



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







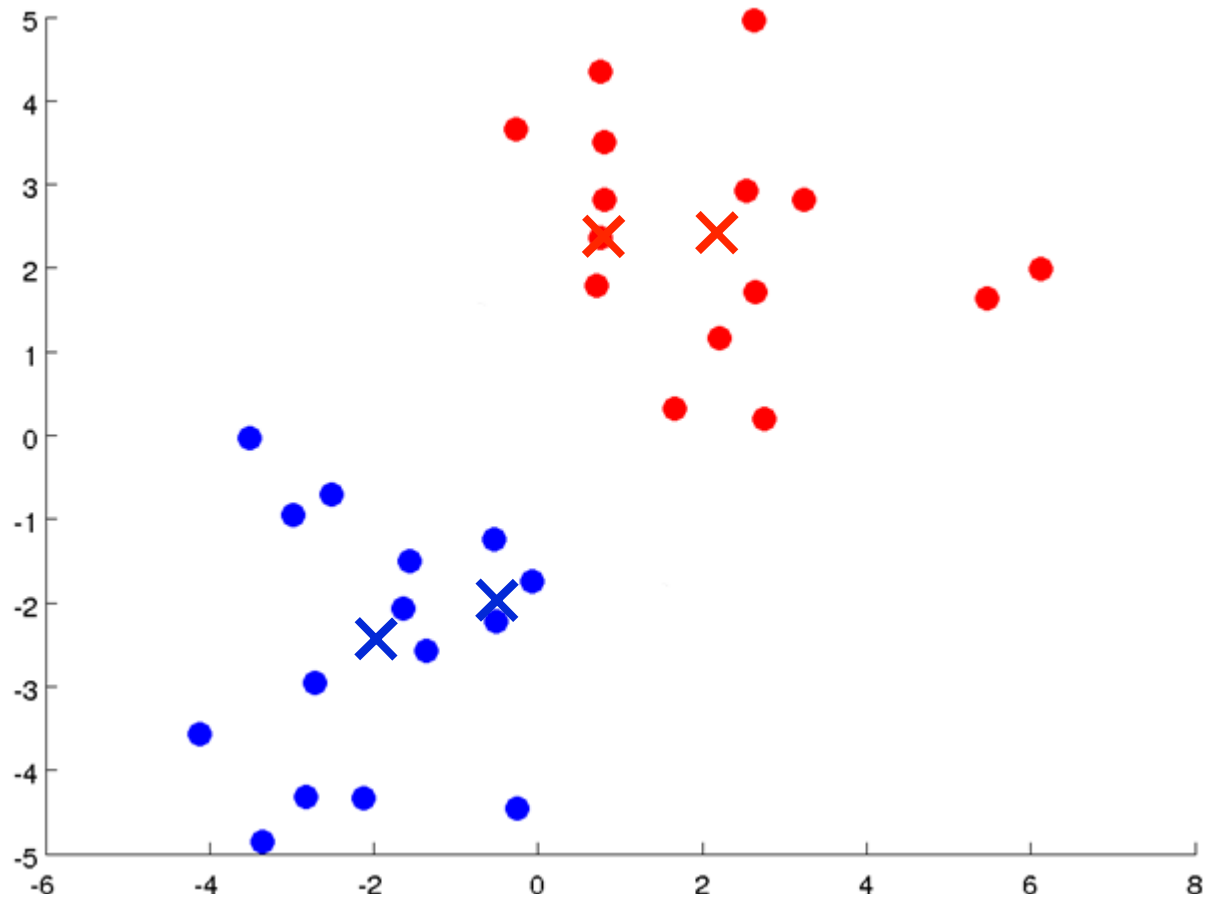














# K-means algorithm

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  $K$

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

Move  
centroid

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

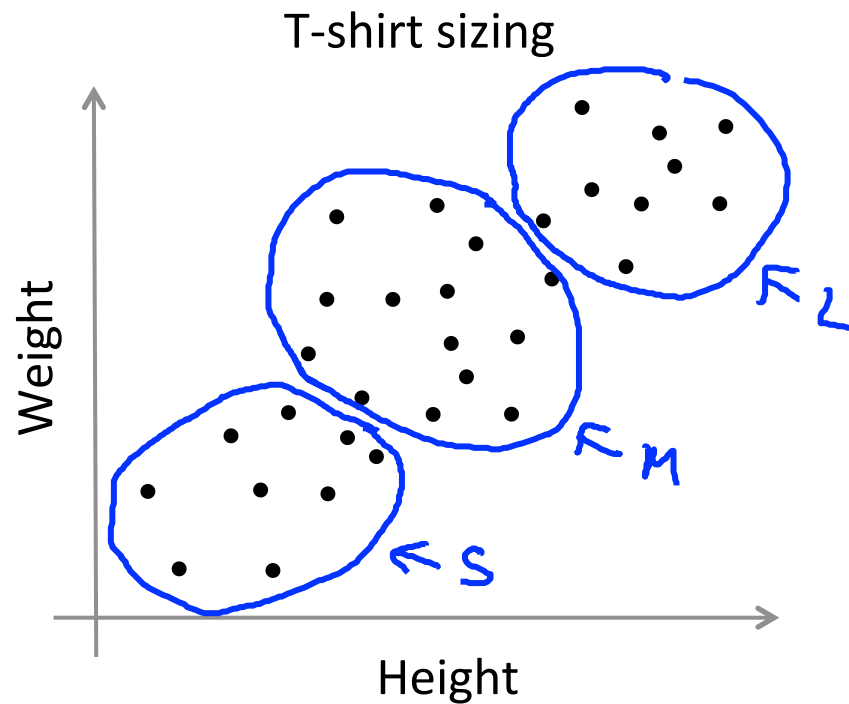
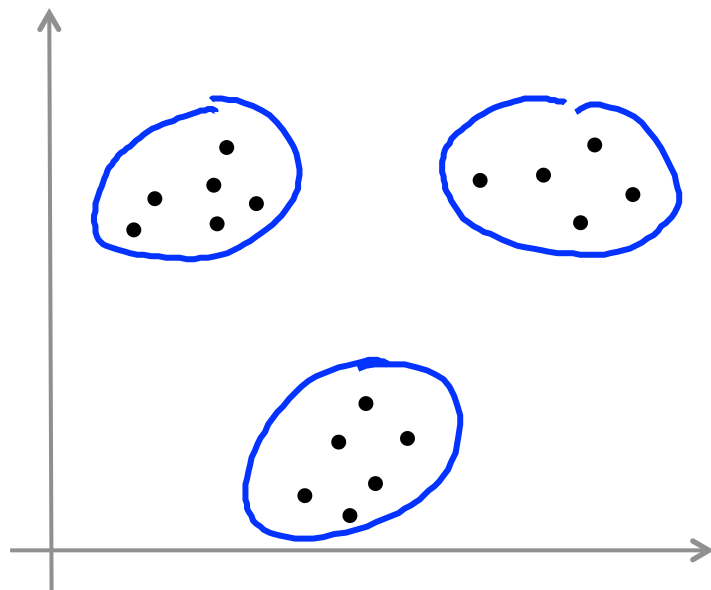
$$\rightarrow c^{(1)}=2, c^{(5)}=2, c^{(6)}=2, c^{(10)}=2$$

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



# 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

→  $\mu_k$  = 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:

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

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

→  $\mu_1, \dots, \mu_K$

Distortion



