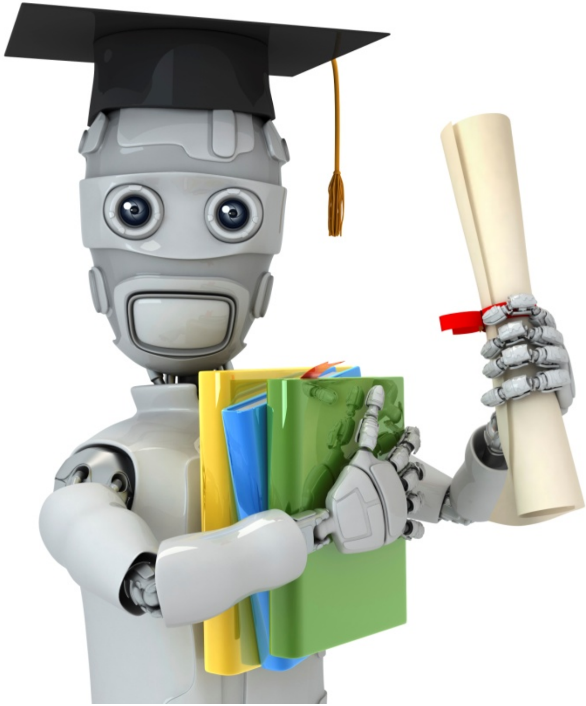
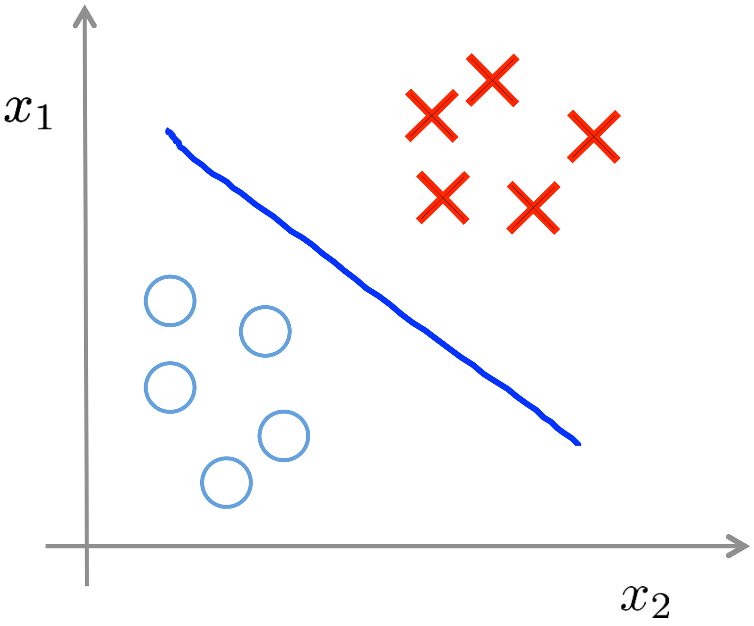


Machine Learning

Clustering

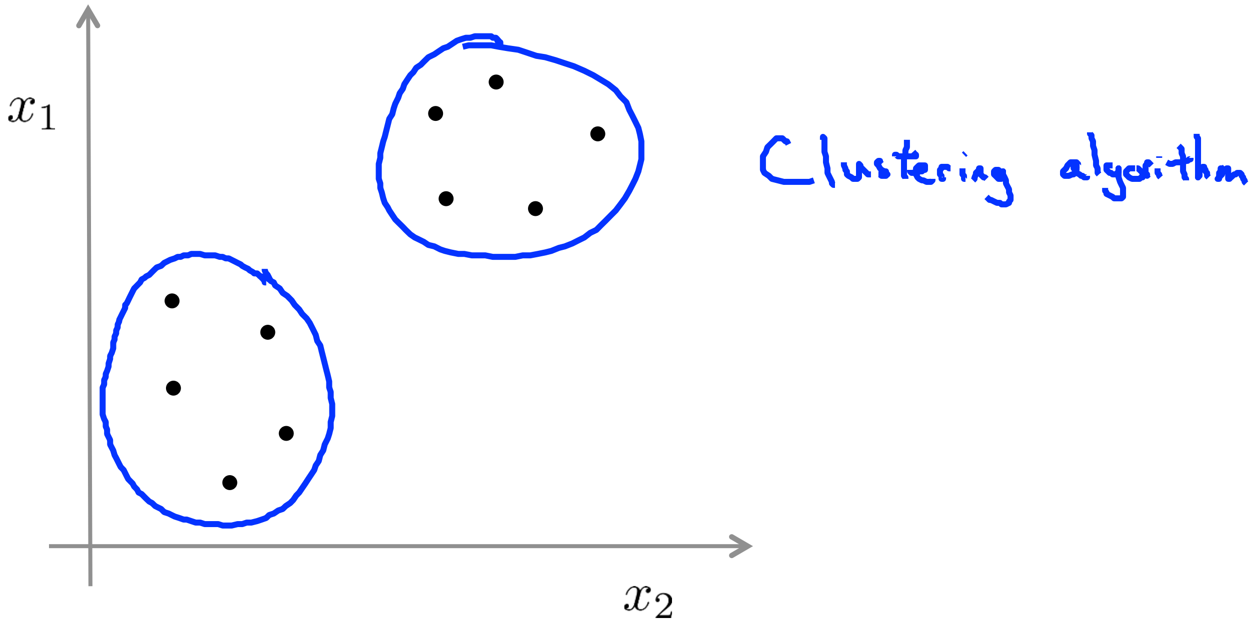
Unsupervised learning introduction

Supervised learning



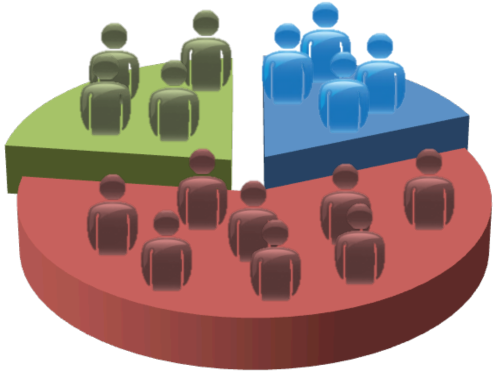
Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}), \ldots, (x^{(m)}, y^{(m)})\}$

