ieeta instituto de engenharia electrónica e telemática de aveiro

universidade de aveiro

Departamento de Eletrónica, Telecomunicações e Informática

Machine Learning

LECTURE 7: UNSUPERVISED LEARNING (K-MEANS CLUSTERING AND PCA)

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Outline

1. K-means clustering

2. Data dimensionality reduction
    - data compression
    - data visualization

3. Principal Component Analysis (PCA)

SUPERVISED vs. UNSUPERVISED LEARNING

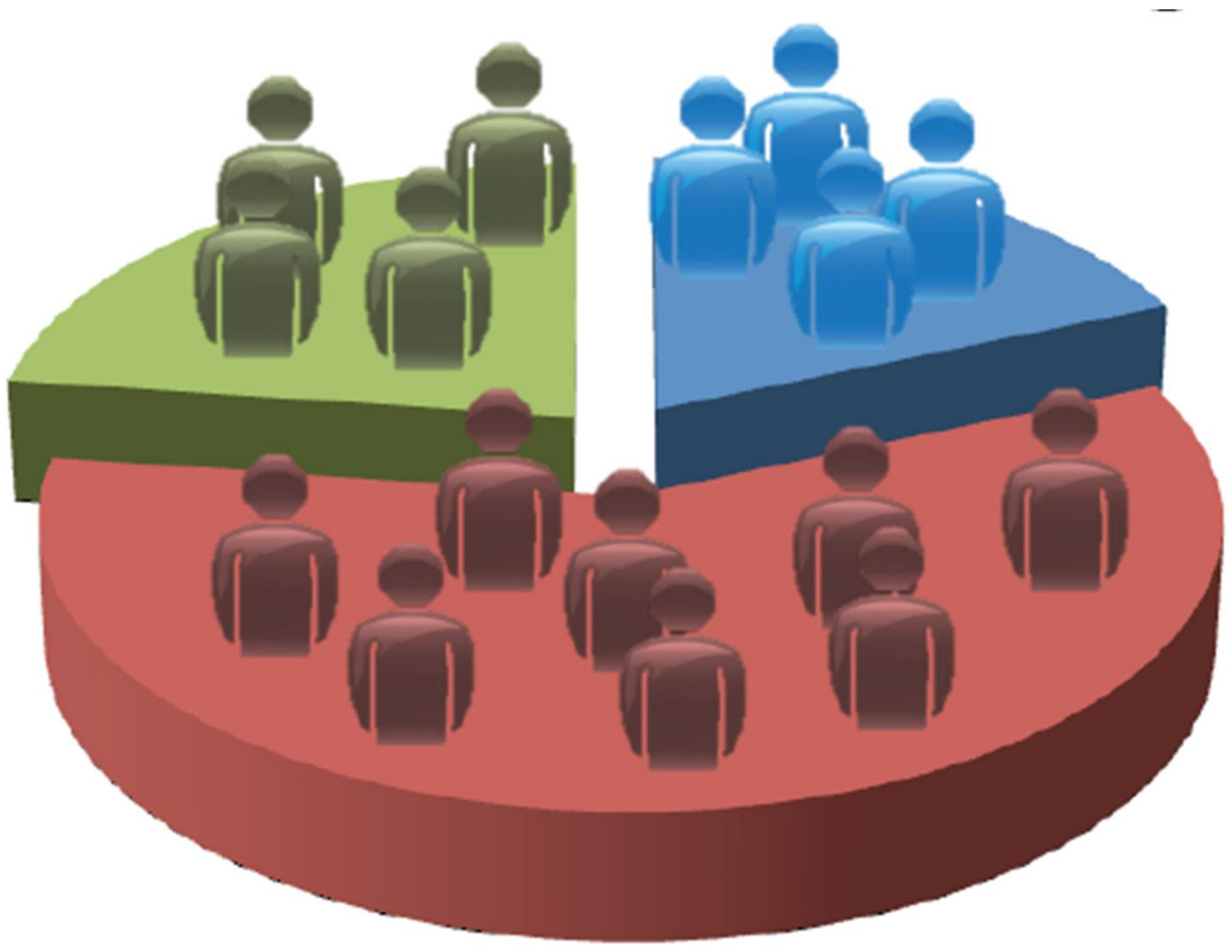
Supervised Learning - (given DATA + LABELS):
ML method is trained with labeled data to predict the labels of new examples (learning by labeled examples)

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

Semi-Supervised Learning – mixture of labeled and unlabeled data

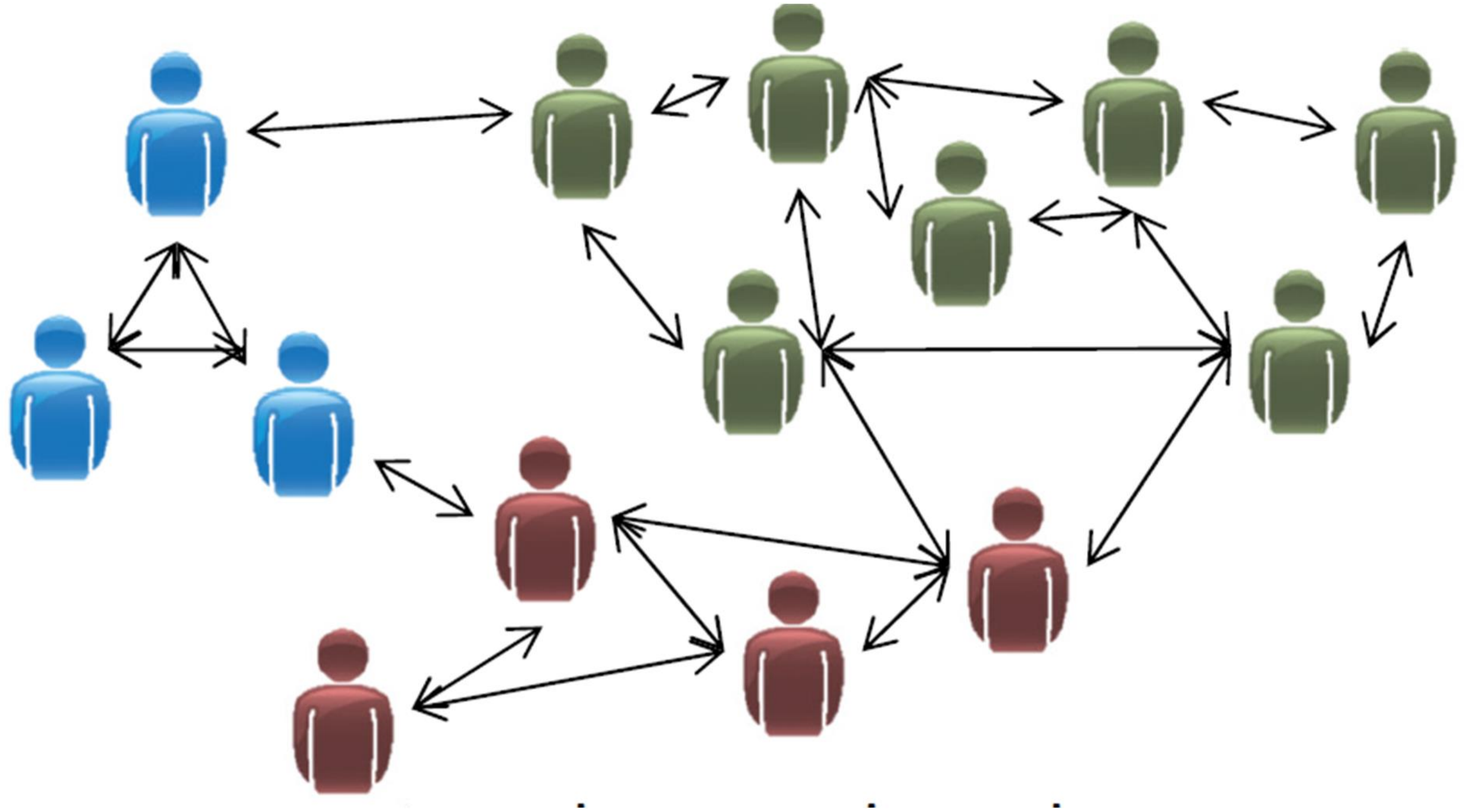
Unsupervised learning -

Market segmentation (data base of customers)

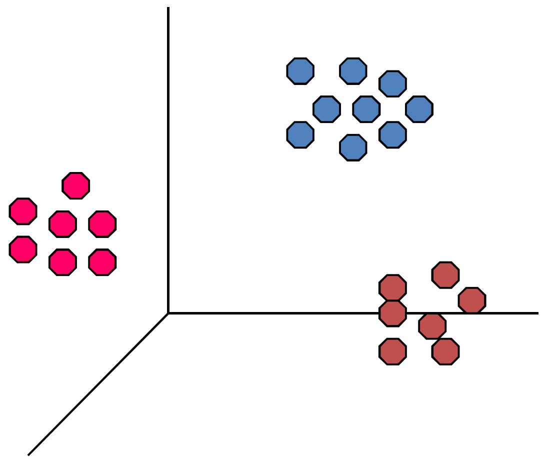


Unsupervised learning

Social network analysis



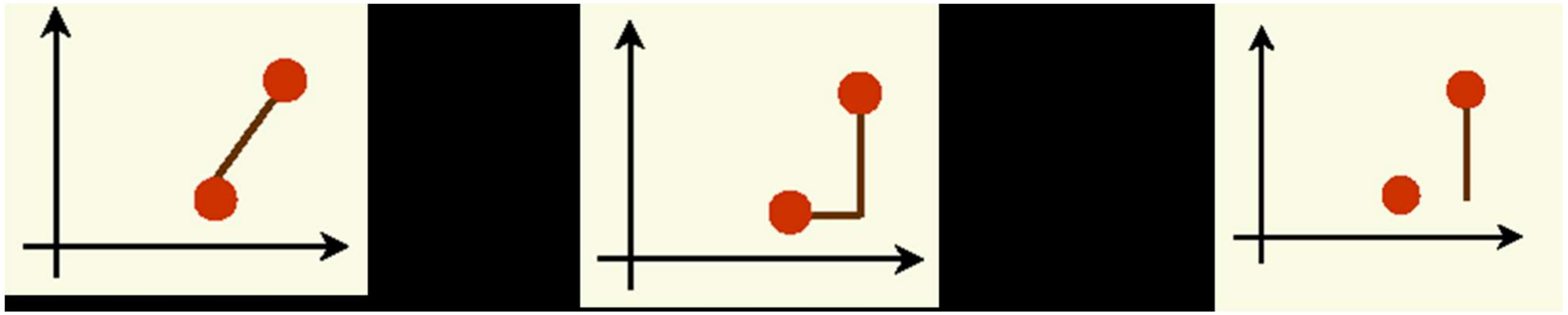
Clustering intuition



- 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)

