

03:32 / 12:32



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## 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

$$\begin{array}{c} \mu_1 \\ \times \end{array} \quad \begin{array}{c} \mu_2 \\ \times \end{array}$$

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  $x^{(i)}$

for  $k = 1$  to  $K$

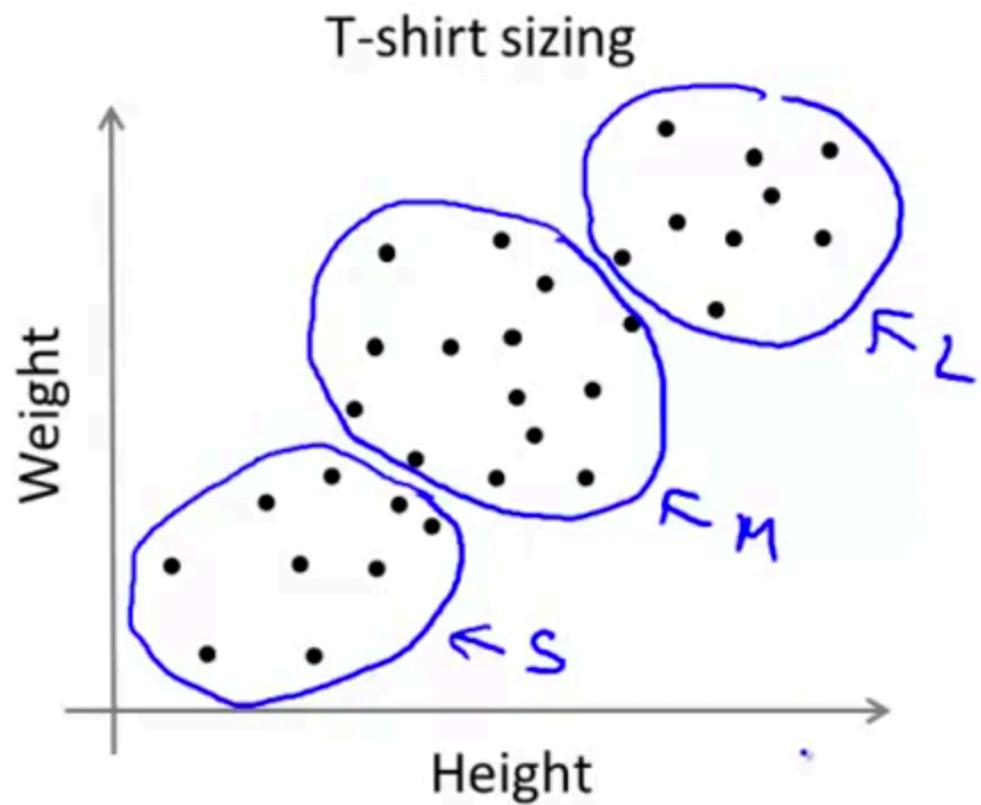
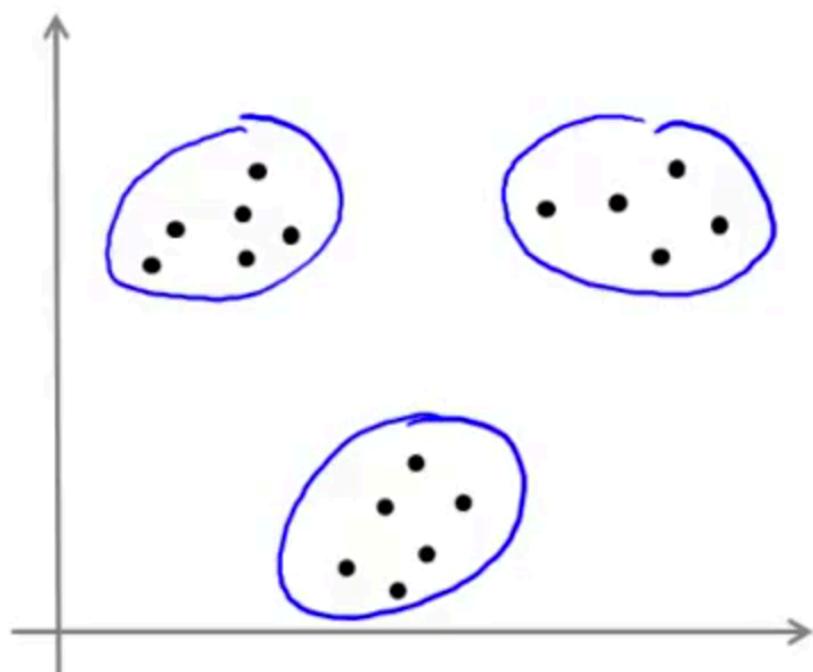
$$\min_k \|\underline{x}^{(i)} - \underline{\mu}_k\|^2$$

