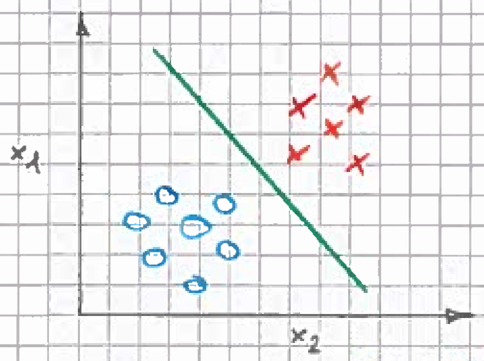
13. CLUSTERING

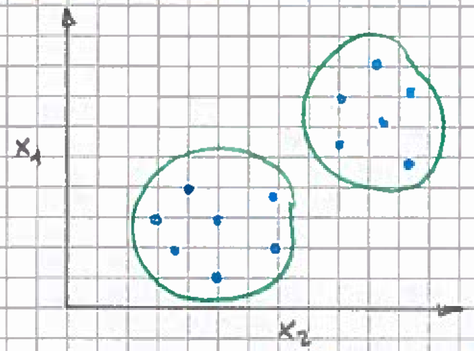
Clustering - Unsupervised learning

Supervised learning:



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

Unsupervised learning:



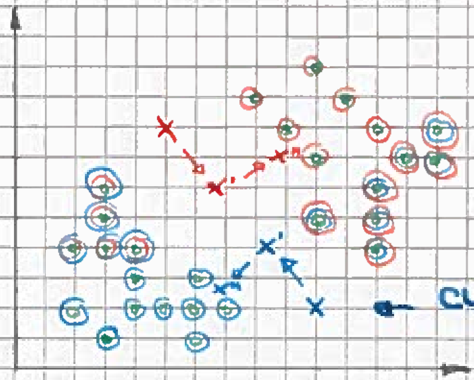
Find some structure in the data

Clustering algorithm

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

Application of clustering:

- Market segmentation
- Social network analysis ⇒ find coherent groups
- Organize computing Clusters
- Astronomical data analysis



→ cluster centroids

choose randomly two cluster centroids

1) cluster assignment step ⇒ cluster points next to centroid

2) move centroid step ⇒ move to new means

set new color of data points

↘ find coherent groups

K-Means → iterative 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)

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

Repeat {

Cluster assignment step:

for $i = 1 : m$

$c^{(i)} :=$ index (from 1 to K) of cluster centroid closest to $x^{(i)}$ $\min_k \Rightarrow \| x^{(i)} - \mu_k \|^2$ ⇒ distance between data point & centroid

$c^{(i)}$

move centroid step:

for $k = 1 : K$

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

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

↳ means all points were assigned to cluster centroid 2

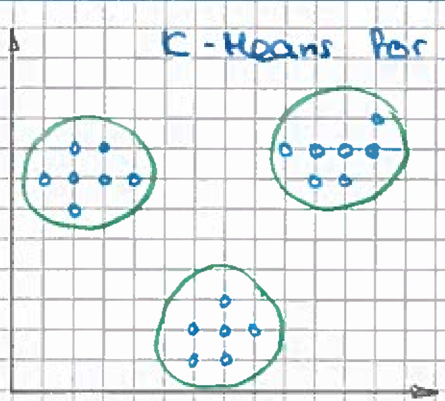
}

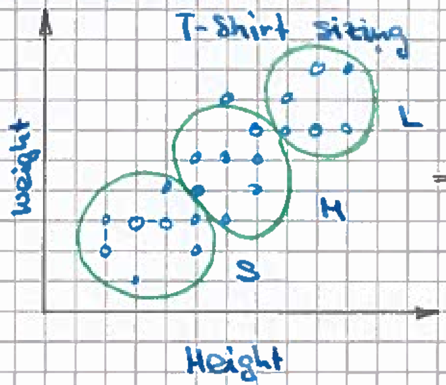
$$\mu_2 = \frac{1}{4} \left[x^{(1)} + x^{(5)} + x^{(6)} + x^{(10)} \right] \in \mathbb{R}^n$$ ⇒ compute the average of these points

