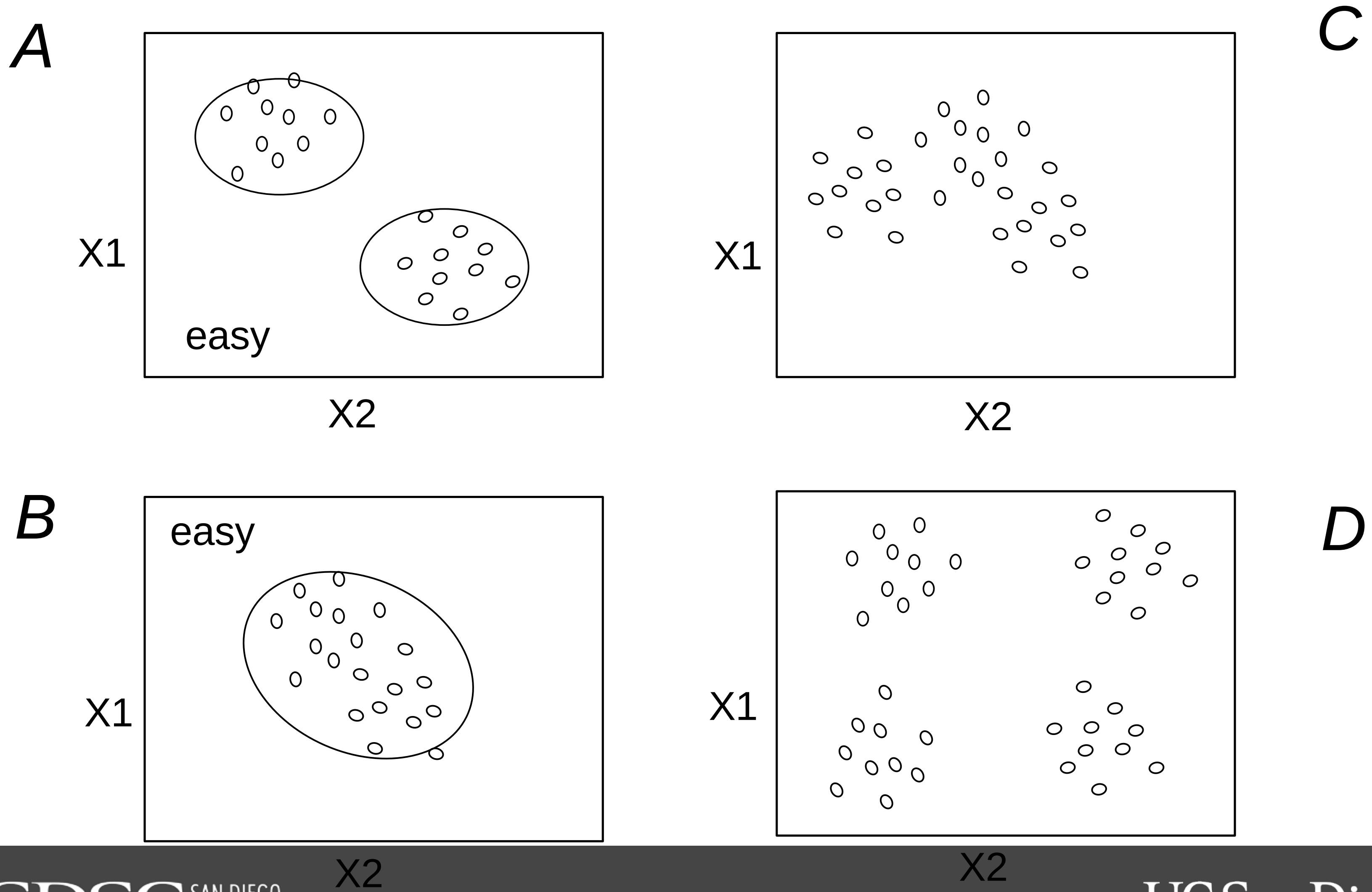