$\underline{\mu}_k$  := average (mean) of points assigned to cluster  $k$

}

## K-means for non-separated clusters

S, M, L



## 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  $k$  ( $\mu_k \in \mathbb{R}^n$ )  $k \in \{1, 2, \dots, K\}$
- $\mu_{c^{(i)}}$  = cluster centroid of cluster to which example  $x^{(i)}$  has been assigned  $x^{(i)} \rightarrow \underline{S}$      $\underline{c^{(i)}} = 5$      $\underline{\mu_{c^{(i)}}} = \mu_5$

Optimization objective:

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

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

## K-means algorithm

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

Repeat {

Cluster assignment step

Minimize  $J(\dots)$  wrt  $c^{(1)}, c^{(2)}, \dots, c^{(n)}$   
(holding  $\mu_1, \dots, \mu_K$  fixed)

for  $i = 1$  to  $m$

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

move  
centroid

for  $k = 1$  to  $K$

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

}

minimize  $J(\dots)$  wrt

$\mu_1, \dots, \mu_K$

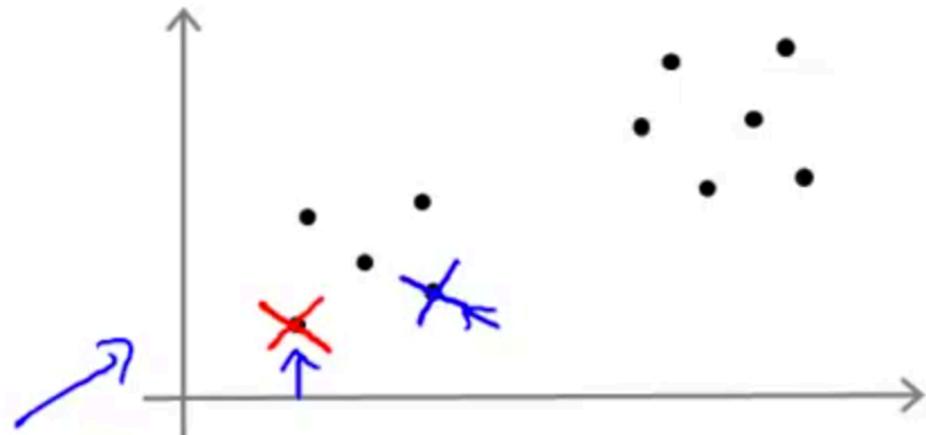
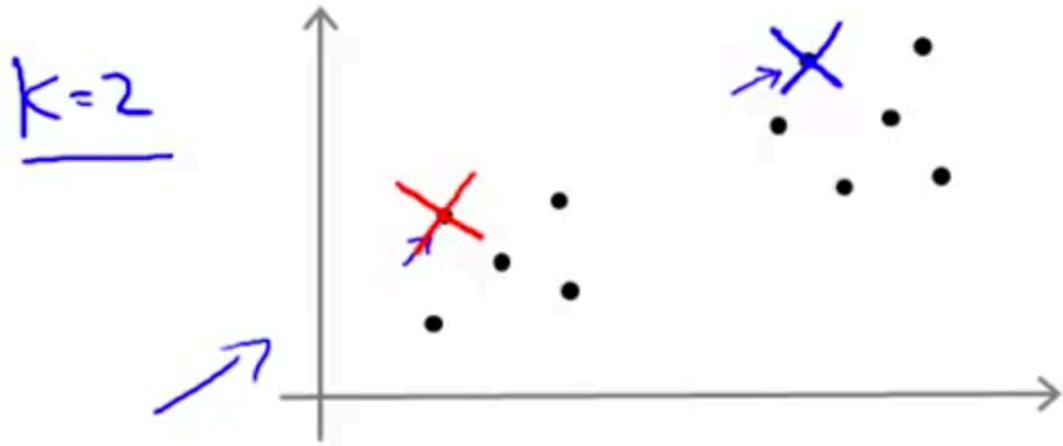
## Random initialization

