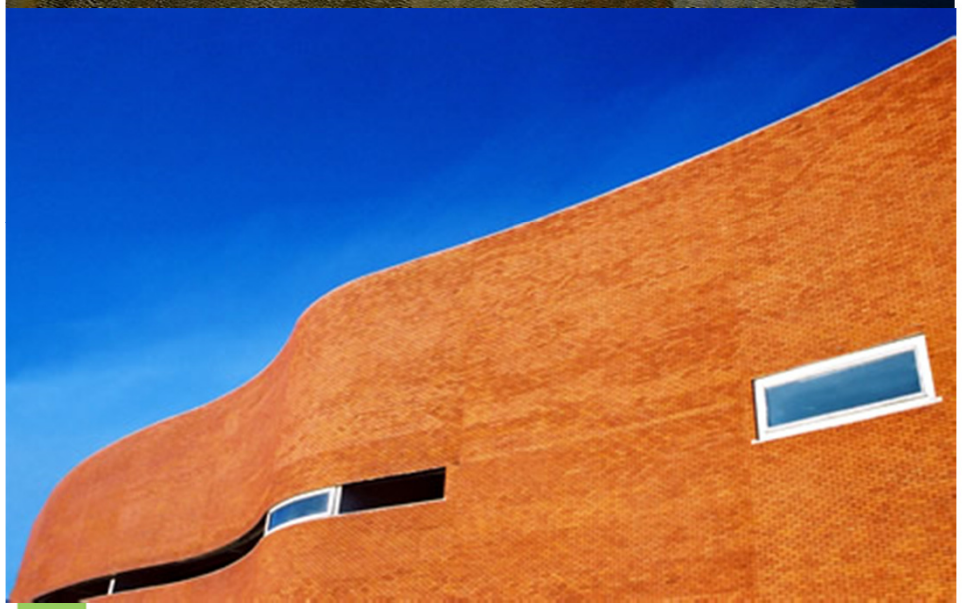
Aprendizagem Aplicada à Segurança

(Mestrado em Cibersegurança-DETI-UA)



LECTURE 5
Unsupervised Learning
(K-means Clustering and PCA)

Petia Georgieva
(petia@ua.pt)

DETI/IEETA – UA

Outline

Unsupervised learning

1. **K-means clustering**

2. **Data dimensionality reduction**
   - data compression /data visualization

3. **Principal Component Analysis (PCA)**

SUPERVISED vs. UNSUPERVISED LEARNING

Supervised Learning - (given DATA + LABELS):
ML method is trained with labeled data to predict the labels of new examples (learning by labeled examples)

Matrix X	feature x_0	feature x_1	.....	feature x_n	Vector y - output (label)
Example 1	1	$x^{(1)}$		$x_n^{(1)}$	$y^{(1)}$
Example 2	1	$x^{(2)}$		$x_n^{(2)}$	$y^{(2)}$
	1				
				$x_n^{(i)}$	
Example m	1	$x^{(m)}$		$x_n^{(m)}$	$y^{(m)}$

Unsupervised Learning - given UNLABELED DATA
ML method to discover the data internal (statistical) structure

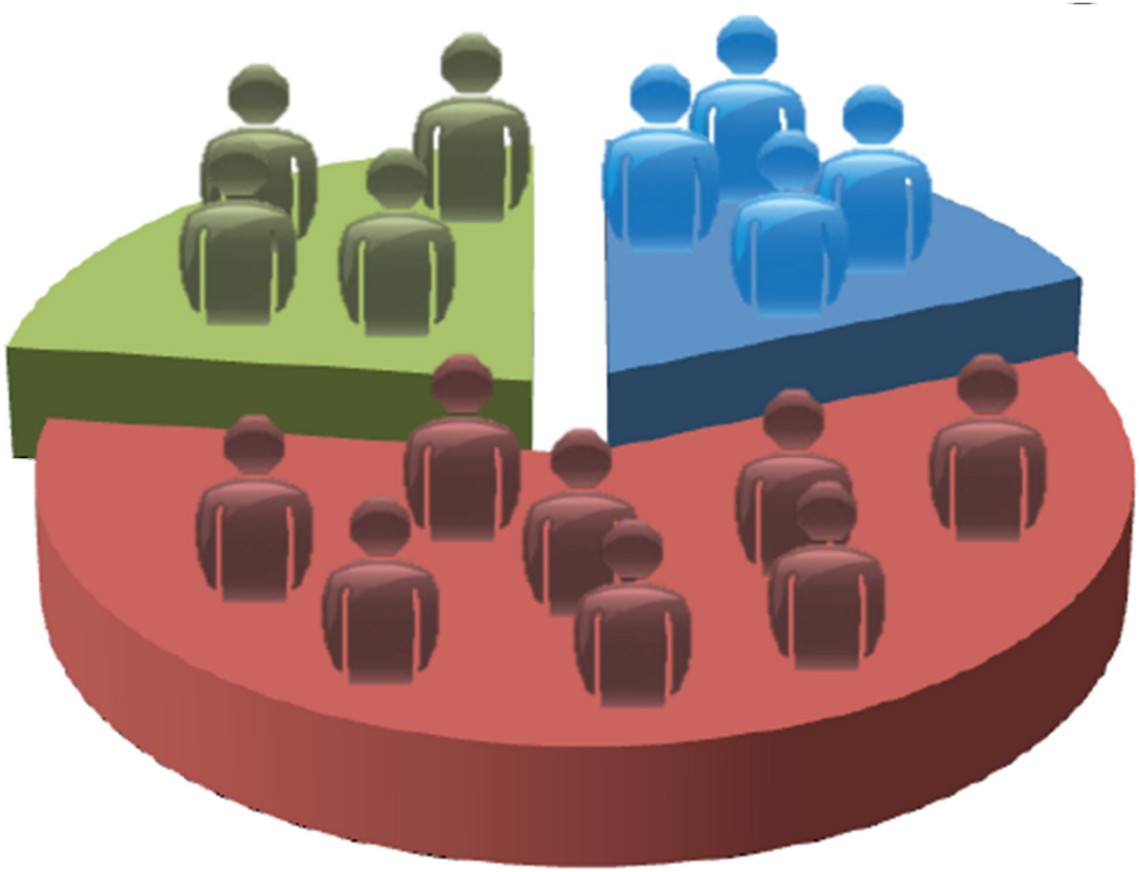
Matrix X	feature x_1	feature x_2	.....	feature x_n
Example 1	$x_1^{(1)}$	$x_2^{(1)}$		$x_n^{(1)}$
Example 2	$x_1^{(2)}$	$x_2^{(2)}$		$x_n^{(2)}$
...				
Example i	$x_1^{(i)}$	$x_2^{(i)}$		$x_n^{(i)}$
...				
...				
Example m	$x_1^{(m)}$	$x_2^{(m)}$		$x_n^{(m)}$

Semi-Supervised Learning – mixture of labeled and unlabeled data

Unsupervised learning -

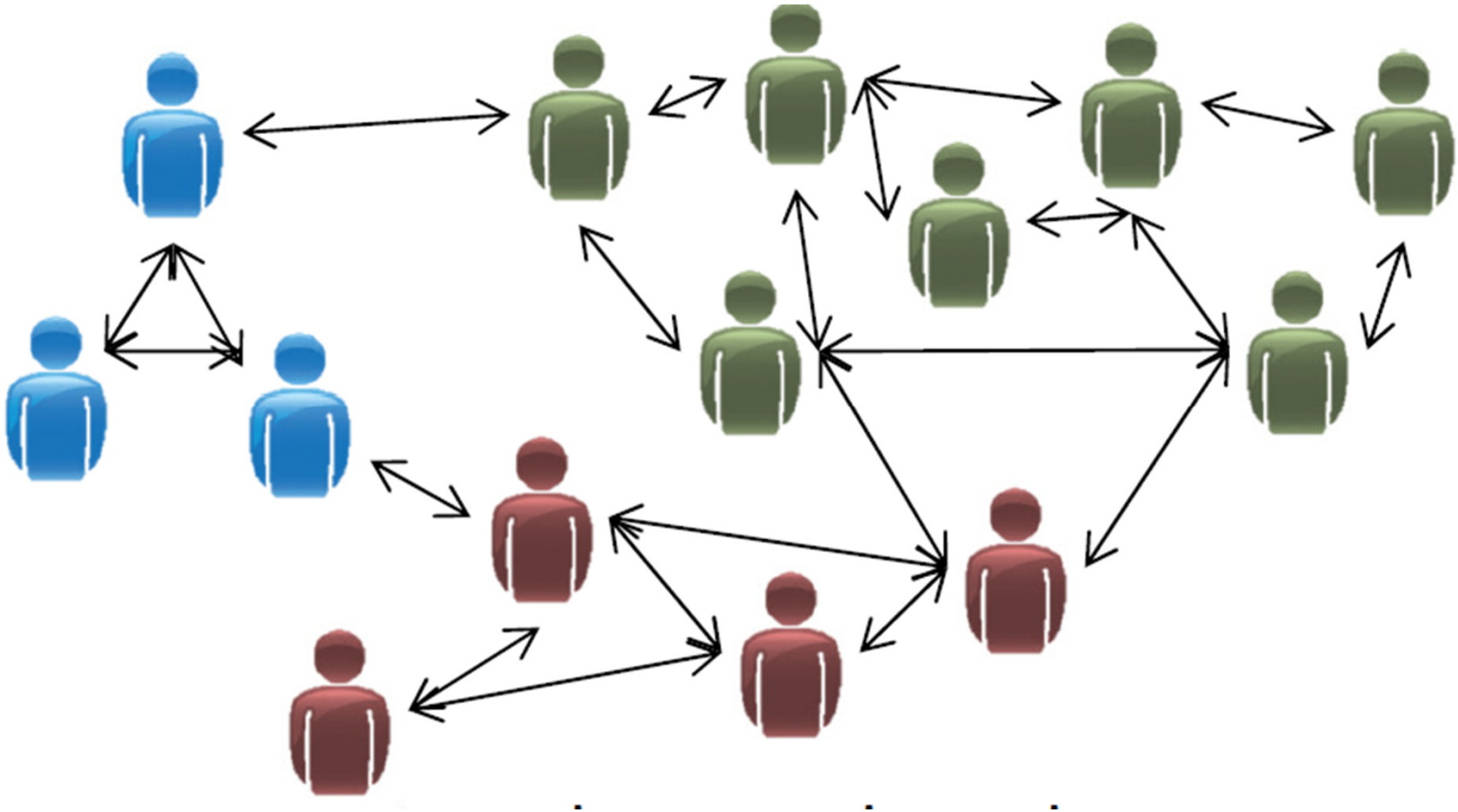
Market segmentation: data base of customers => division in target groups

Features: education, job, age, marital status, etc.