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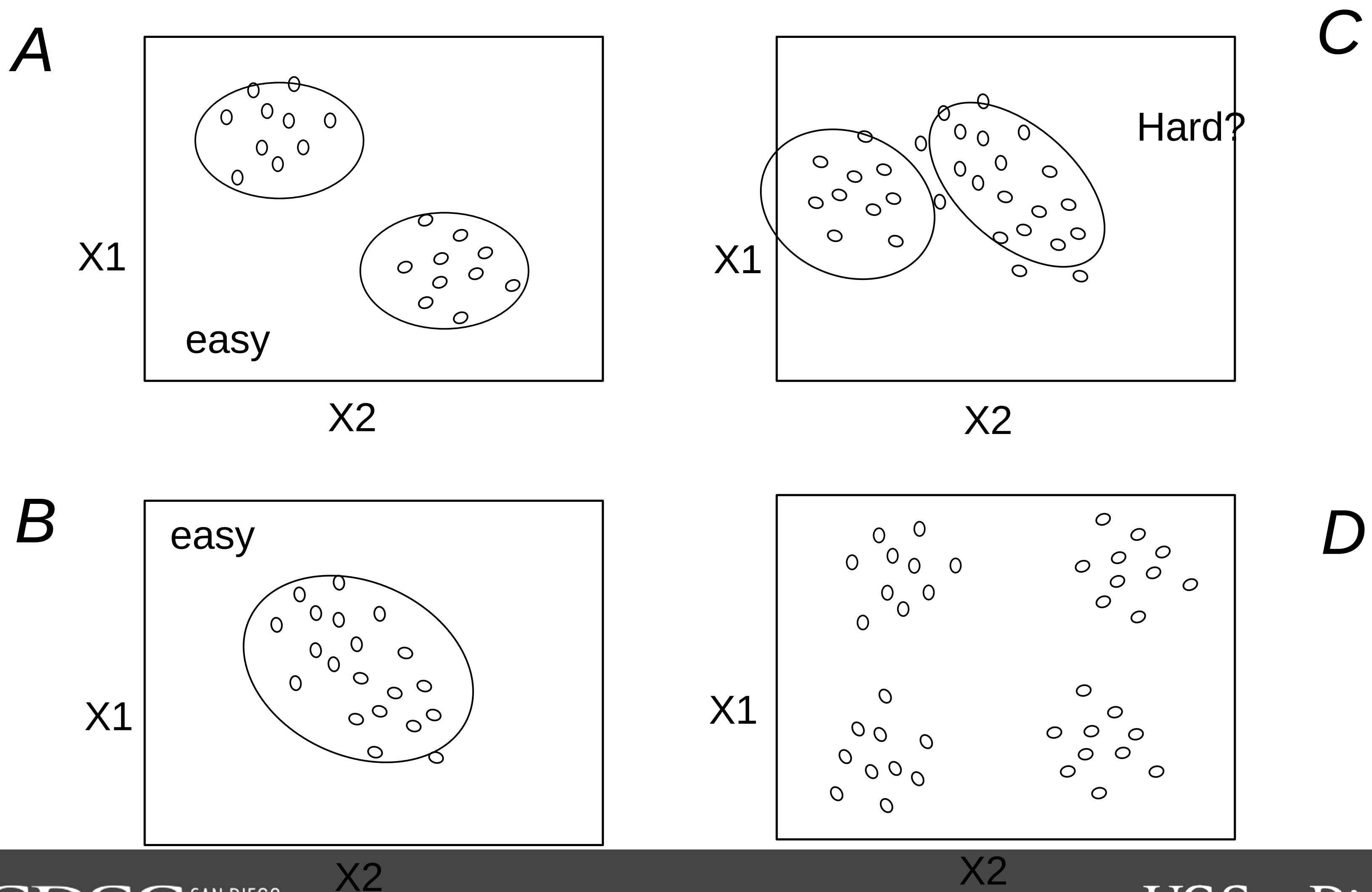