Should have  $K < m$

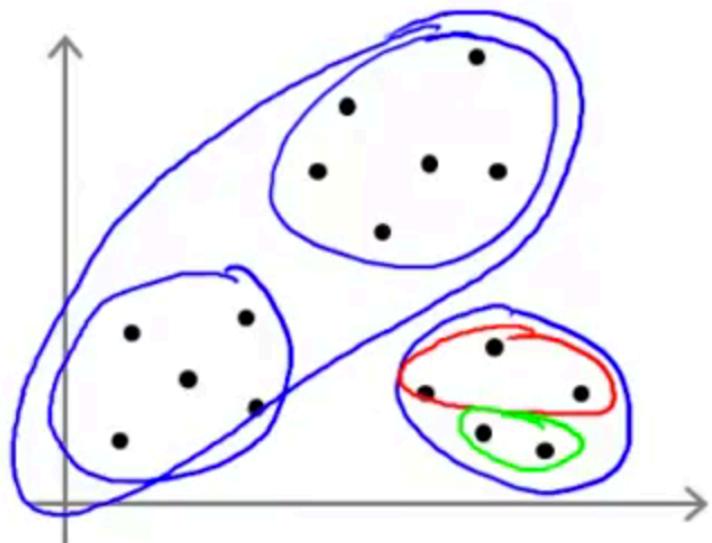
Randomly pick  $K$  training examples.

