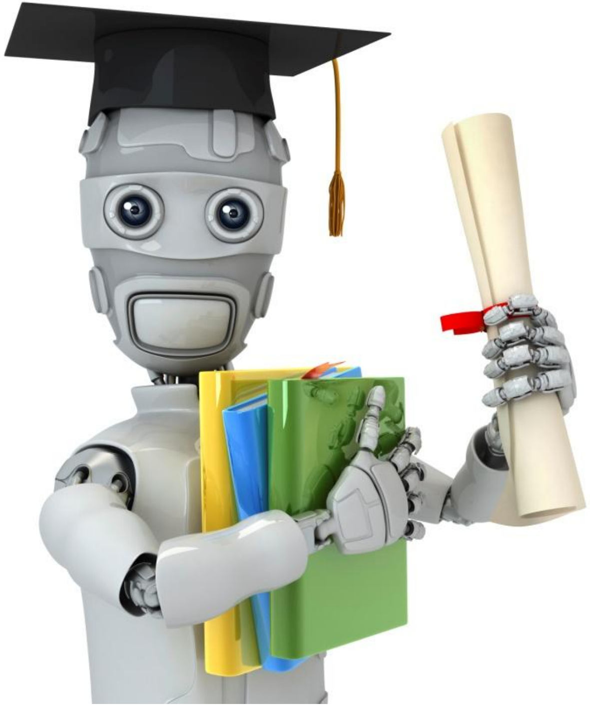
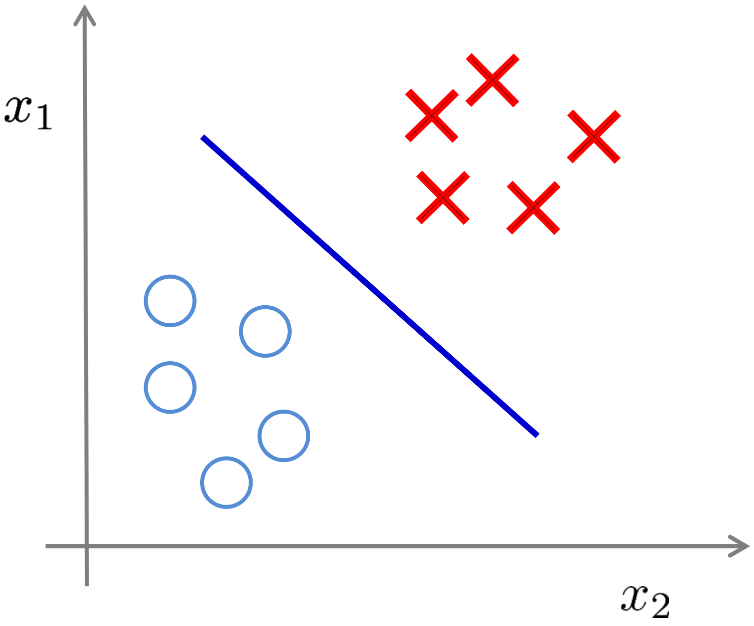


Machine Learning

Clustering

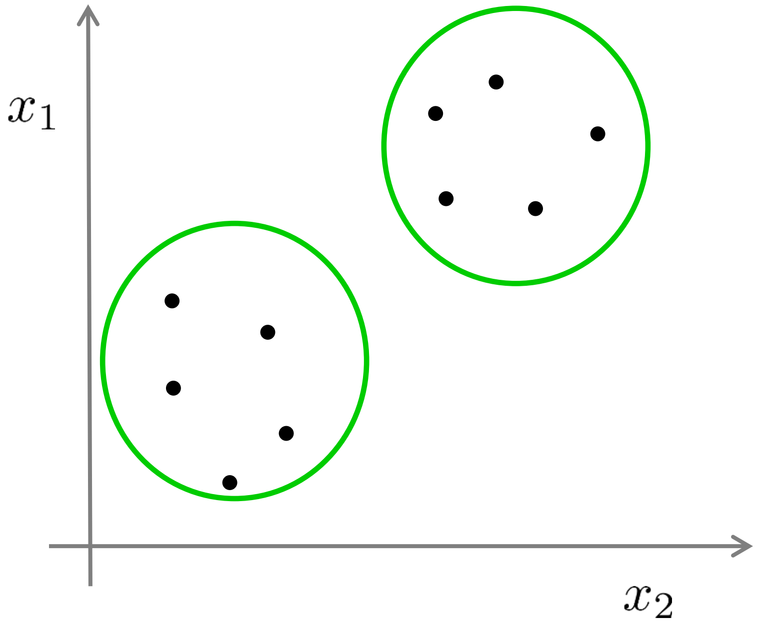
Unsupervised learning introduction

Supervised learning



Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}), \ldots, (x^{(m)}, y^{(m)})\}$

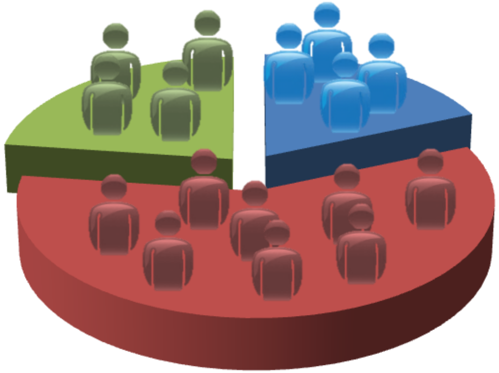
Unsupervised learning



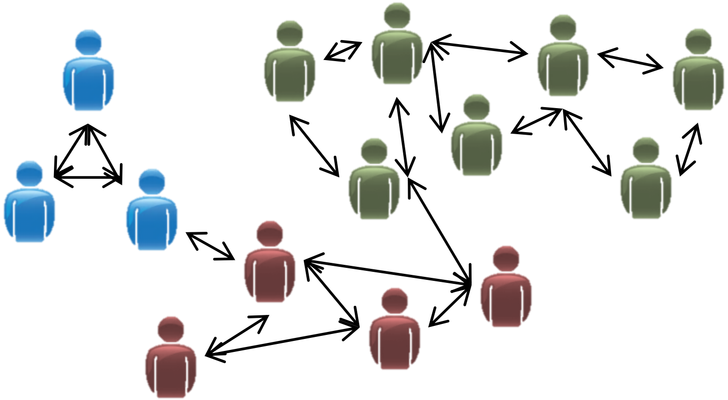
Clustering algorithm

Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$

Applications of clustering



Market segmentation

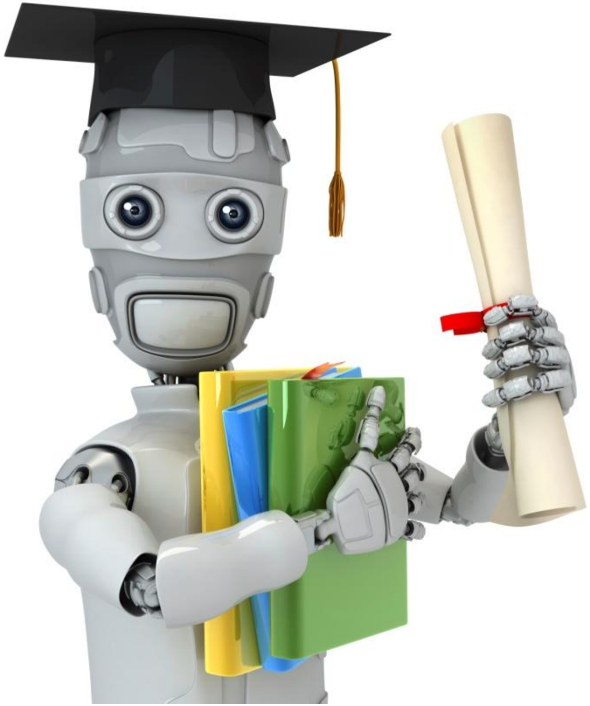


Social network analysis

Organize computing clusters

Image credit: NASA/JPL-Caltech/E. Churchwell (Univ. of Wisconsin, Madison)