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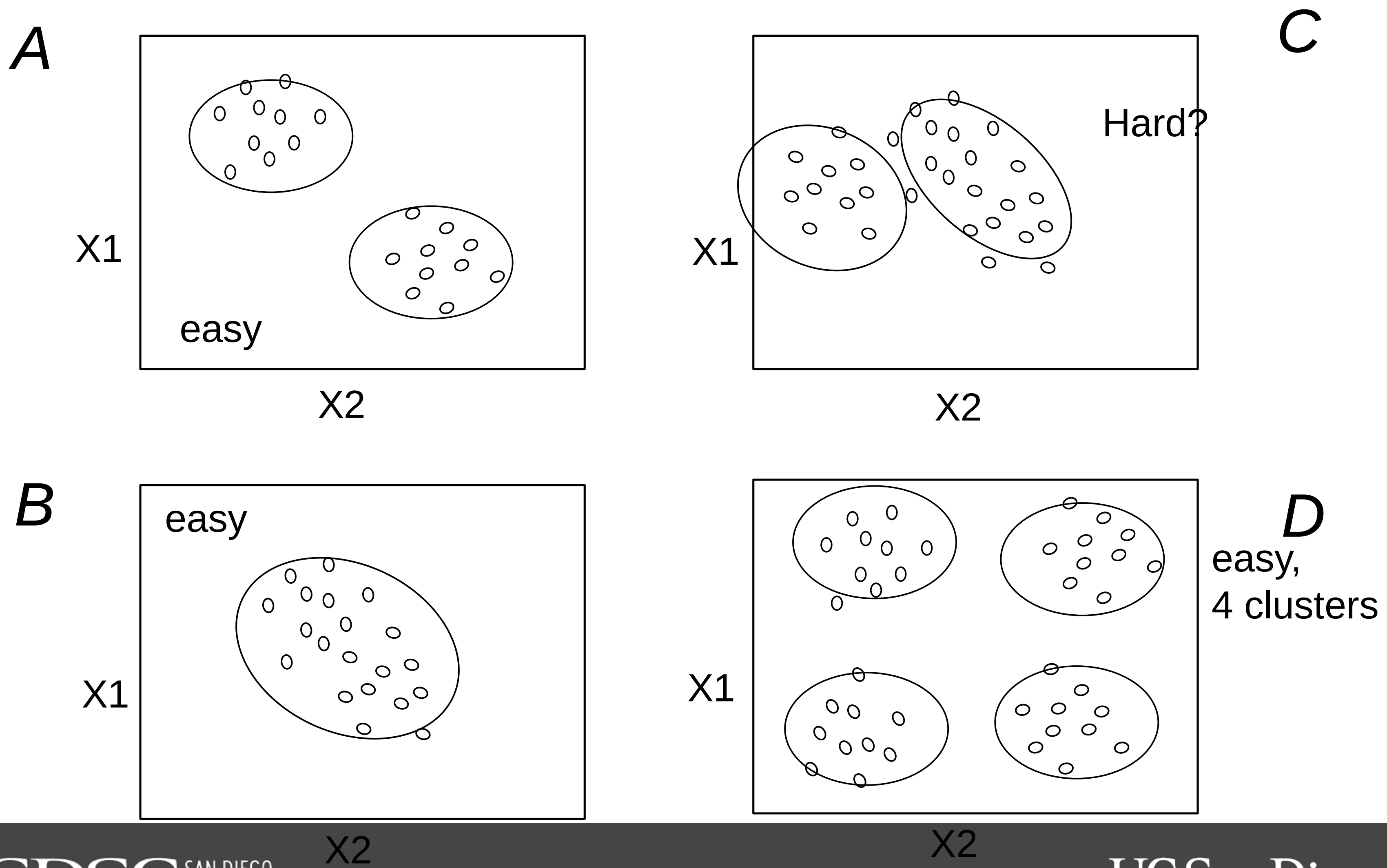
