

Optimization objective (Distortion of k-means algorithm)

Minimize  $J(c^{(1)}, \dots, c^{(m)}, \underbrace{\mu_1, \dots, \mu_k}_{\text{centroids}}) = \frac{1}{n} \sum_{i=1}^m \|x^{(i)} - \underbrace{\mu_{c^{(i)}}}_{\substack{\text{centroid to which } x^{(i)} \text{ was} \\ \text{assigned}}}\|^2$

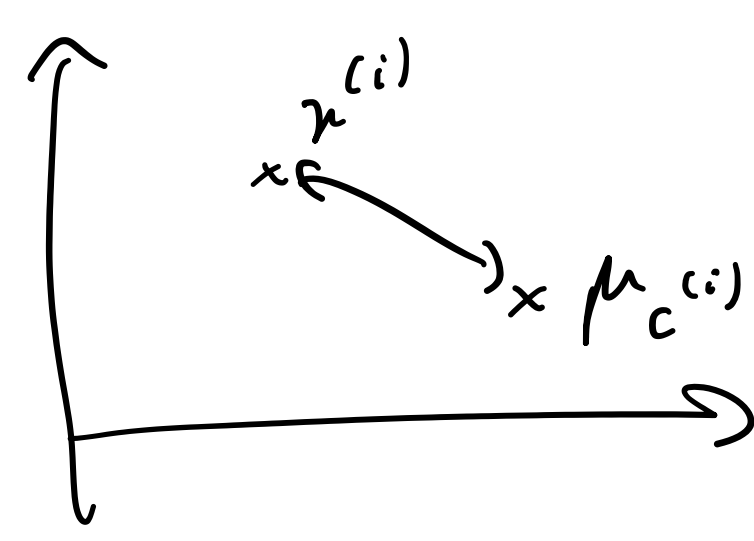
2 steps of k-means algorithm:

1. Cluster assignment step

$\min J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k)$   
 wrt  $c^{(1)}, \dots, c^{(m)}$   
 while fixing  $\mu_1, \dots, \mu_k$

2. Move centroids step.

$\min J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k)$   
 wrt.  $\mu_1, \dots, \mu_k$   
 while fixing  $c^{(1)}, \dots, c^{(m)}$