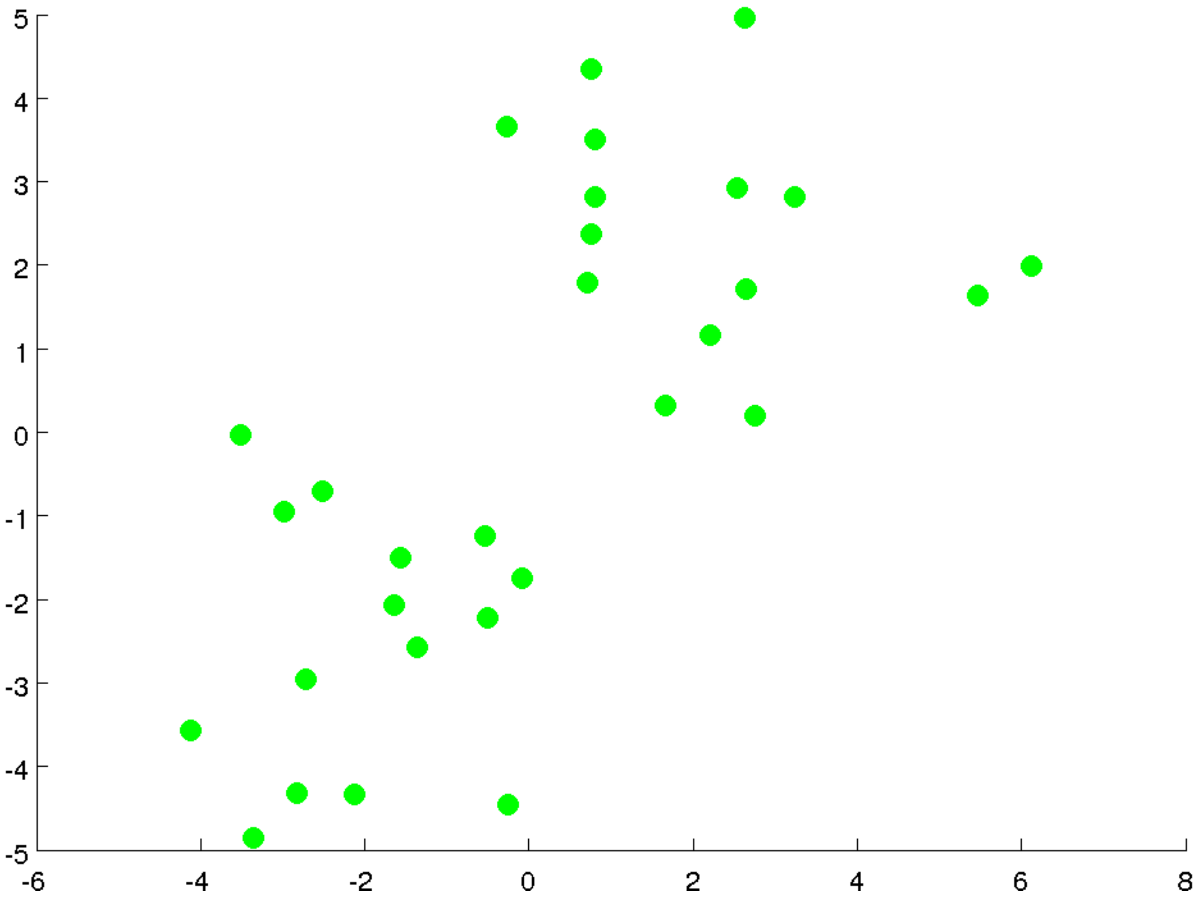
Astronomical data analysis



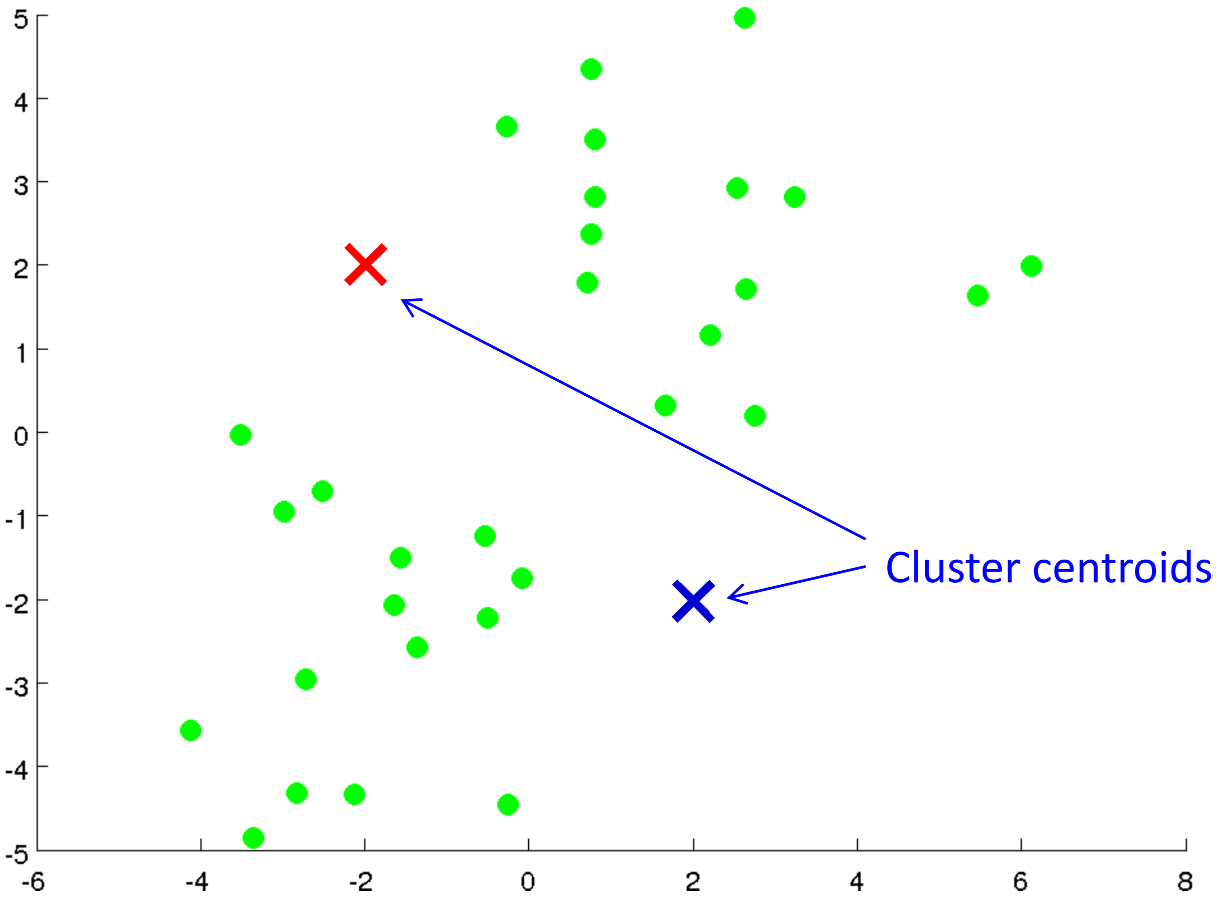
Machine Learning

Clustering