Unsupervised learning

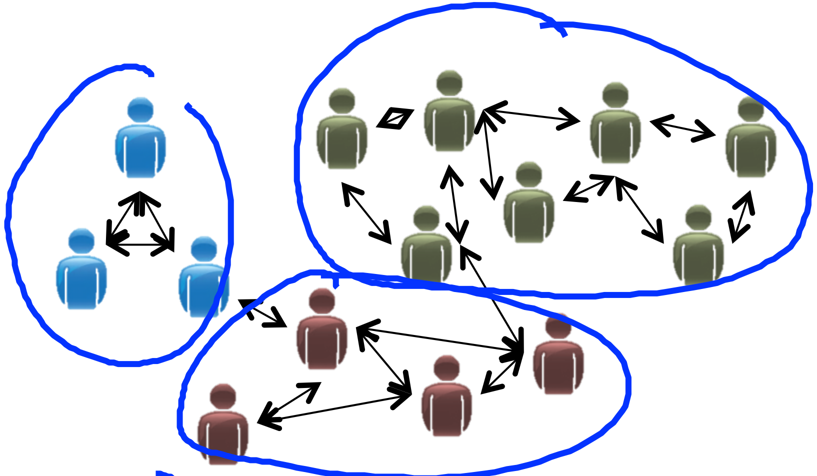


Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$ ←

Applications of clustering



Market segmentation

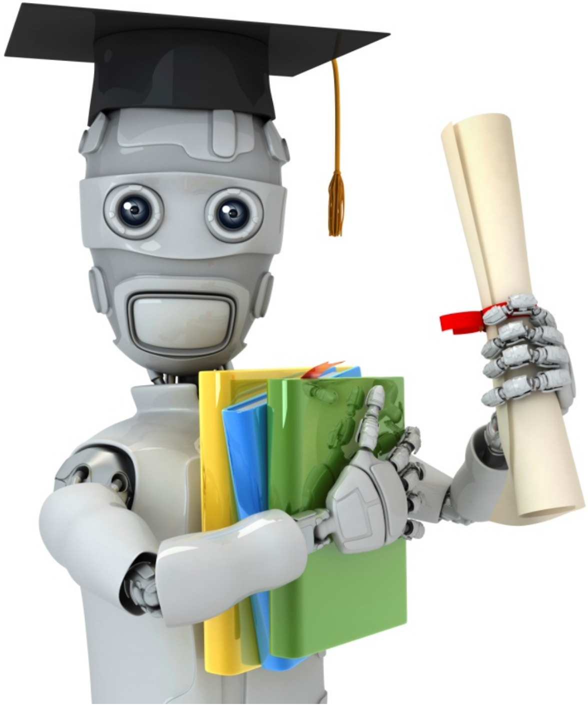


Social network analysis

Organize computing clusters

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

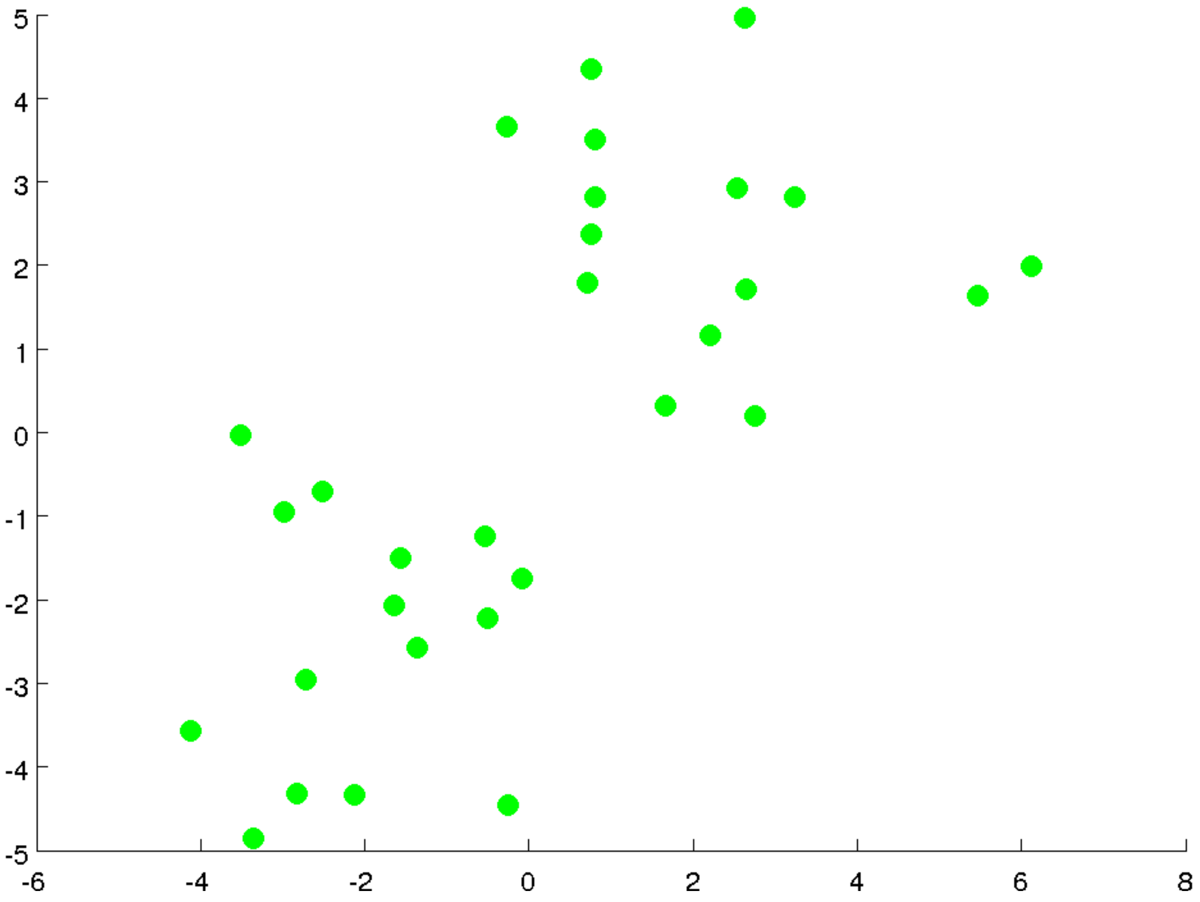
Astronomical data analysis



Machine Learning

Clustering

K-means algorithm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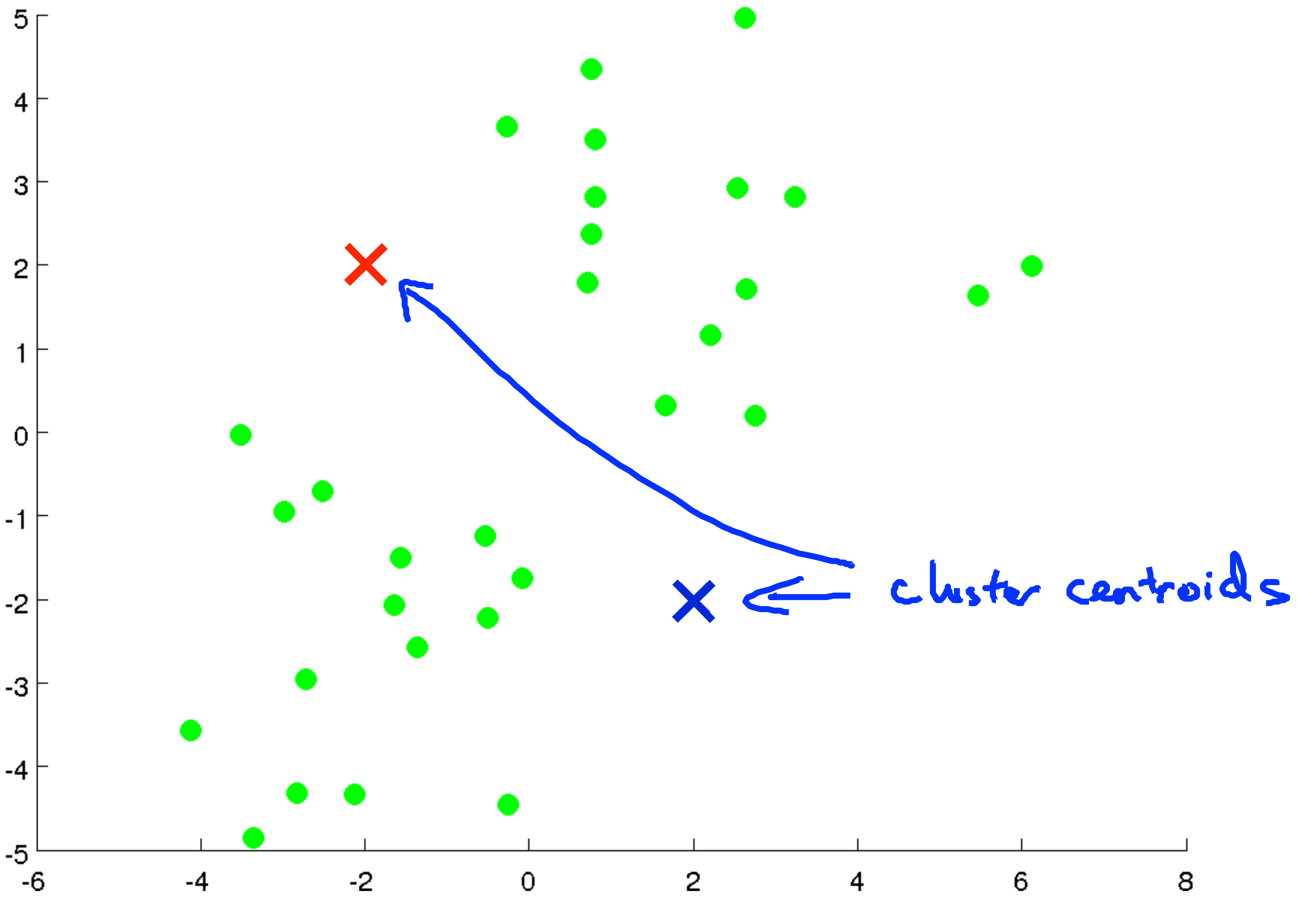