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

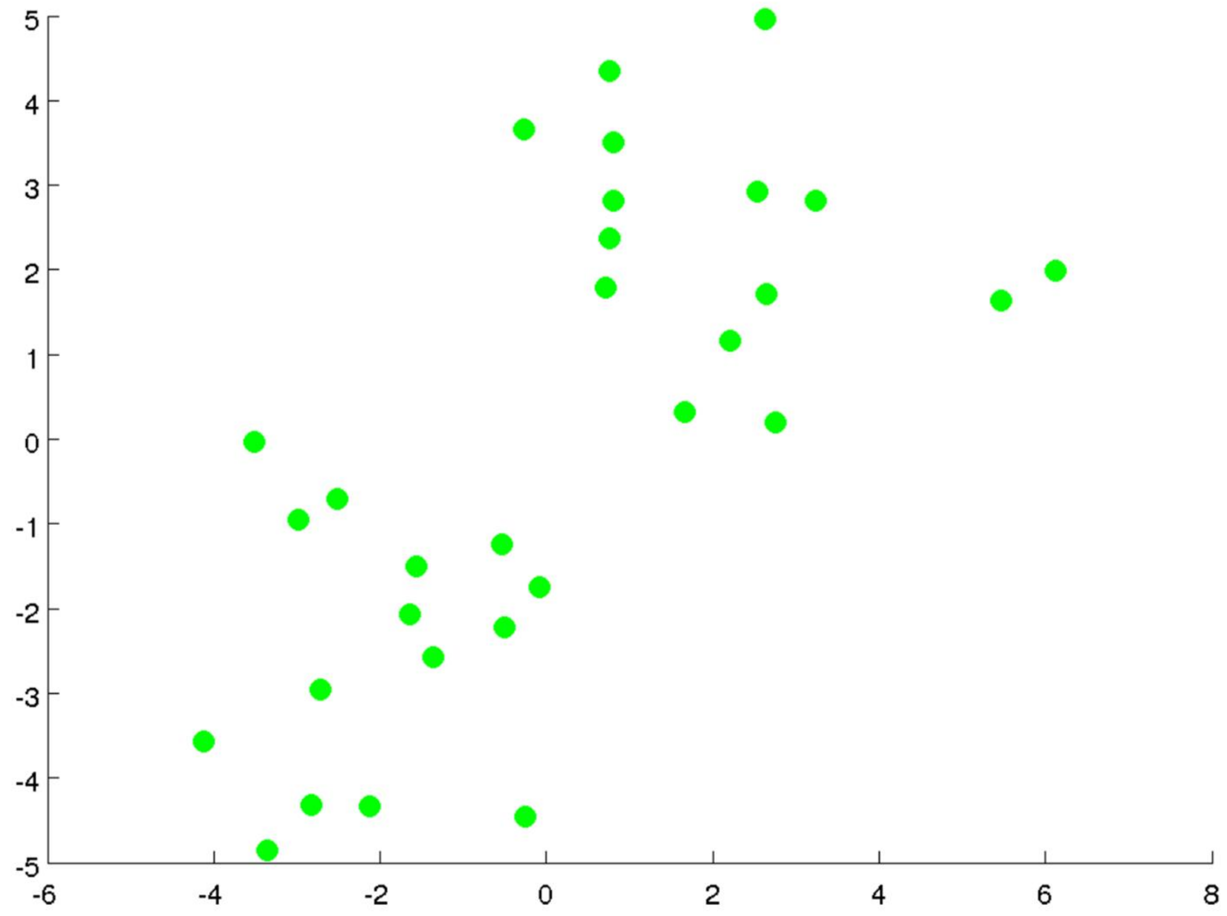
Chebyshev distance

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

K-means algorithm

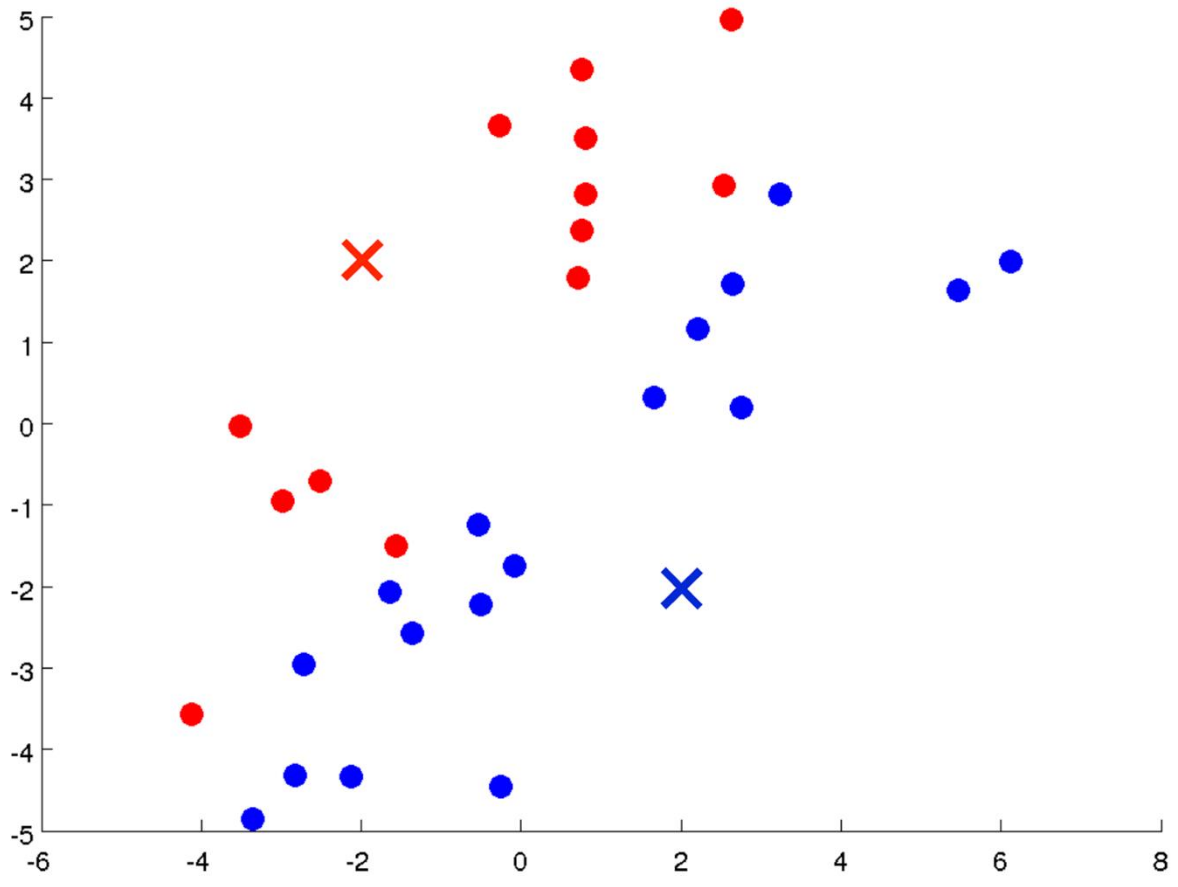
Given input:

- **K (number of clusters)**
- **Training set (no labels)**



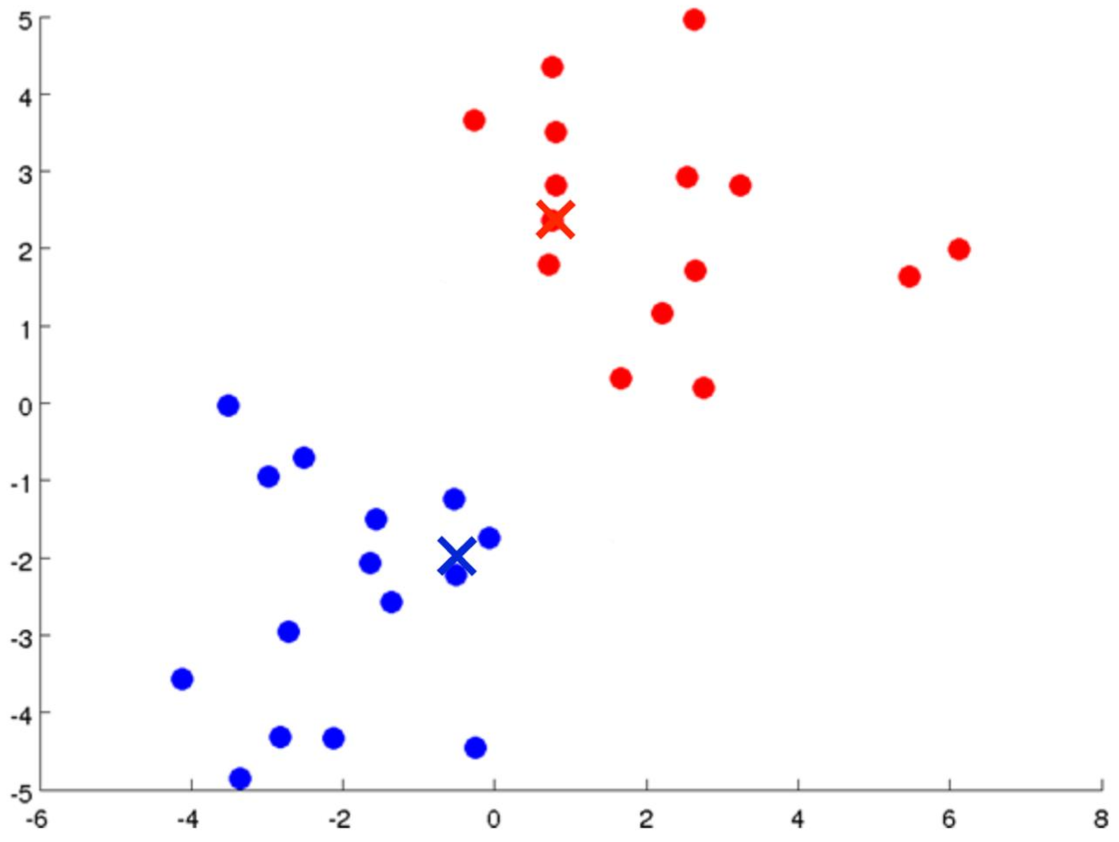
K-means algorithm

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



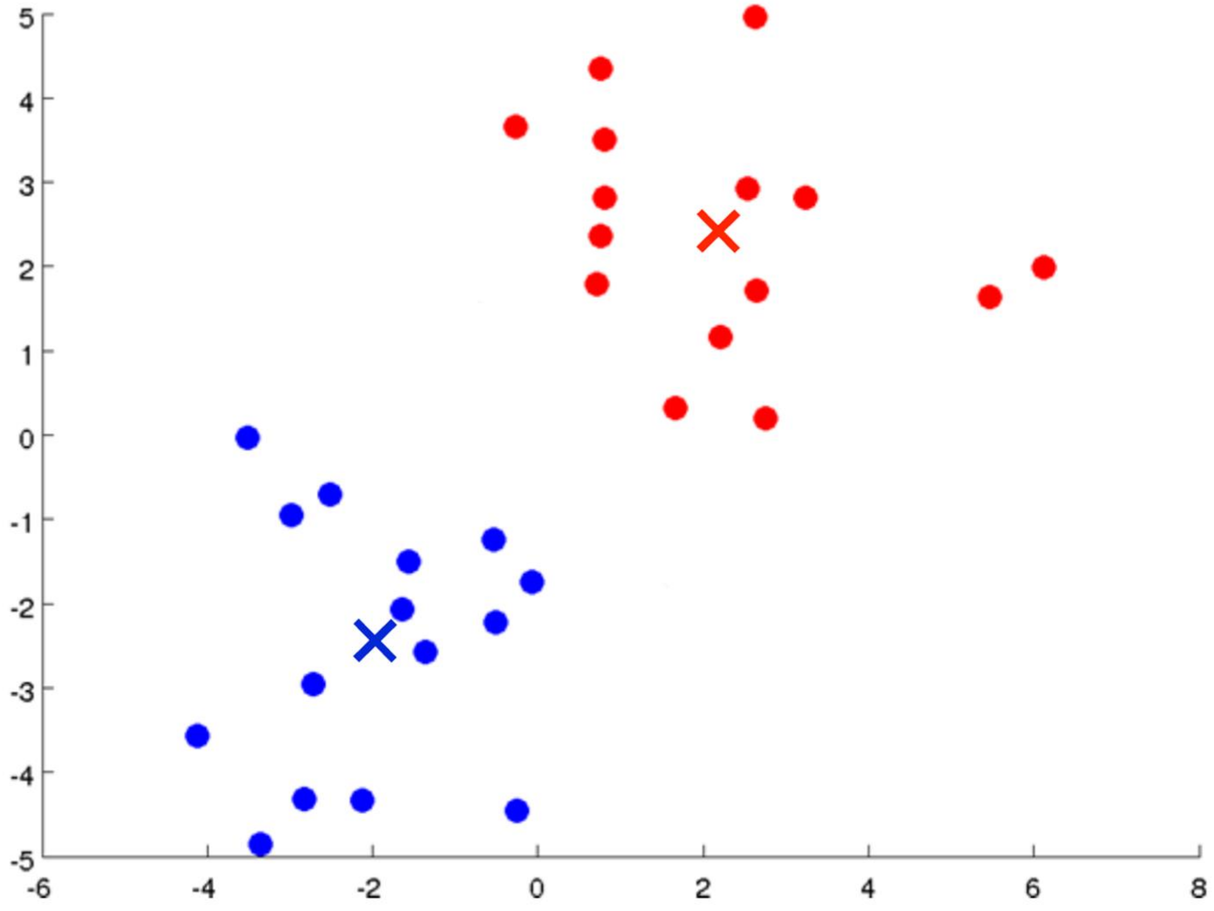
K-means algorithm

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

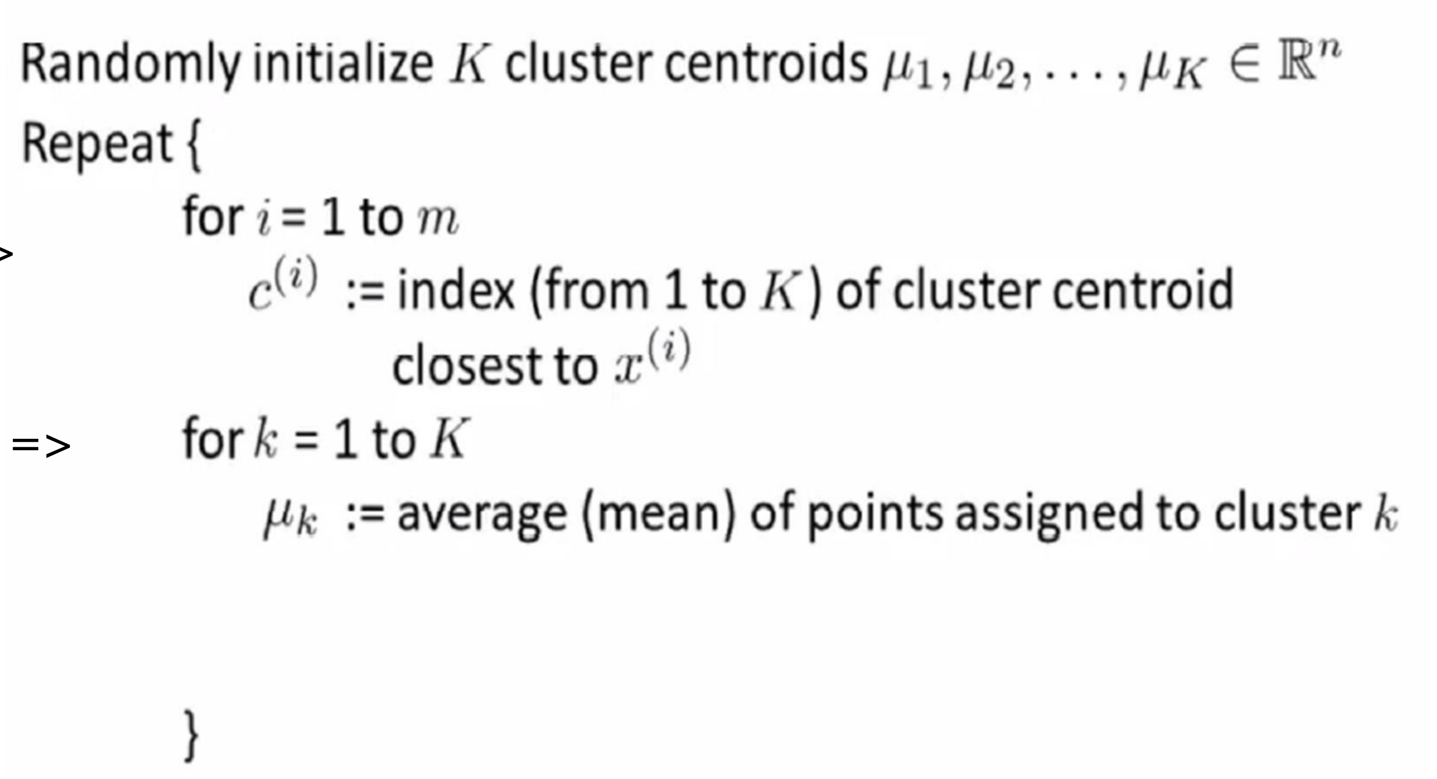


K-means algorithms

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 $K$
            $\mu_k$ := average (mean) of points assigned to cluster $k$
        }
```

K-means optimization objective (distortion = average distance)

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

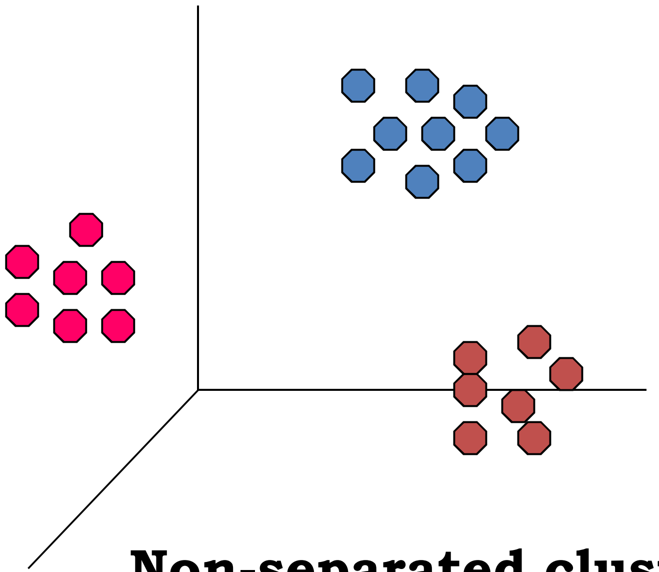
$$\min_{\substack{c^{(1)}, \dots, c^{(m)}, \\ \mu_1, \dots, \mu_K}} J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)$$

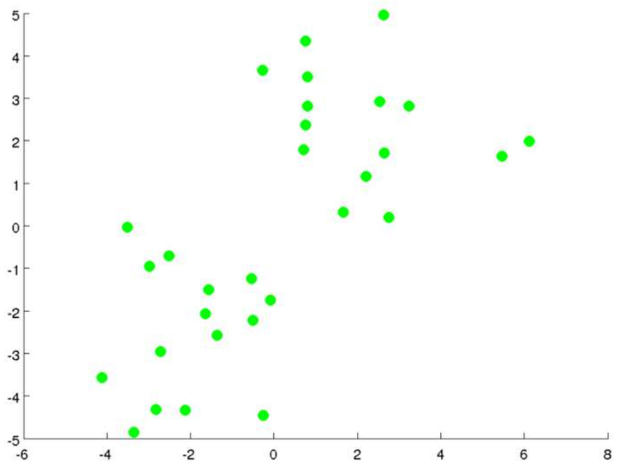
Stop K-means learning (different criteria):

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

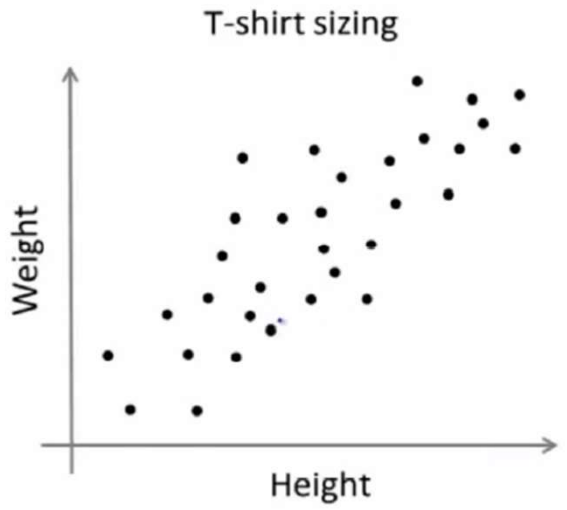
K-means for non-separated clusters

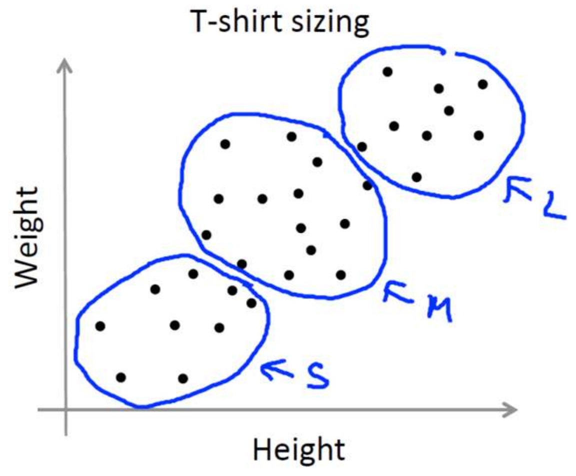
Separated clusters





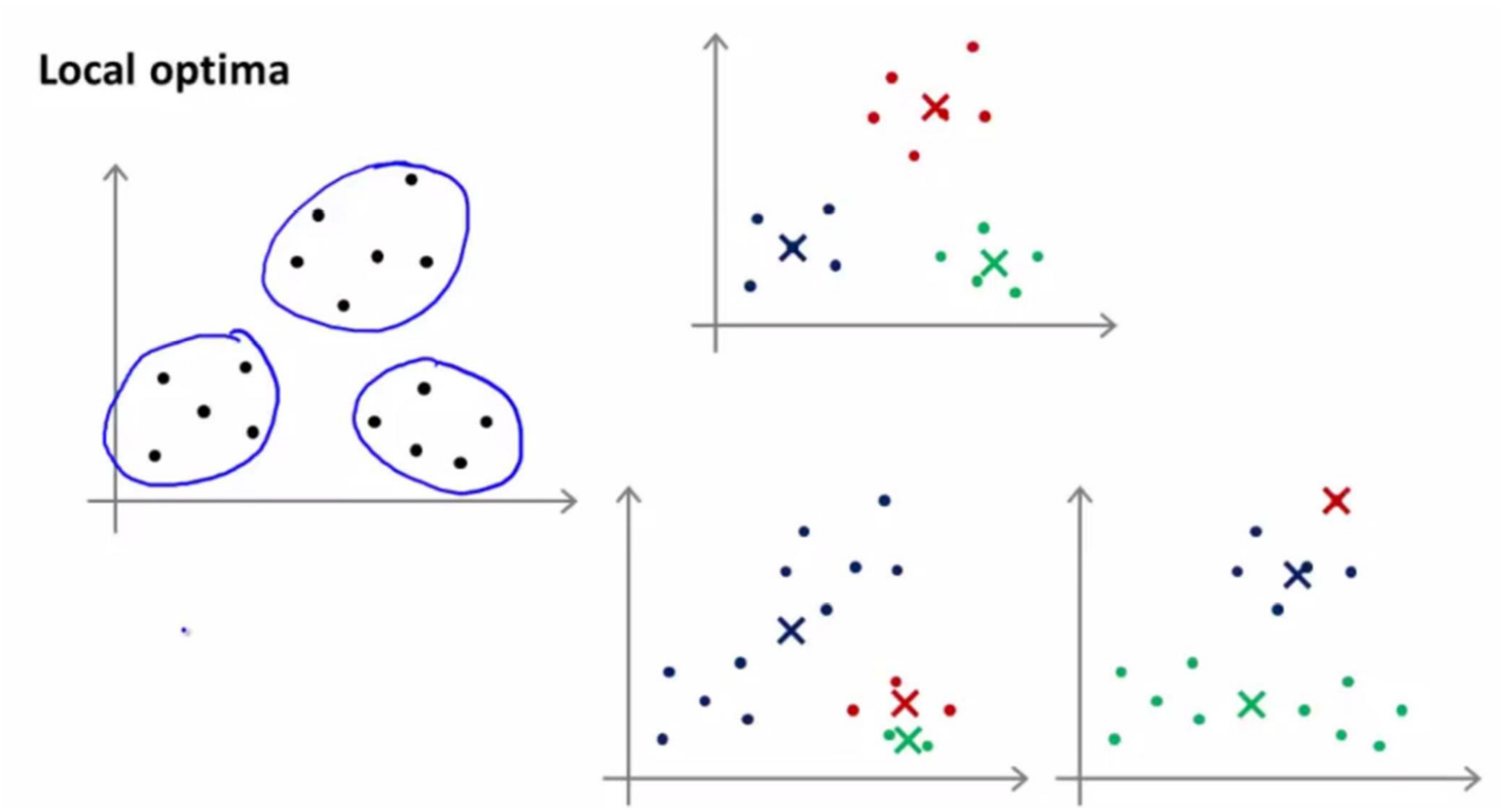
Non-separated clusters (find problem specific criteria)





Single (Random) Initialization

Choose # of clusters K <m (# of examples)
Inicialize K cluster centroids = randomly picked K training examples



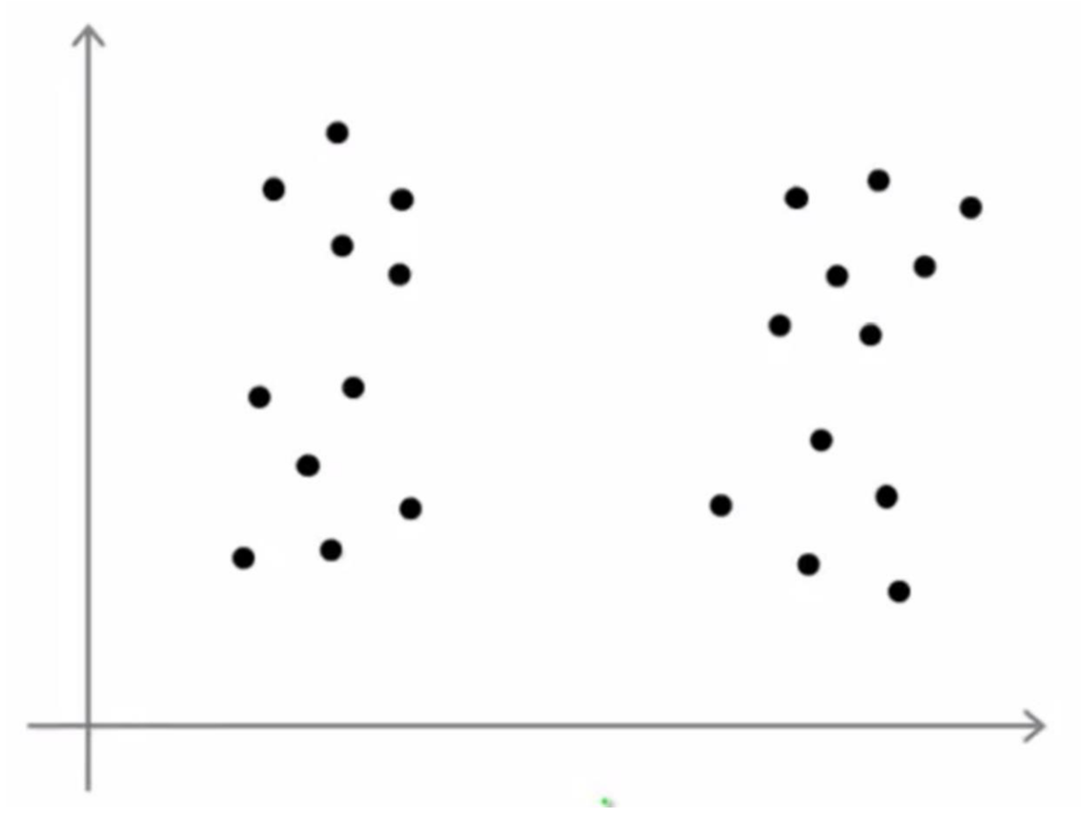
Repeat Random Initializations

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

Repeat random inicializations works well for relatively small number of cluster e.g. K = (2,…10) .

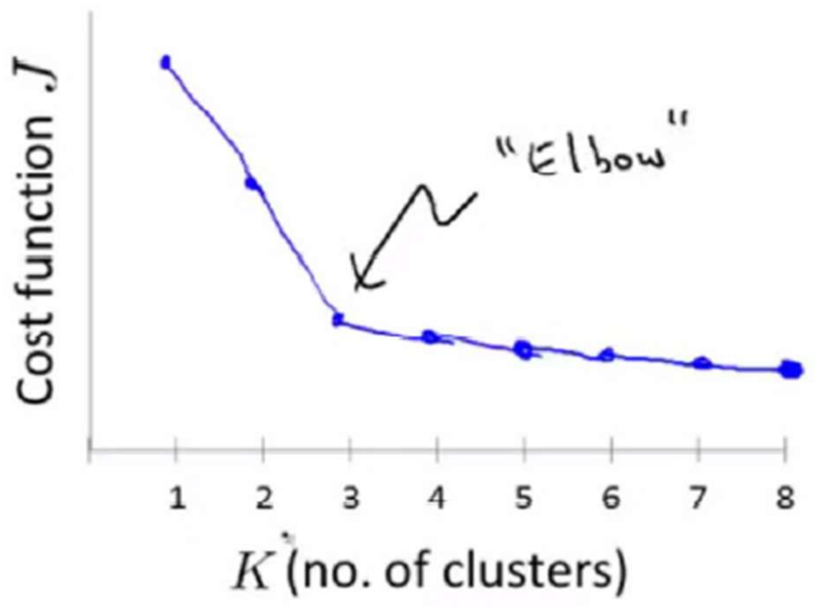
Choosing the number of clusters



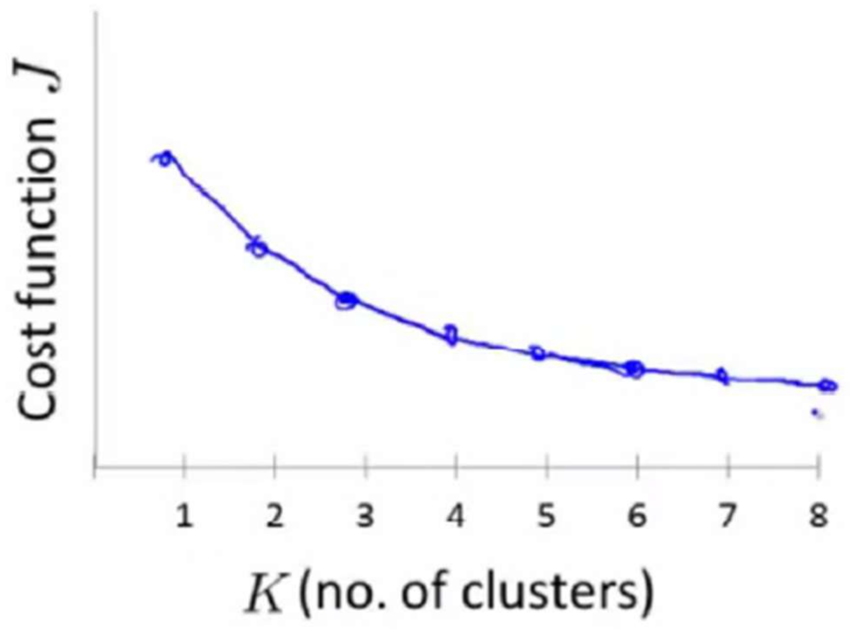
- Choose K by data visualisation (if possible)
- Ask domain experts (highly recommendable) , e.g. anomaly detection (experts should know how many types of anomalies are expected)
- Choose K automatically (e.g. Elbow method)