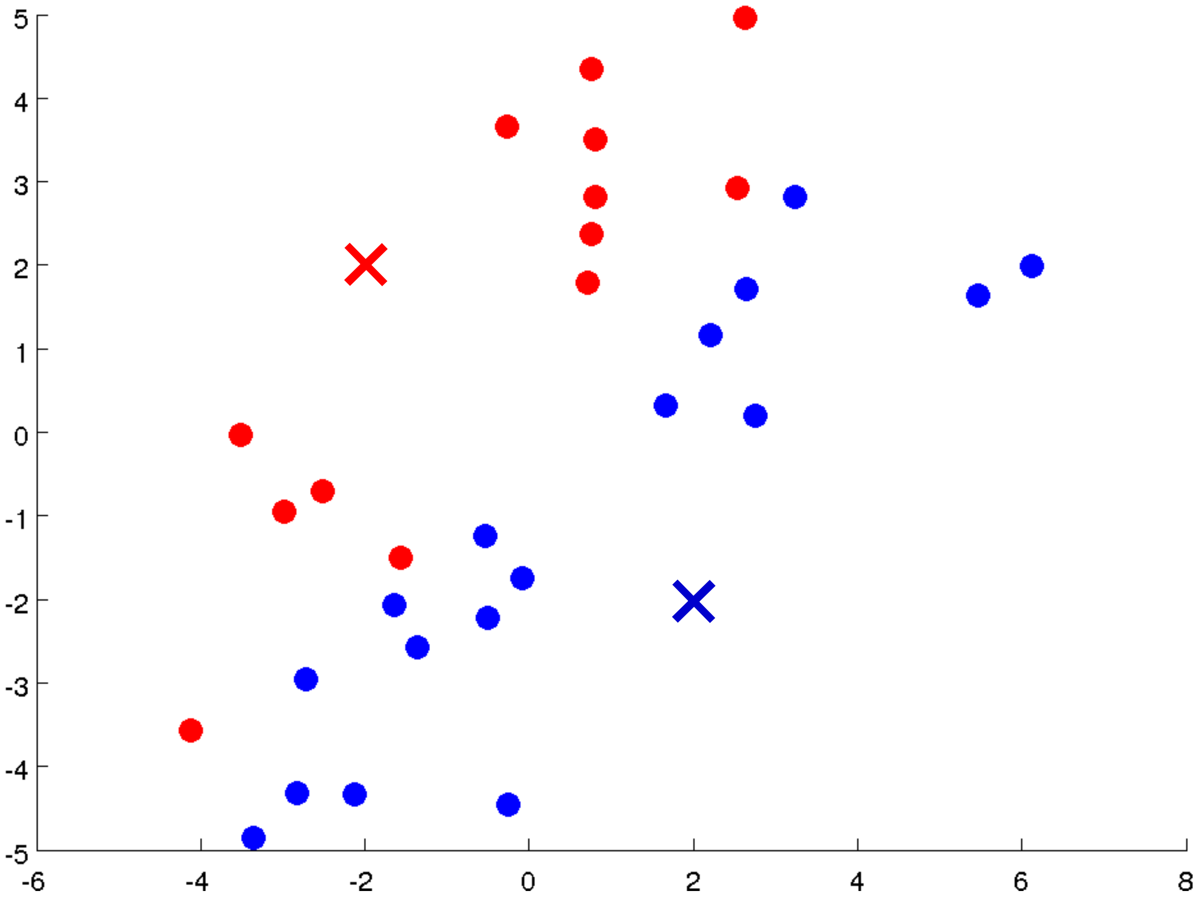
K-means algorithm



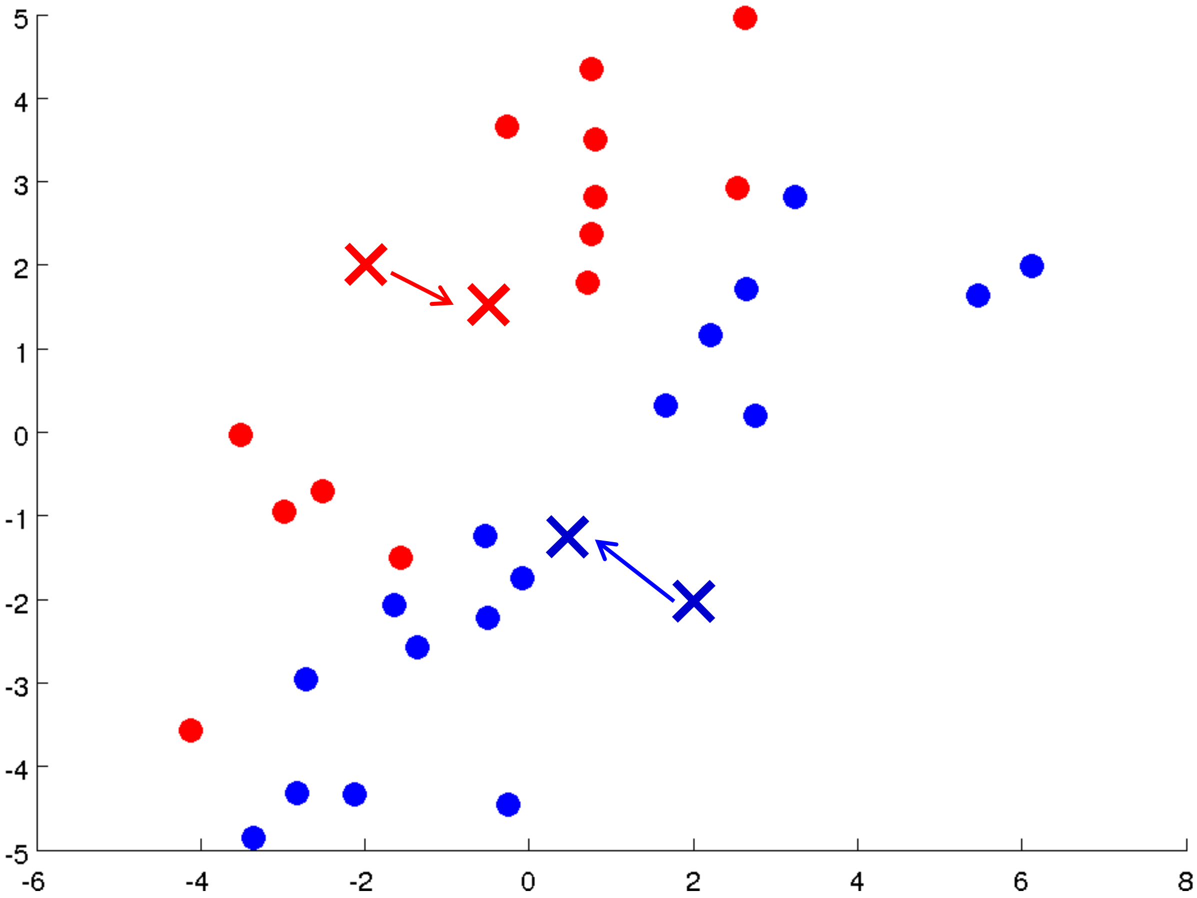
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