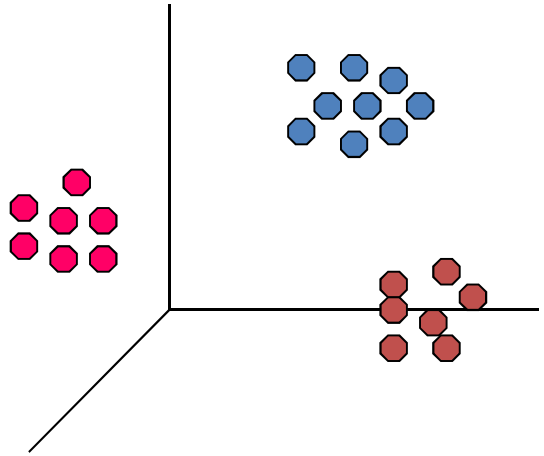


Unsupervised learning

Social network analysis: user grouping, group-specific advertising



Clustering intuition



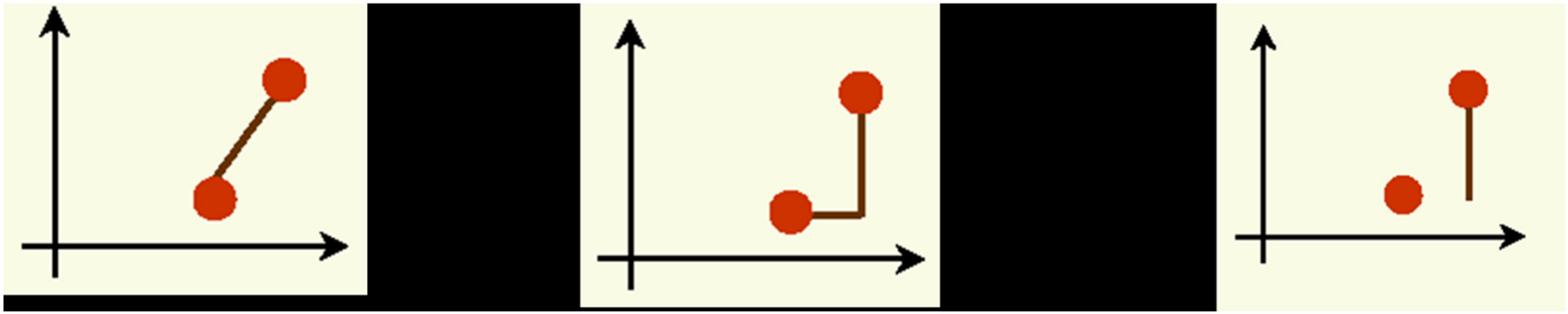
- Given a set of not labeled examples

- Find a relevant grouping of the examples into clusters such that:

  - Examples in the same cluster have **high similarity**
  - Examples from different clusters have **high dissimilarity**

Similarity measures –
Euclidian distance; Chebyshev distance; Manhattan distance

Distance (similarity) measures



Euclidian Distance (L2 norm)

$$d(p,q)=\sqrt{(x_p-x_q)^2+(y_p-y_q)^2}$$

Manhattan Distance (L1 norm)

$$d(p,q)=|x_p-x_q|+|y_p-y_q|$$

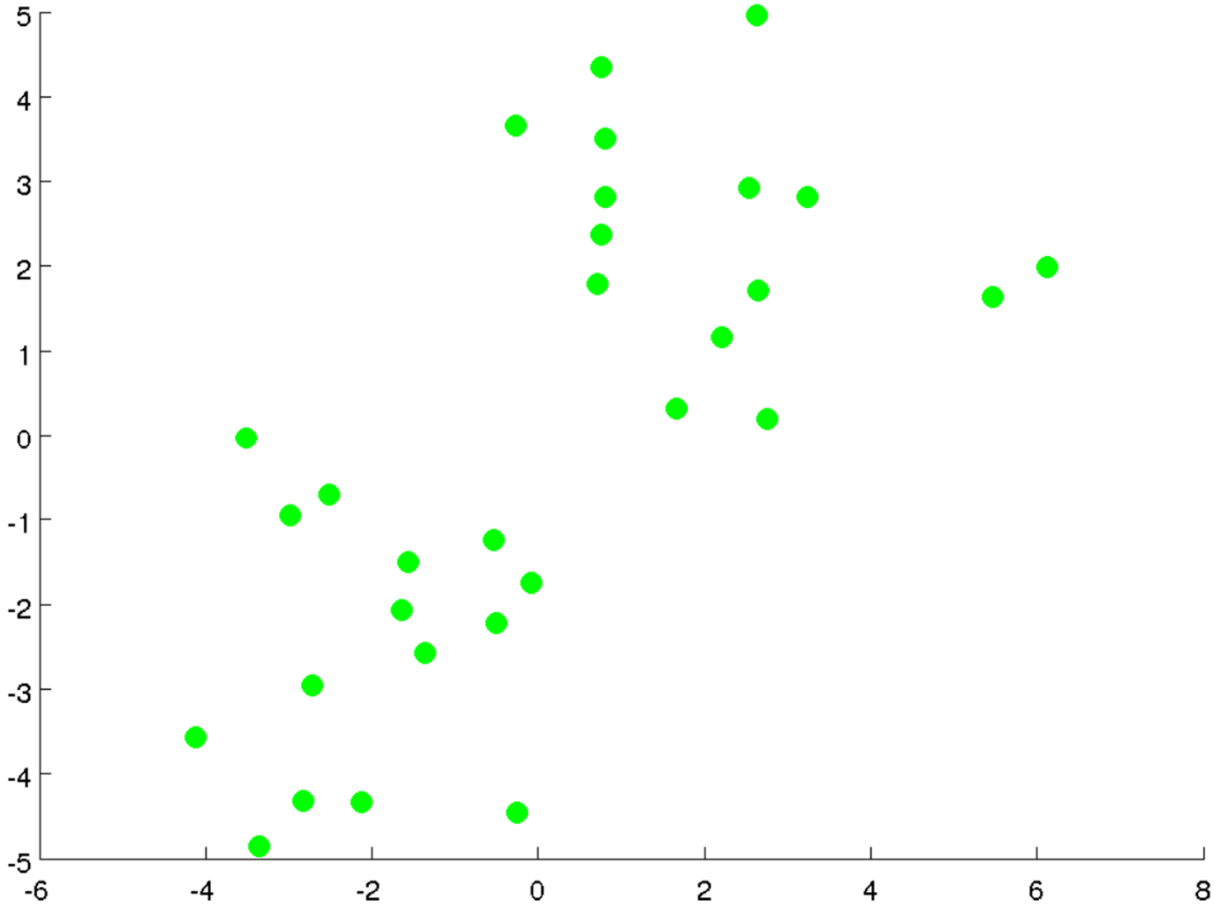
Chebyshev distance

$$d(p,q)=\max|(x_p-x_q),(y_p-y_q)|$$

K-means algorithm

Given:

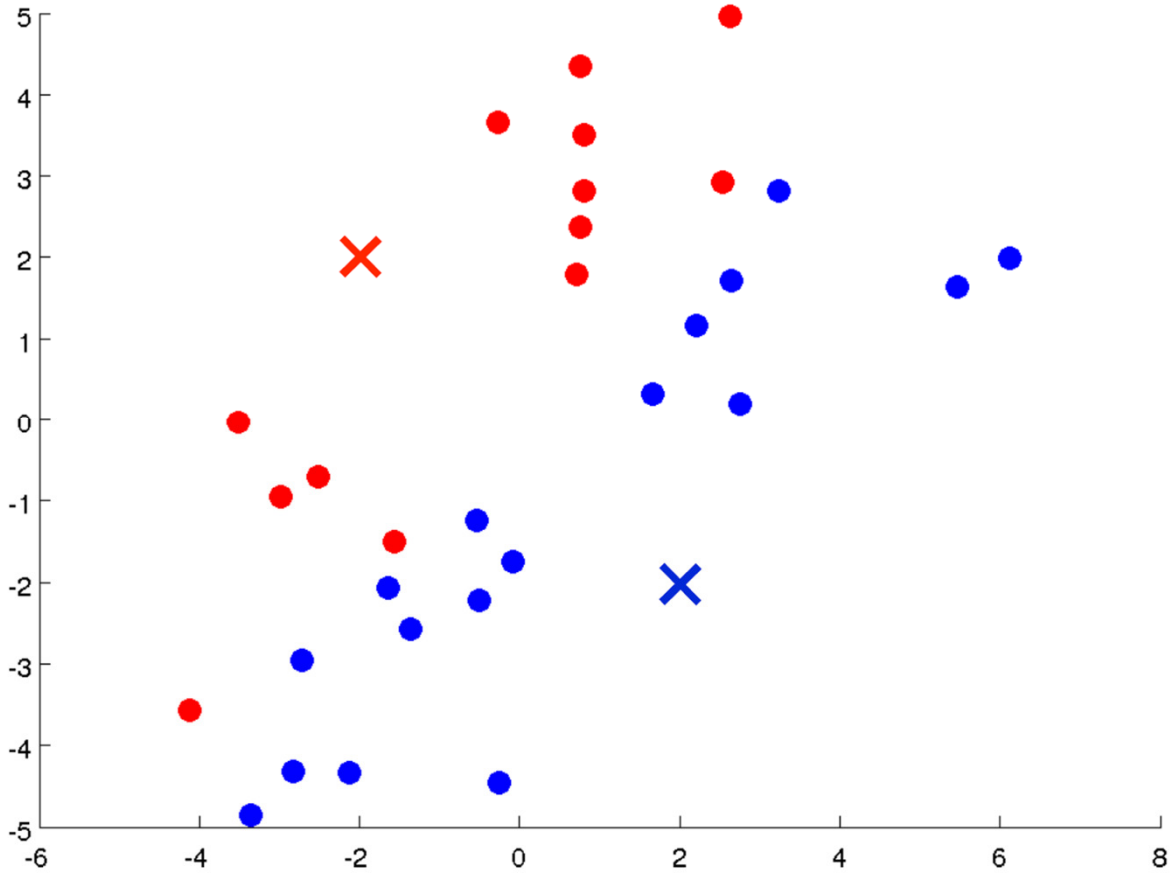
- **K – the number of clusters**
- **Training set - no labels**