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

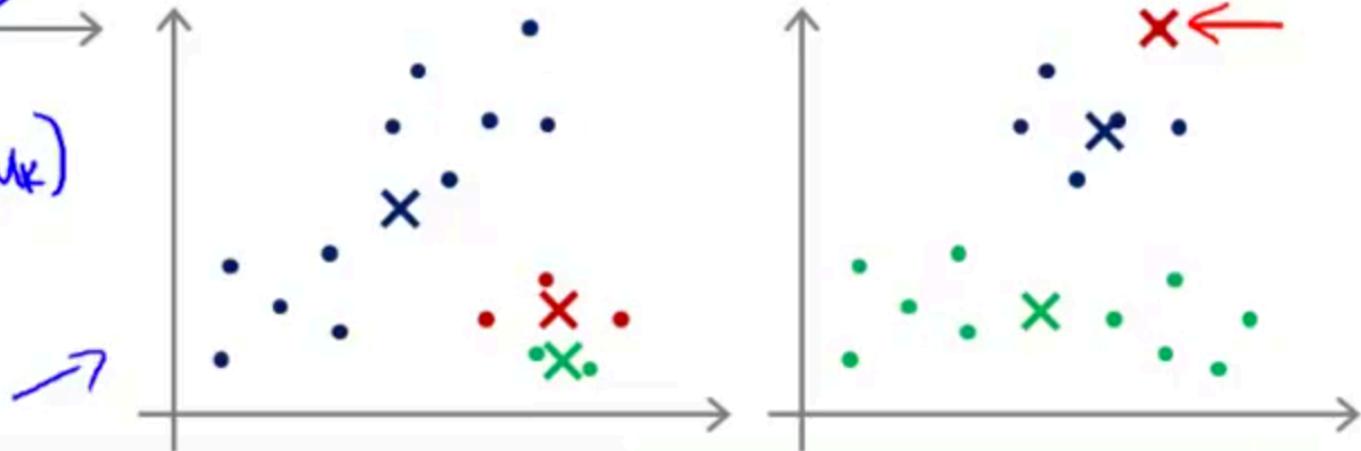
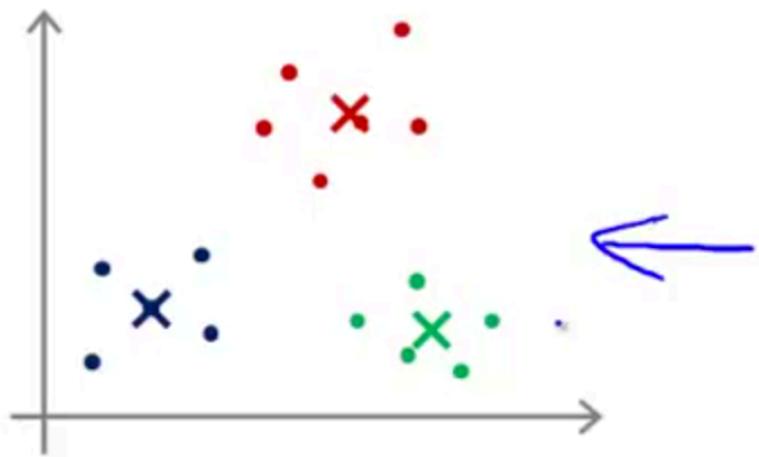
$$\begin{aligned}\mu_1 &= x^{(1)} \\ \mu_2 &= x^{(2)} \\ &\vdots\end{aligned}$$