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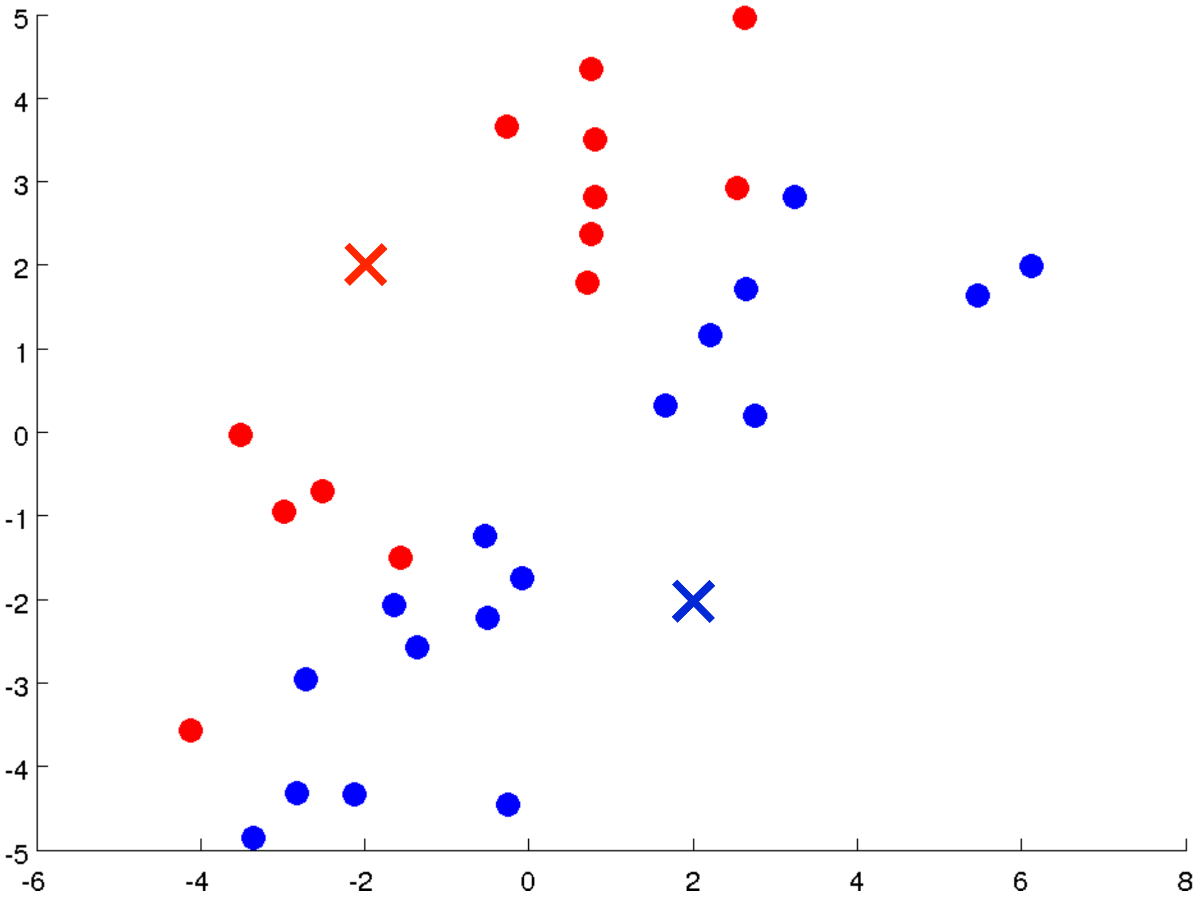
cluster centroids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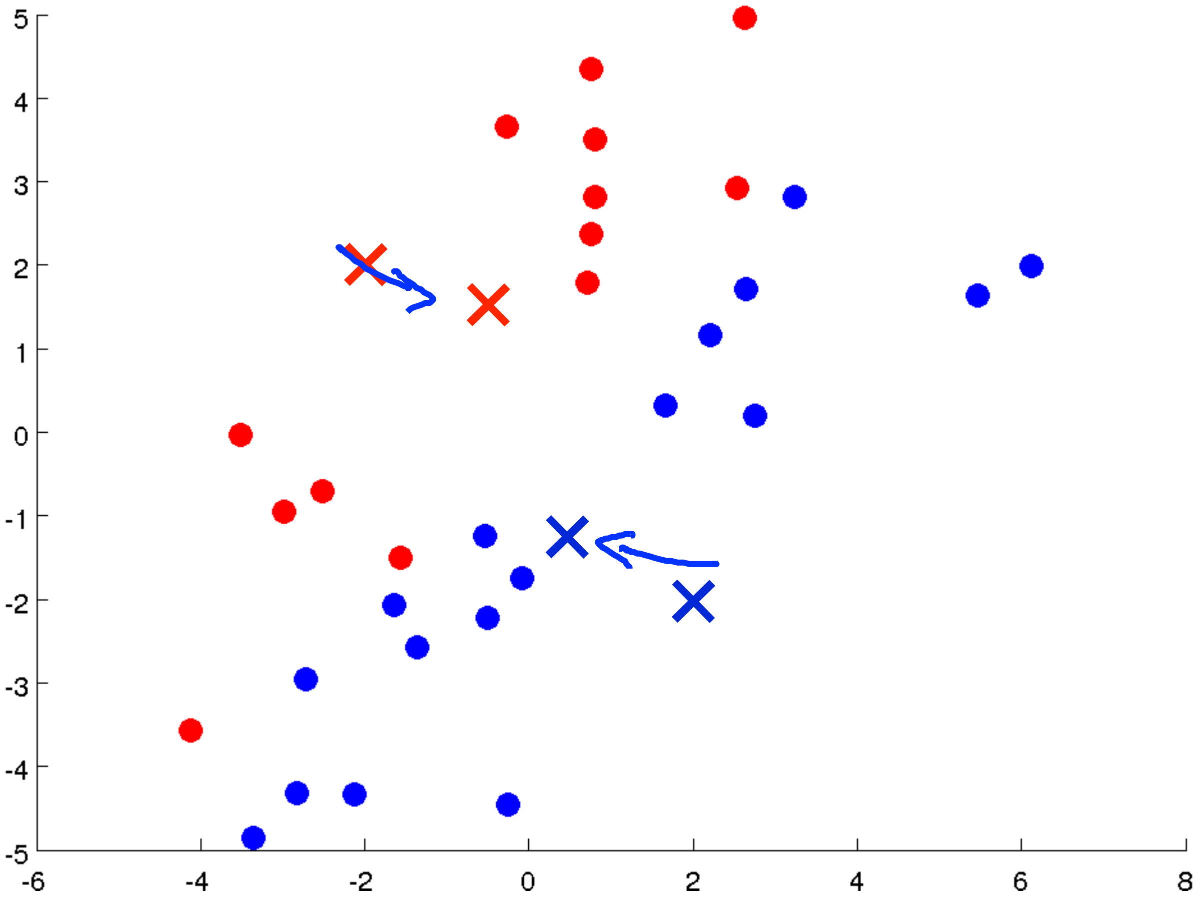