universidade de aveiro

K-means algorithm

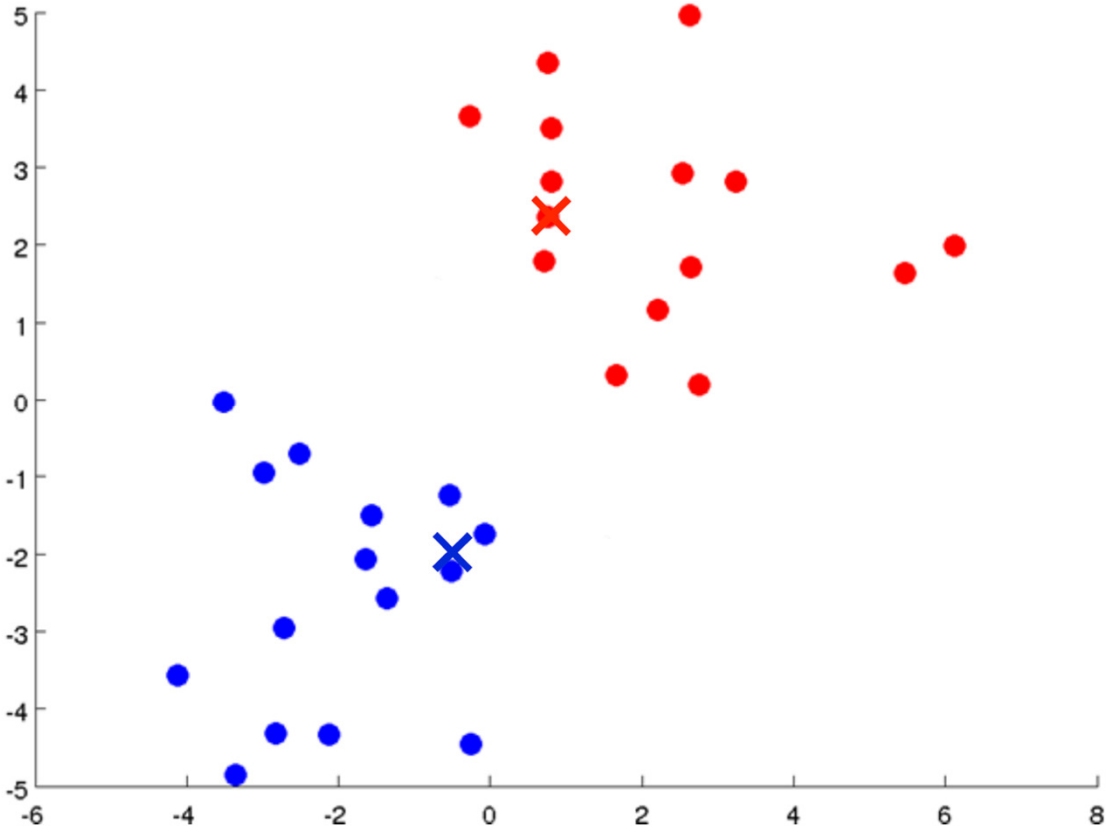
Randomly initialize K cluster centroids (e.g. K=2)
Assign data points to their closest centroid (Euclidian distance)



universidade de aveiro

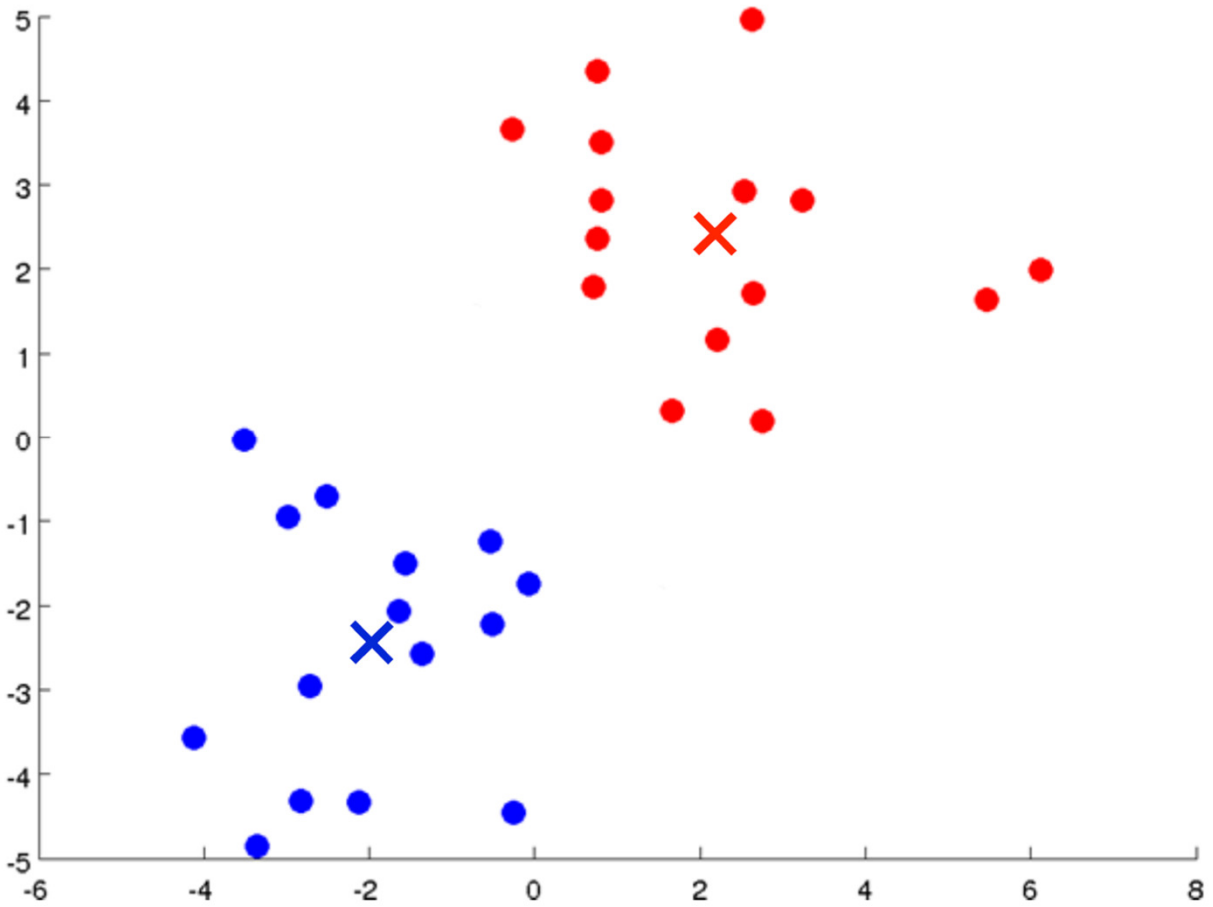
K-means algorithm

Compute new centroids = mean of the points assigned to that cluster.
Assign data points to the new closest centroid.



K-means algorithm

Repeat until convergence



K-means algorithms

Input:
- K (number of clusters)
- Training set (no labels)

Cluster assignment => step

Move centroid => step

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to cluster k

}

K-means optimization objective (distortion = average distance)

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2$$

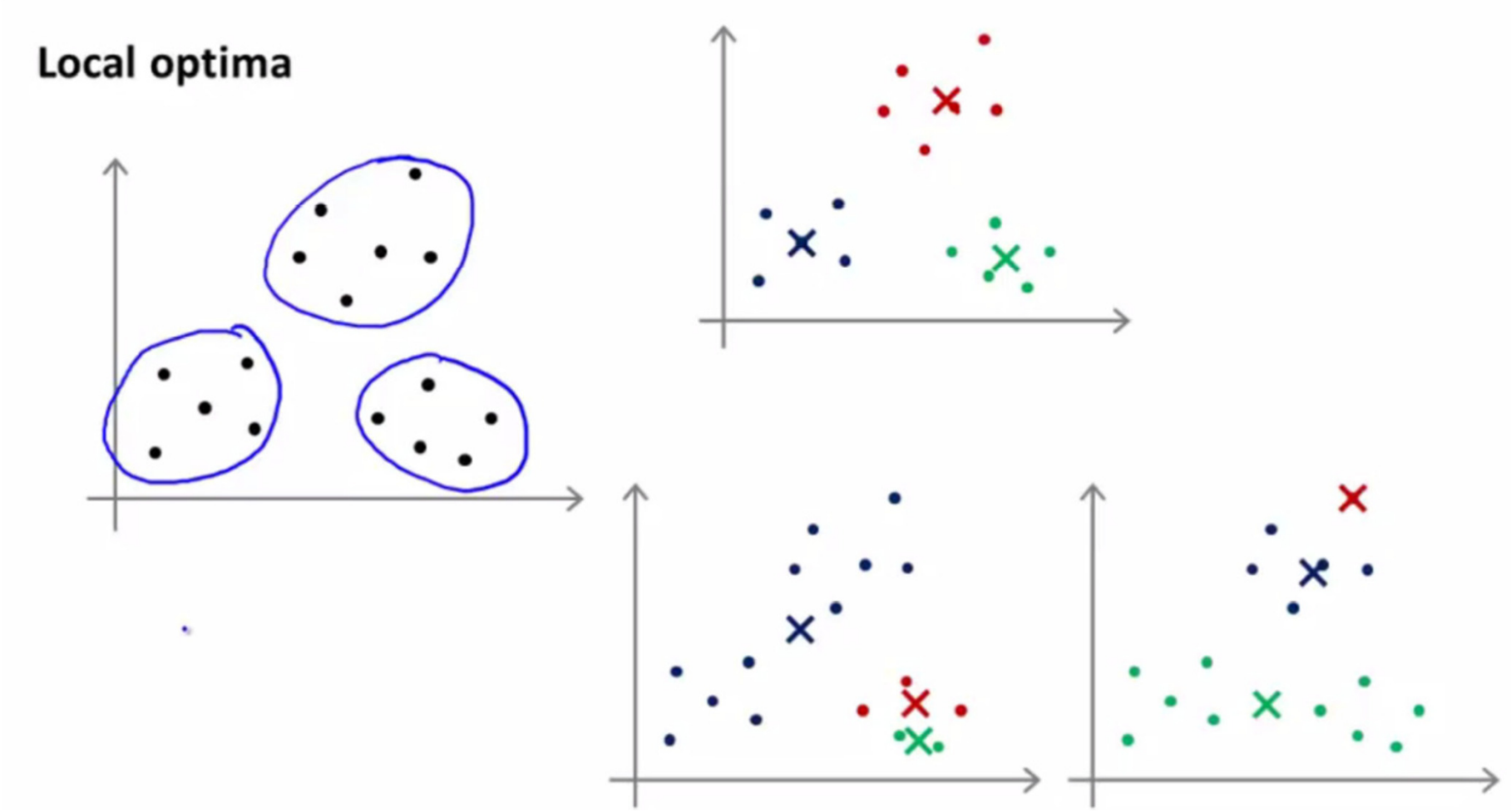
$$\min_{\substack{c^{(1)},\ldots,c^{(m)}, \\ \mu_1, \ldots, \mu_K}} J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