Choosing the number of clusters (Elbow method)

Appropriate for Elbow method

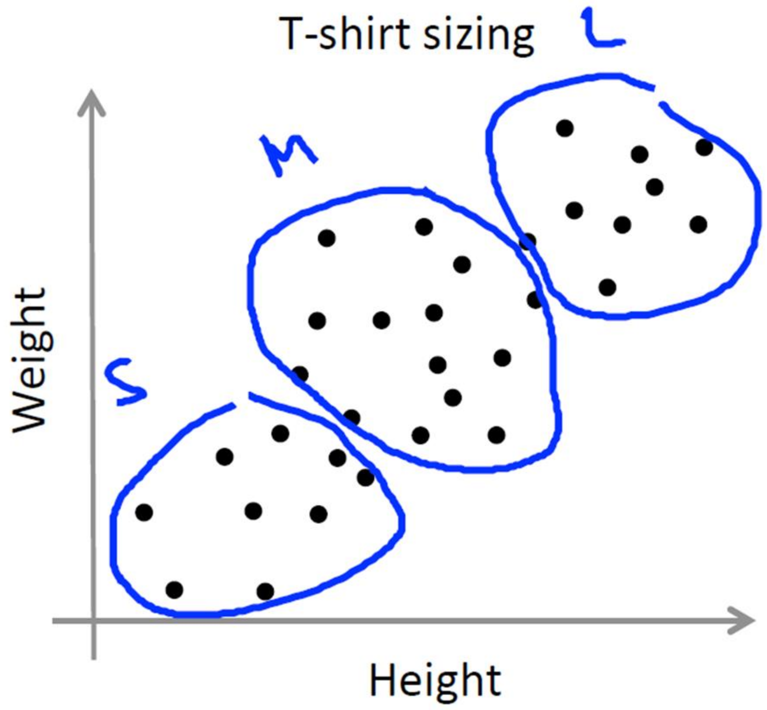


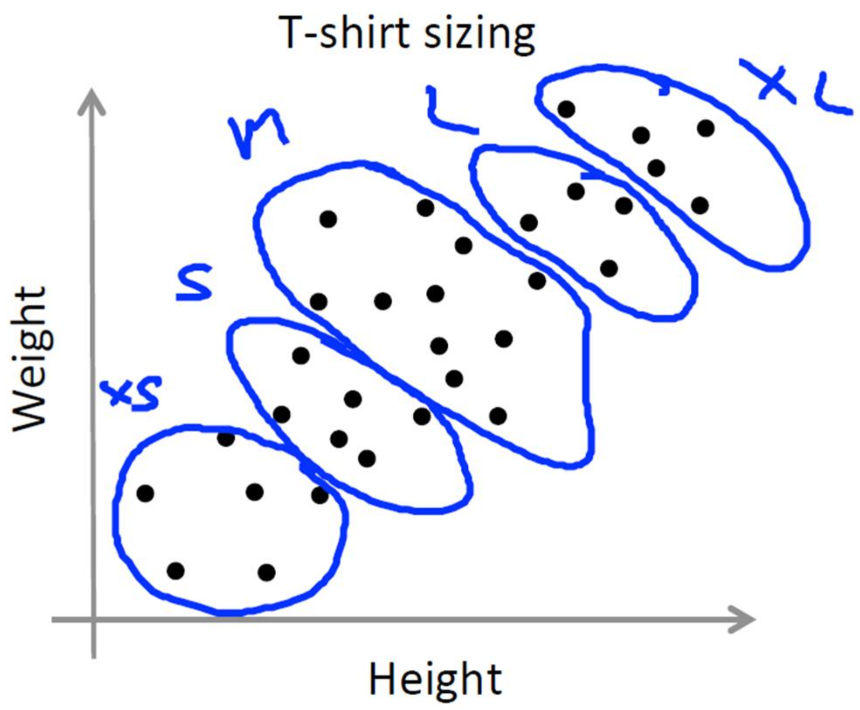
Not Appropriate for Elbow method



Choosing the number of clusters

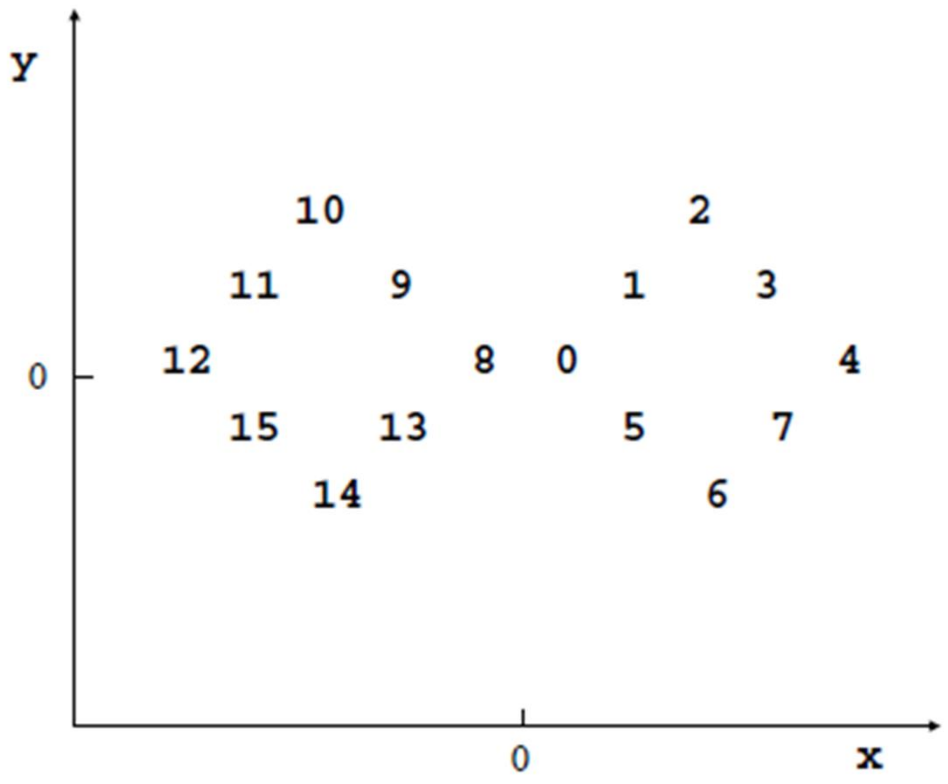
Run K-means to get clusters according to a particular purpose.
(S, M, L type of t-shirts) or (XS, S, M, L, XL, of t-shirts))





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

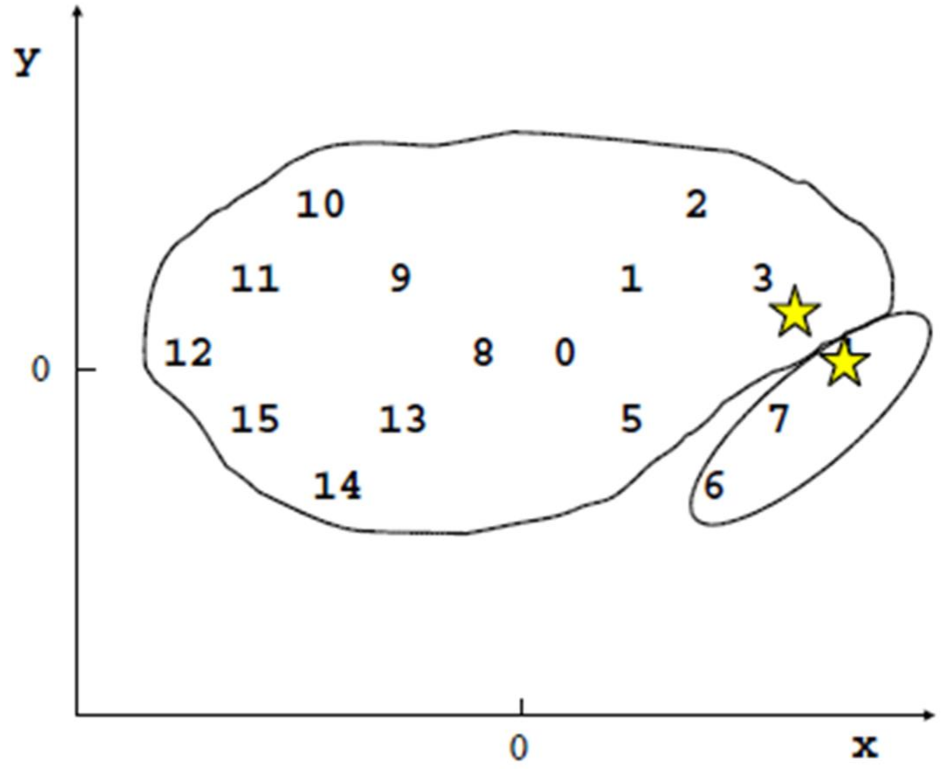


- find the best 2 clusters

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

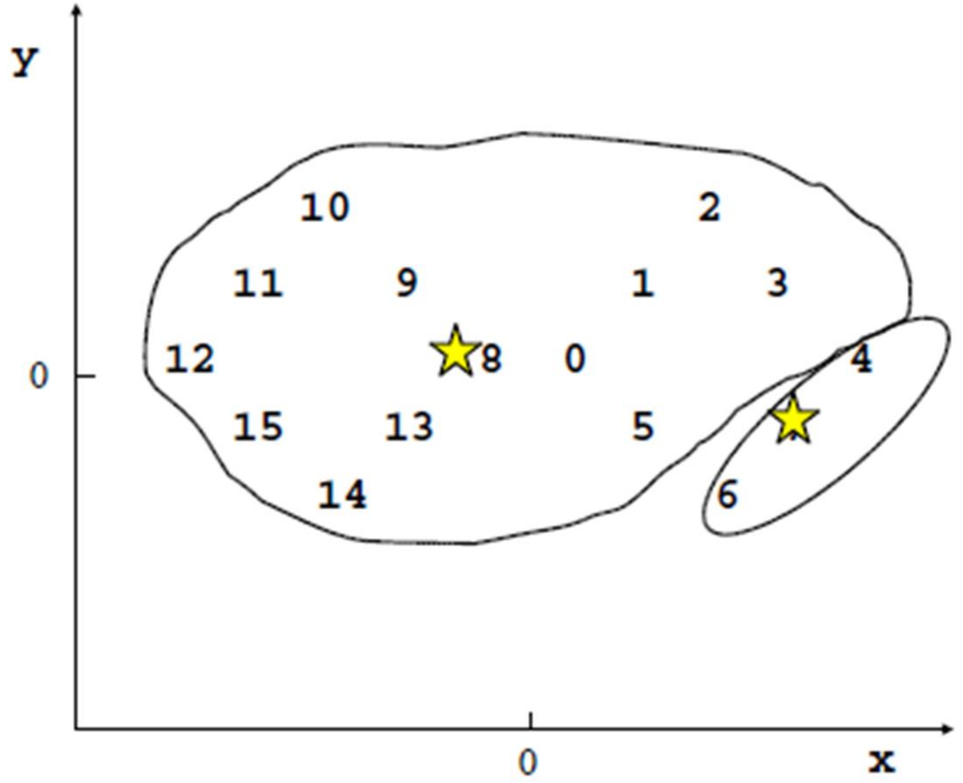


K-MEANS CLUSTERING – Example

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)

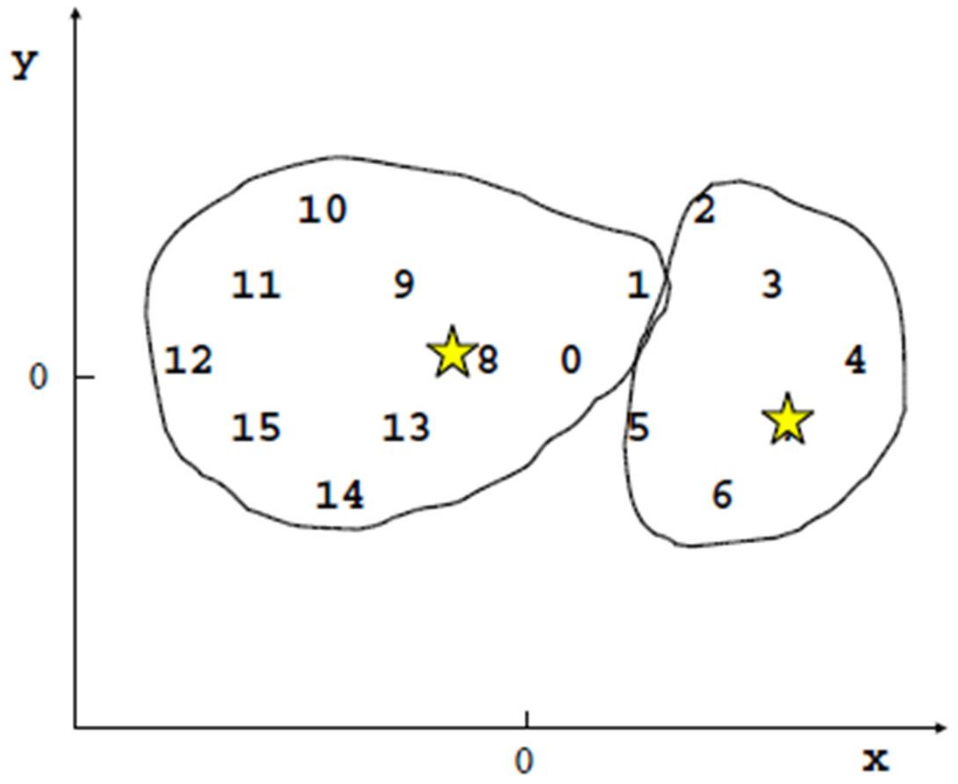


K-MEANS CLUSTERING – Example

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)

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Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
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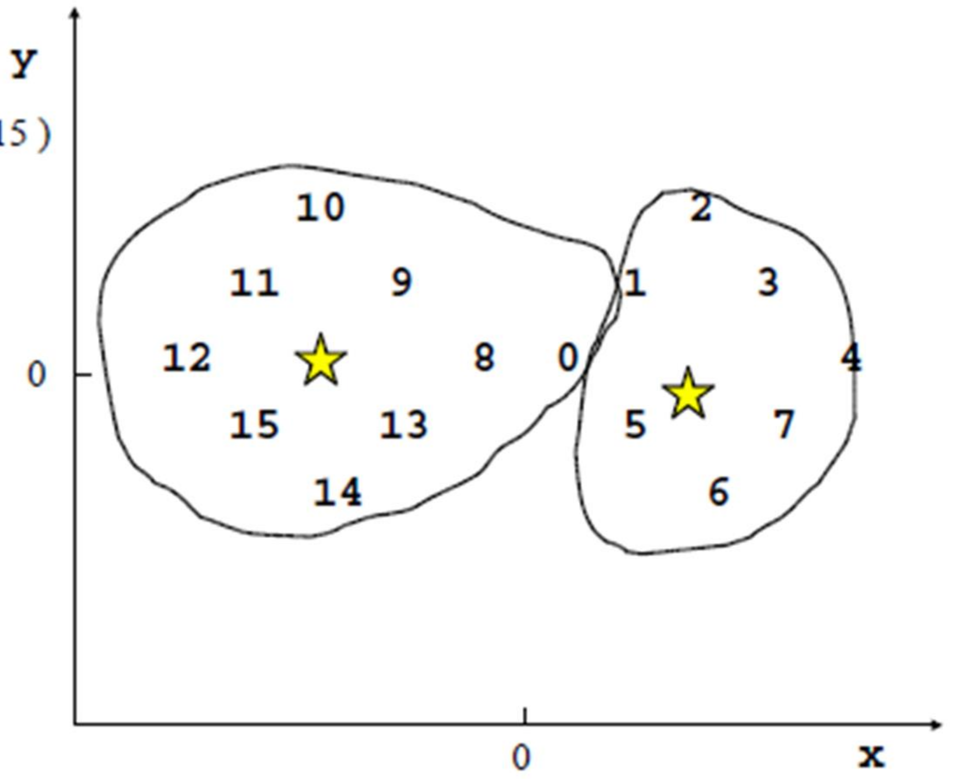
Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

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



K-MEANS CLUSTERING – Example

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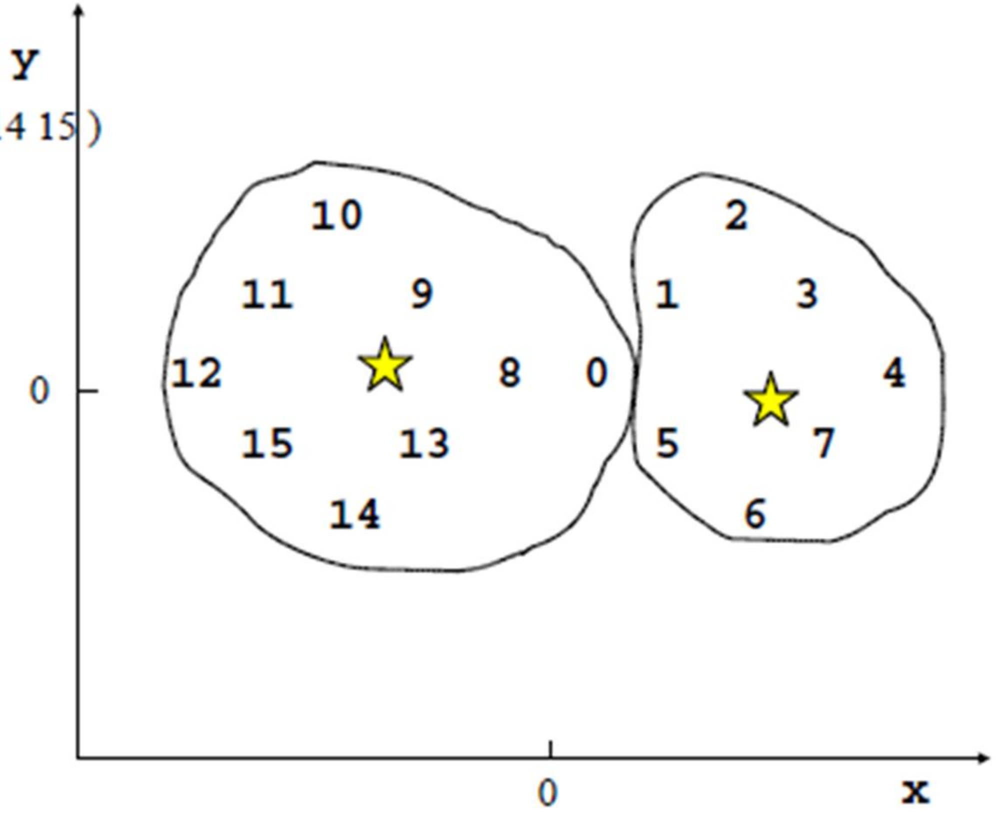
Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115



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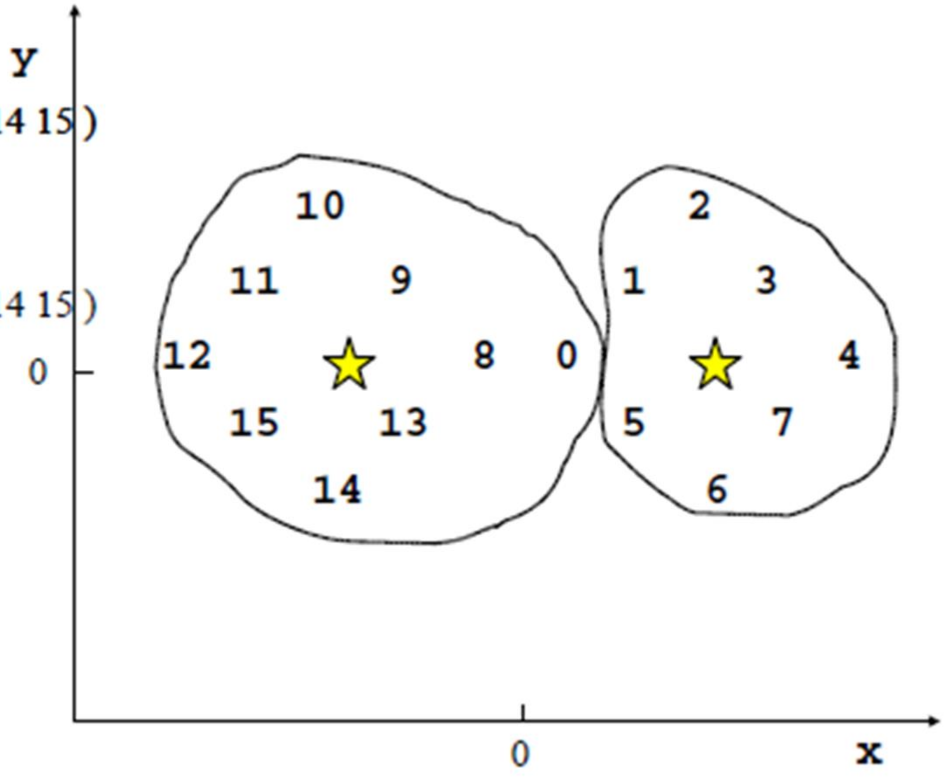
Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115

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



K-MEANS CLUSTERING – Example

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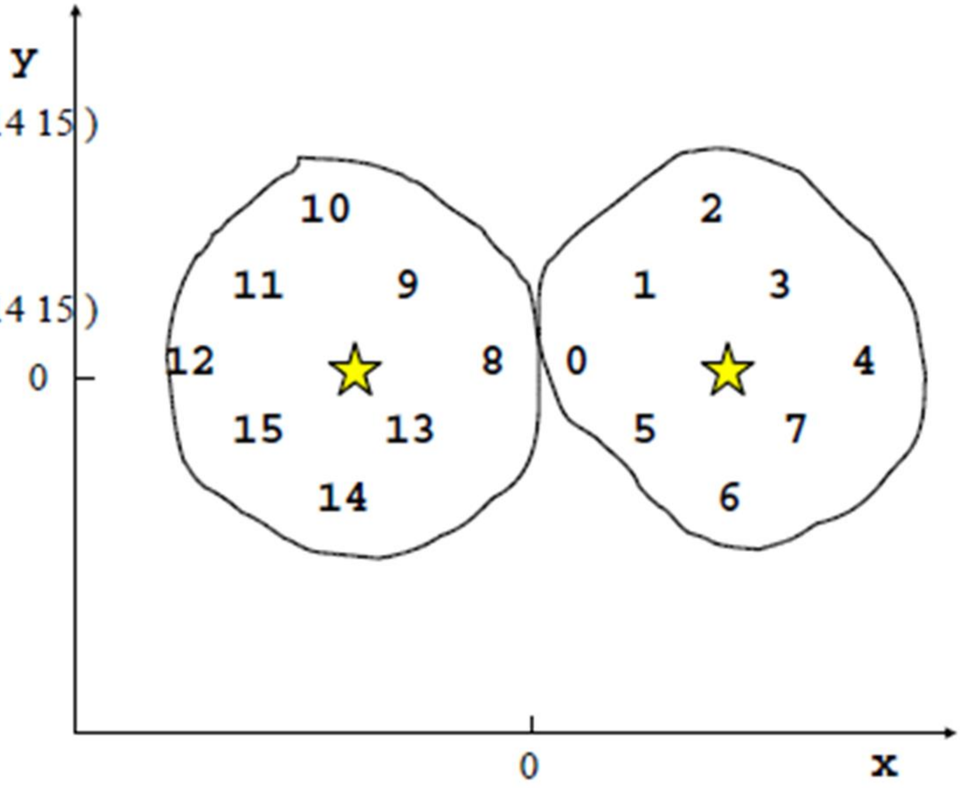
Average Distance: 3.6928

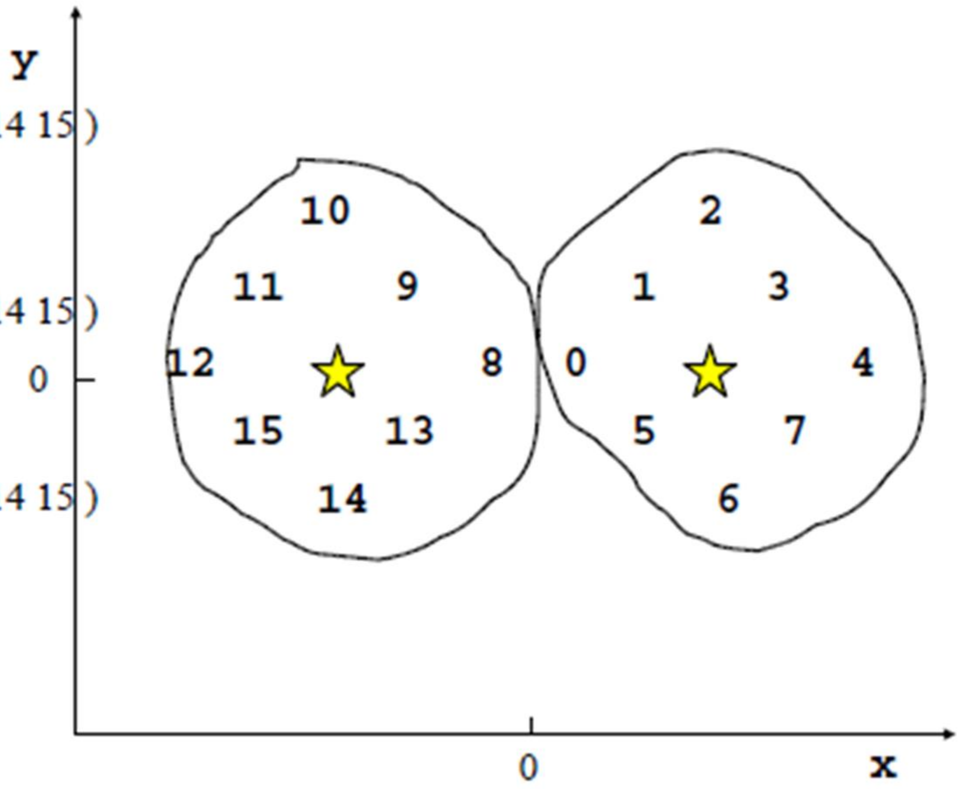
Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115

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.
```