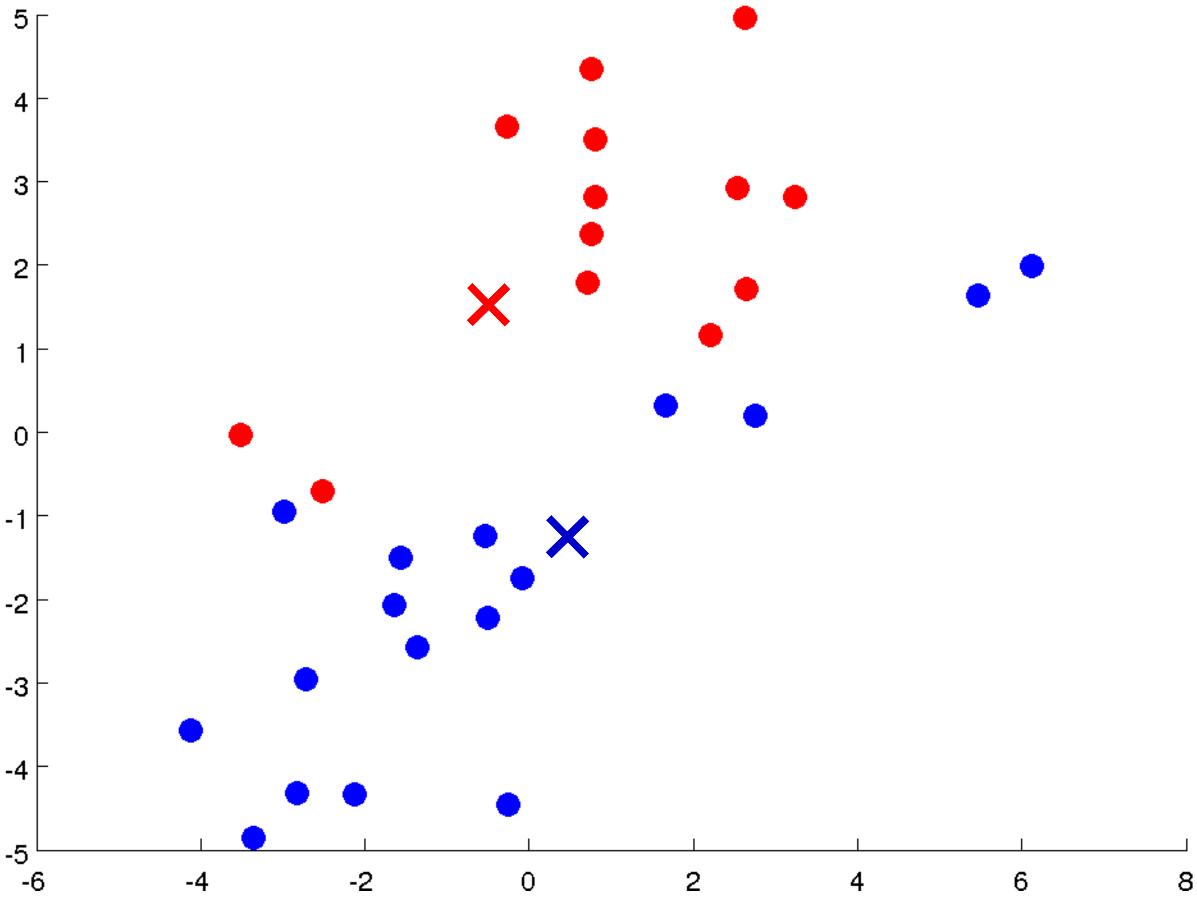
Andrew Ng



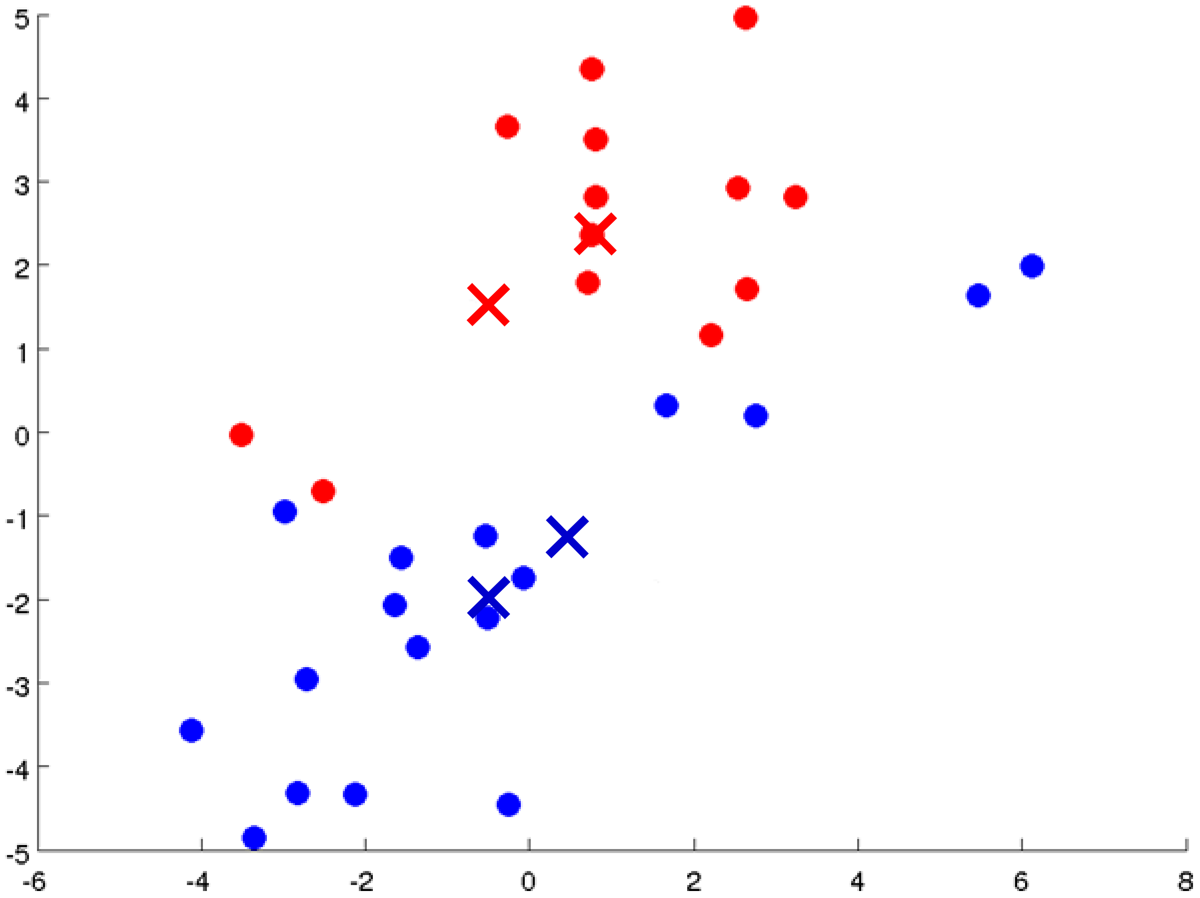
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



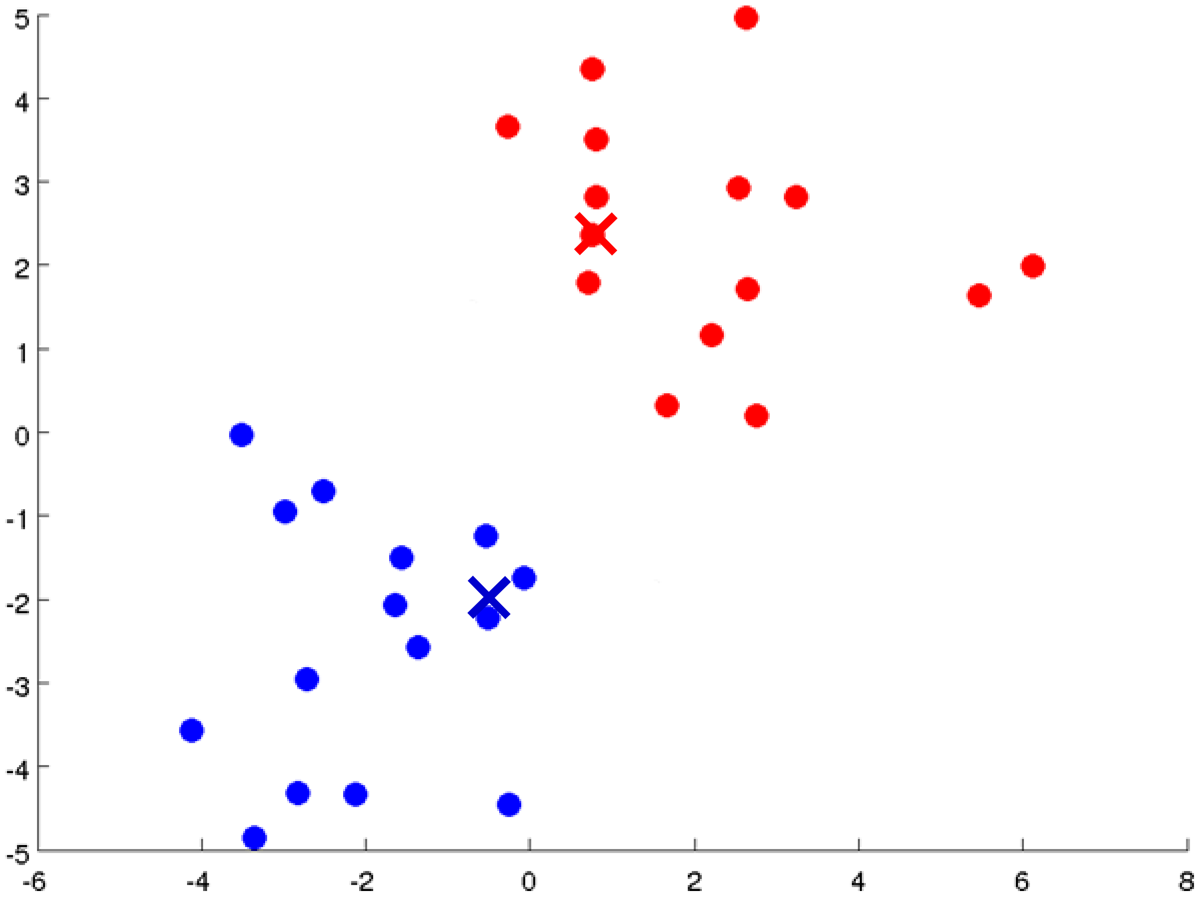
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