## Local optima



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



## Random initialization

For  $i = 1$  to 100 {  $50 - 1000$

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

$k = 2 - 10$



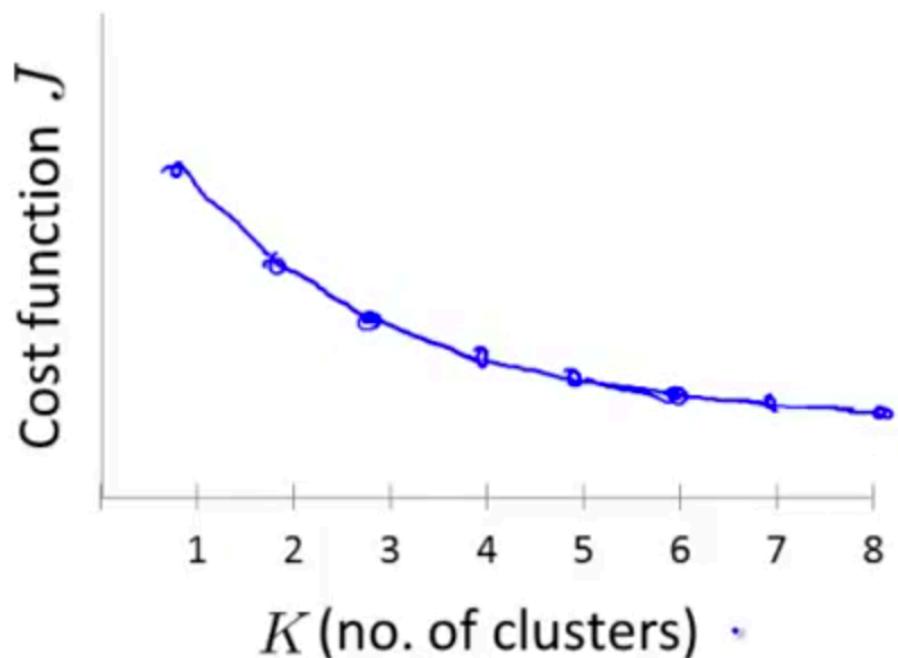
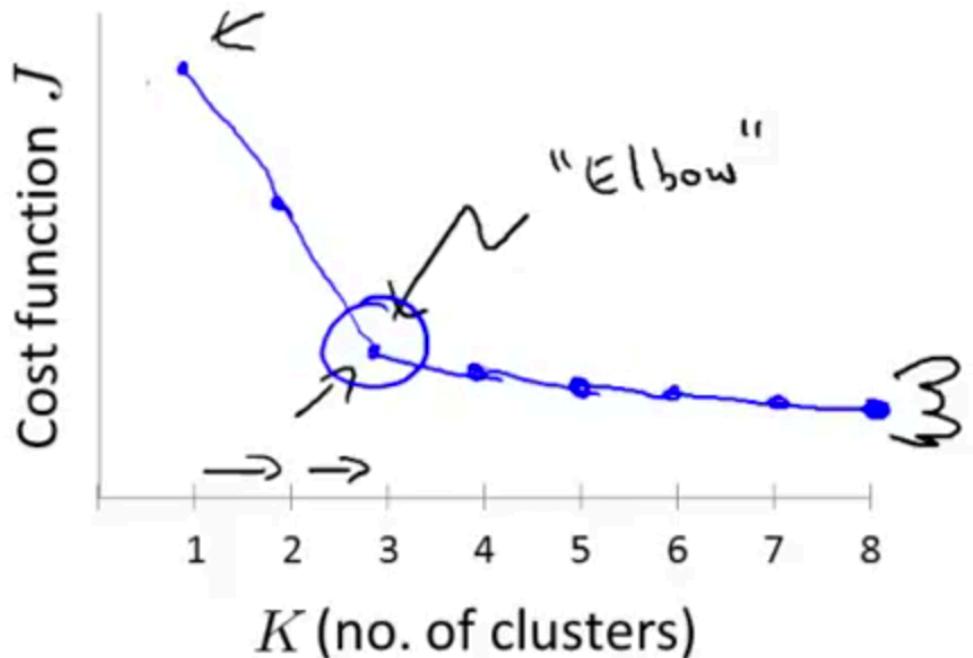
7:12 / 7:49



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## Choosing the value of K

Elbow method:

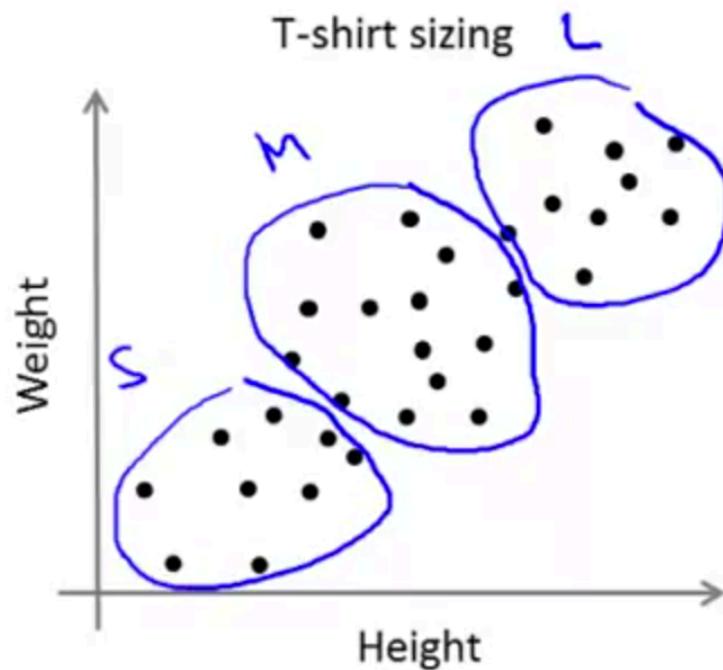


## Choosing the value of K

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.

$$K=3 \quad S, M, L$$

E.g.



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

