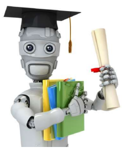
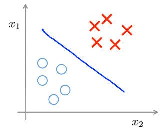


Machine Learning

Clustering

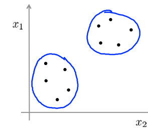
Unsupervised learning introduction

Supervised learning



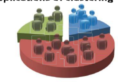
Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}), \ldots, (x^{(m)}, y^{(m)})\}$

Unsupervised learning

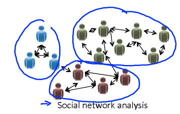


Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$

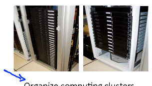
Applications of clustering



Market segmentation



Social network analysis



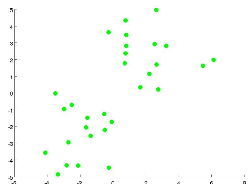
Organize computing clusters

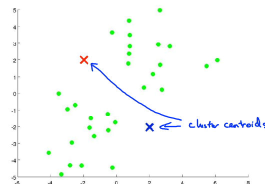
Astronomical data analysis

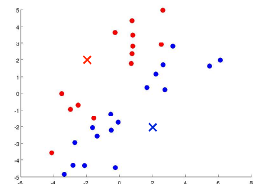
Machine Learning

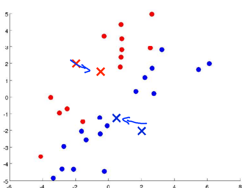
Clustering

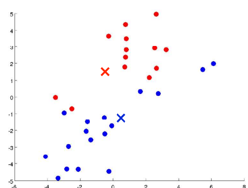
K-means algorithm

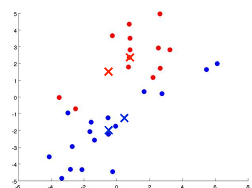


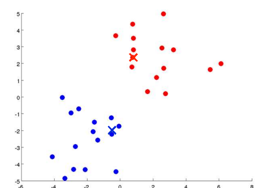


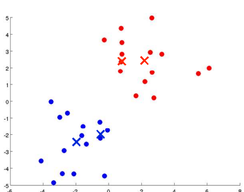


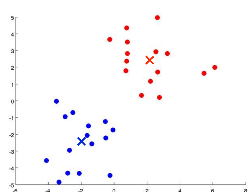












K-means algorithm

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 μ_2

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 $x^{(i)}$

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

Move centroid

for k = 1 to K

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

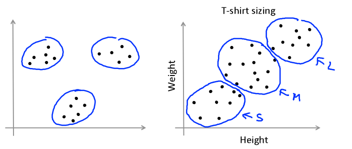
$x^{(1)}, x^{(5)}, x^{(6)}, x^{(10)} \rightarrow c^{(1)}=2, c^{(5)}=2, c^{(6)}=2, c^{(10)}=2$

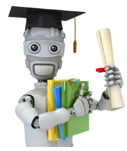
$\mu_2 = \frac{1}{4}\left[x^{(1)} + x^{(5)} + x^{(6)} + x^{(10)}\right] \in \mathbb{R}^n$

}

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 k ($\mu_k \in \mathbb{R}^n$)

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

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

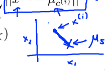
$x^{(i)} \rightarrow 5 \quad c^{(i)} = 5 \quad \mu_{c^{(i)}} = \mu_5$

Optimization objective:

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

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

Distortion



K-means algorithm

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

Repeat {

Cluster assignment step: Minimize $J(\ldots)$ wrt $c^{(1)}, c^{(2)}, \ldots, c^{(m)}$ (holding $\mu_1, \ldots, \mu_K$ fixed)

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 $J(\ldots)$ wrt $\mu_1, \ldots, \mu_K$

Clustering

Random initialization

Machine Learning

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

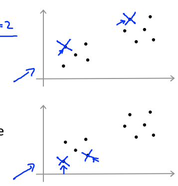
$K = 2$

Should have $K < m$

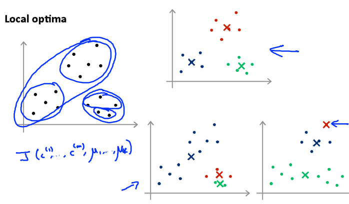
Randomly pick K training examples.

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

$\mu_1 = x^{(i)}$
$\mu_2 = x^{(j)}$



Local optima



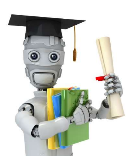
Random initialization

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

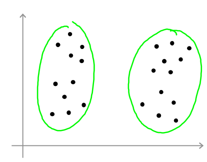


Clustering

Choosing the number of clusters

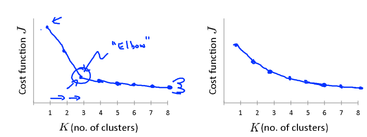
Machine Learning

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.