



Machine Learning

Clustering

Unsupervised learning
introduction

Supervised learning



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

Unsupervised learning



Clustering algorithm

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

Applications of clustering



→ Market segmentation



→ Social network analysis



→ Organize computing clusters



→ Astronomical data analysis



Machine Learning

Clustering

K-means algorithm





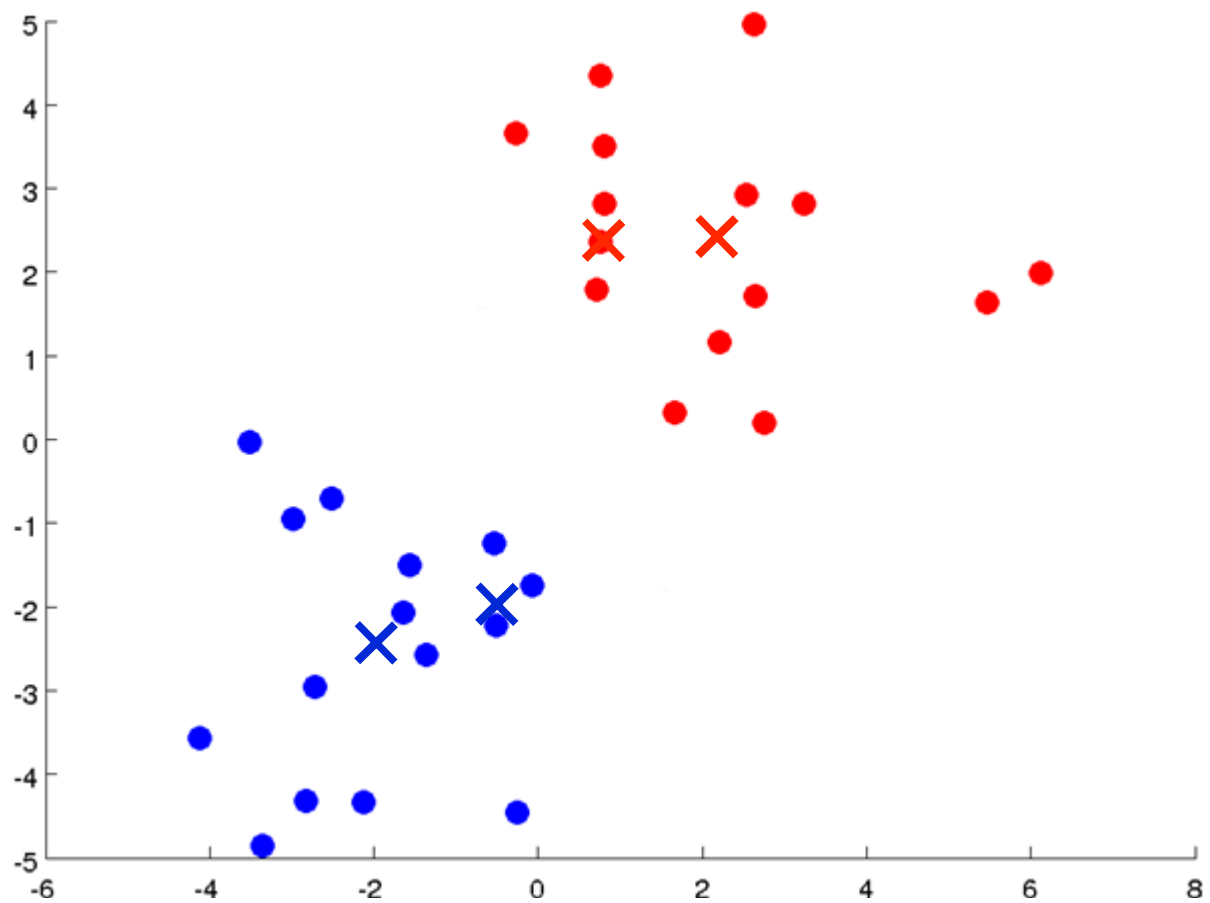














K-means algorithm

Input:

