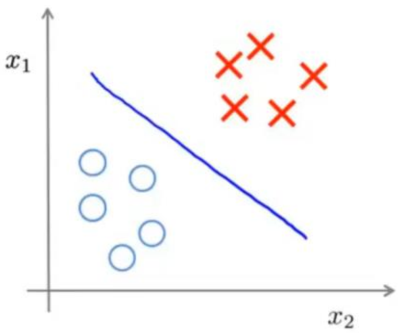
Clustering

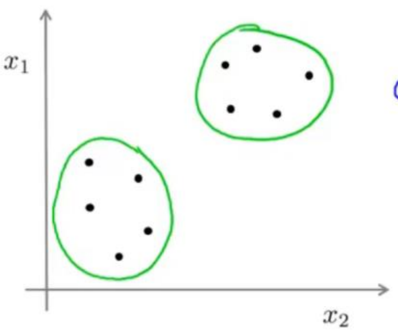
1 Unsupervised learning introduction

Supervised learning



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

Unsupervised learning

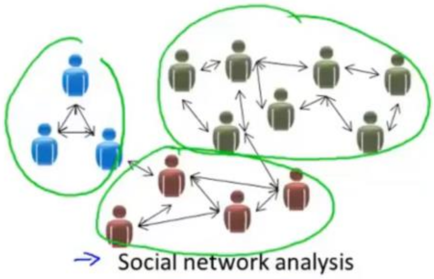


Clustering algorithm

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

Applications of clustering

Market segmentation

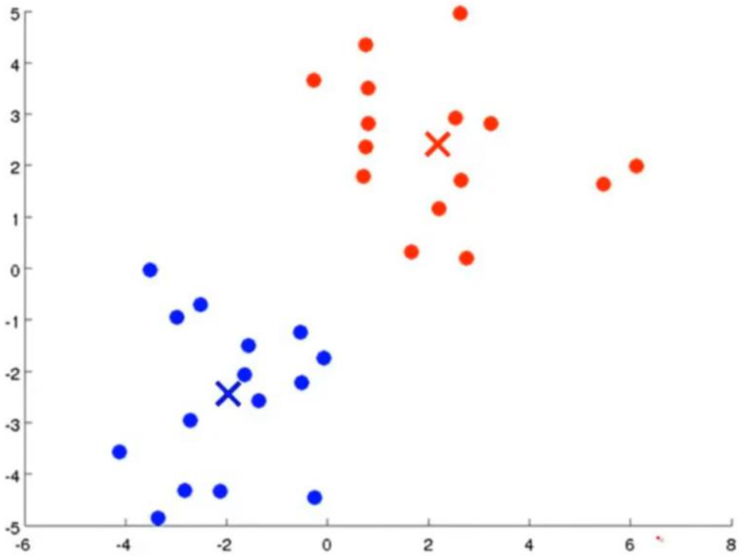


Social network analysis

Organize computing clusters

Astronomical data analysis

2 K-means algorithm



K-means algorithm

Input:

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

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

K-means algorithm

μ_1 × μ_2 ×

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

Repeat {

Cluster assignment step

for i = 1 to m

$\underline{c^{(i)}}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$ $\quad \min_k \|x^{(i)} - \mu_k\|^2 \rightarrow c^{(i)}$

Move centroid

for k = 1 to K

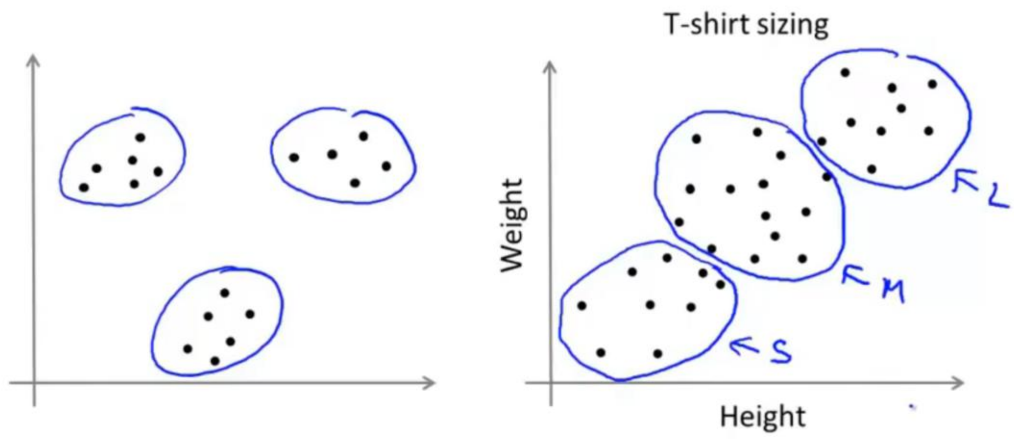
→ μ_k := average (mean) of points assigned to cluster k

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

}

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

K-means for non-separated clusters



3 Optimization objective

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

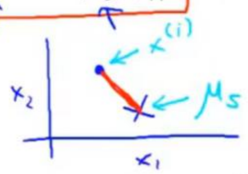
$\mu_{c^{(i)}}$ = cluster centroid of cluster to which example $x^{(i)}$ has been assigned $x^{(i)} \rightarrow \underline{5}$ $\underline{c^{(i)} = 5}$ $\underline{\mu_{c^{(i)}}} = \mu_5$

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



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K-means algorithm

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

Cluster assignment step

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

(holding $\mu_1, \ldots, \mu_K$ 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 $J(\ldots)$ wrt $\boxed{\mu_1, \ldots, \mu_K}$

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4 Random initialization

Random initialization

Should have $K < m$

$K=2$

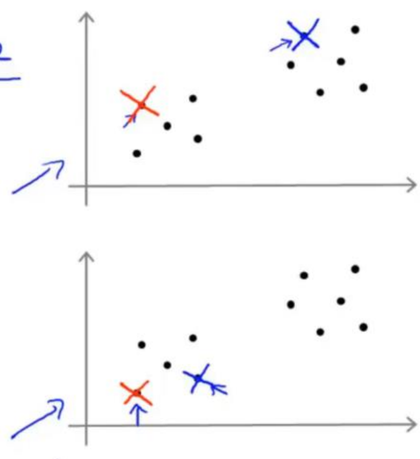
Randomly pick K training examples.