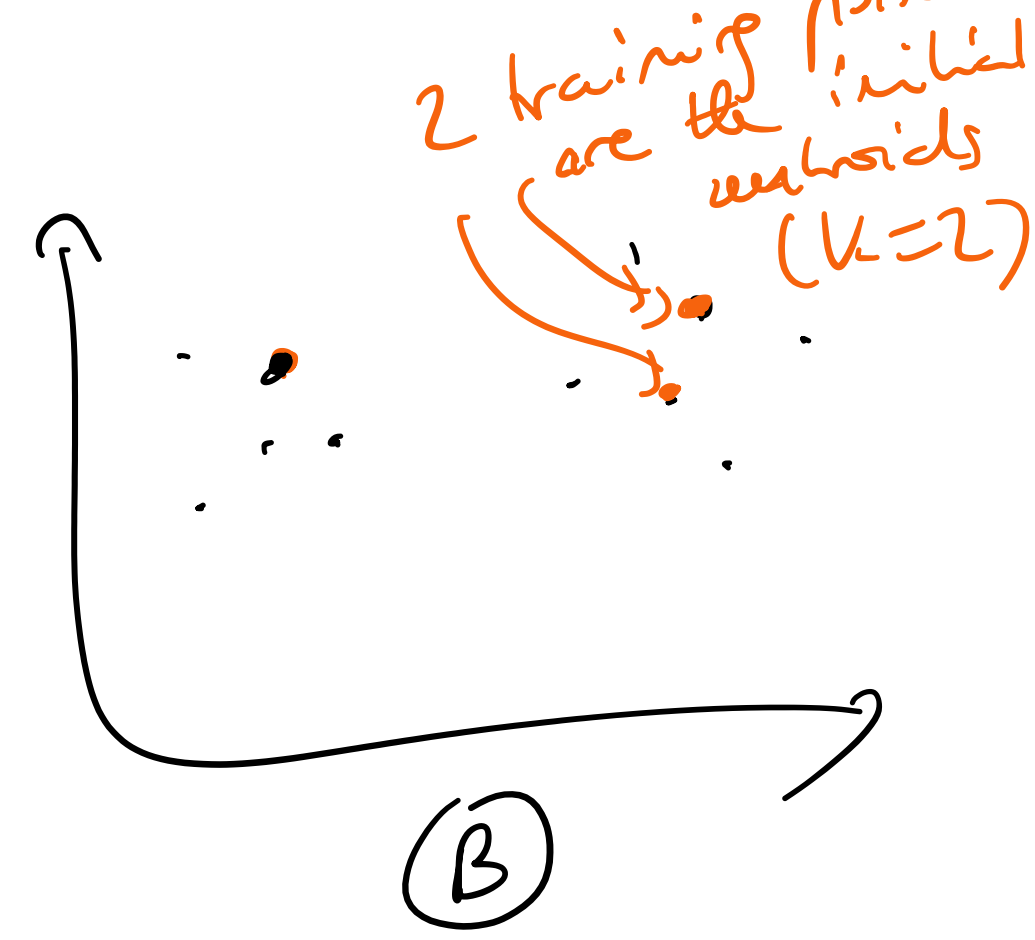
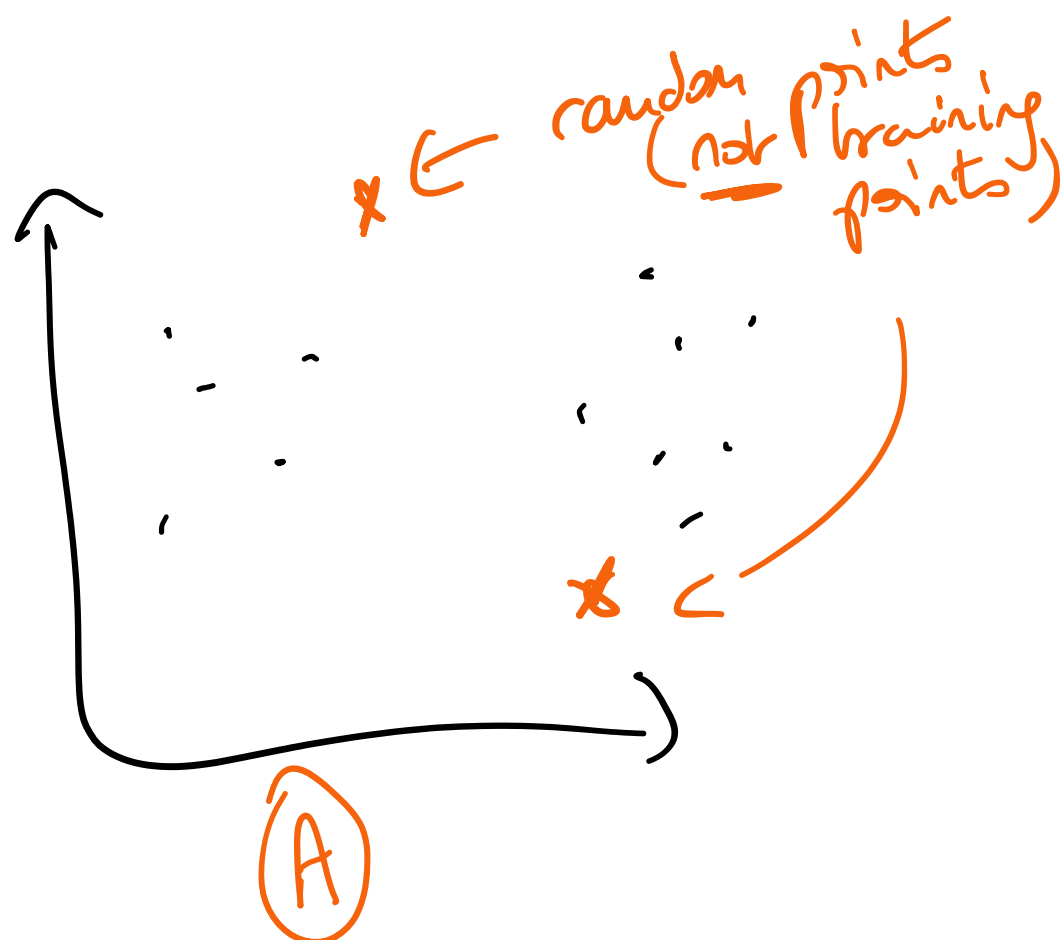