Stop K-means learning (different criteria):

- Achieved Max number of iterations
- J < some threshold
- No improvement of *J* between subsequent iterations

Single (Random) Initialization

Choose number of clusters K
Inicialize K cluster centroids = randomly picked K training examples



Repeat Random Initializations

For i = 1 to 100 {

Randomly initialize K-means.

Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.

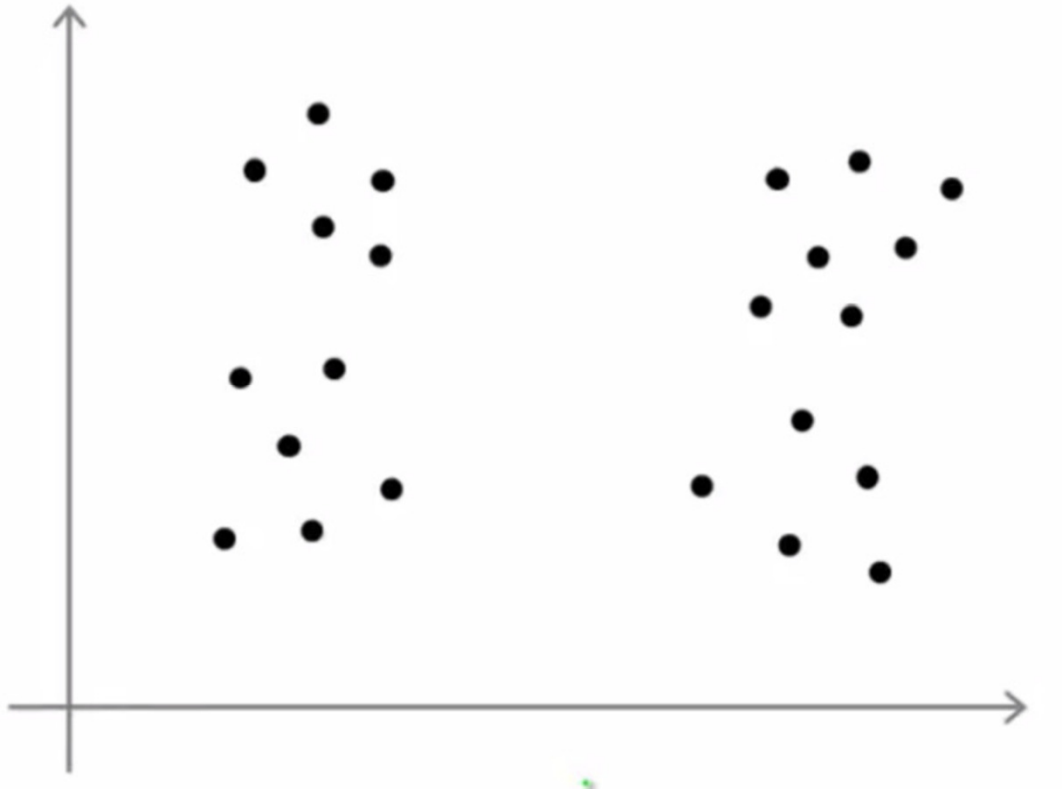
Compute cost function (distortion)

$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

}

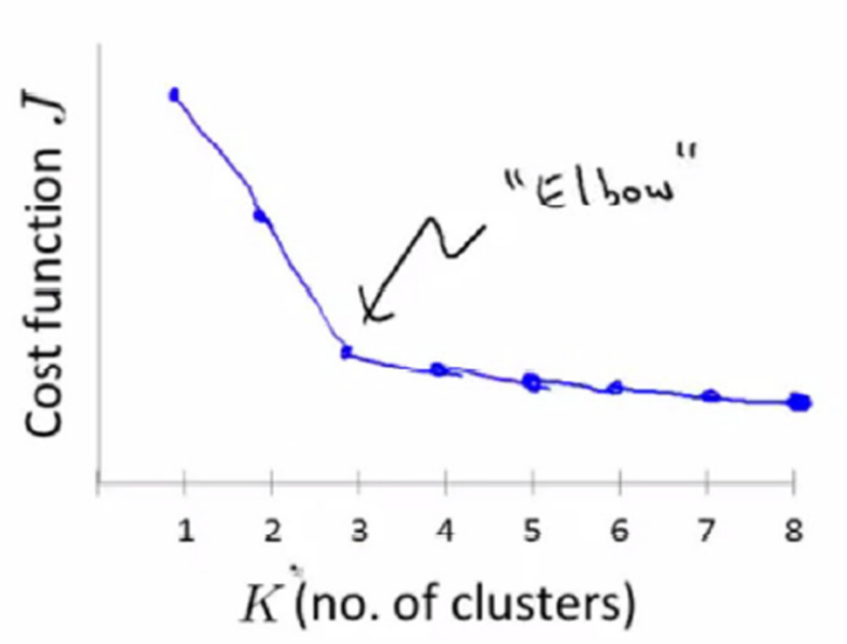
Pick clustering that gave lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

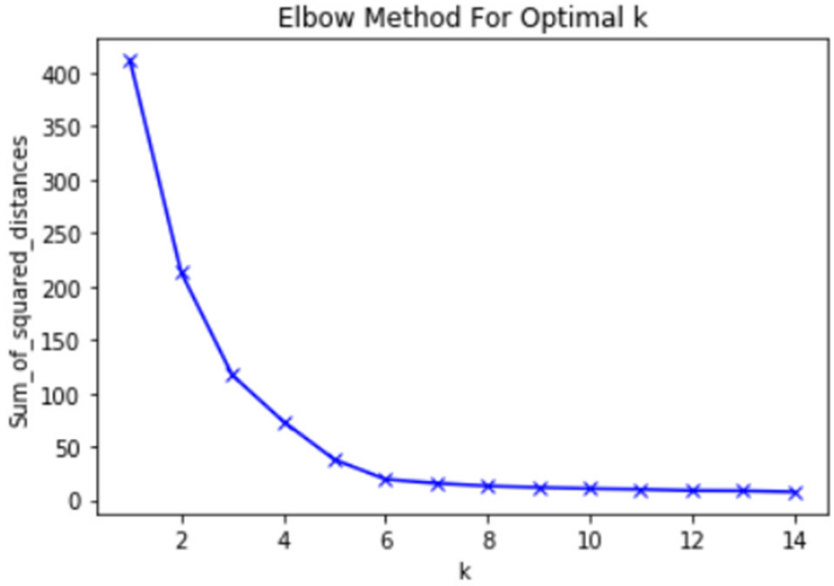
How to Choose # of clusters



- Choose K by data visualisation (if possible)
- Ask domain experts (highly recommendable) , e.g. anomaly detection (experts should know how many types of anomalies are expected)
- Choose K automatically (e.g. Elbow method)

Choosing the number of clusters (Elbow method)

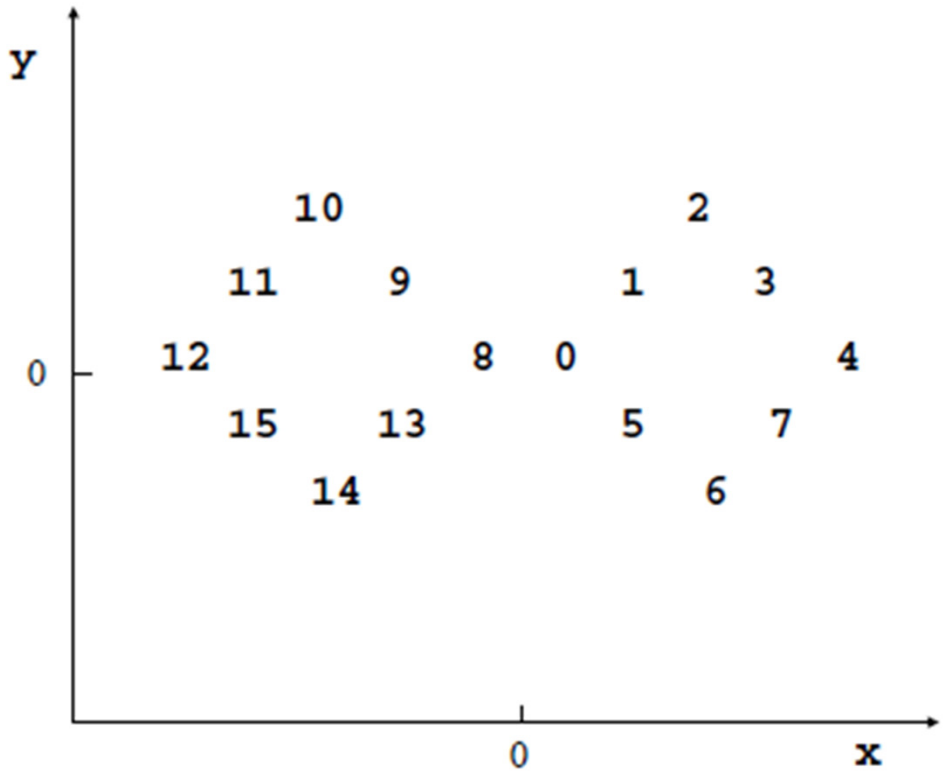




[Tutorial: How to determine the optimal number of clusters for k-means clustering | by Tola Alade | Cambridge Spark]
https://blog.cambridgespark.com/how-to-determine-the-optimal-number-of-clusters-for-k-means-clustering-14f27070048f