HIERARCHICAL CLUSTERING

● Two approaches

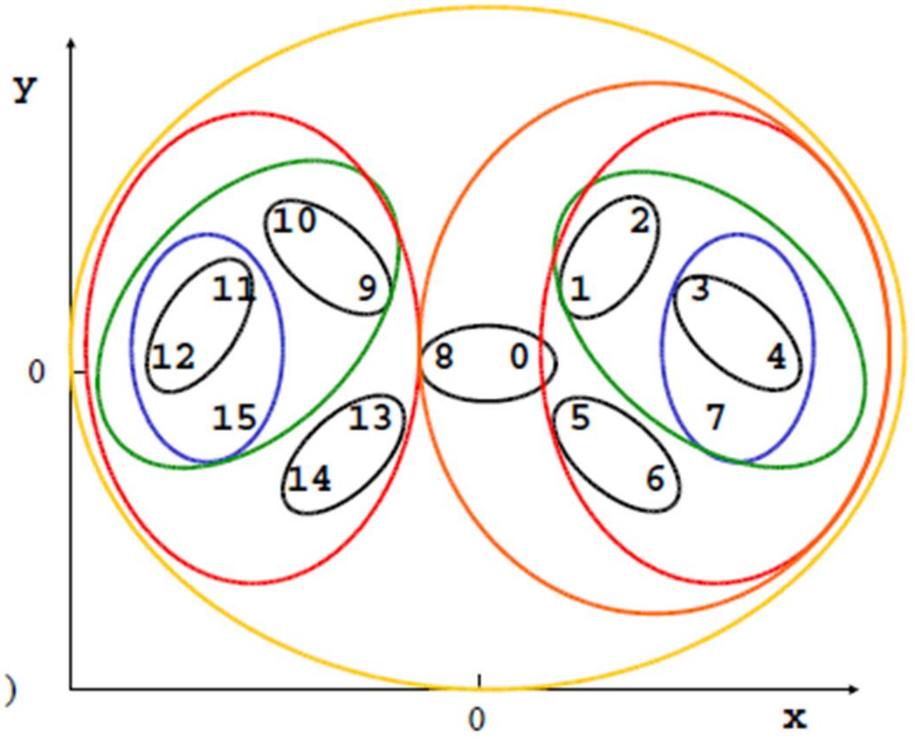
➢ **Top-down:**
- start with 1 cluster (all examples belong to one cluster)
- successively split into new sub clusters (based on some threshold max distance between the centroid and the examples)