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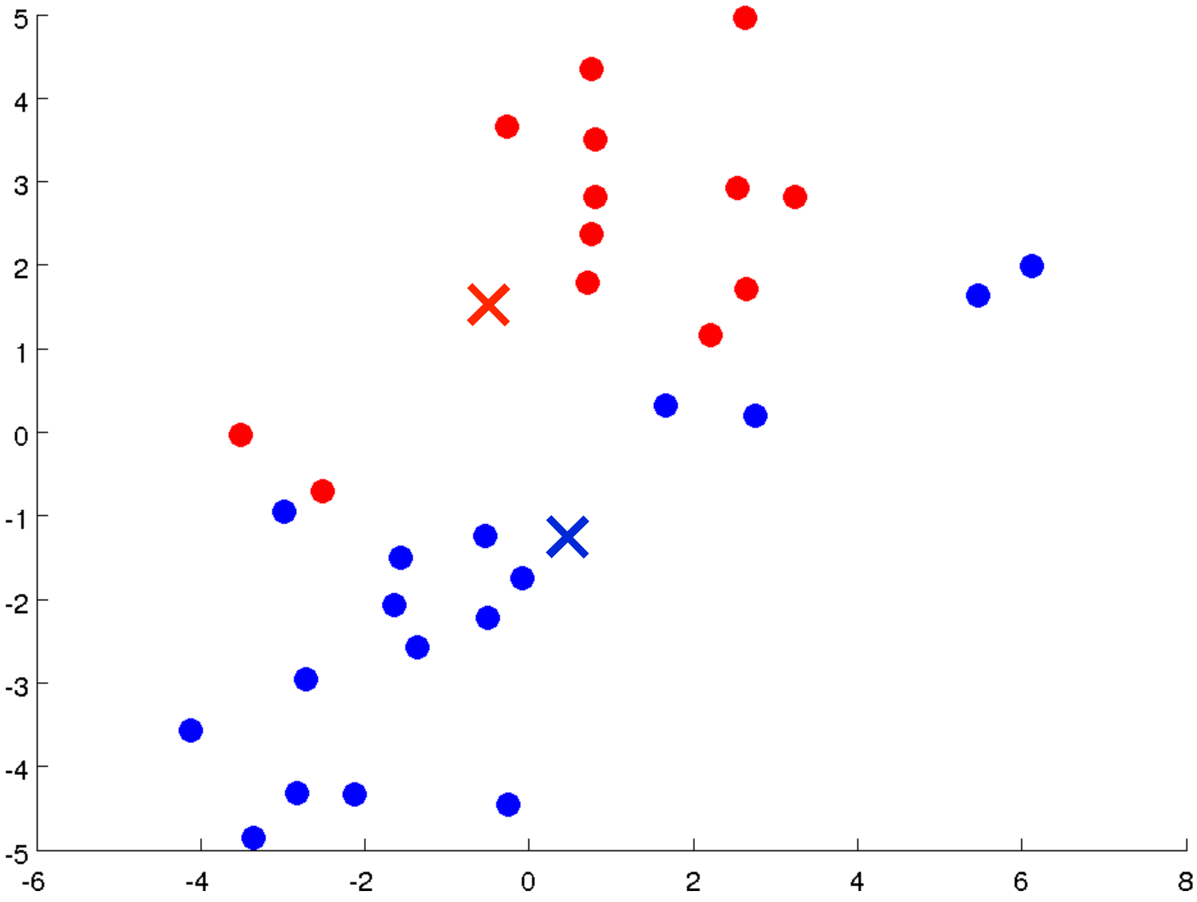
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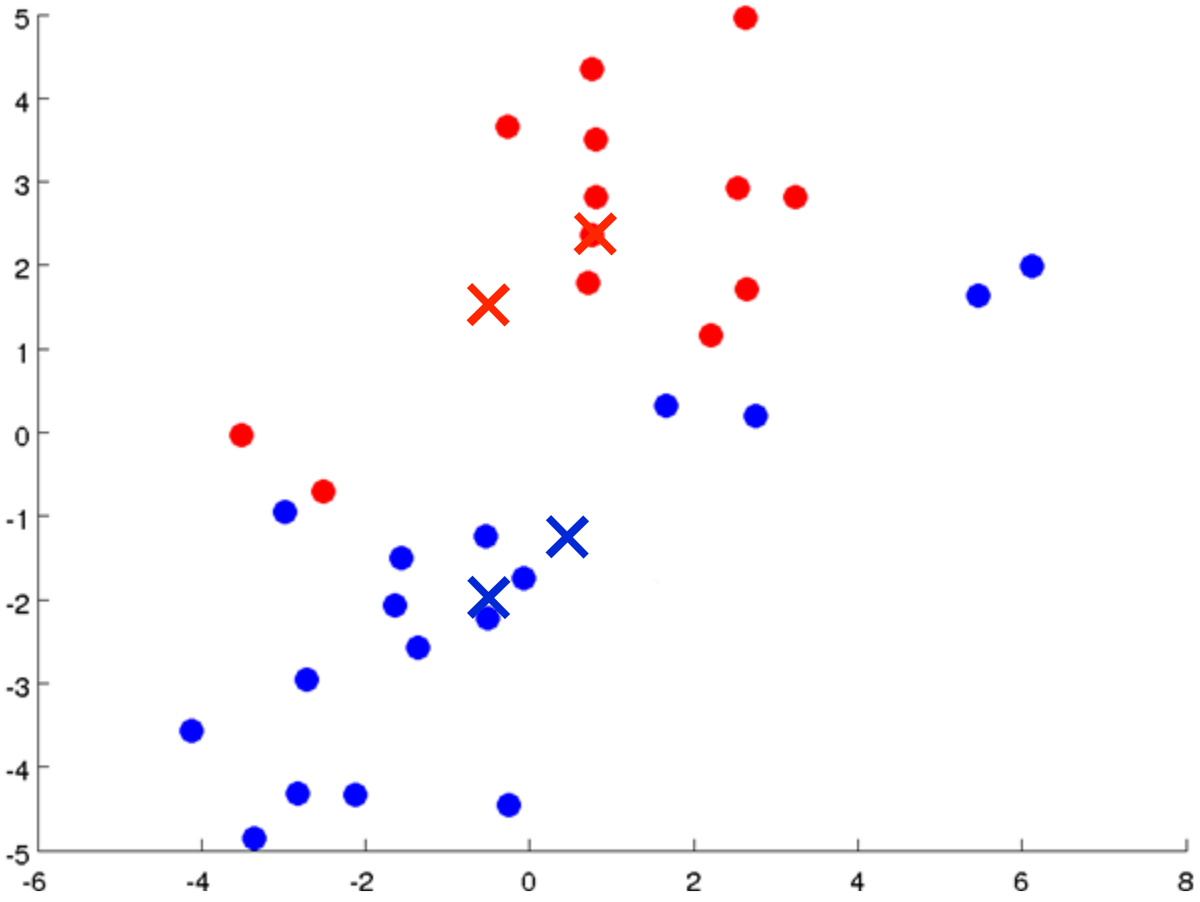