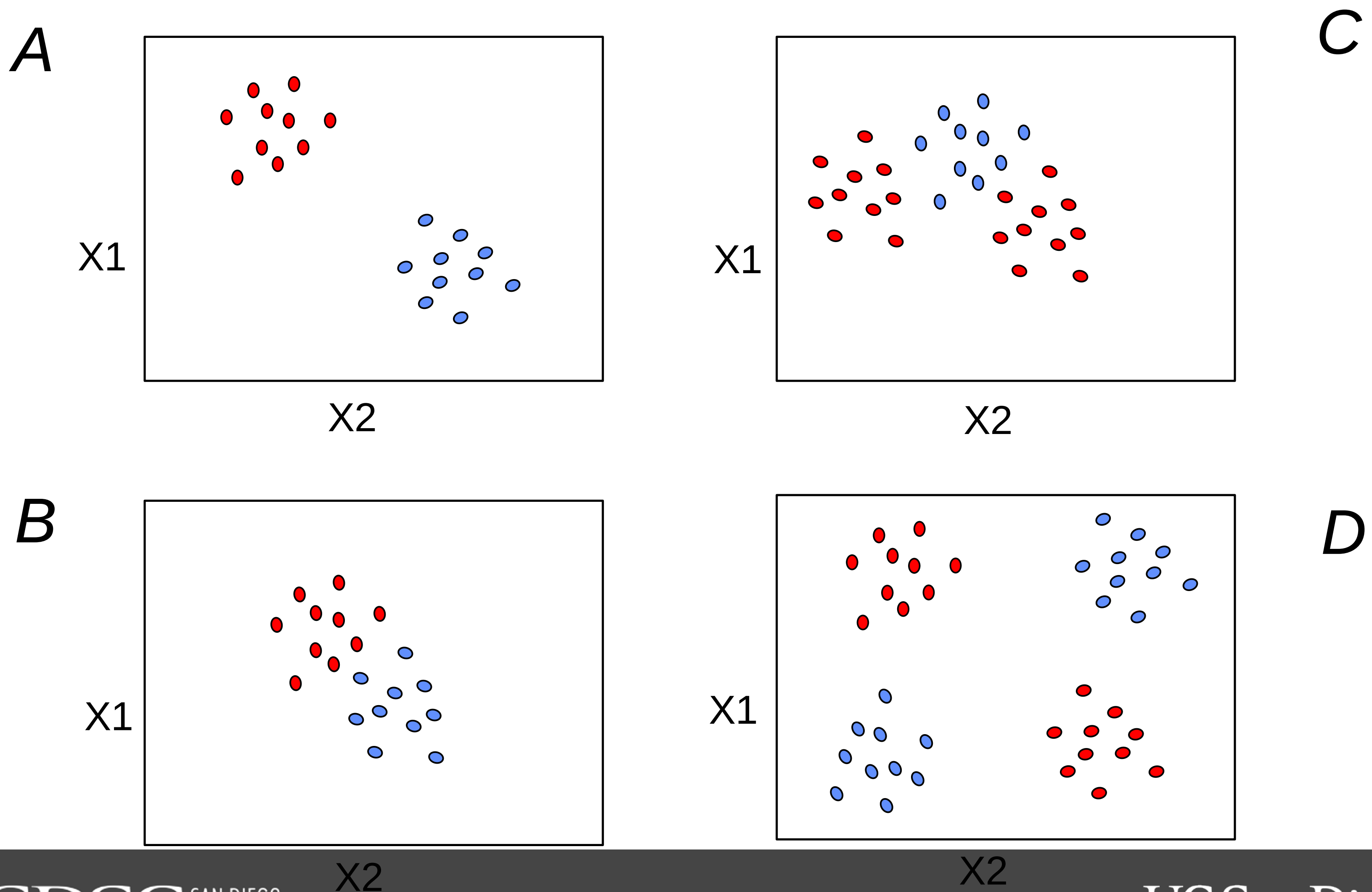
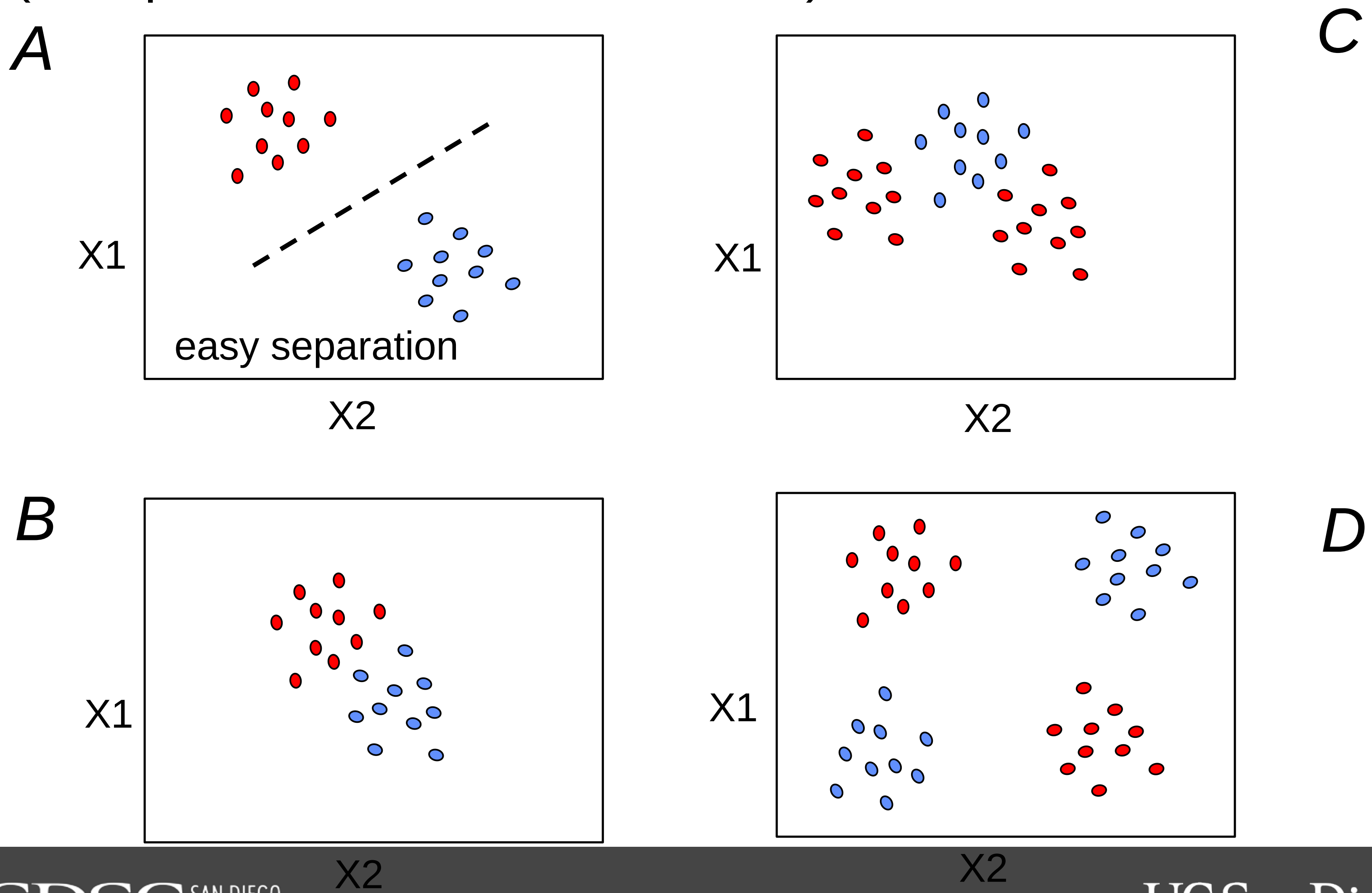