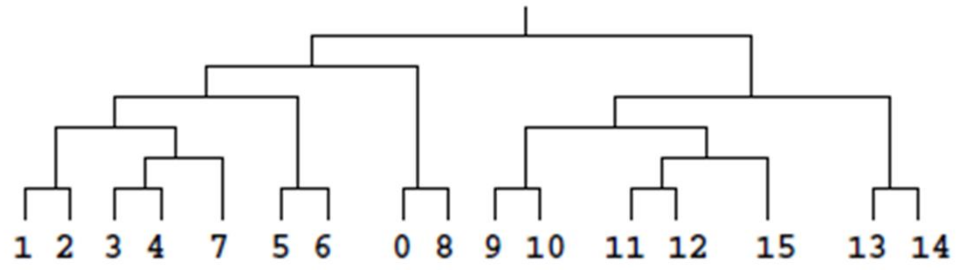
➢ **Bottom-up:**
- start with as many clusters as examples
- successively merge existing clusters
(based on some similarity measure between clusters)

SIMILARITY BETWEEN CLUSTERS

Bottom-up clustering (average-link):

```
min distance = 2.00000   ( 8 ) ( 0 )
min distance = 2.82843   ( 2 ) ( 1 )
min distance = 2.82843   ( 4 ) ( 3 )
min distance = 2.82843   ( 6 ) ( 5 )
min distance = 2.82843   ( 10 ) ( 9 )
min distance = 2.82843   ( 12 ) ( 11 )
min distance = 2.82843   ( 14 ) ( 13 )
min distance = 3.16228   ( 7 ) ( 3 4 )
min distance = 3.16228   ( 15 ) ( 11 12 )
min distance = 4.73756   ( 3 4 7 ) ( 1 2 )
min distance = 4.73756   ( 11 12 15 ) ( 9 10 )
min distance = 4.74131   ( 1 2 3 4 7 ) ( 5 6 )
min distance = 4.74131   ( 9 10 11 12 15 ) ( 13 14 )
min distance = 5.57143   ( 0 8 ) ( 5 6 1 2 3 4 7 )
min distance = 9.90476   ( 13 14 9 10 11 12 15 ) ( 5 6 1 2 3 4 7 0 8 )
```





K-MEANS -summary

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

Expectation Maximization (EM)

Expectation Maximization (EM) is a generalization of K-Means.

Probabilistic approach, that assumes data from each cluster has a certain distribution (for example Gaussian Distribution).
Search for the Gaussian Distribution parameters (mean and standard deviation) that maximise the likelihood of data.

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Hard vs. Fuzzy CLUSTERING

Hard Clustering: Each point belongs to a single cluster.

Fuzzy clustering: Each example *xi* belongs to any cluster *cj* up to some degree depending on the values of membership function *Mcj(xi)* .

- If *Mcj(xi)* close to 1, the membership of *xi* to cluster *cj* is high
- If *Mcj(xi)* close to 0, the membership of *xi* to cluster *cj* is low

K-means for dimensionality reduction

dimensionality reduction is useful for:

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

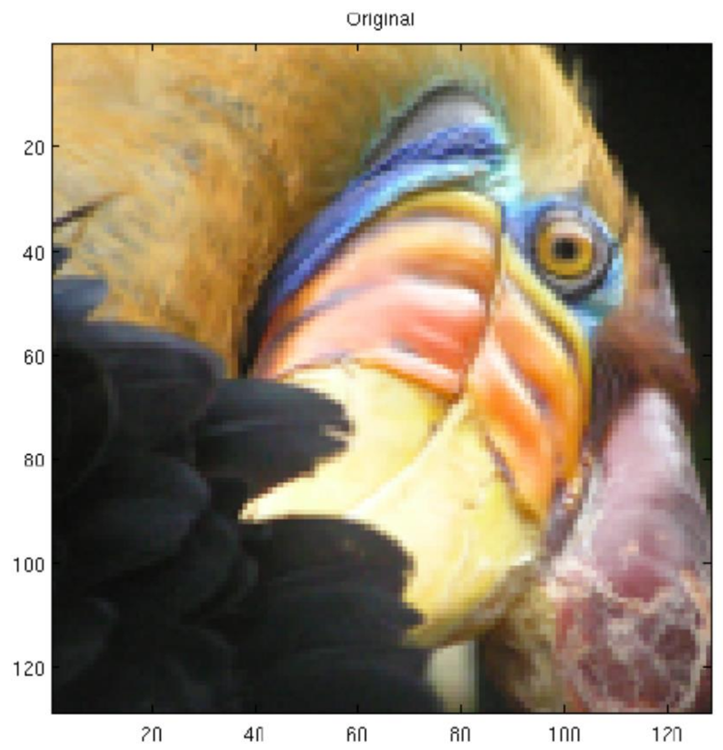
Reduce memory/ disk needed to store data
Speed up learning algorithm

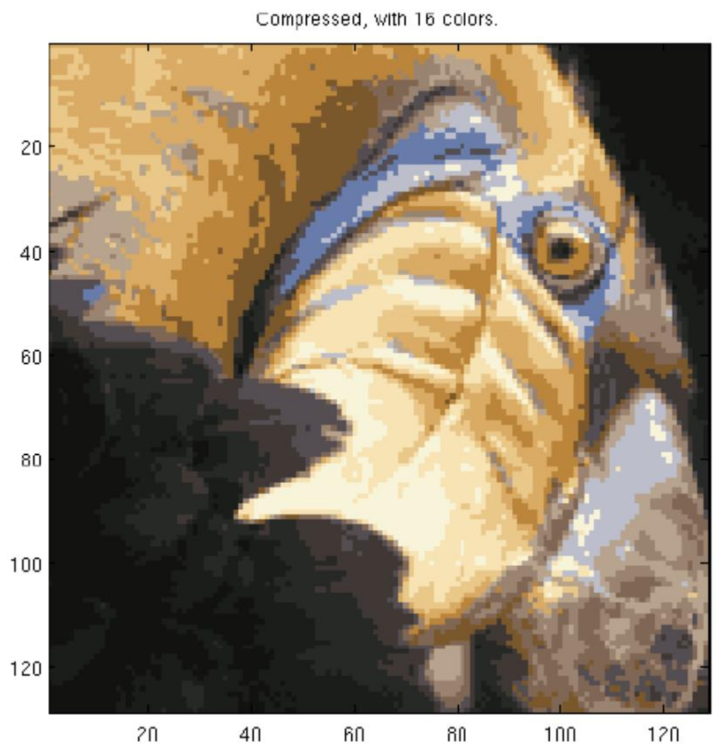
Data visualization (from 100-50D to 2-3D)

Remark: kernel methods do the opposite, from the original low dimensional features (nonlinear models) go to a higher dimensional feature space (linear models)

Image compression with K-means

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





SEMI-SUPERVISED LEARNING
Google Street View and clustering

How to extrapolate concepts and label new objects in millions of unlabeled pictures. Feed a massive database of pictures to a machine, and use clustering to understand what is composed of, what are the elements in the pictures.

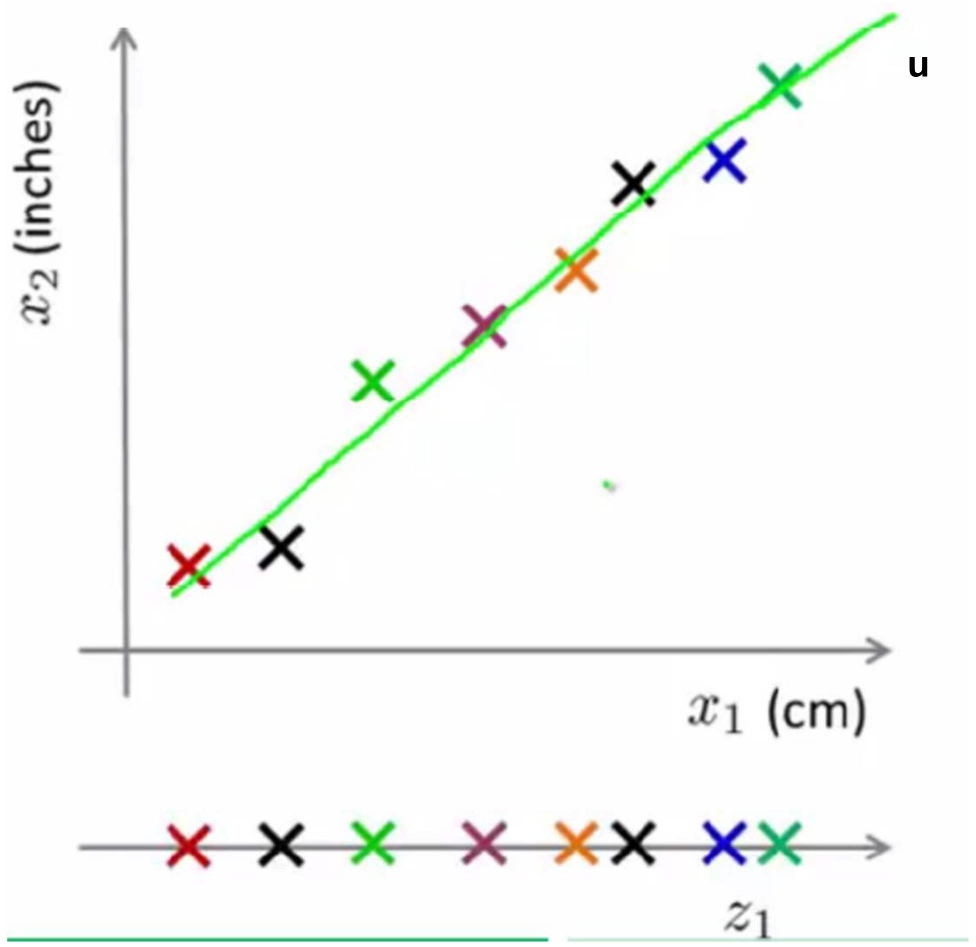
SEMI-SUPERVISED LEARNING

DARPA self-driving car http://cs.stanford.edu/group/roadrunner/

DATA COMPRESSION

Example: reduce data from 2D to 1D

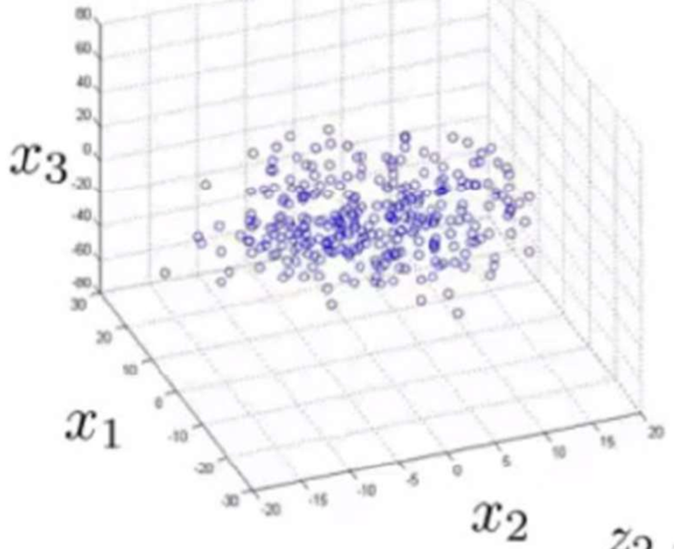
If 2D data is located along a line, the second dimension is redundant