↳ move μ_2 to average

if cluster centroid has no points assigned to it → eliminate that ⇒ $K-1$ cluster

K-Means for non separated clusters





S, M, L

=> Market segmentation

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

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

K = # number of clusters

$k = \{1, 2, \dots, K\}$

$x^{(i)} \to 5 \qquad c^{(i)} = 5$

$\Downarrow$ assigned to cluster #5

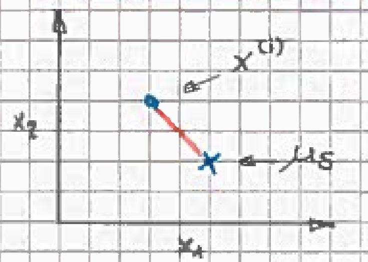
$\mu_{c^{(i)}} = \mu_5$

Optimization Objective:

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

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

also called Distortion of cost function



K-Means algorithm

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

Repeat {

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

$\Rightarrow$ min $J(\dots)$ wrt $c^{(1)}, c^{(2)}, \dots, c^{(m)}$ (holding $\mu_1, \dots, \mu_K$ fixed)

move centroid step:
for $k = 1 : K$
μ_k := average (mean) of points assigned to cluster k

}

$\Rightarrow$ min $J(\dots)$ wrt $\mu_1 \dots \mu_K$

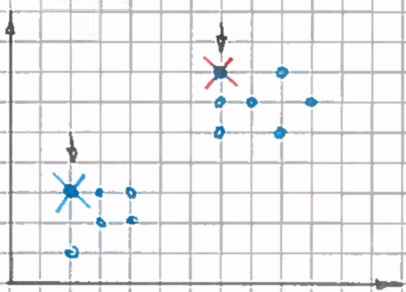
Random initialization:

K = 2

Should have $K < m$

Randomly pick K training examples

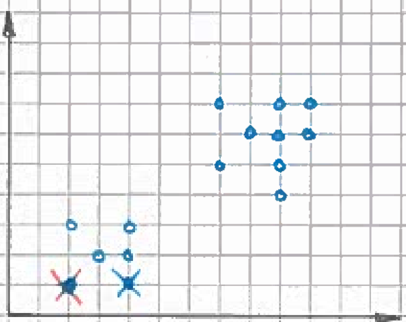
Set $\mu_1 \dots \mu_K$ equal to these K examples



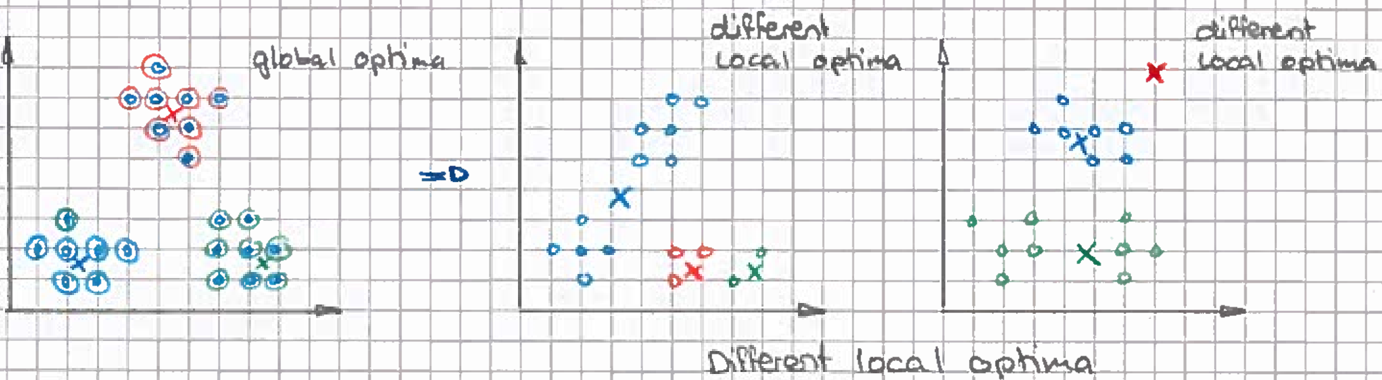
$\mu_1 = x^{(i)}$

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

$\vdots$



Local optima:



to prevent K-Means getting stuck at local optima, try multiple initializations

Random initialization:

for i = 1 : 100 { → typically 50 - 1000

Random initialize K-Means

Run K-Means. Get $c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K$

Compute cost function (distortion)