Now imaging there are two classes



Which are easy or hard to classify?
(ie separate red or blue with lines)



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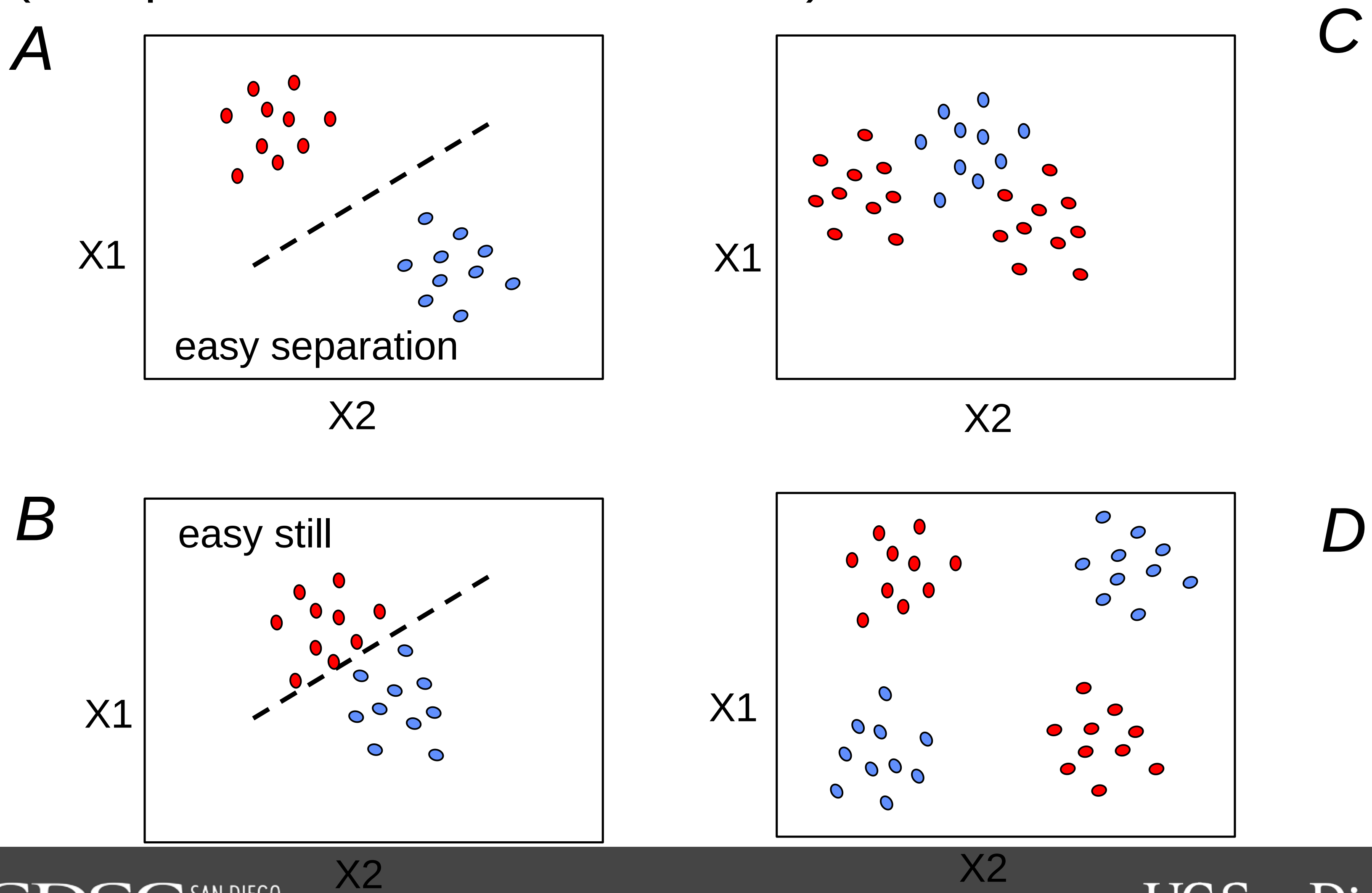