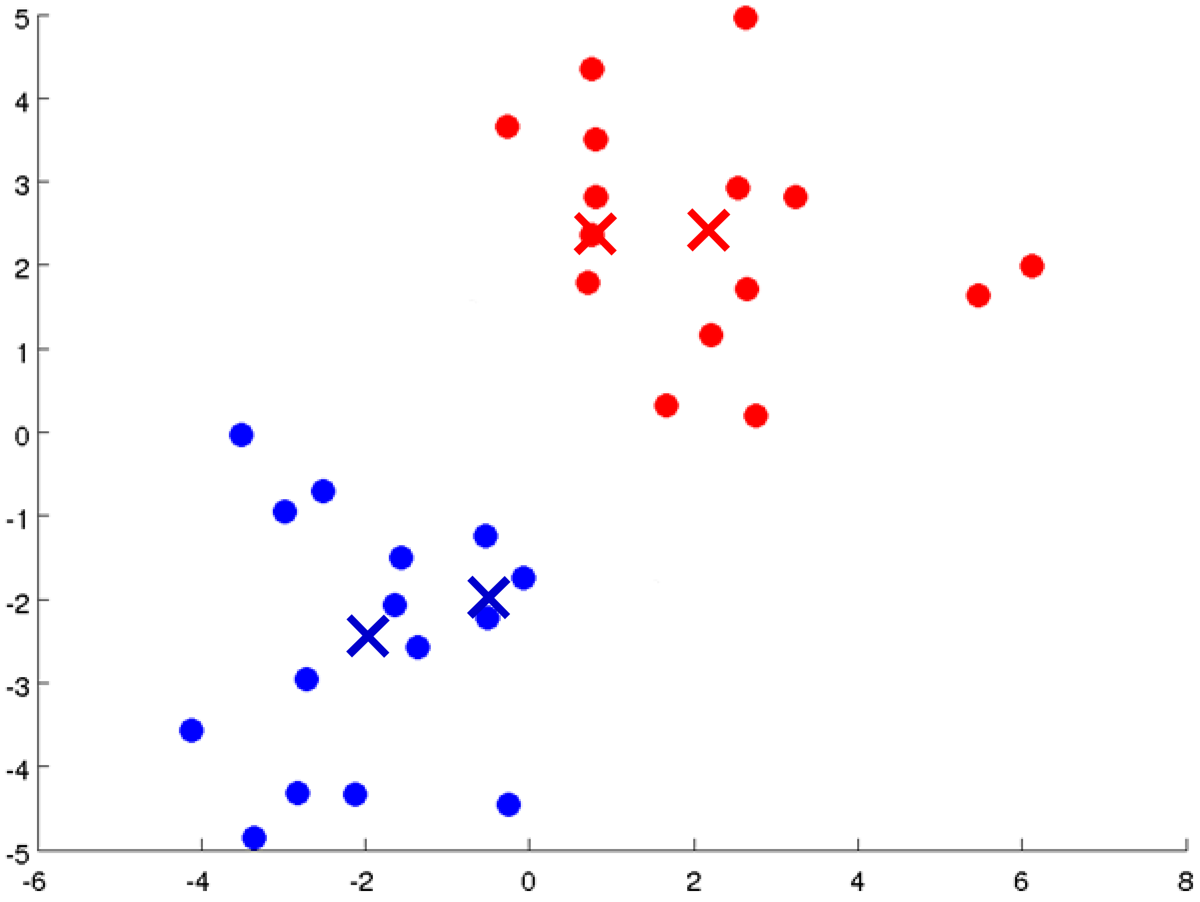
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



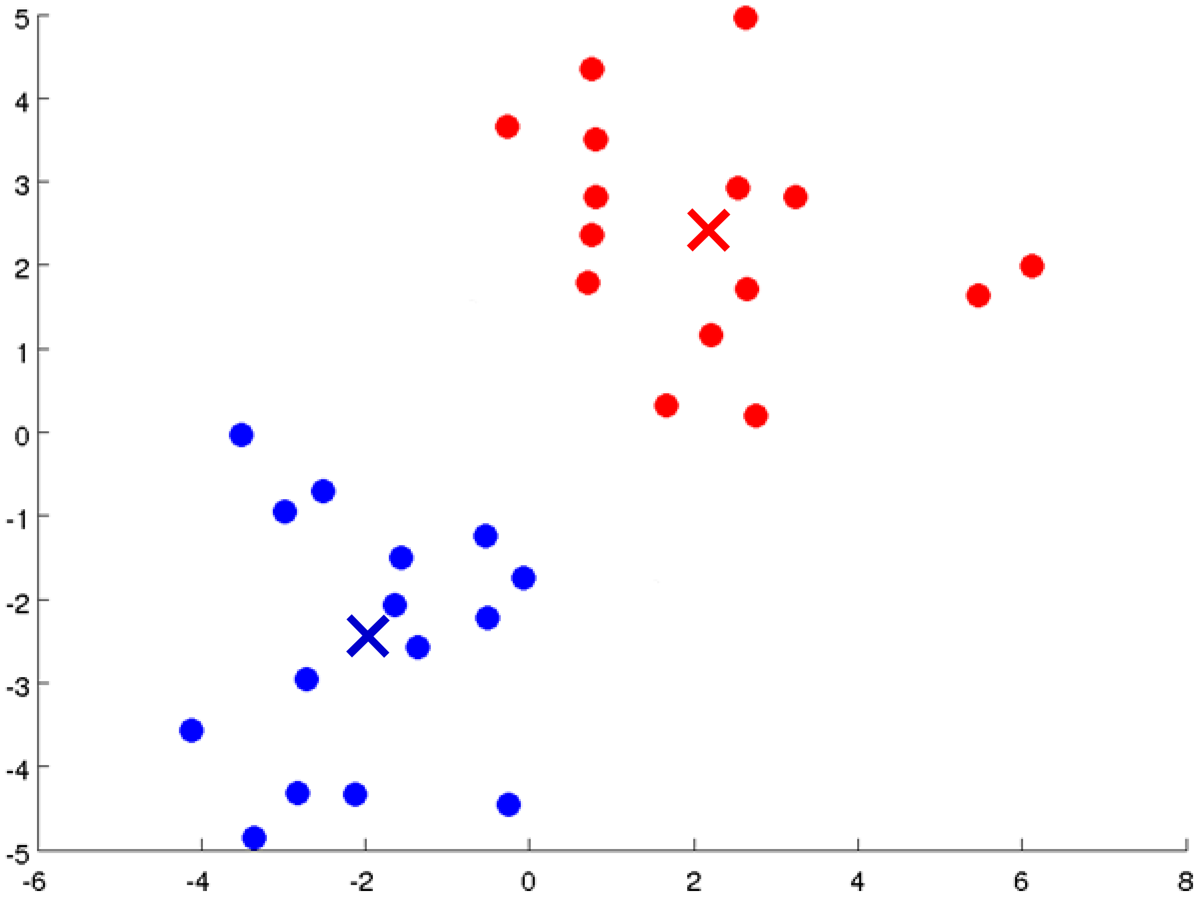
5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