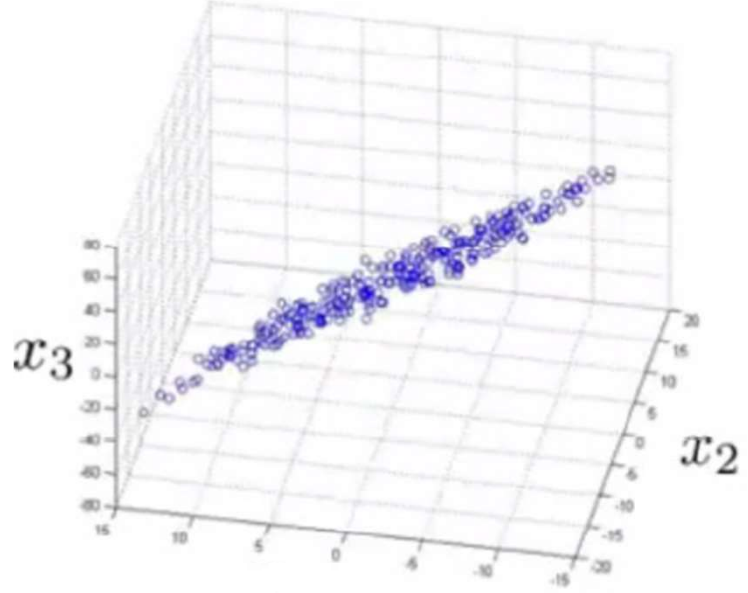


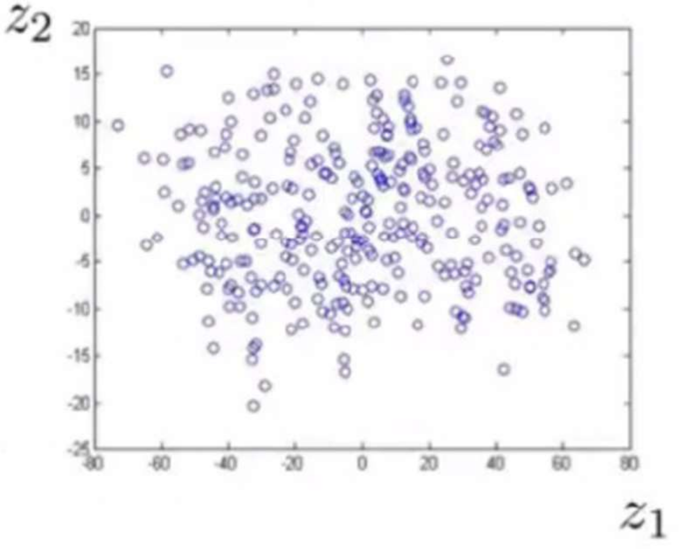
DATA COMPRESSION

Example: reduce data from 3D to 2D

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

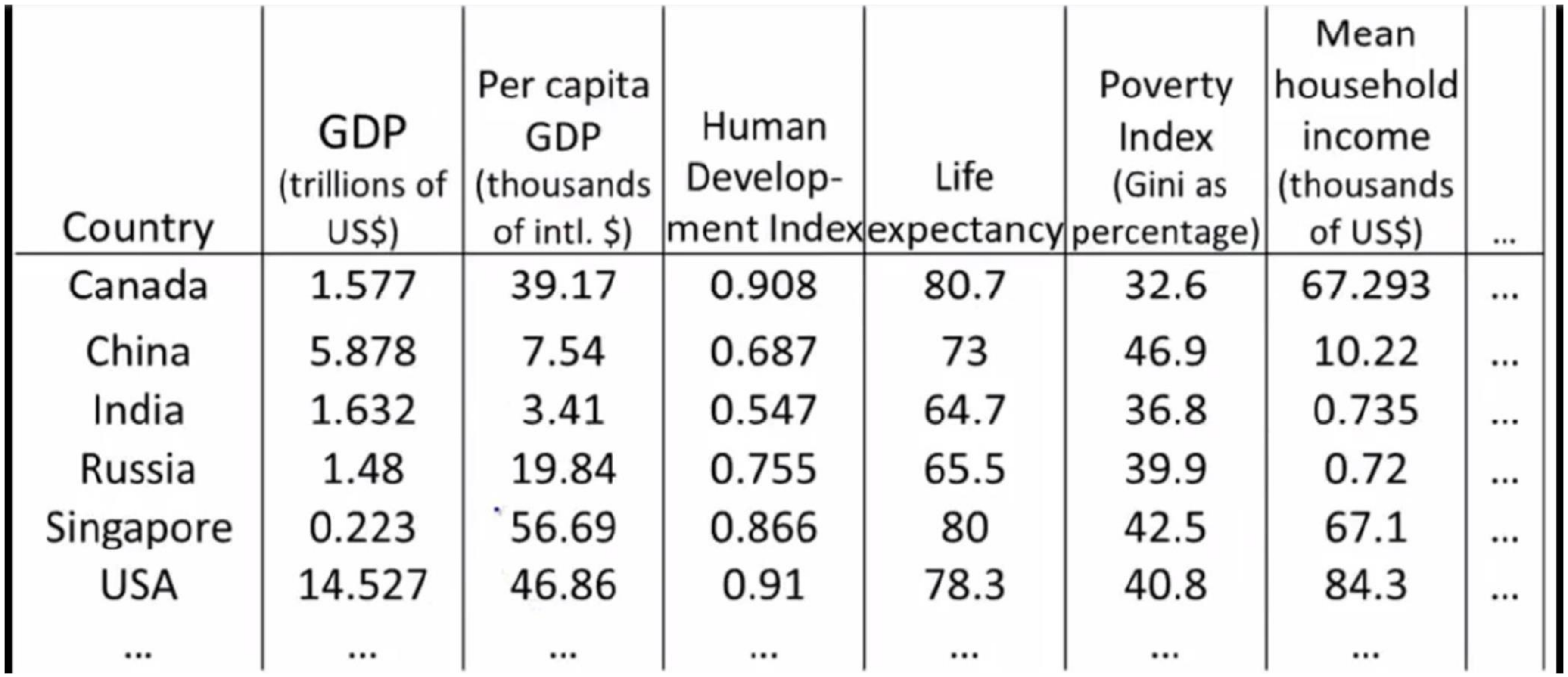






DATA VISUALIZATION

Example: Reduce data from high dimension to 2D or 3D

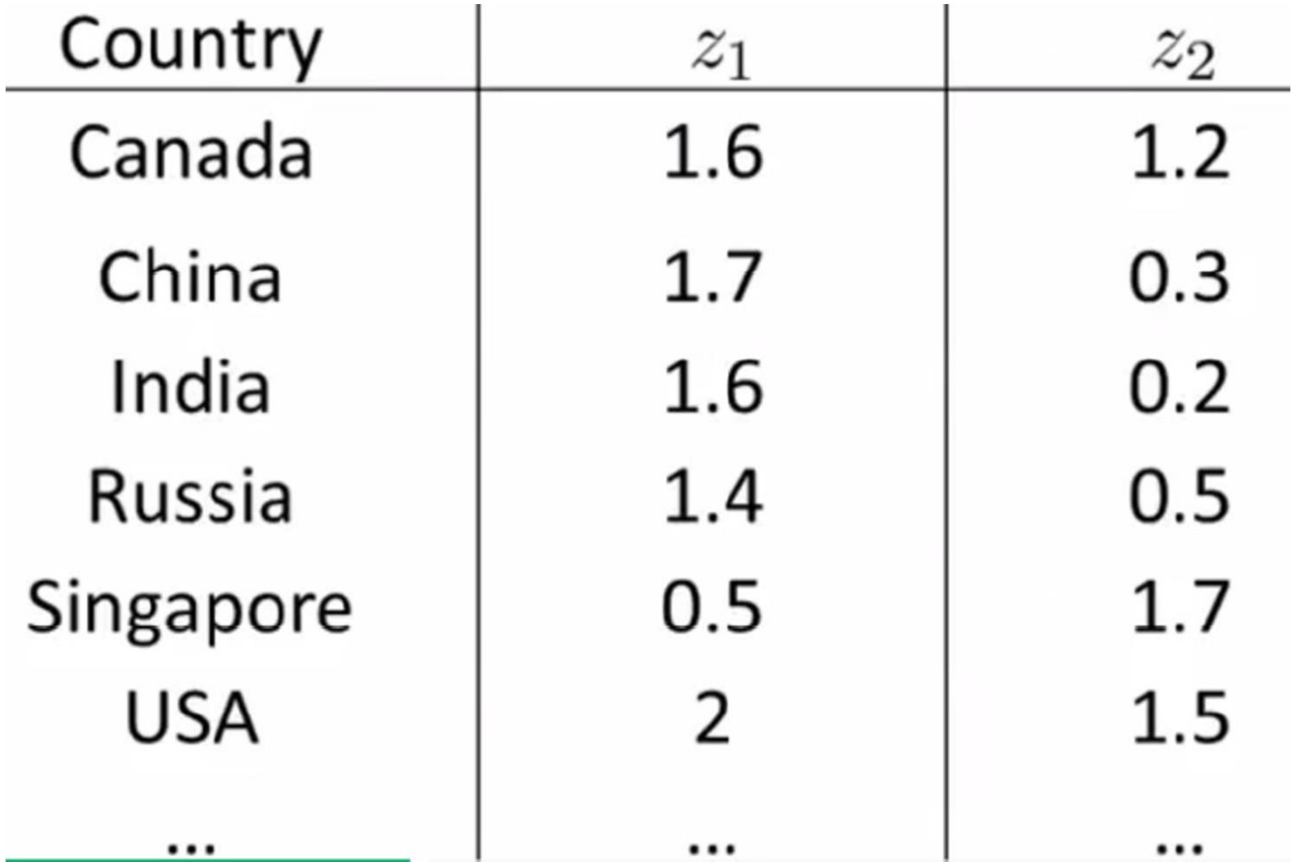


Country	GDP (trillions of US$)	Per capita GDP (thousands of intl. $)	Human Develop-ment Index	Life expectancy	Poverty Index (Gini as percentage)	Mean household income (thousands of US$)	...
Canada	1.577	39.17	0.908	80.7	32.6	67.293	...
China	5.878	7.54	0.687	73	46.9	10.22	...
India	1.632	3.41	0.547	64.7	36.8	0.735	...
Russia	1.48	19.84	0.755	65.5	39.9	0.72	...
Singapore	0.223	56.69	0.866	80	42.5	67.1	...
USA	14.527	46.86	0.91	78.3	40.8	84.3	...
...	...	...	...	...	...	...	

DATA VISUALIZATION

Reduce data from high dimension to 2D or 3D

for example: z1(country size/GDP) and z2 (GDP/per person)

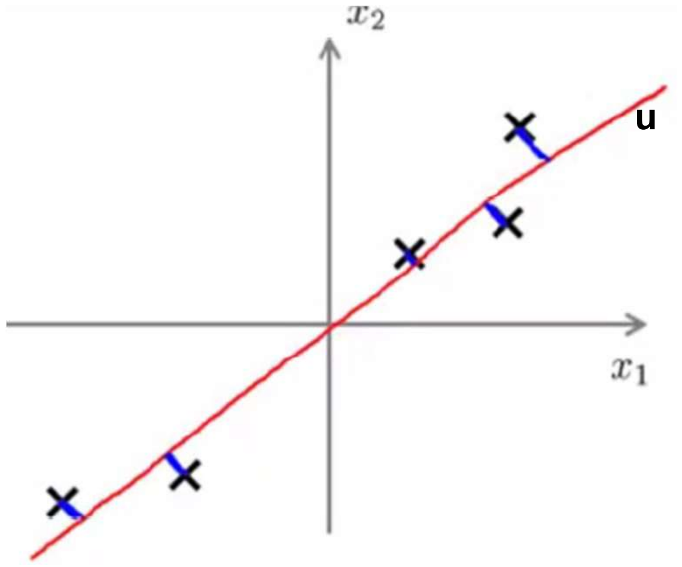


Country	z_1	z_2
Canada	1.6	1.2
China	1.7	0.3
India	1.6	0.2
Russia	1.4	0.5
Singapore	0.5	1.7
USA	2	1.5
...	...	...

PRINCIPAL COMPONENT ANALYSIS (PCA)

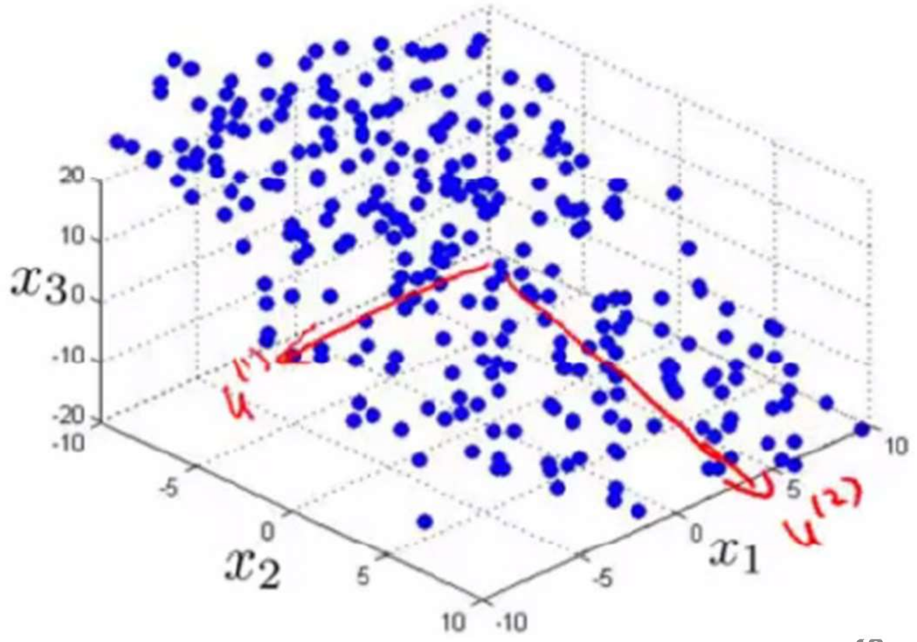
Reduce from 2D to 1D:

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

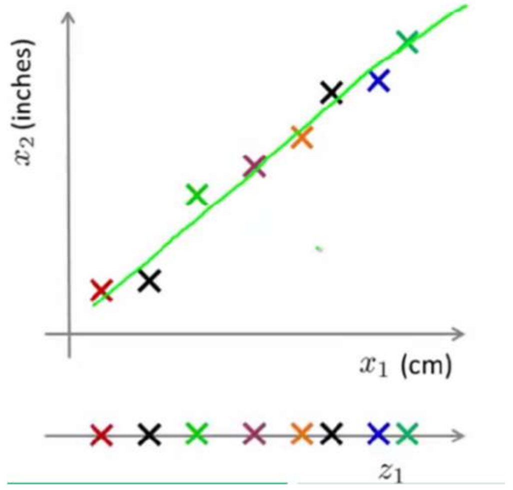


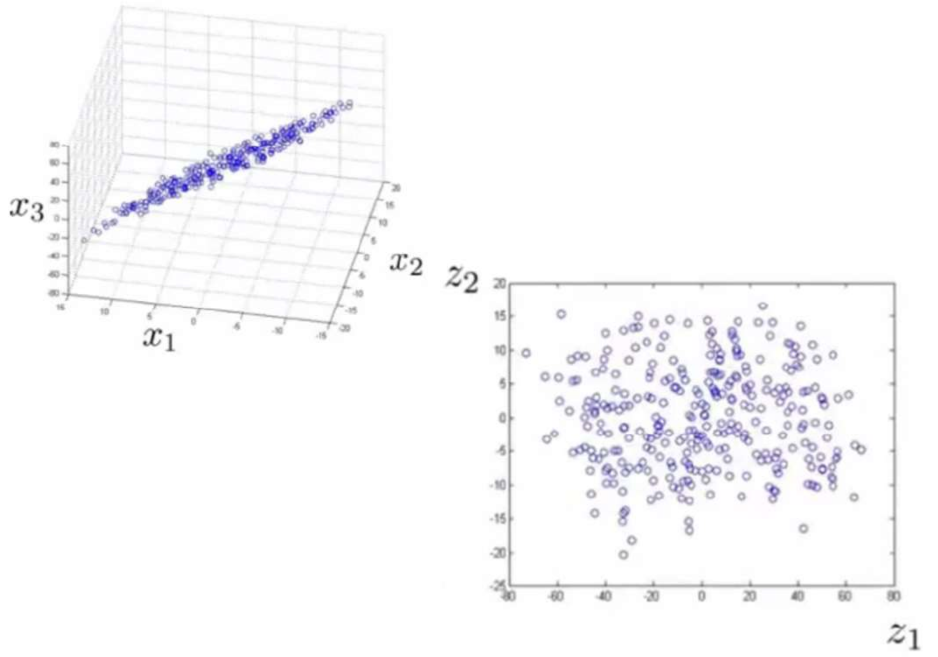
PRINCIPAL COMPONENT ANALYSIS (PCA)