K-MEANS CLUSTERING – Example

Id	x	y
0:	1.0	0.0
1:	3.0	2.0
2:	5.0	4.0
3:	7.0	2.0
4:	9.0	0.0
5:	3.0	-2.0
6:	5.0	-4.0
7:	7.0	-2.0
8:	-1.0	0.0
9:	-3.0	2.0
10:	-5.0	4.0
11:	-7.0	2.0
12:	-9.0	0.0
13:	-3.0	-2.0
14:	-5.0	-4.0
15:	-7.0	-2.0

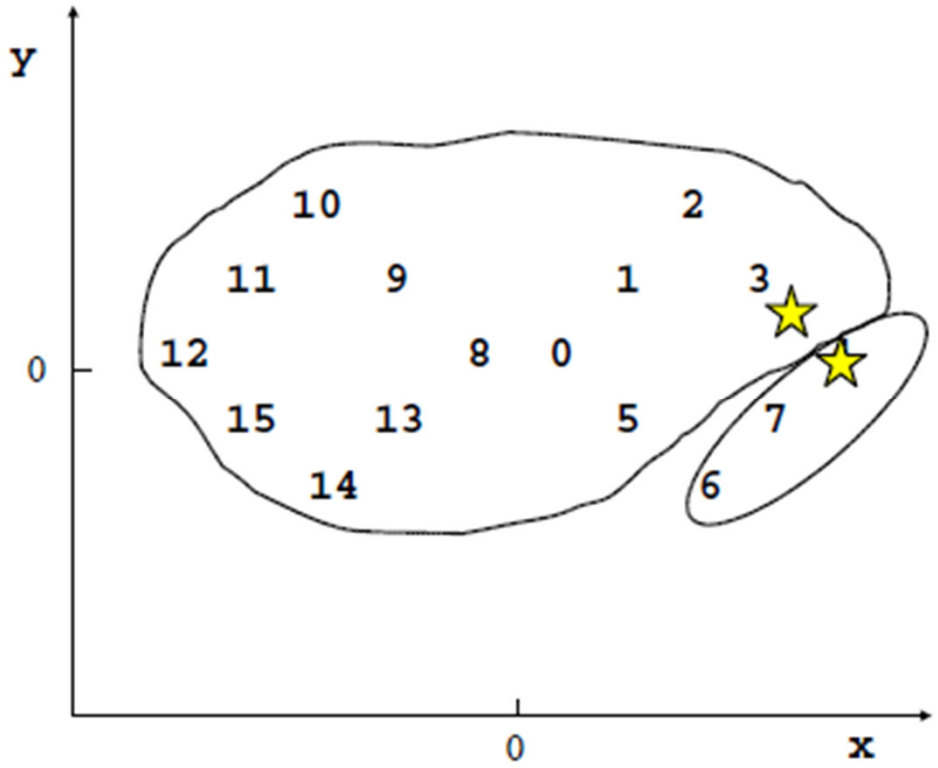


- find the best 2 clusters

K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

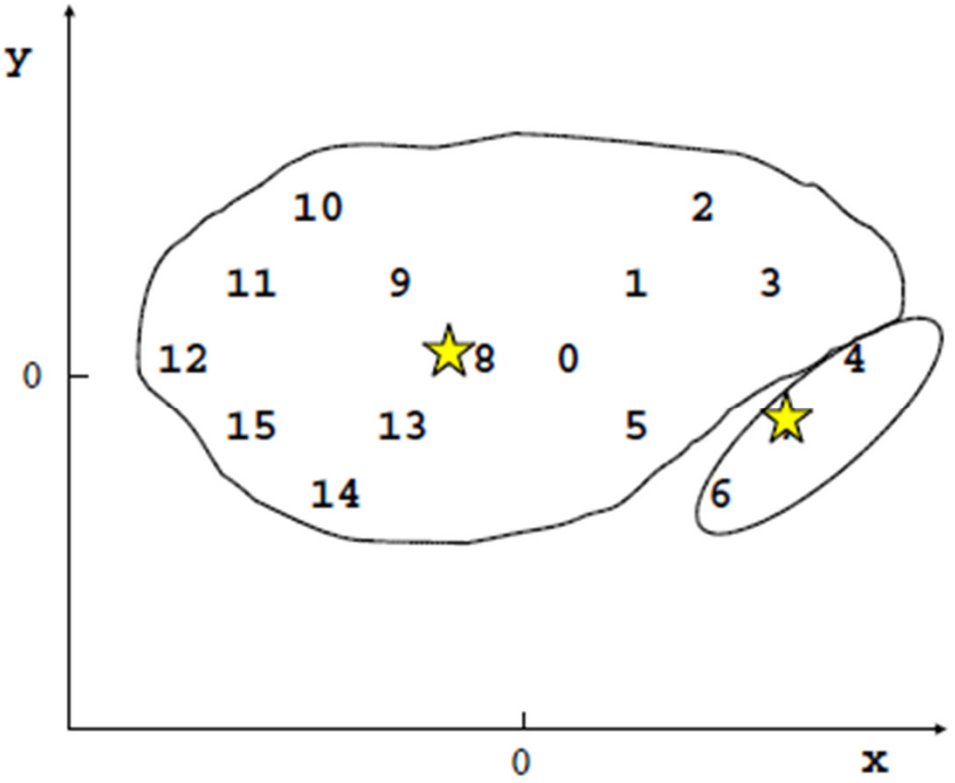


K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)

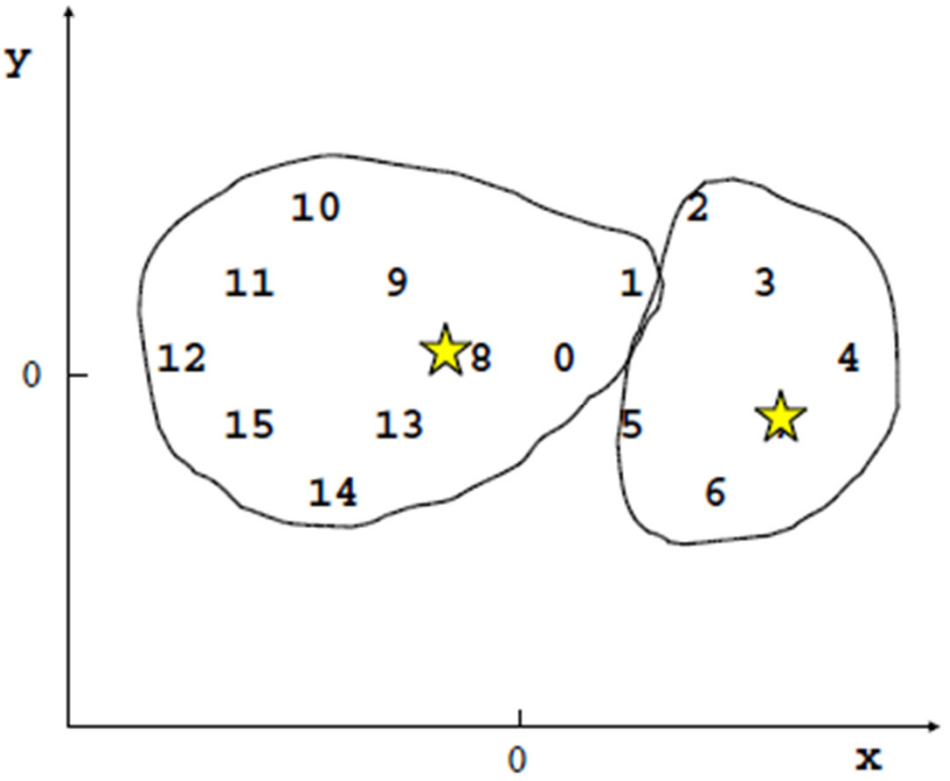


K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928



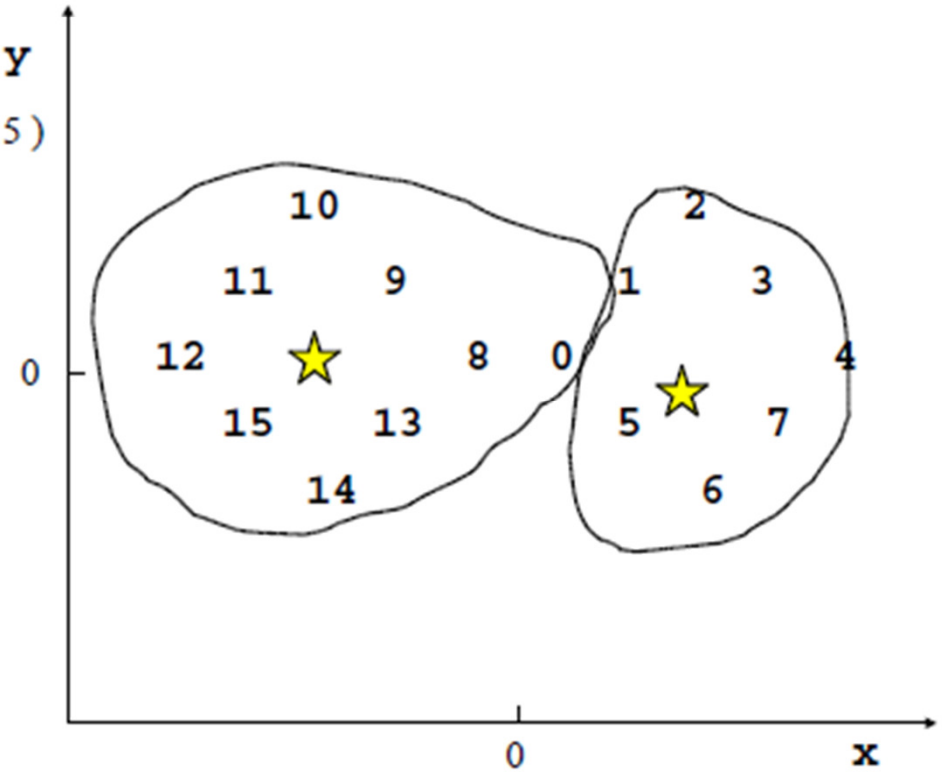
K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)