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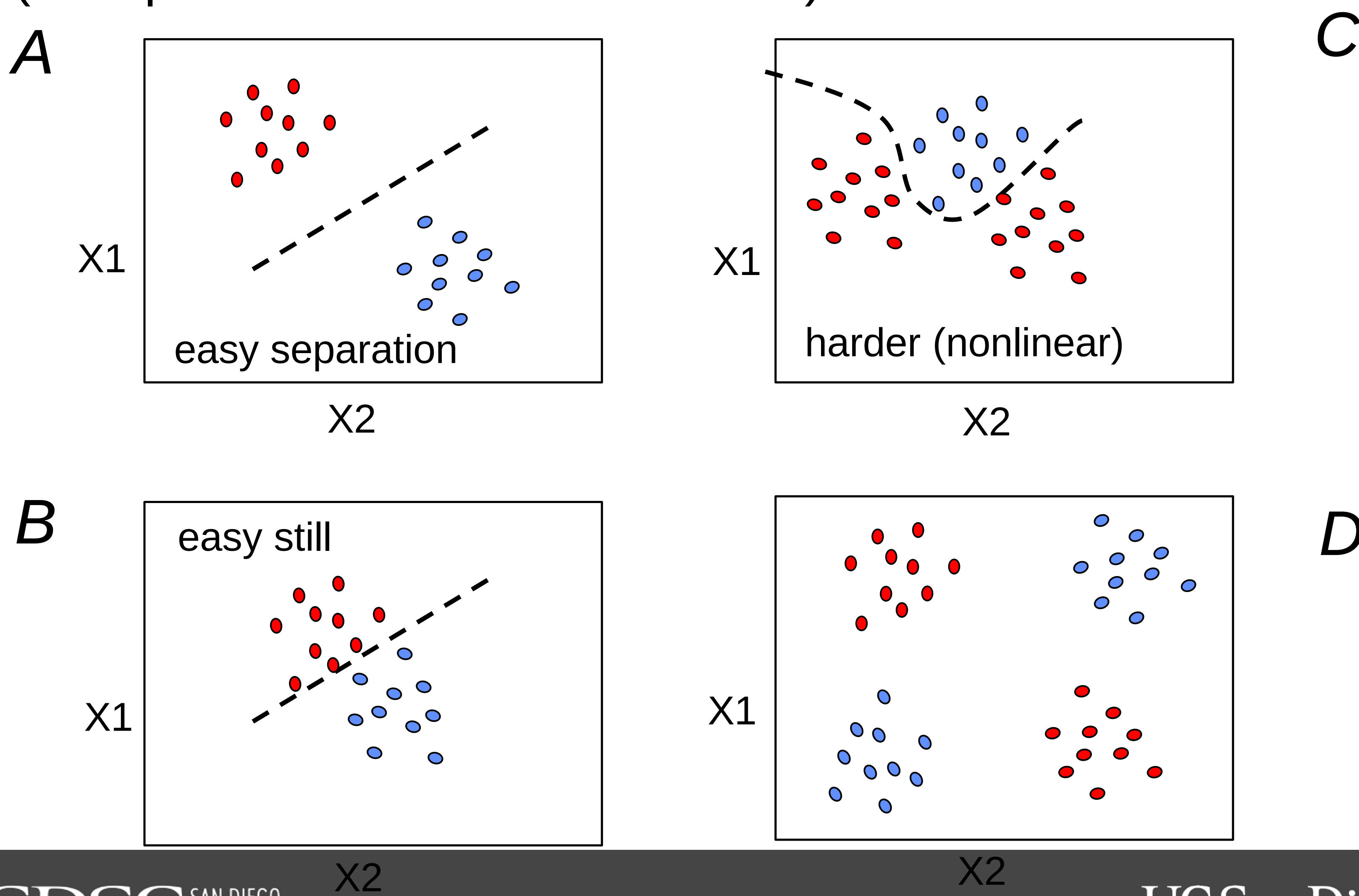

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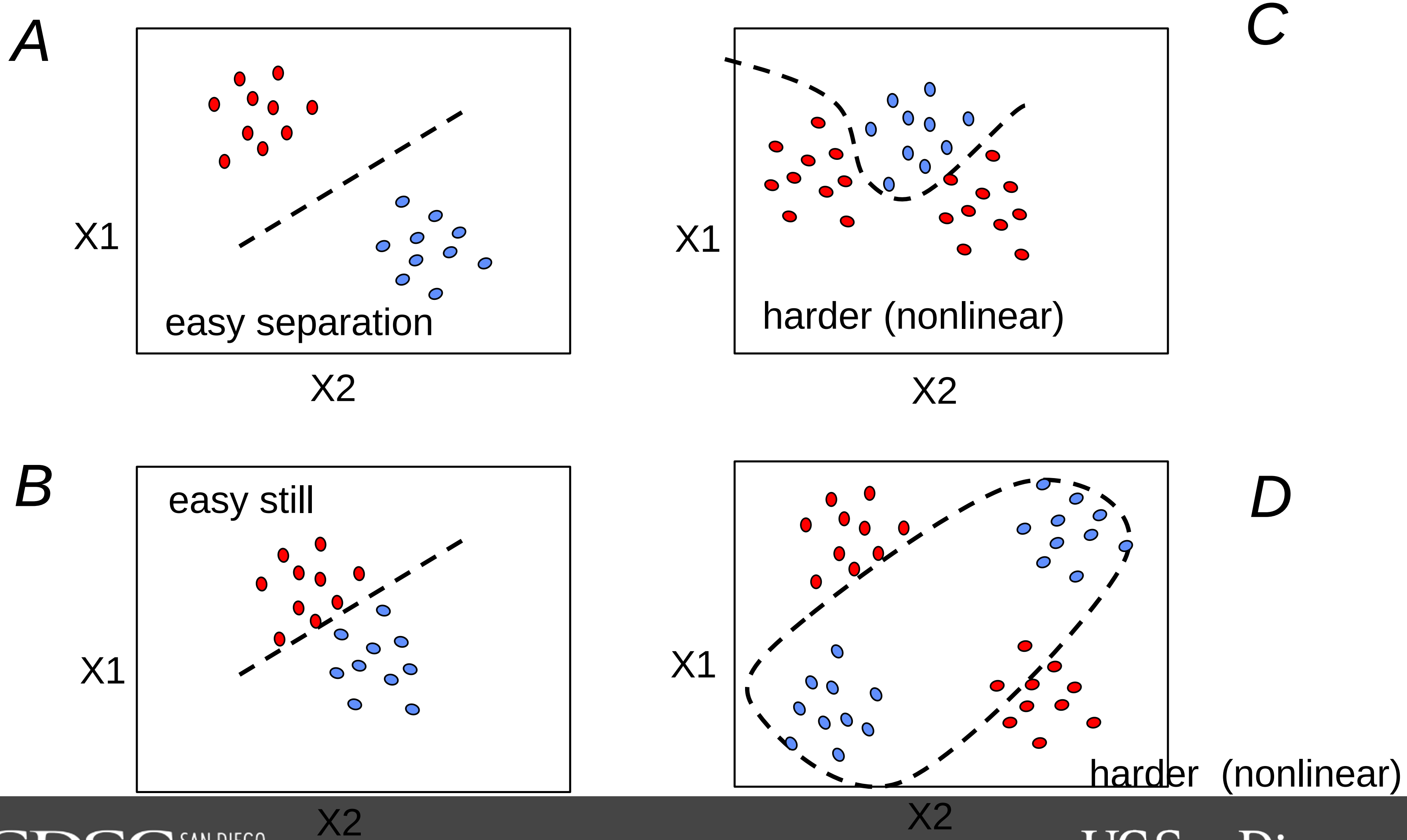