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

Two tasks:

- 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.
- Compute the values of the projected data in the lower dimensional space (z values)





PRINCIPAL COMPONENT ANALYSIS (PCA)

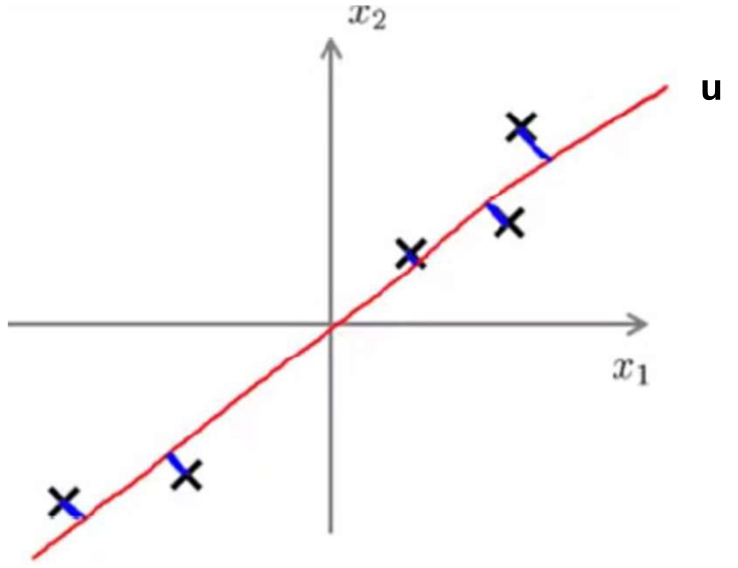
PCA is not Linear Regression !!!

Linear Regression minimizes the vertical distance.

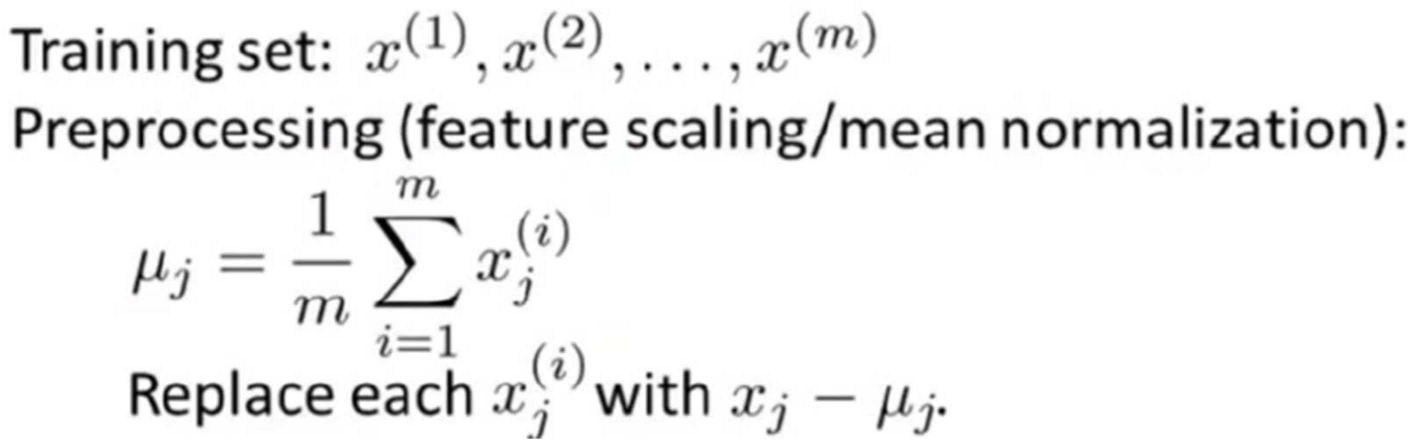
LR is a supervised learning method, it has a given output y.

PCA minimizes the ortogonal distance between the points and the projection surface (line, plane, etc.)

PCA is an unsupervised method, it has no output y.



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].

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:

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

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.

Use linear algebra libraries to compute SVD => [U,S,V]=svd(Cov)

PCA

The projection vectors are the first k columns of U (k<n):

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \dots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n} \qquad Ureduce_{nxk} = U(:,1:k)$$

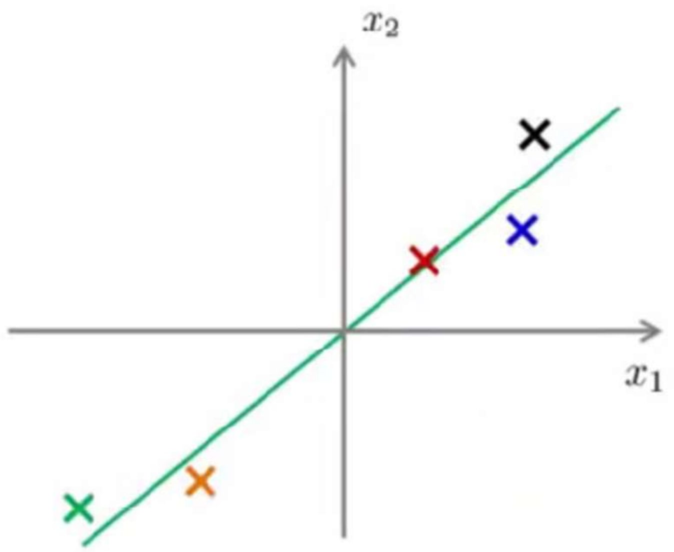
Step 3: Compute the new (projected) data matrix Z (m examples, k features):

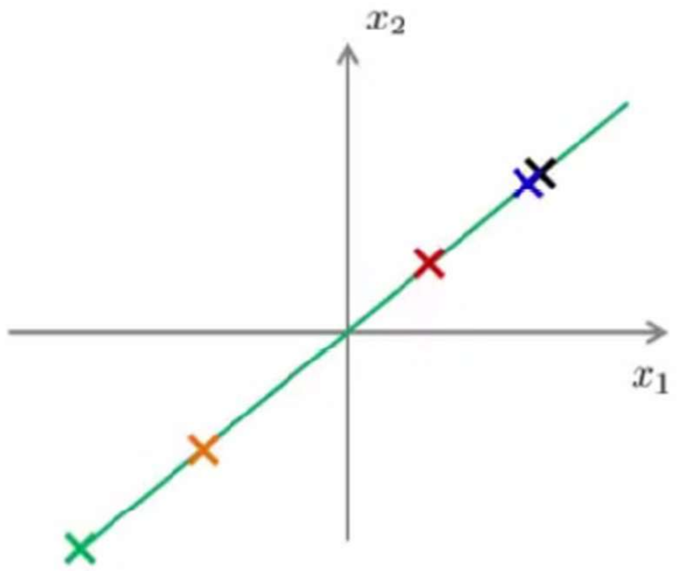
$$Z_{mxk} = X_{mxn} * Ureduce_{nxk}$$

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

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

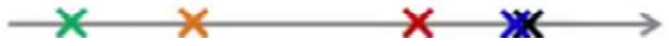
Reconstruction from compressed representation





$$z = U_{reduce}^T x$$

$$x_{approx} = U_{reduce} z$$



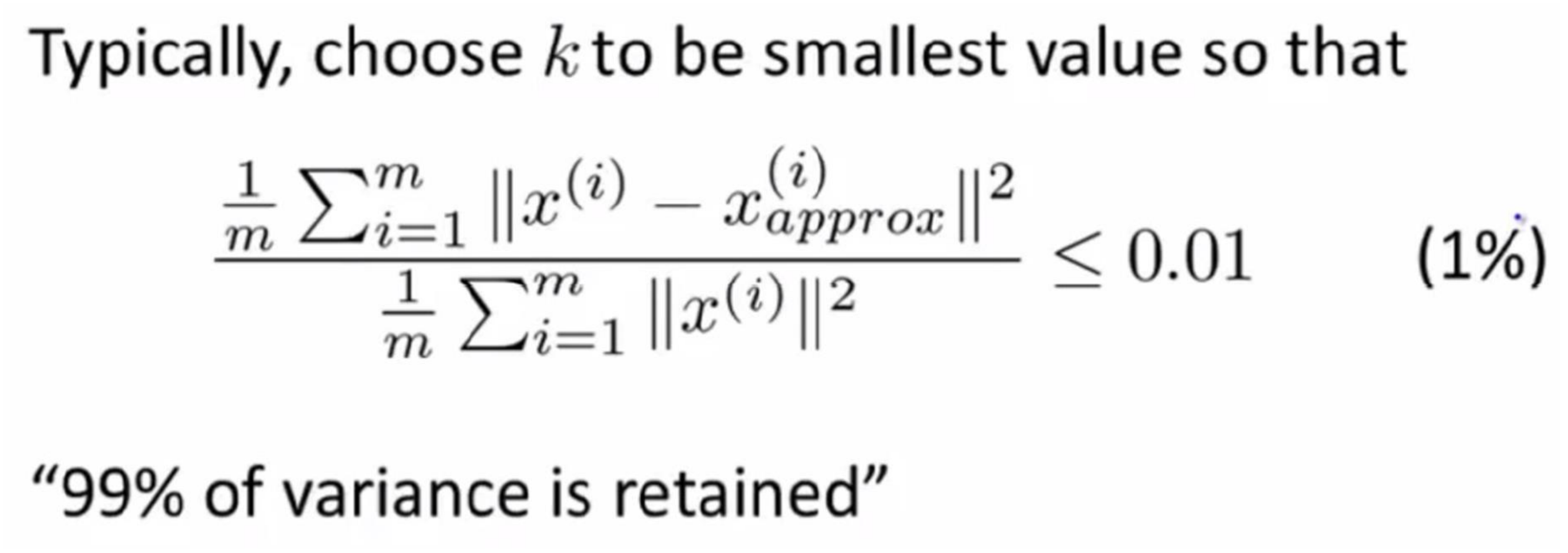
Choosing k (number of principal components)

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

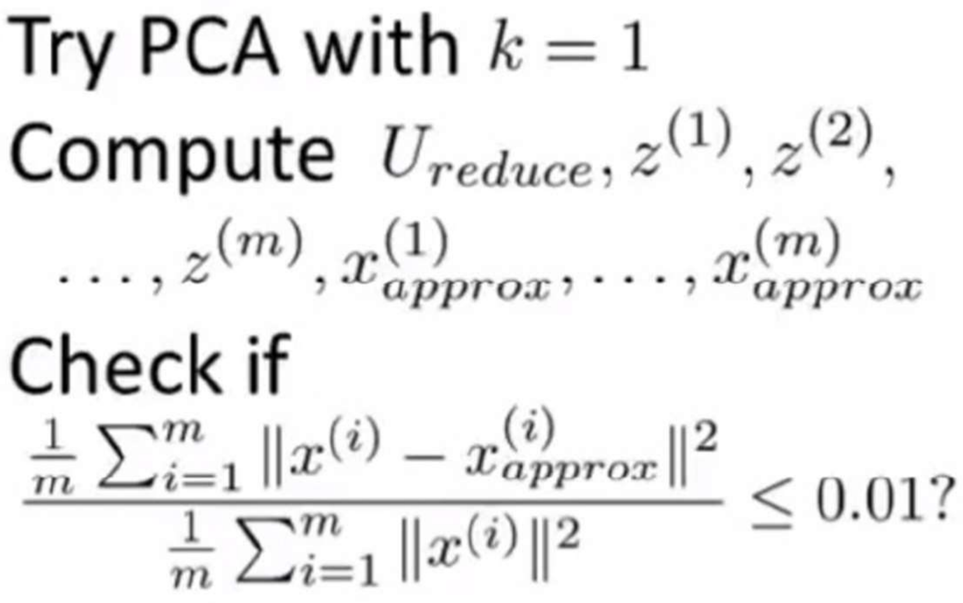
$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2} \leq 0.01 \qquad (1\%)$$

“99% of variance is retained”

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

Choosing k (number of principal components)

Algorithm 1 (highly inefficient, need to compute SVD several times):



Try PCA with $k = 1$

Compute $U_{reduce}, z^{(1)}, z^{(2)}, \ldots, z^{(m)}, x_{approx}^{(1)}, \ldots, x_{approx}^{(m)}$

Check if

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

If not ok, try with k=2, 3,.. until get desired retained variance

Choosing k (number of principal components)

Algorithm 2 (Compute SVD once): [U,S,V]=svd(Cov)

Increase *k* (starting from *k*=1) until get the desired retained variance (e.g. 99 %):

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

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

PCA application

To speed-up the supervised learning algorithm:

- Get training set $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$
- Run PCA to reduce $x^{(i)}$ in dimension to get $z^{(i)}$

Run learning algorithm on the new training set with less features:

$$\{(z^{(1)}, y^{(1)}), \ldots, (z^{(m)}, y^{(m)})\}$$

Note: The projection matrix *Ureduce* is computed only once with the training data matrix *X*. This mapping is then applied to the cross validation and test examples.

Bad use of PCA: if the reason for applying PCA is not to speed-up learning but to prevent overfiting (less features less likely to overfit), better use regularization !!!