Initialization

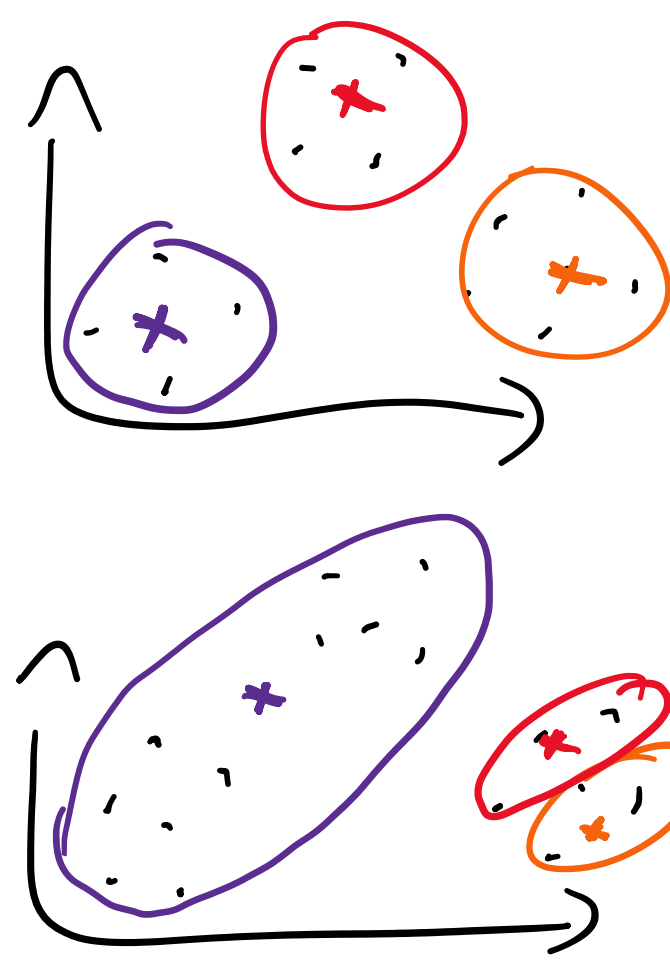
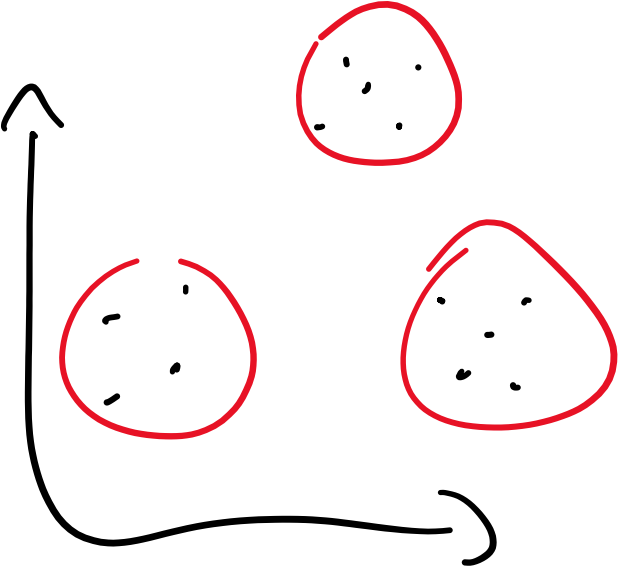
Pick the value of k

Strategy: (A) pick random points as the k initial cluster centroids.

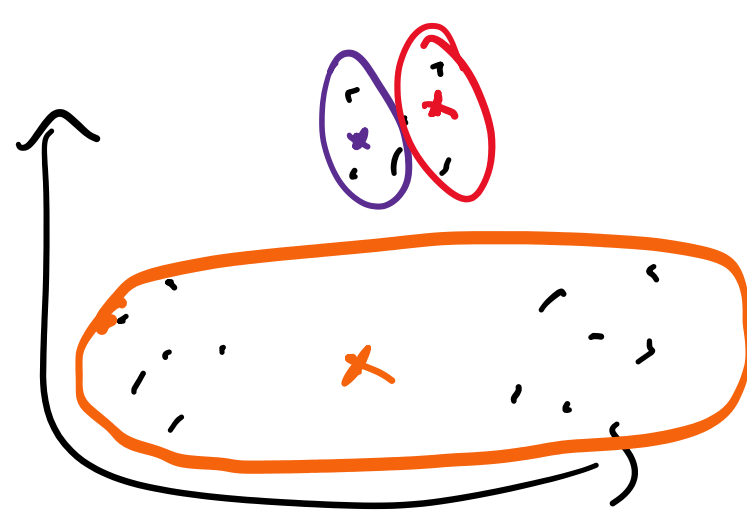
(B) pick randomly k training points as the k initial cluster centroids.



Local Optima



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



for some number of trials:

randomly initialize k centroids  $\mu_1, \dots, \mu_k$

Run k-means to obtain

$c^{(1)}, \dots, c^{(m)}$  } assignments  
 $\mu_1, \dots, \mu_k$  } centroids

compute distortion (cost)  $J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k)$

Pick random initialization that yields min J

$\hookrightarrow \mu_1, \dots, \mu_k$   
 $c^{(1)}, \dots, c^{(m)}$  } keeps the outputs of that trial of k-means.

Heuristic works well when k is small.

Choosing the no of centroids/clusters: k