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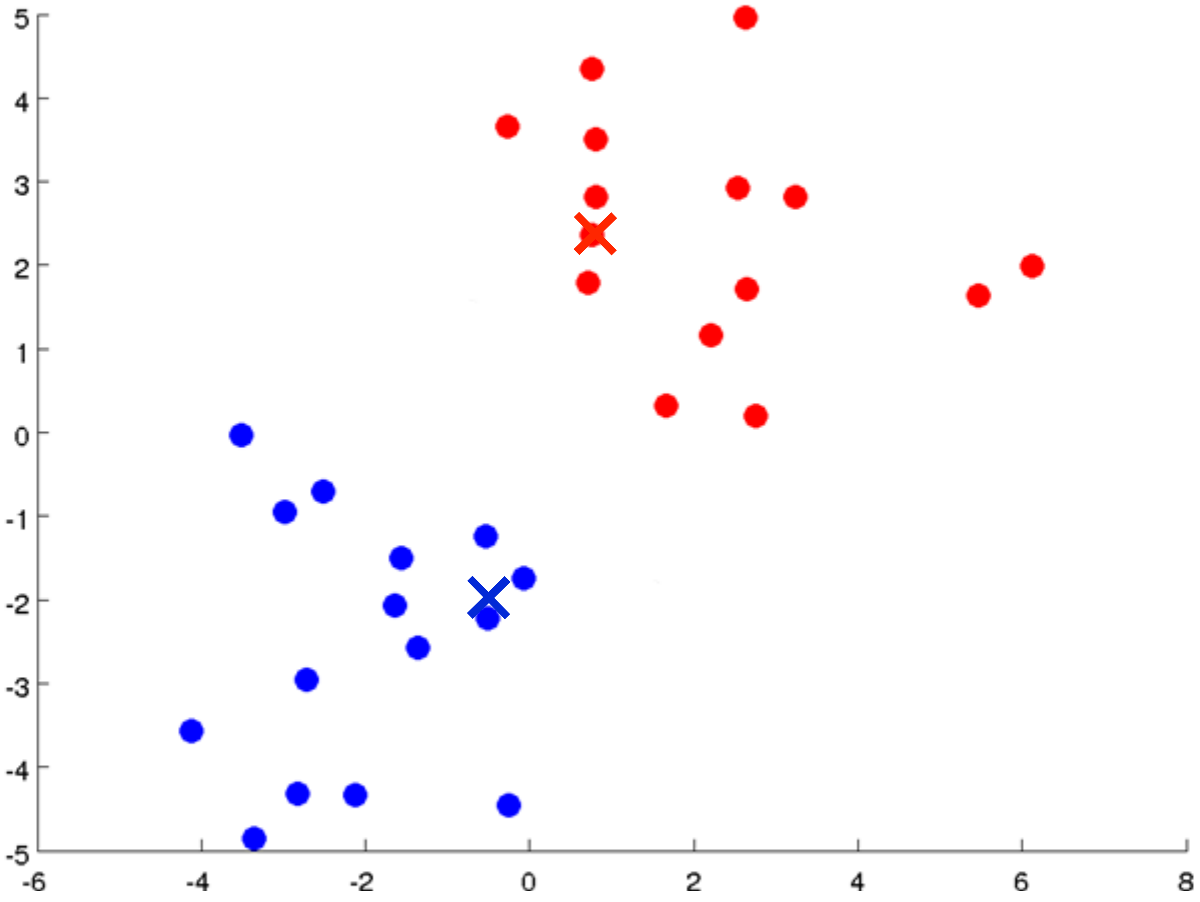
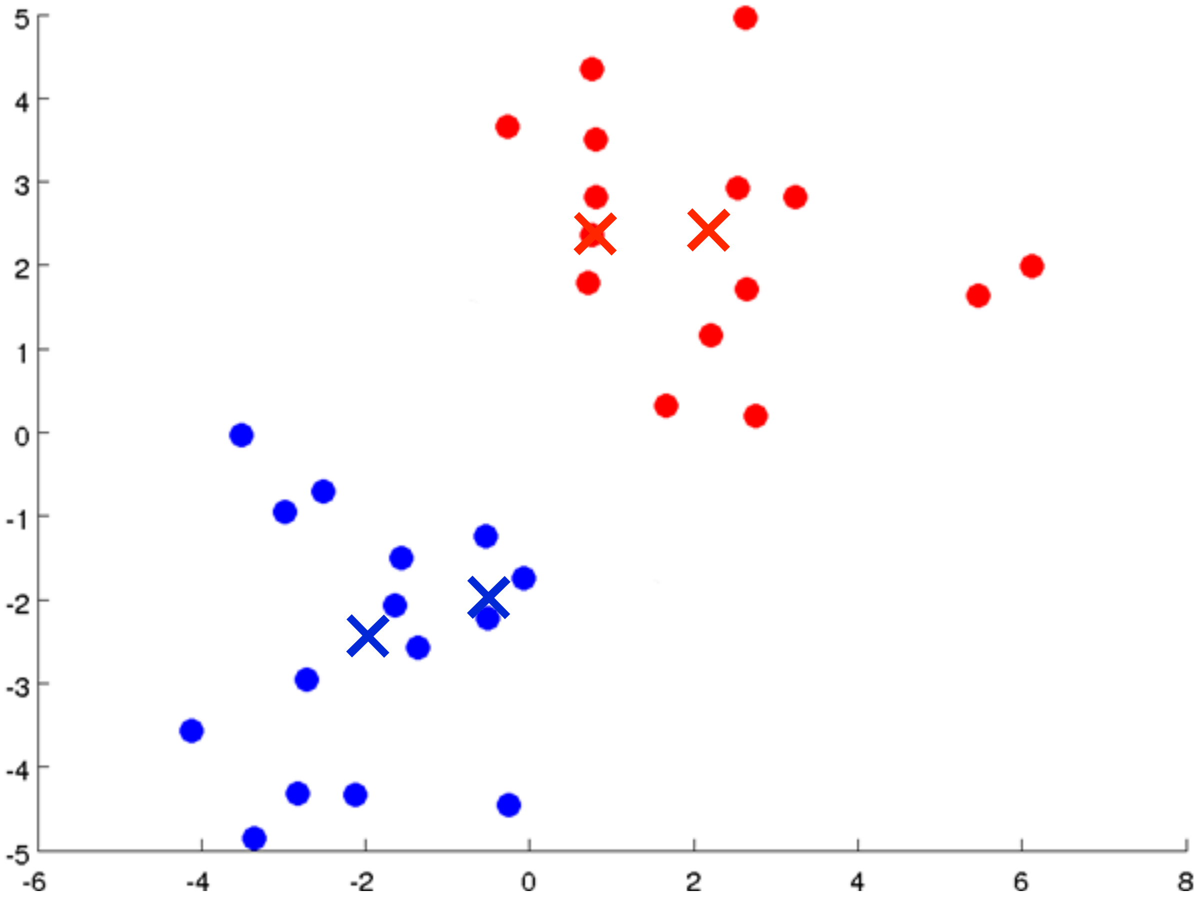