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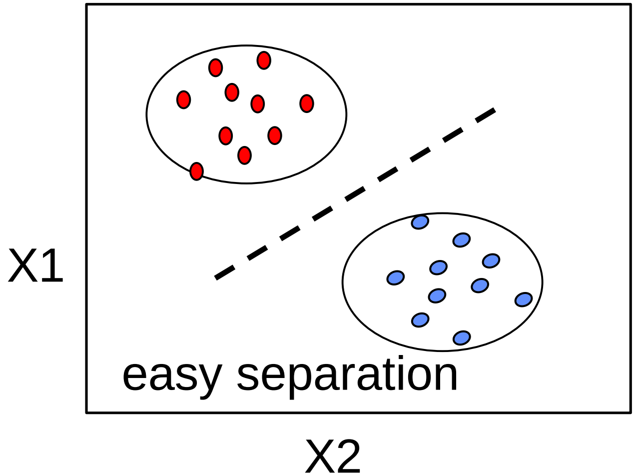
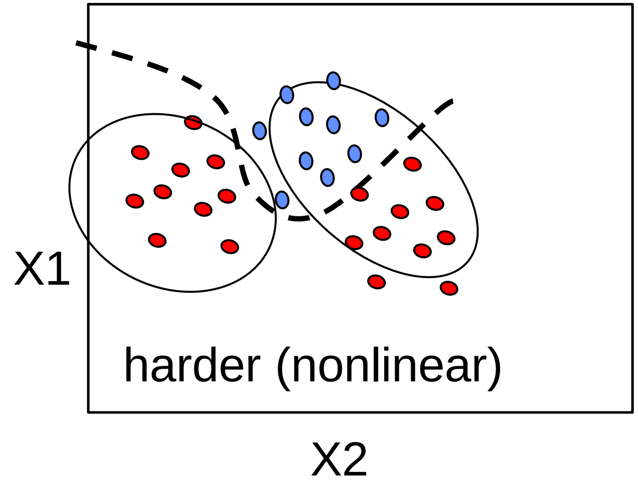
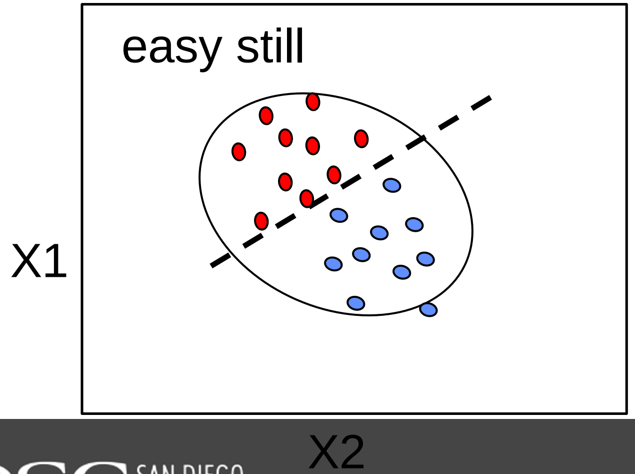


C

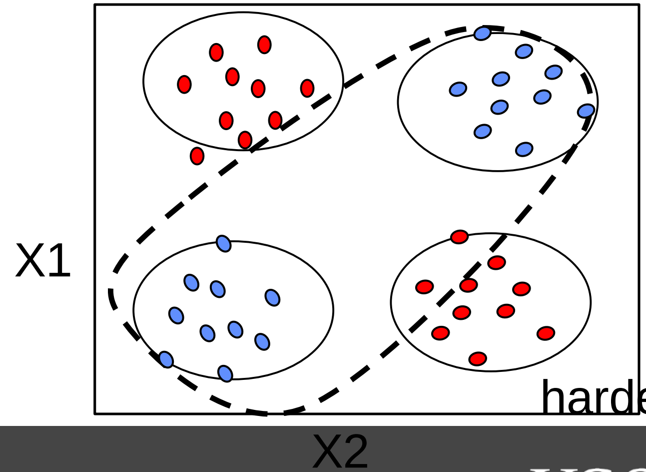


In summary:
No easy relationship between clusters and classification

B



D



harder (nonlinear)

Pause

Exercise, Kmeans and visualization in 2-D using SVD

- Using same data from SVD exercise, and SVD reduced matrix
- Run Kmeans
- Project data points onto first 2 SVD factors and plot them colored by cluster

(Which 2 factors?