$J(c^{(1)}, c^{(2)} \dots c^{(m)}, \mu_1 \dots \mu_K)$

}

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

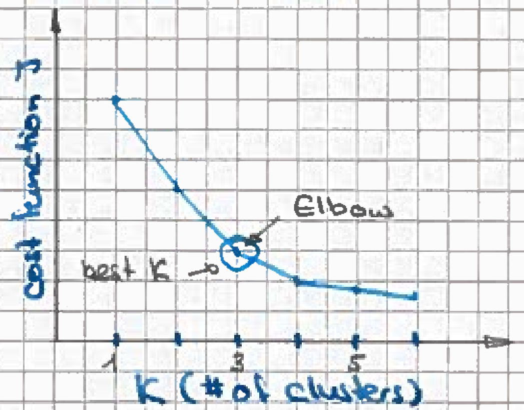
if we have $K = 2 - 10$ random init can make difference, but not so much a problem with K large.

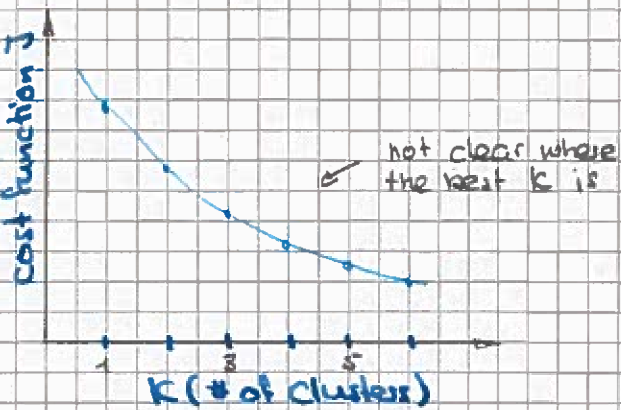
Choosing the number of clusters

What is the write value of k?

Choosing the value of k

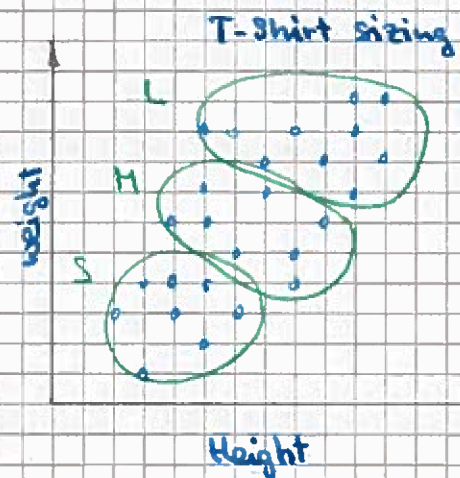
Elbow method



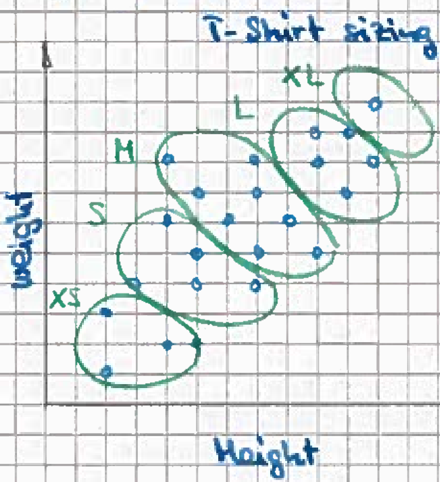


=> no high expectation with this approach.

Sometimes you are running K-Means to get clusters to use for some later/downstream purposes. 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

Choosing K
deciding by looking at clustered output => chosen by human inside