Andrew Ng



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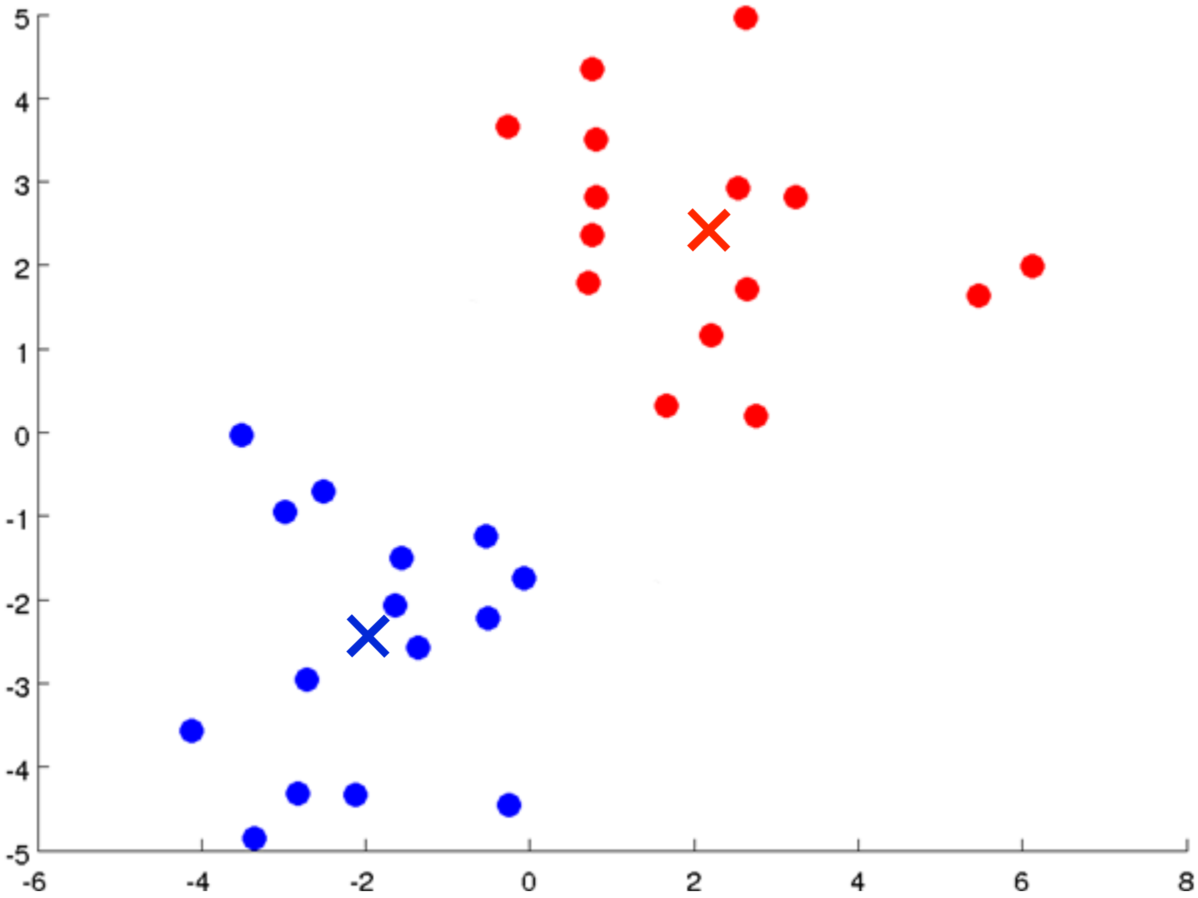


Andrew Ng

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

μ_1 $\times$ $\quad$ μ_2 $\times$

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

Repeat {

Cluster assignment step

for i = 1 to m

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

$\min_k \|x^{(i)} - \mu_k\|^2 \rightarrow c^{(i)}$

Move centroid

for k = 1 to K

$\rightarrow \mu_k$:= average (mean) of points assigned to cluster k

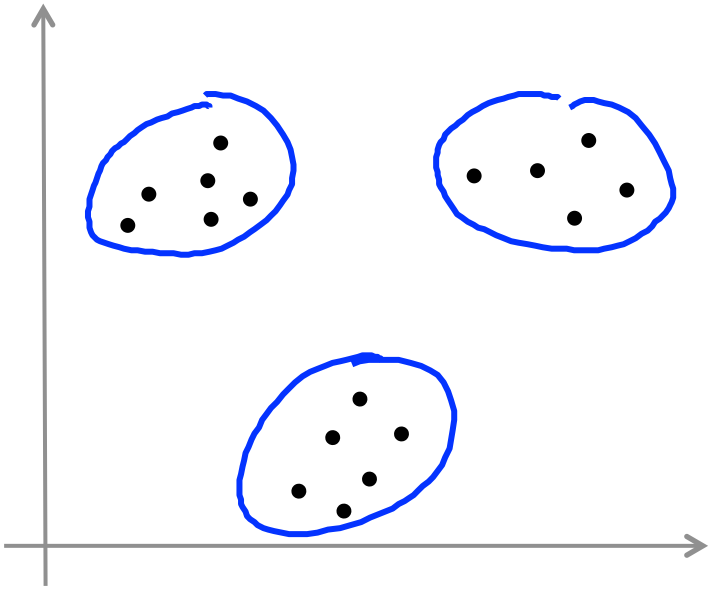
$x^{(1)}, x^{(5)}, x^{(6)}, x^{(10)} \rightarrow c^{(1)} = 2, c^{(5)} = 2, c^{(6)} = 2, c^{(10)} = 2$

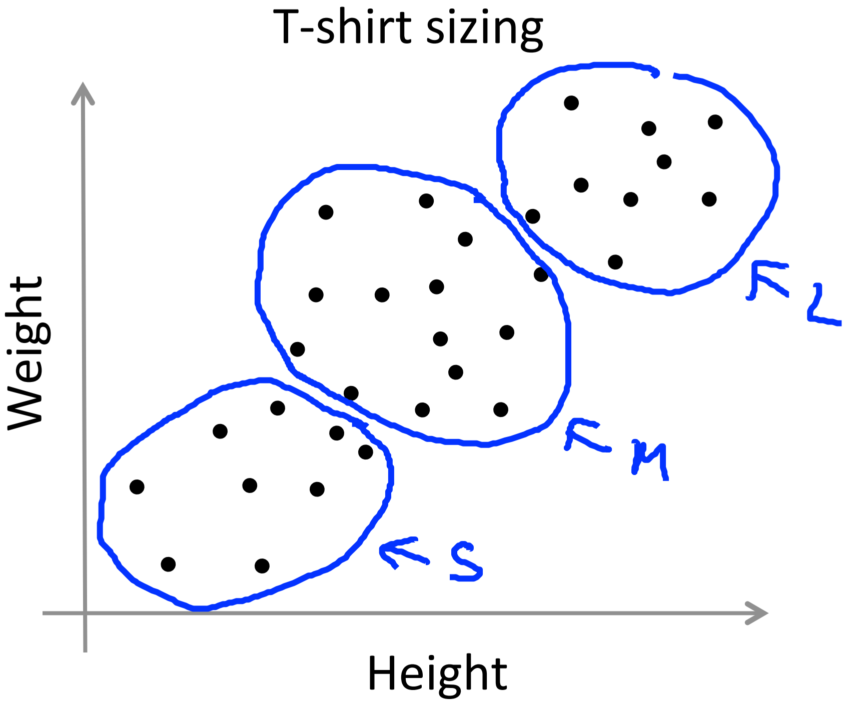
$$\mu_2 = \frac{1}{4}\left[x^{(1)} + x^{(5)} + x^{(6)} + x^{(10)}\right] \in \mathbb{R}^n$$

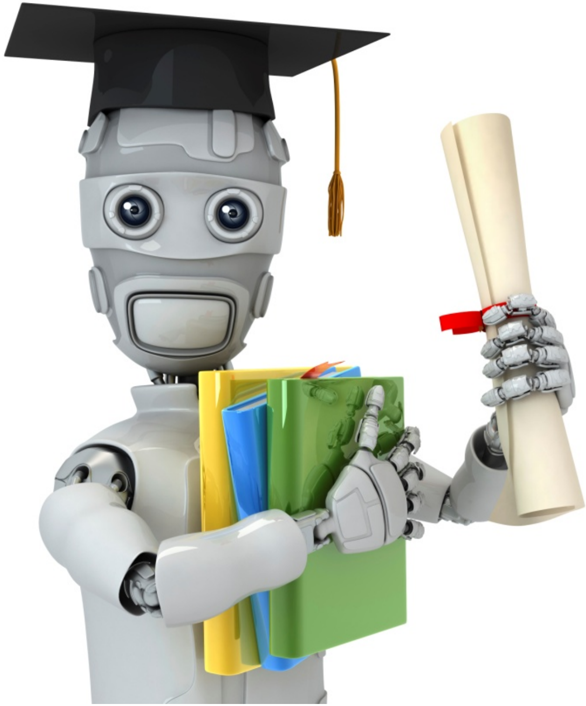
}

K-means for non-separated clusters

S, M, L







Clustering

Optimization objective

Machine Learning

K-means optimization objective

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

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

K $\quad$ $k \in \{1,2,\ldots,K\}$

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

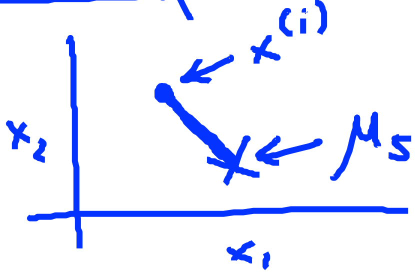
$x^{(i)} \to \underline{5}$ $\quad$ $\underline{c^{(i)} = 5}$ $\quad$ $\underline{\mu_{c^{(i)}}} = \mu_5$