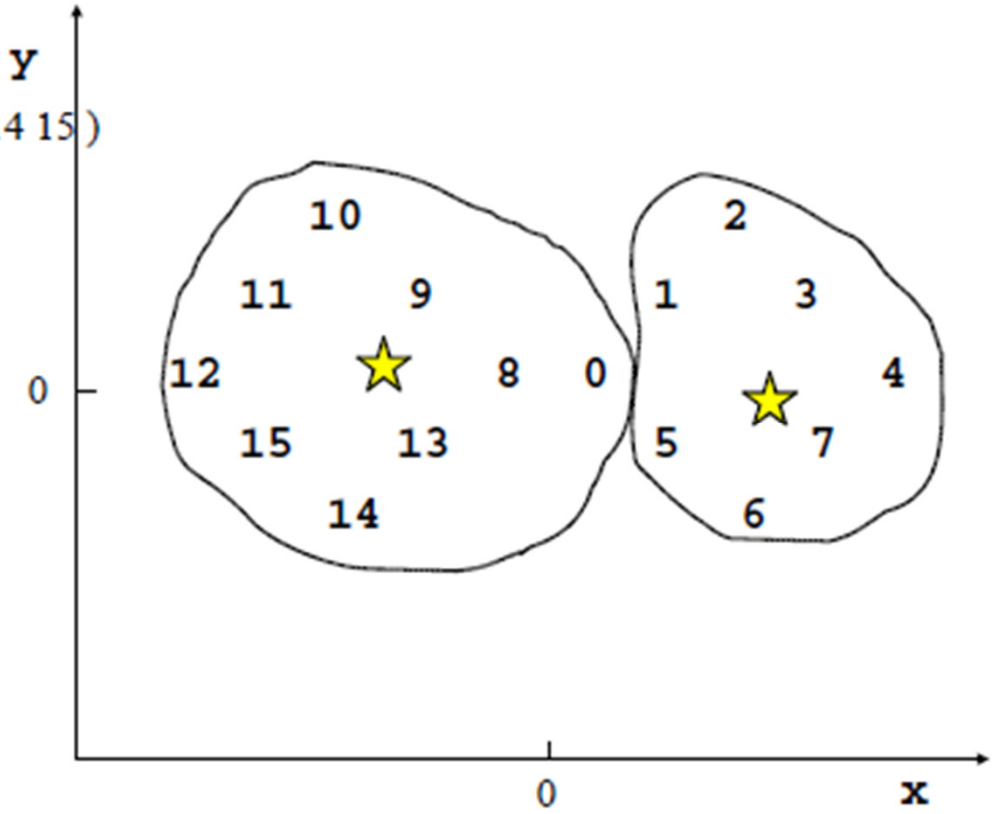
K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115



K-MEANS CLUSTERING – Example

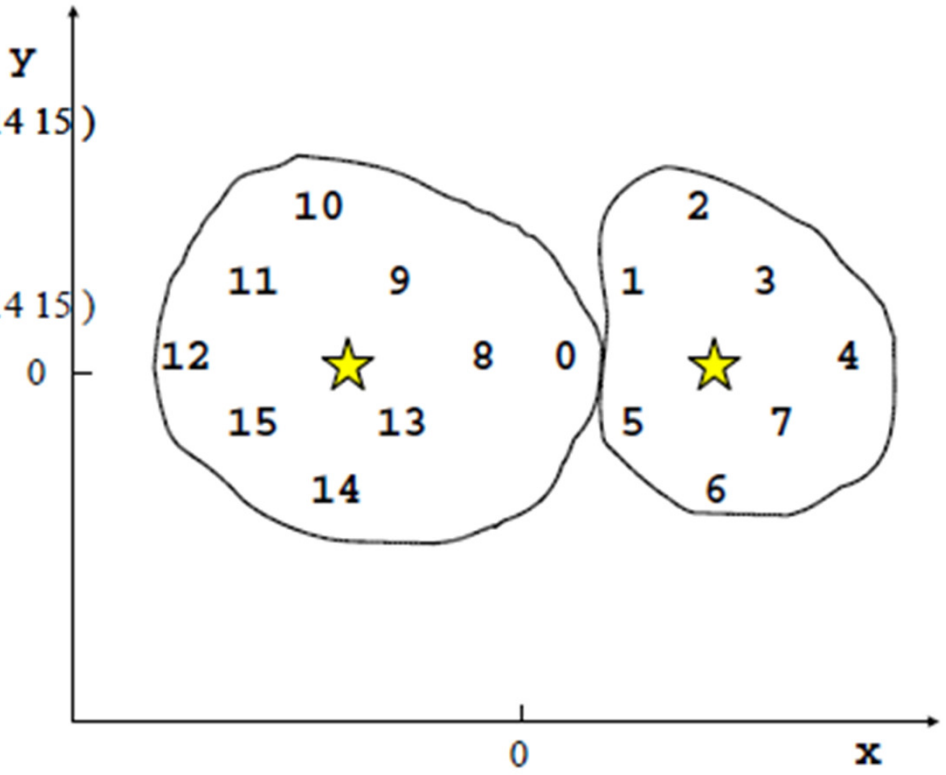
Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)



K-MEANS CLUSTERING – Example

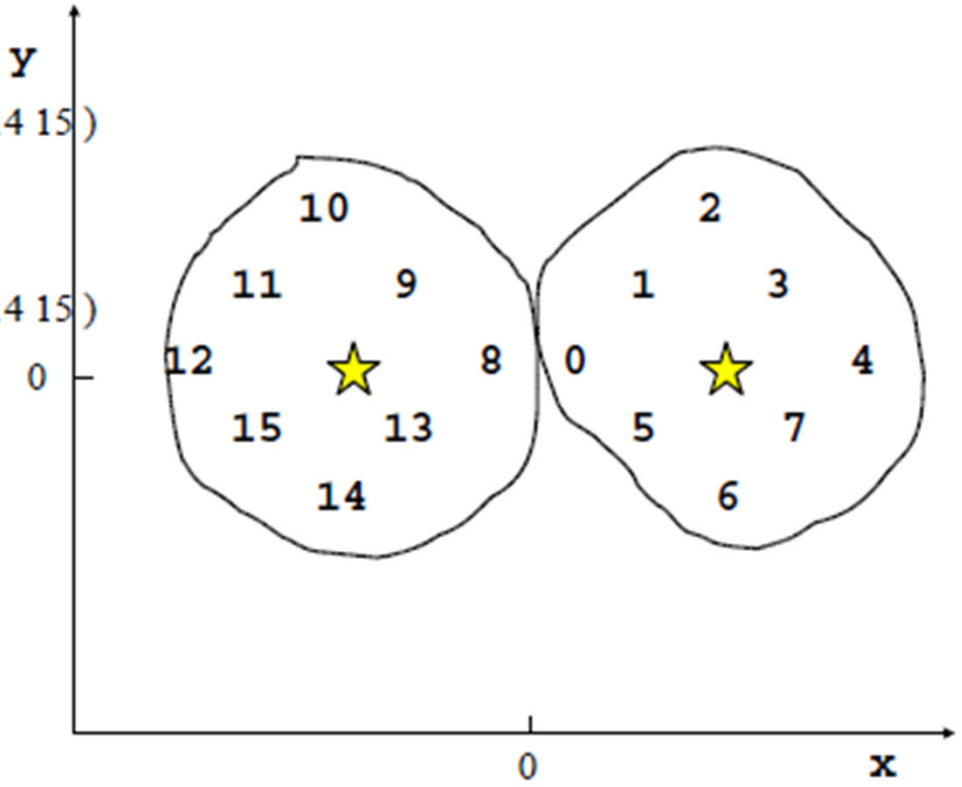
Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
Cluster Centers: (5.0 0.0) (-5.0 0.0)
Average Distance: 3.41421



K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

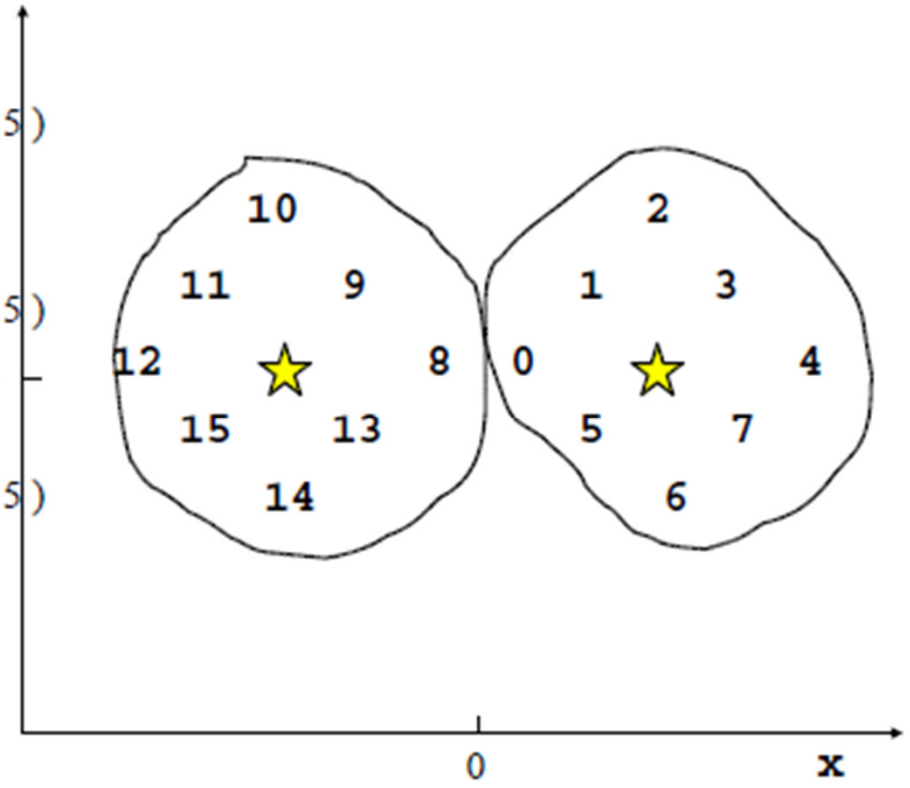
Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
Cluster Centers: (5.0 0.0) (-5.0 0.0)
Average Distance: 3.41421

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
No improvement.