5
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-4
-2
0
2
4
6
8



Andrew Ng



Andrew Ng

K-means algorithm

Input:

- K (number of clusters)
- Training set $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$

$x^{(i)} \in \mathbb{R}^n$ (drop $x_0 = 1$ convention)

K-means algorithm

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

Repeat {

Cluster assignment step

for i = 1 to m

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

$\min_{k} = ||x^{(i)} - u_k||^2$

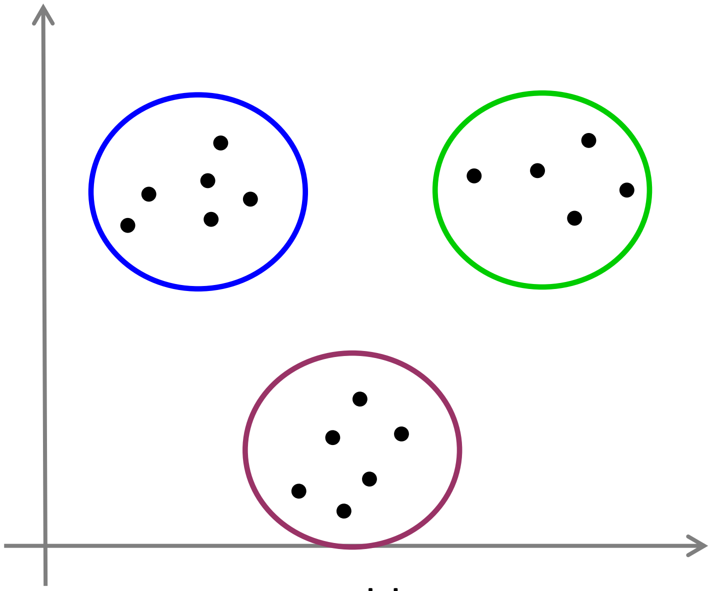
Move centroids step

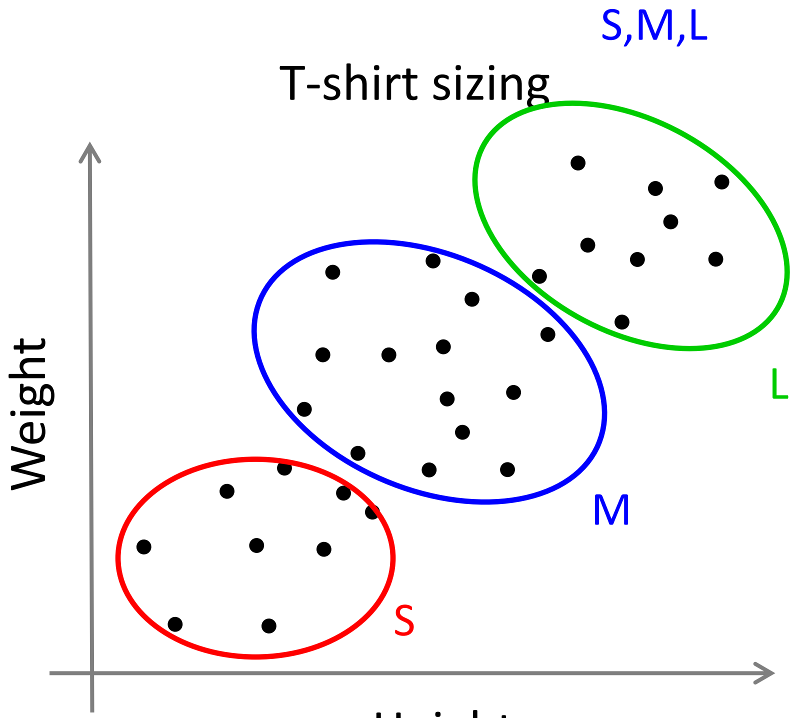
for k = 1 to K

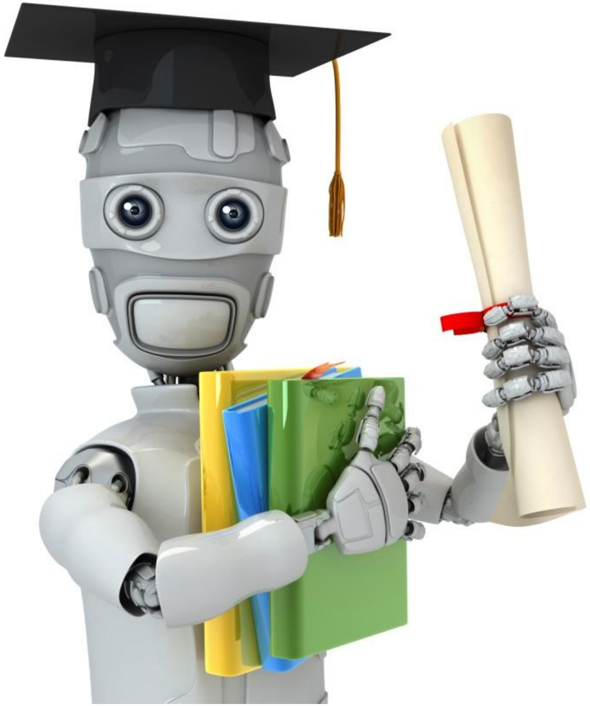
μ_k := average (mean) of points assigned to cluster k

}

K-means for non-separated clusters







Machine Learning

Clustering

Optimization objective

K-means optimization objective

$c^{(i)}$ = index of cluster (1,2,…,K) to which example $x^{(i)}$ is currently assigned

μ_k = cluster centroid k ($\mu_k \in \mathbb{R}^n$)

$\mu_{c^{(i)}}$ = cluster centroid of cluster to which example $x^{(i)}$ has been assigned

$x^{(i)} \to 5 \quad c^{(i)} = 5 \quad \mu_{c^{(i)}} = \mu_5$

Optimization objective:

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

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

K-means algorithm

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

$Minimize\ J(\ldots)\ w.r.t\ \ c^{(1)}, c^{(2)}, \ldots, c^{(k)}$
$(holding\ \ \mu_1, \ldots, \mu_k\ fixed)$

Cluster assignment step

Repeat {

for i = 1 to m

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

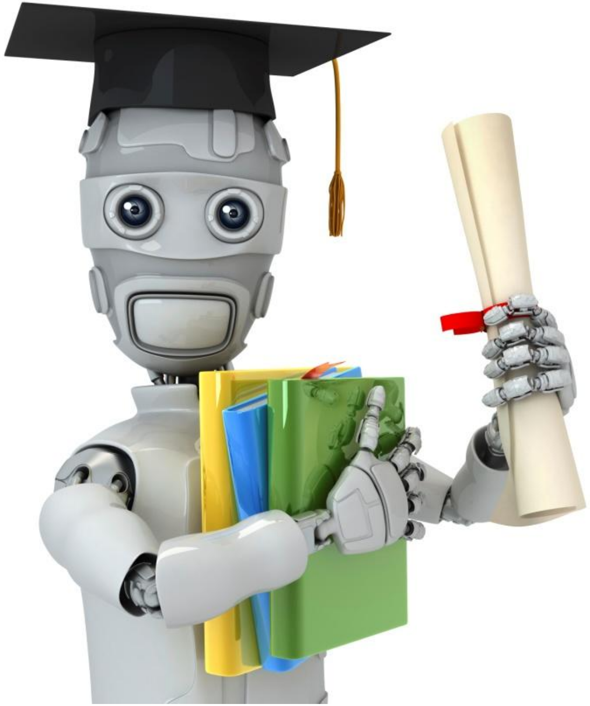
for k = 1 to K

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

}

Move centroids step

$Minimize\ J(\ldots)\ w.r.t\ \ \mu_1, \ldots, \mu_k$



Machine Learning

Clustering

Random initialization

K-means algorithm

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

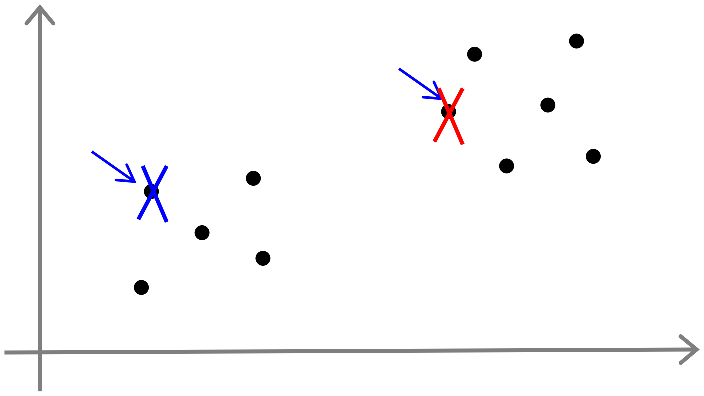
μ_k := average (mean) of points assigned to cluster k