Optimization objective:

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

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

Distortion



K-means algorithm

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

Cluster assignment step

Minimize $J(\dots)$ wrt $\boxed{c^{(1)}, c^{(2)}, \dots, c^{(m)}}$ ←

(holding $\mu_1, \dots, \mu_K$ fixed)

Repeat {

for i = 1 to m

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

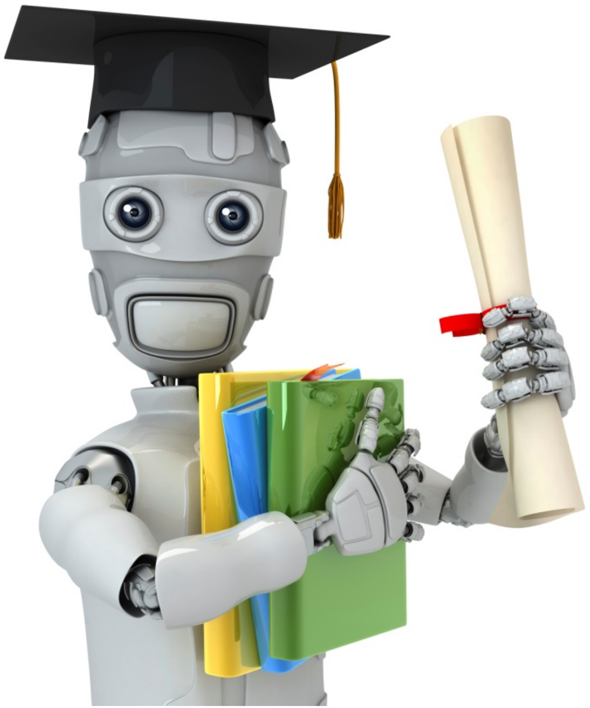
move centroid

for k = 1 to K

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

}

minimize $J(\dots)$ wrt $\boxed{\mu_1, \dots, \mu_K}$



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 $K < m$

$K=2$

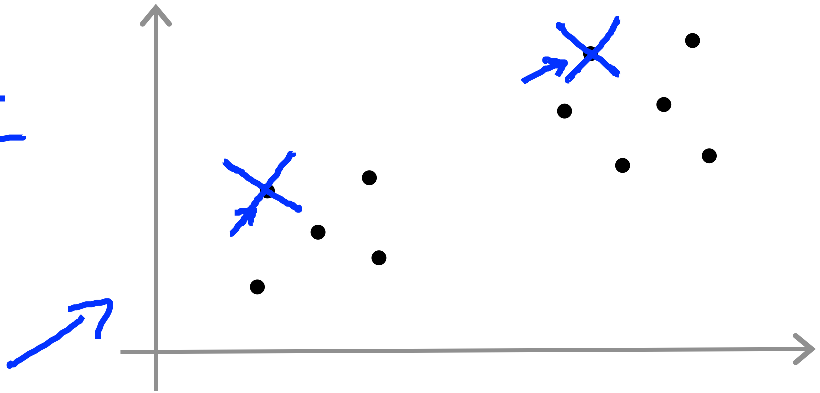
Randomly pick K training examples.

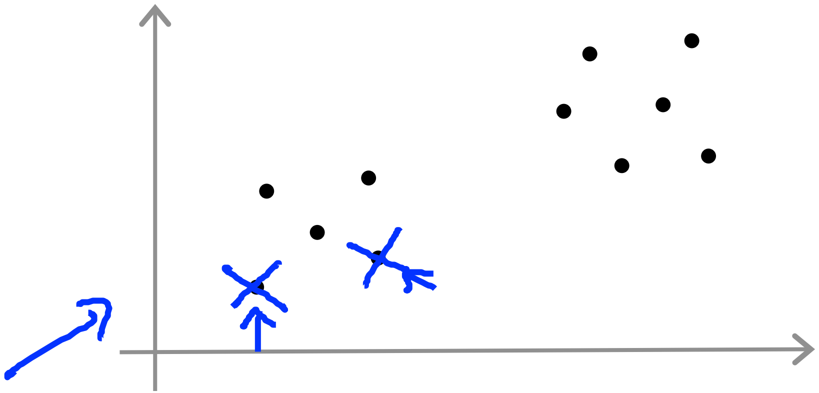
Set $\mu_1, \ldots, \mu_K$ equal to these K examples.