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

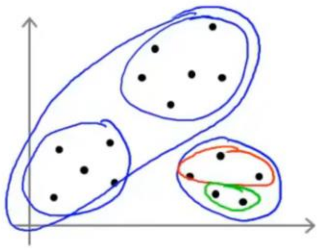
$\mu_1 = x^{(i)}$

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

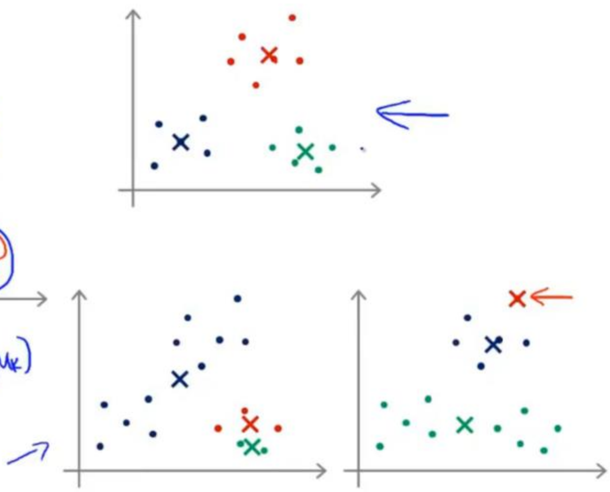
$\vdots$



Local optima



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



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Random initialization

For i = 1 to 100 { 50 - 1000

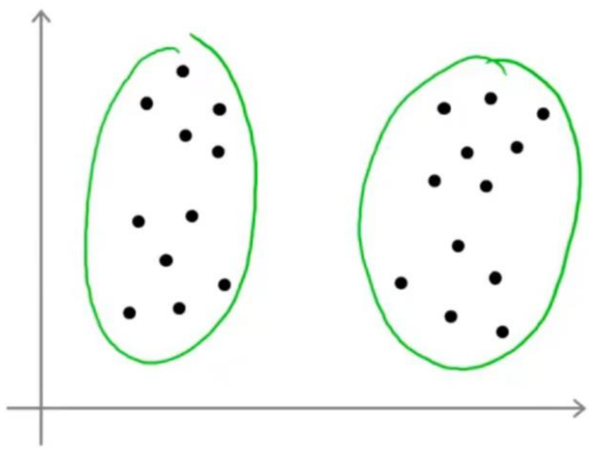
Randomly initialize K-means.
Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.
Compute cost function (distortion)
$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$
}

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

k=2-10

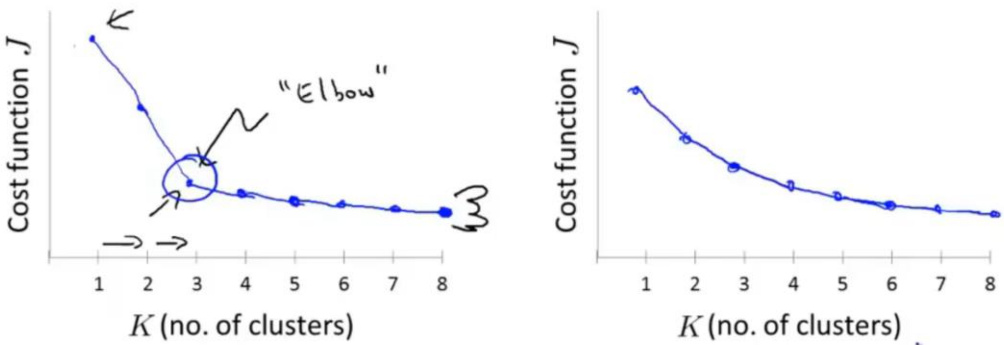
5 Choosing the number of clusters

What is the right value of K?



Choosing the value of K

Elbow method:

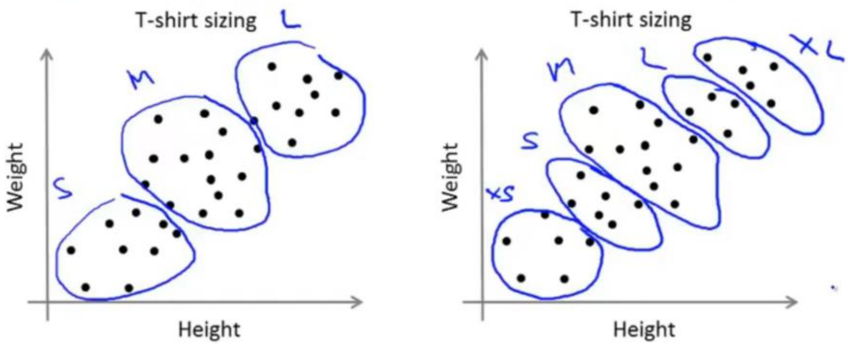


Choosing the value of K

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.



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