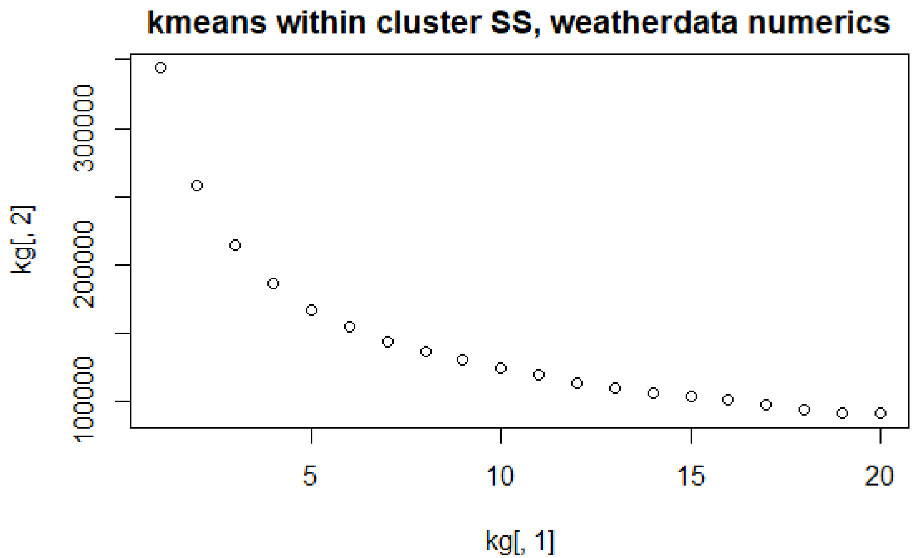
Keep in mind that:

Wsvd$U is N rows x P cols

Wsvd$V is PxP,

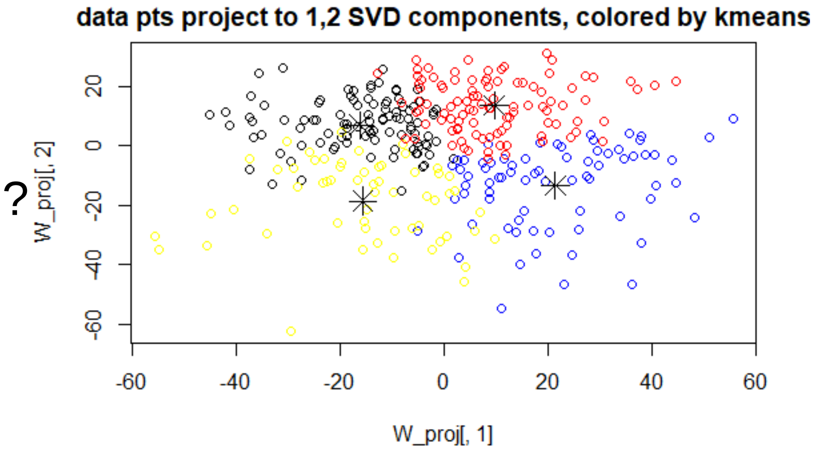
Data point is Px1 in original space and 2x1 in reduced space)

See clustering_exercise Rmd file
Rerun the SVD exercise if you need to, to get the W_mncntr and Wsvd matrices
Run Kmeans



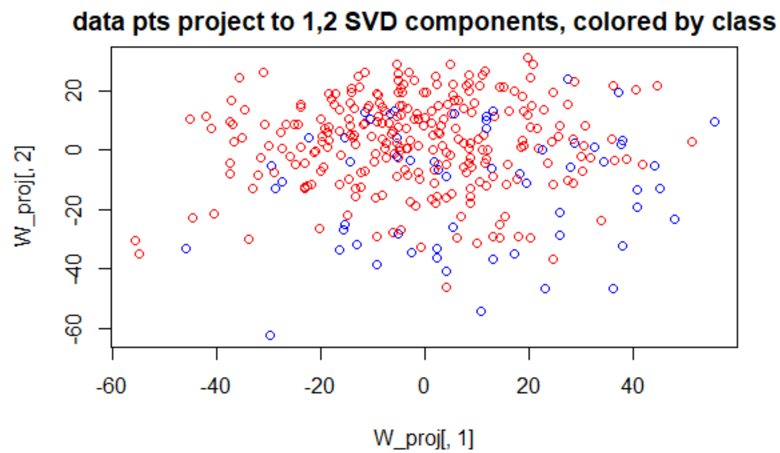
Run Kmeans with k=4
Plot data points onto 2-D space, use colors determined by Kmeans
Plot cluster centers

Are points well separated in 2-D projection?
Should they be?



Plot using colors determined by class (raintomorrow)

Are classes well separated?



Principle Components vs Clustering

- **PCA, SVD reduces dimensions, Clustering reduces to categorical groups**

- **In some cases, *k* PCs $\Leftrightarrow$ *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