$\mu_1 = x^{(i)}$

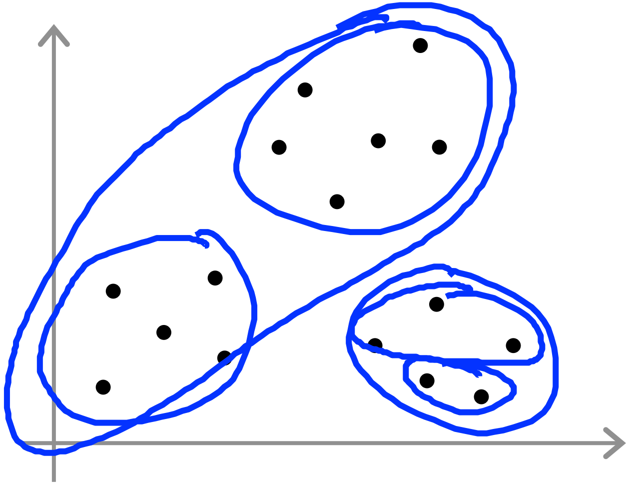
$\mu_2 = x^{(j)}$

$\vdots$

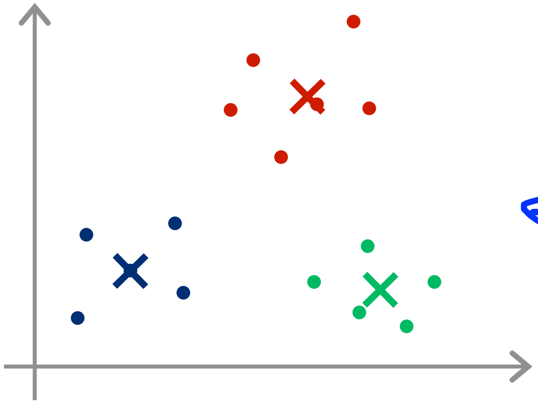


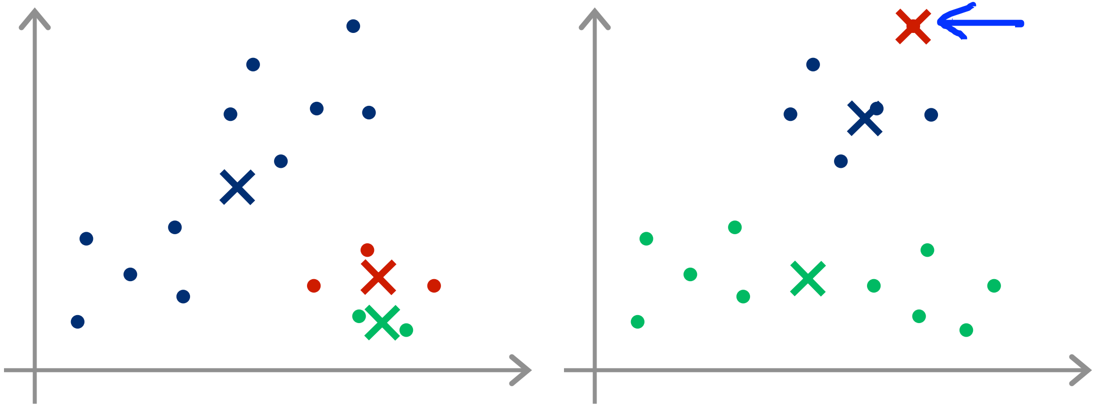


Local optima



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





Random initialization

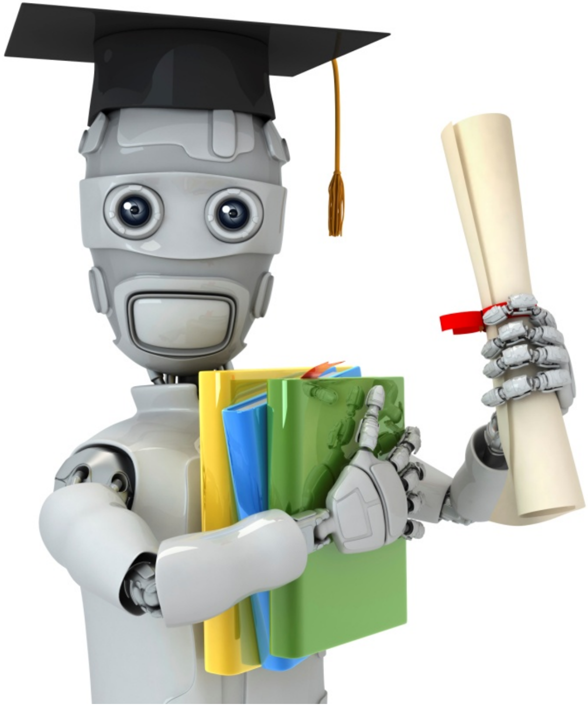
For i = 1 to 100 {

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

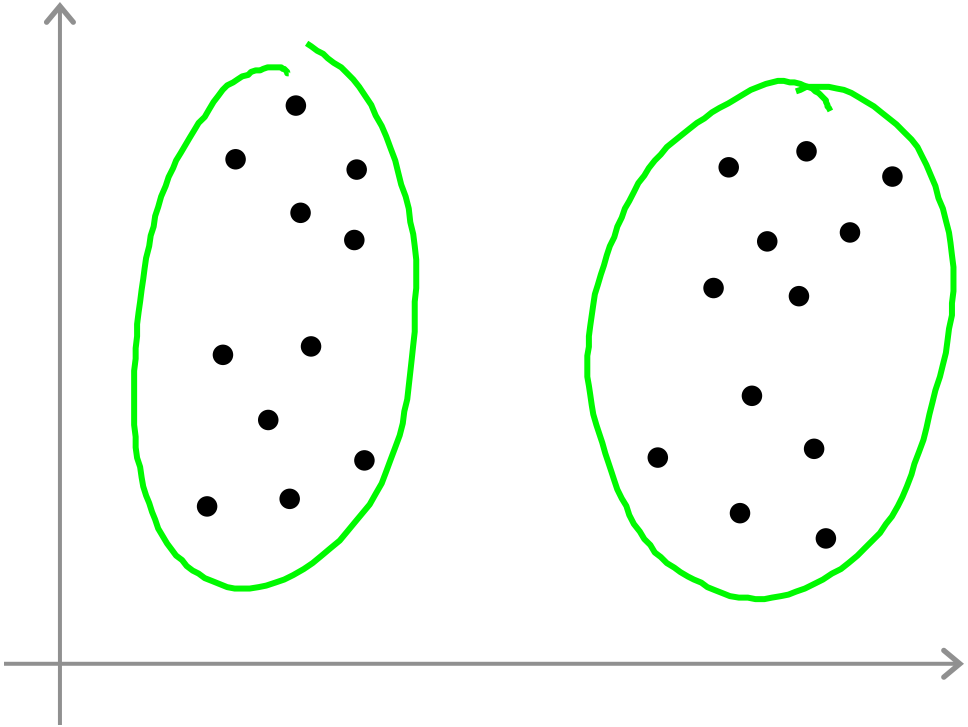


Machine Learning

Clustering

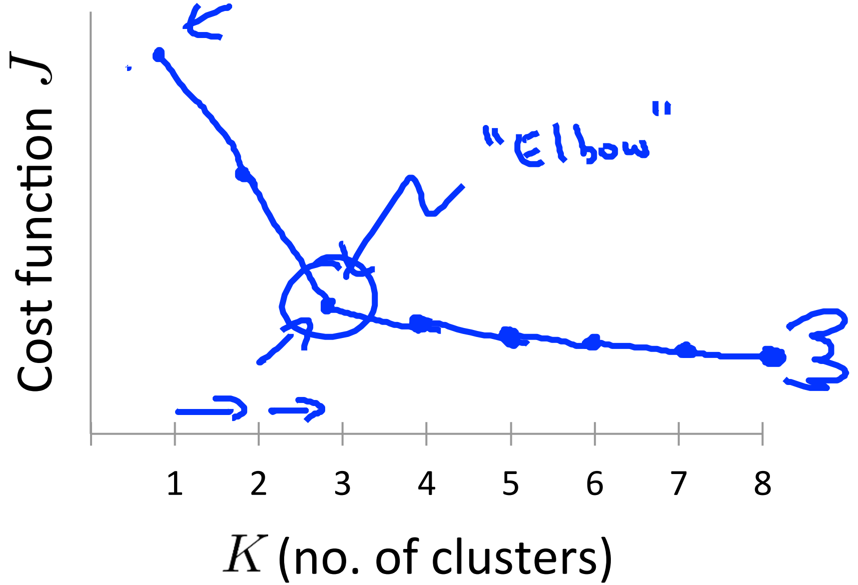
Choosing the number of clusters

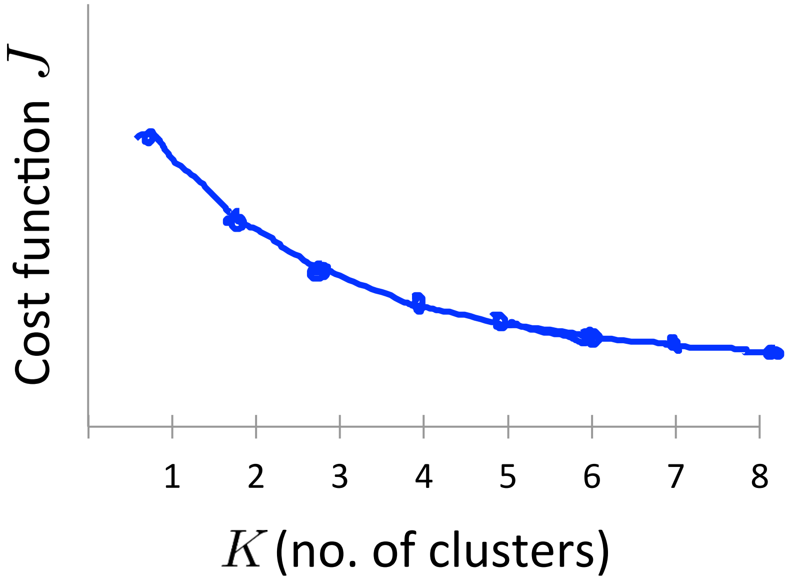
What is the right value of K?



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.

K=3 S, M, L

K=5 XS, S, M, L, XL

E.g.