# K-means algorithm

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

Repeat {

*Cluster assignment step*  
Minimize  $J(\dots)$  w.r.t.  $c^{(1)}, c^{(2)}, \dots, c^{(m)} \leftarrow$   
(holding  $\mu_1, \dots, \mu_K$  fixed)

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  $k$

} *minimize  $J(\dots)$  w.r.t.  $\mu_1, \dots, \mu_K$*

*move centroid*



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  $K < m$

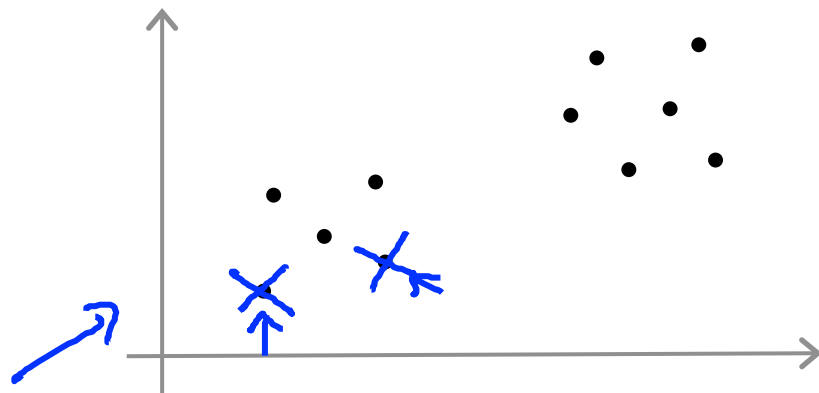
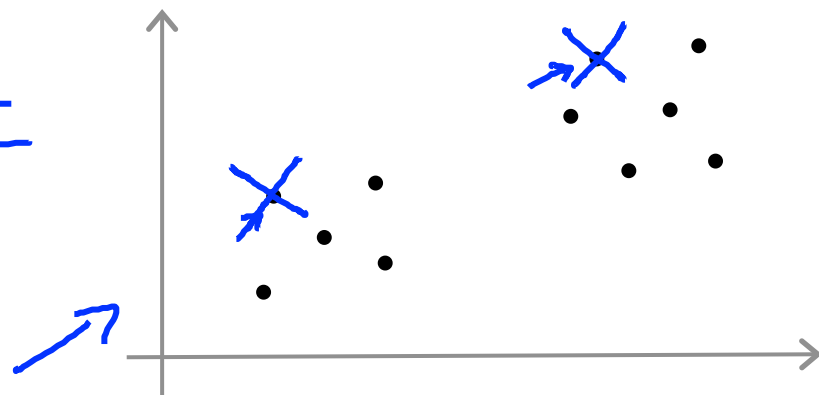
Randomly pick  $K$  training examples.

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

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

Randomly select any examples to be initial points

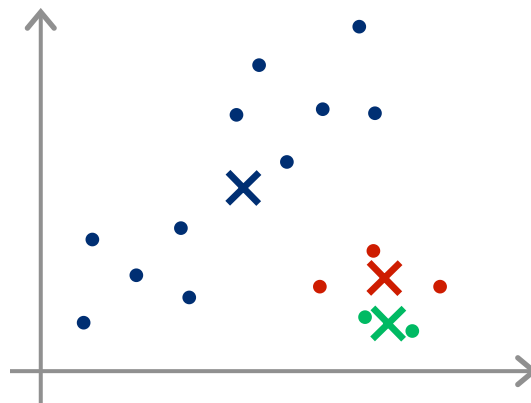
$K=2$



# 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