}

Random initialization

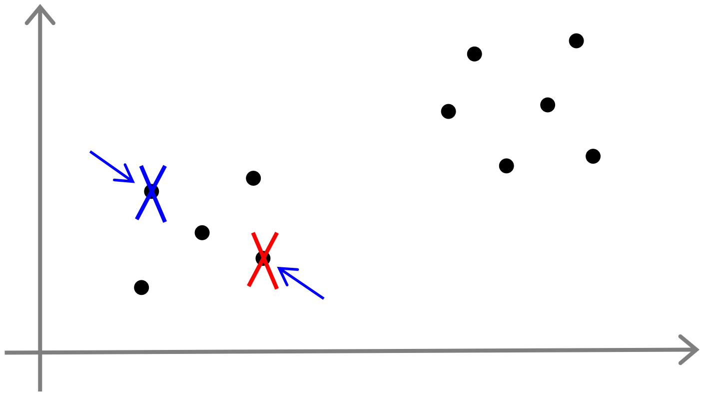
Should have $K < m$

Example:
K=2



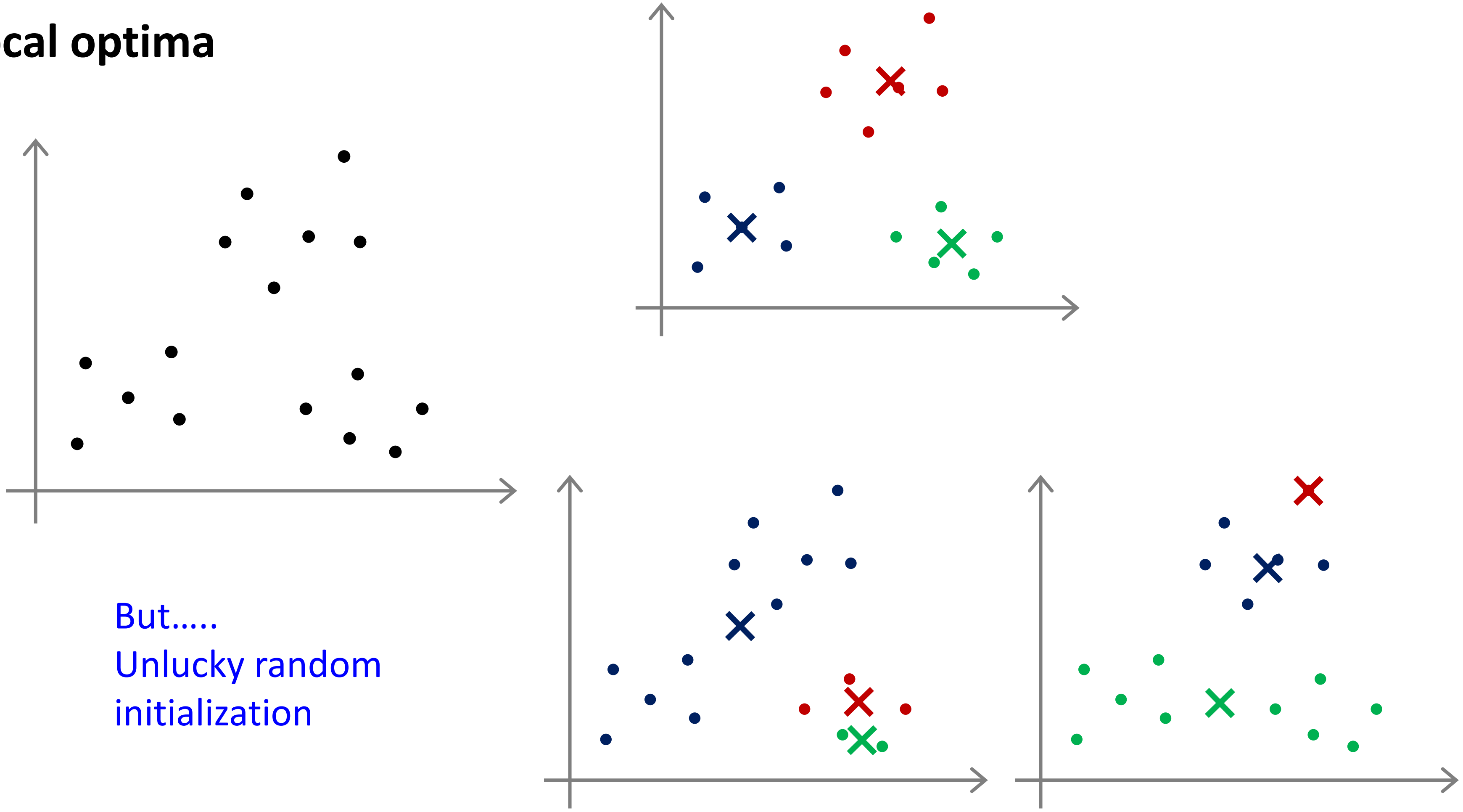
Randomly pick K training examples.

Set $\mu_1, \ldots, \mu_K$ equal to these K examples.



Andrew Ng

Local optima



But.....
Unlucky random initialization

Andrew Ng

Random initialization

For i = 1 to 100 {

Randomly initialize K-means.

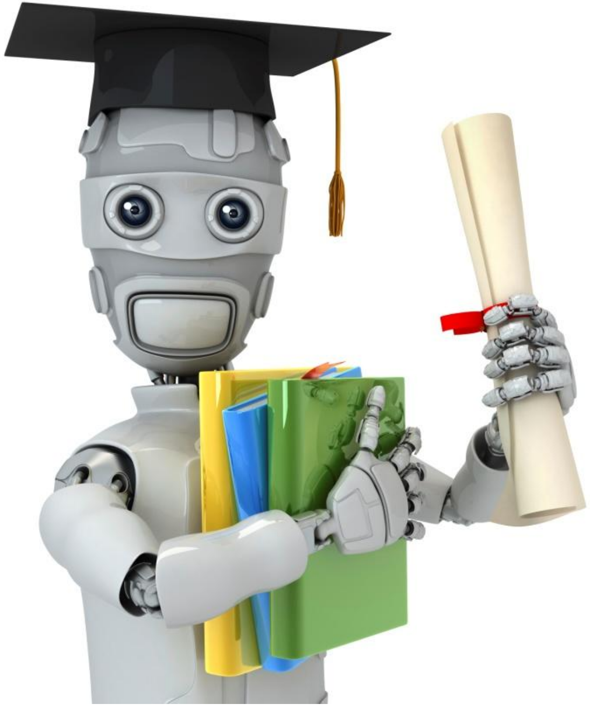
Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.