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

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

K-means algorithm

$$\mu_1 \quad \mu_2$$

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

Repeat {

Cluster assignment step

for $i = 1$ to m

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

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

\uparrow
 $c^{(i)}$

for $k = 1$ to K

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

Move centroid

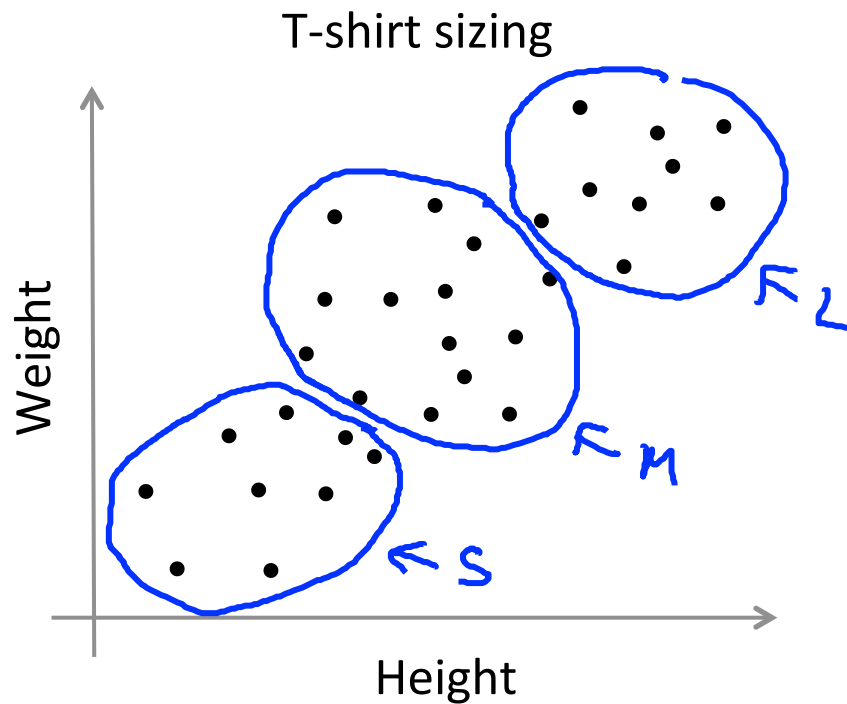
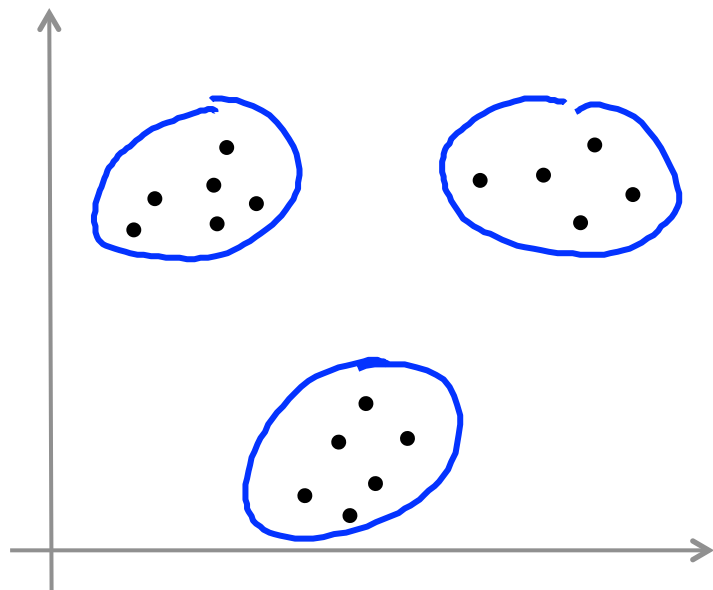
$$x^{(1)}, x^{(5)}, x^{(6)}, x^{(10)}$$

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

$$\mu_2 = \frac{1}{4} \begin{bmatrix} x^{(1)} + x^{(5)} + x^{(6)} + x^{(10)} \\ - \end{bmatrix} \in \mathbb{R}^n$$

K-means for non-separated clusters

S, M, L





Machine Learning

Clustering Optimization objective

K-means optimization objective

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

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

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

K $k \in \{1, 2, \dots, K\}$
 $x^{(i)} \rightarrow 5$ $\underline{c^{(i)} = 5}$ $\underline{\mu_{c^{(i)}}} = \mu_5$

Optimization objective:

$$\rightarrow \underline{J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)} = \frac{1}{m} \sum_{i=1}^m \left[\|x^{(i)} - \mu_{c^{(i)}}\|^2 \right] \leftarrow$$

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

→ μ_1, \dots, μ_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 $J(\dots)$ w.r.t

$c^{(1)}, c^{(2)}, \dots, c^{(m)}$ ←

(holding μ_1, \dots, μ_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

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

}

Minimize $J(\dots)$ w.r.t μ_1, \dots, μ_K



Machine Learning

Clustering Random initialization

K-means algorithm

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

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
}

Random initialization

Should have $K < m$

Randomly pick K training examples.

Set μ_1, \dots, μ_K equal to these K examples.

$$\begin{aligned}\mu_1 &= x^{(i)} \\ \mu_2 &= x^{(j)} \\ &\vdots\end{aligned}$$

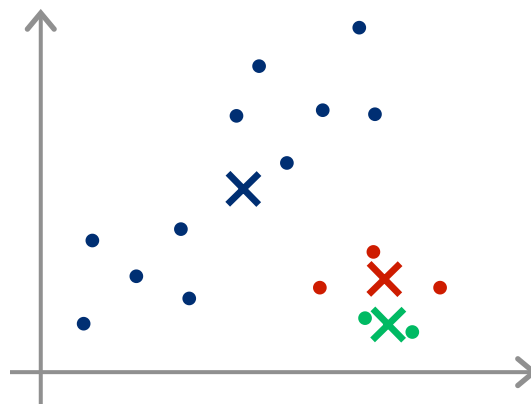
$K=2$



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

Compute cost function (distortion)

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

}

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



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

E.g.



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