K-MEANS -summary

- The most popular clustering method.
- Need to know K.
- May converge to a Local Minimum .
- High number of computations.

K-means for dimensionality reduction

dimensionality reduction is useful for:

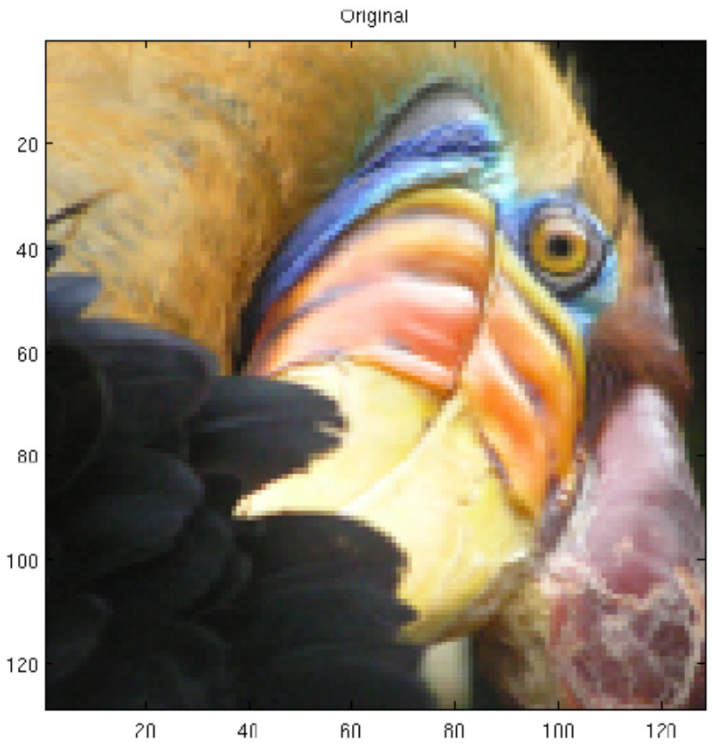
Data compression (from 10000-1000 D to) 100 D

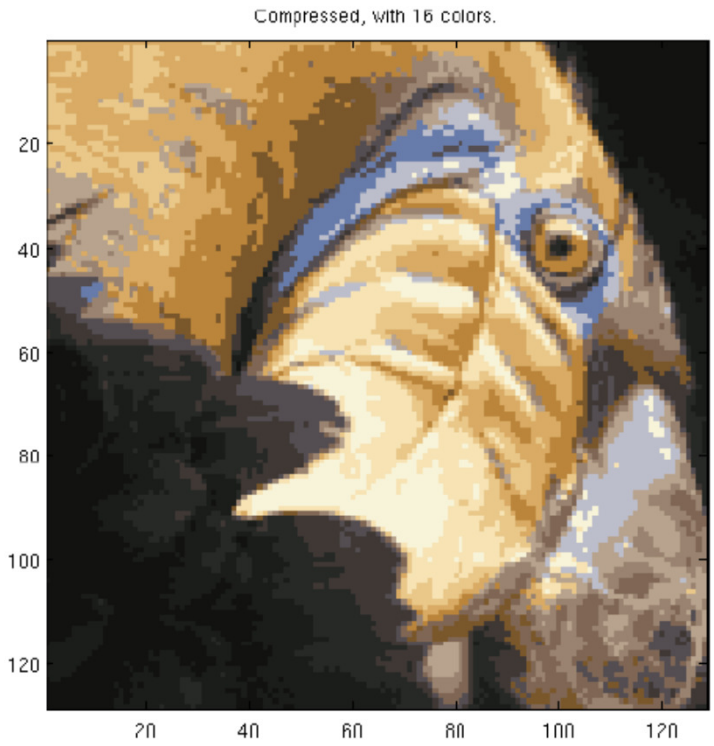
Reduce memory/ disk needed to store data
Speed up learning algorithm

Data visualization (from 100-50D to 2-3D)

Image compression with K-means

RGB image: 3*8 bits/pixel Compressed image: 16 colors(clusters) => 4 bits

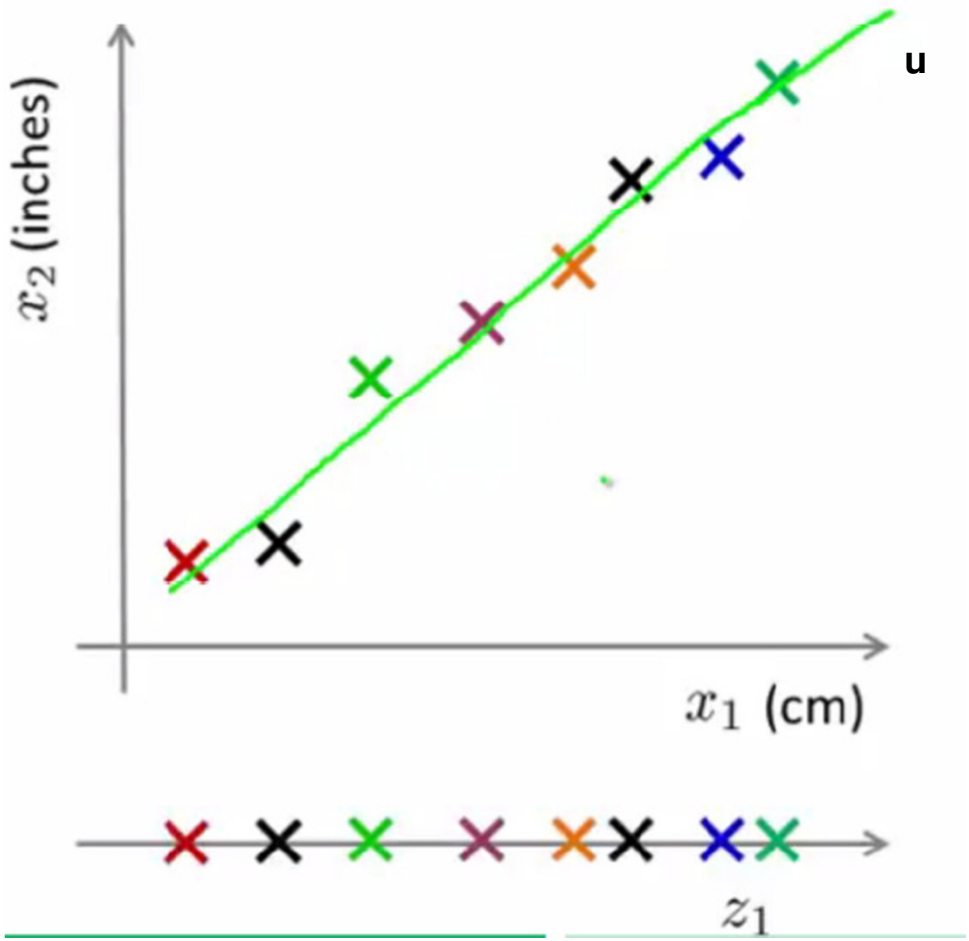




DATA COMPRESSION

Example: reduce data from 2D to 1D

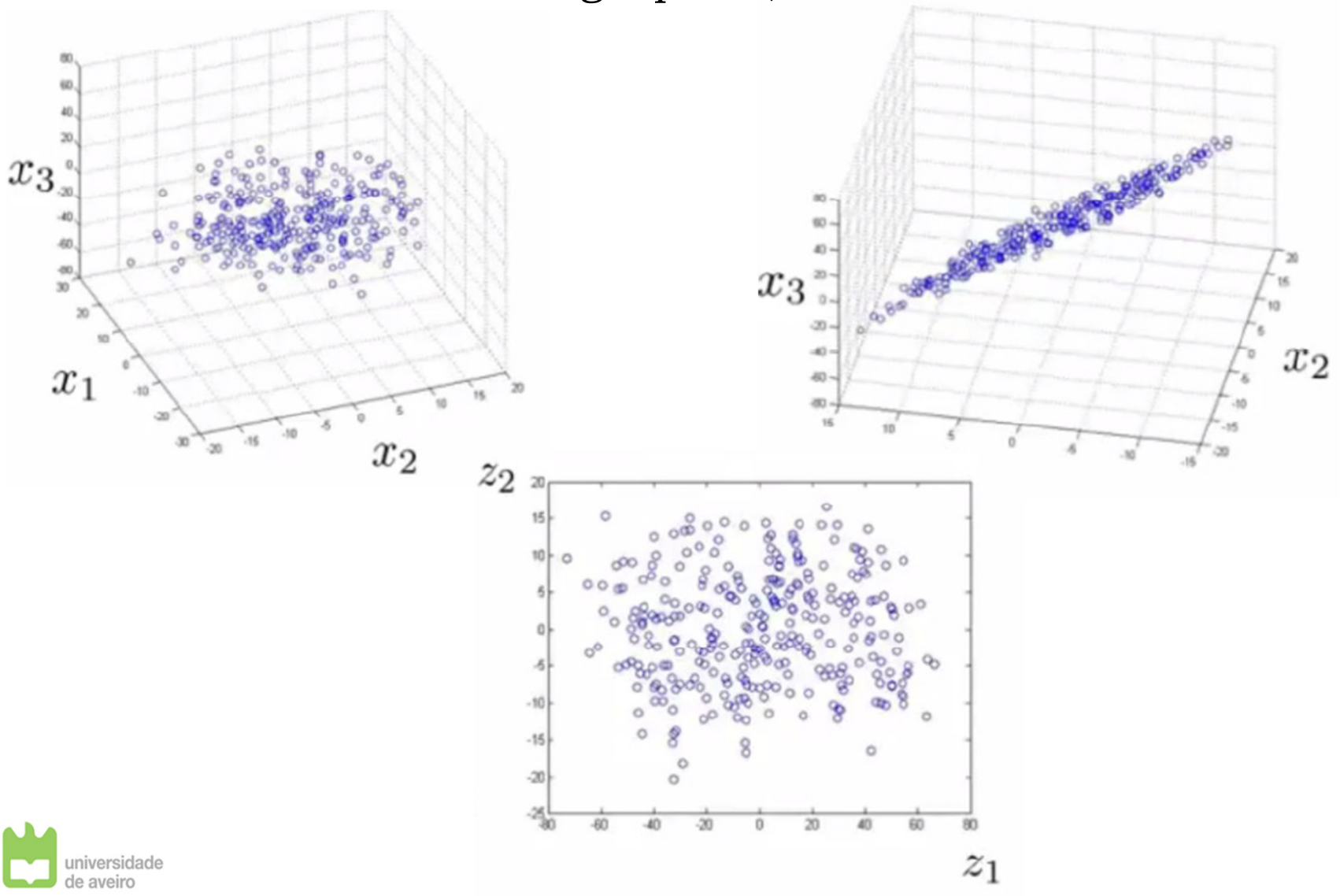
If 2D data is located along a line, the second dimension is redundant