Compute cost function (distortion)

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

}

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

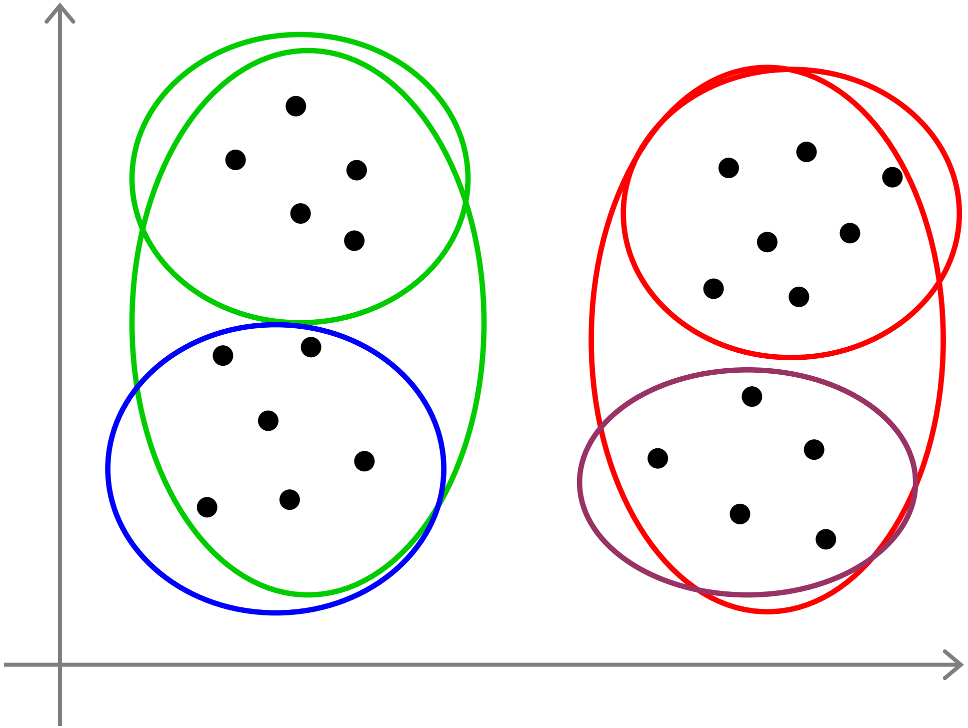


Machine Learning

Clustering

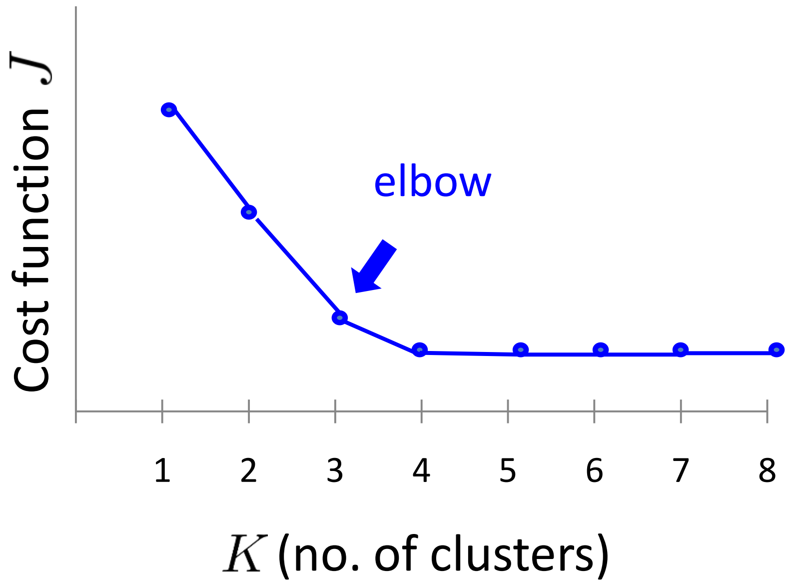
Choosing the number of clusters

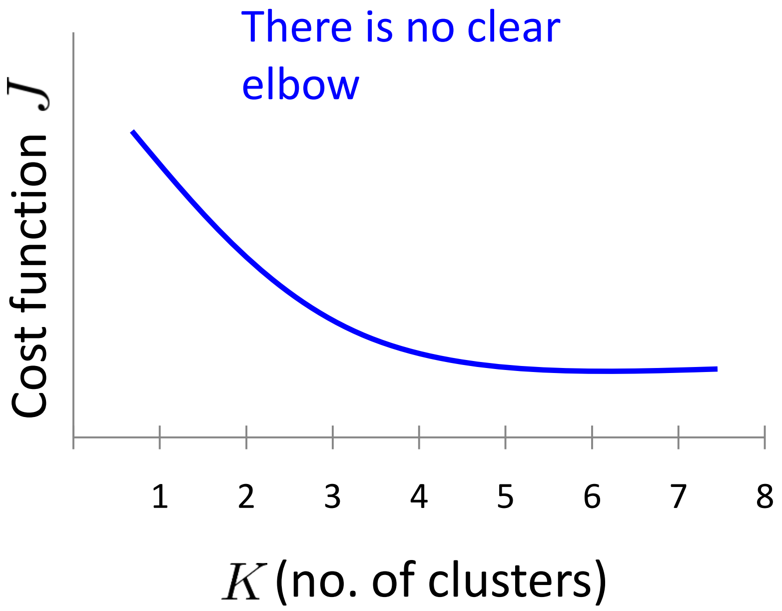
What is the right value of K?



Choosing the value of K

Elbow method:

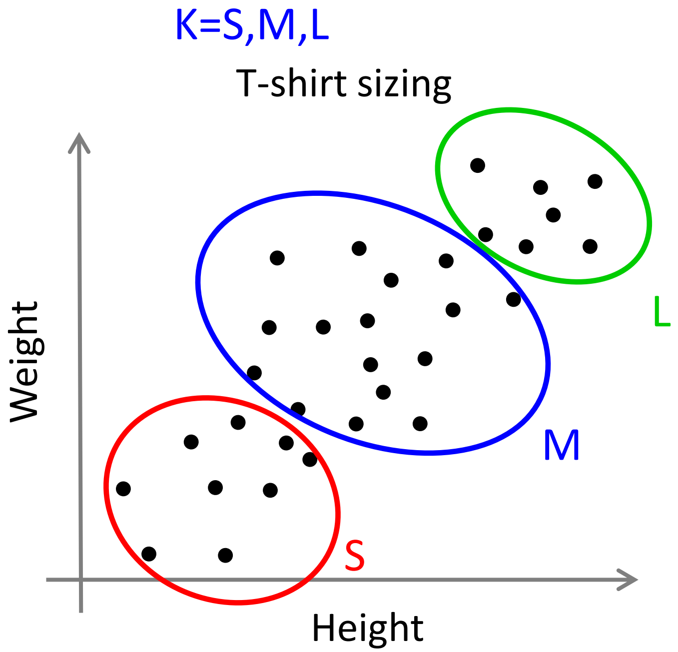


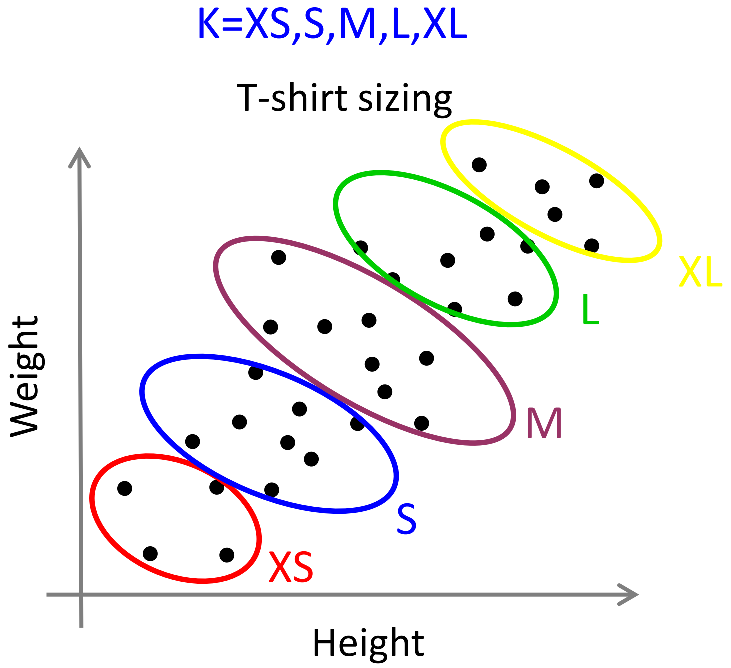


Choosing the value of K

Sometimes, you're running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose.

E.g.





Andrew Ng