DATA COMPRESSION

Example: reduce data from 3D to 2D

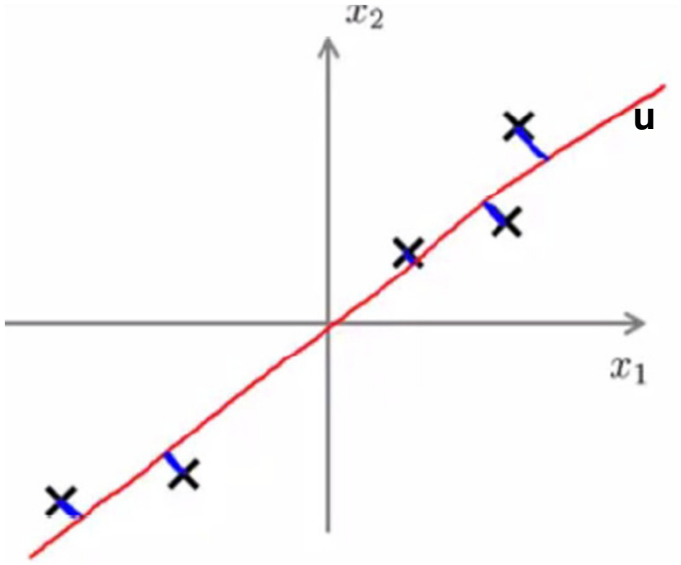
If 3D data is located along a plane, the 3rd dimension is redundant



PRINCIPAL COMPONENT ANALYSIS (PCA)

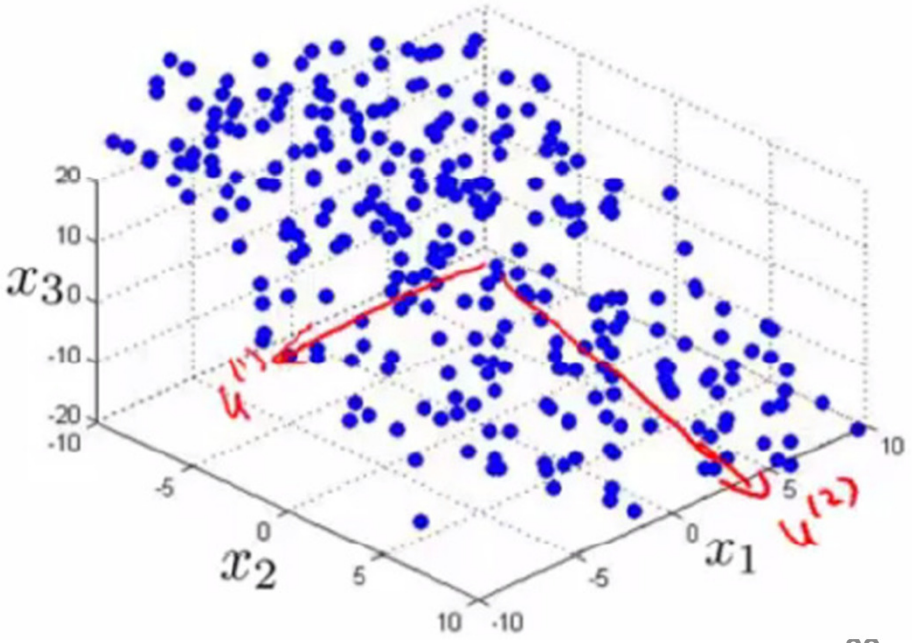
Reduce from 2D to 1D:

find the best direction (vector u) onto which to project data such that to minimize the projection error



Reduce from 3D to 2D:

find the orientation of the best plane (vectors u1, u2) onto which to project data such that to minimize the projection error

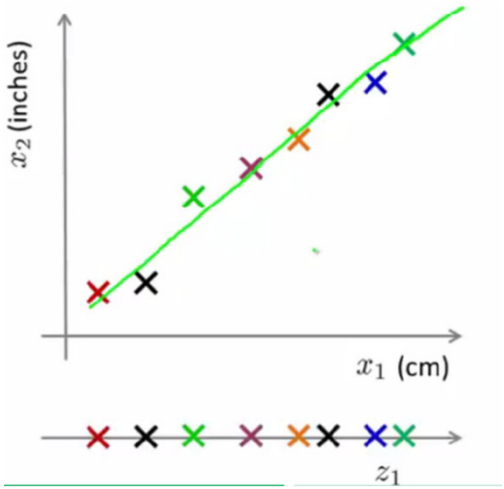


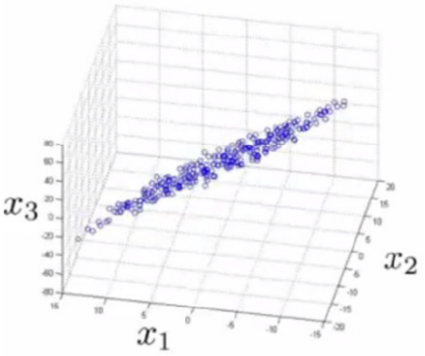
PRINCIPAL COMPONENT ANALYSIS (PCA)

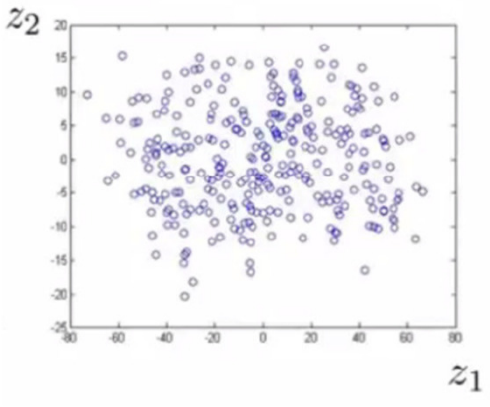
Reduce from n-dimension to k-dimension (k<n):

Two tasks:

- ***Task 1:*** Compute the coordinate system of the best k-dimensional surface (represented by vectors u1,..uk) onto which to project data such that to minimize the projection error.
- ***Task 2:*** Compute the values of the projected data in the lower dimensional space (z values)







PCA – DATA PREPROCESSING (step 1)

Training set: $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$

Preprocessing (feature scaling/mean normalization):

$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

Thus, all features have zero mean !

If the features have significantly different range of values, normalize them., e.g. in the interval [0,1] or [-1,1] or mean=0 & std=1

matrix X (mxn)	feature x_1	feature x_2	.....	feature x_n
Example 1	$x_1^{(1)}$	$x_2^{(1)}$		$x_n^{(1)}$
Example 2	$x_1^{(2)}$	$x_2^{(2)}$		$x_n^{(2)}$
...				
Example i	$x_1^{(i)}$	$x_2^{(i)}$		$x_n^{(i)}$
...				
...				
Example m	$x_1^{(m)}$	$x_2^{(m)}$		$x_n^{(m)}$

DATA NORMALIZATION

from sklearn.preprocessing import MinMaxScaler

```
mms = MinMaxScaler()
mms.fit(data)
data_transformed = mms.transform(data)
```

MinMaxScaler?

MinMaxScaler(feature_range=(0, 1), copy=True)

Transforms features by scaling each feature to a given range.

from sklearn.preprocessing import StandardScaler

```
sc=StandardScaler()
sc.fit(data)
data_transformed =sc.transform(data)
```

Standardize features by removing the mean and scaling to unit variance.

PCA – Singular Value Decomposition (step 2)

- Compute Covariance matrix of the mean normalized data matrix *X* (dimension *mxn* - m examples, n features):

$$\mathbf{Cov = X^T * X}$$

- Compute Singular Value Decomposition(SVD) of Covariance matrix:

$$\mathbf{Cov = U * S * V}$$

U (*nxn*) - matrix of eigenvectors:

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \cdots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}$$

S (*nxn*)– diagonal matrix of singular values in decreasing order:

$$S_{nxn} = \begin{bmatrix} S_{11} & 0 & \cdots & 0 \\ 0 & S_{22} & \vdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & S_{nn} \end{bmatrix}$$

SVD is equivalent to eigen-values/eigen-vector decomposition.

PCA

The projection vectors are the first k columns of U (k<n): -***Task 1***

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \cdots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$Ureduce_{nxk} = U(:,1:k)$$

Step 3: Compute the new (projected) data matrix Z (m examples, k features): - ***Task 2***

$$Z_{mxk} = X_{mxn} * Ureduce_{nxk}$$

Step 4: Reconstruct data matrix X from the projected Z matrix :

$$X_{approx(mxn)} = Z_{mxk} * Ureduce^{T}_{kxn}$$

Choosing k (number of principal components)

Average squared approximation error:

$$\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{approx}^{(i)}\|^2$$

Total data variation:

$$\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2$$

Typically, choose k to be smallest value so that

$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2} \leq 0.01 \qquad (1\%)$$

"99% of variance is retained"

(typically the desired retained variance is between 90-99%)

Choosing k (number of principal components)

Compute SVD once: [U,S,V]=svd(Cov)

Choose k<n such that you get the desired retained variance

(e.g. 99 %):

$$\frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{n} S_{ii}} \geq 0.99$$

$$S_{nxn} = \begin{bmatrix} S_{11} & 0 & \cdots & 0 \\ 0 & S_{22} & \vdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & S_{nn} \end{bmatrix}$$