

Clustering - Random Initialization

How to initialize K-means, and more importantly how to make K-means avoid local optima as well.

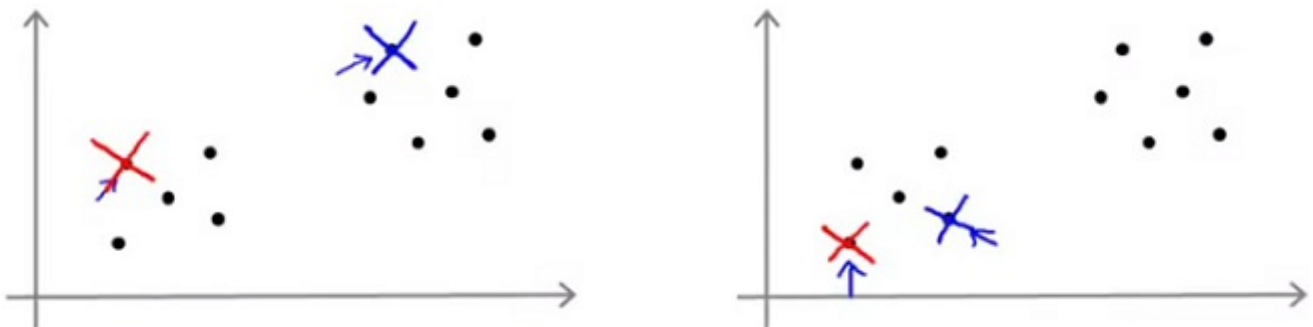
Consider clustering algorithm:

- 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  $k$ 
}
```

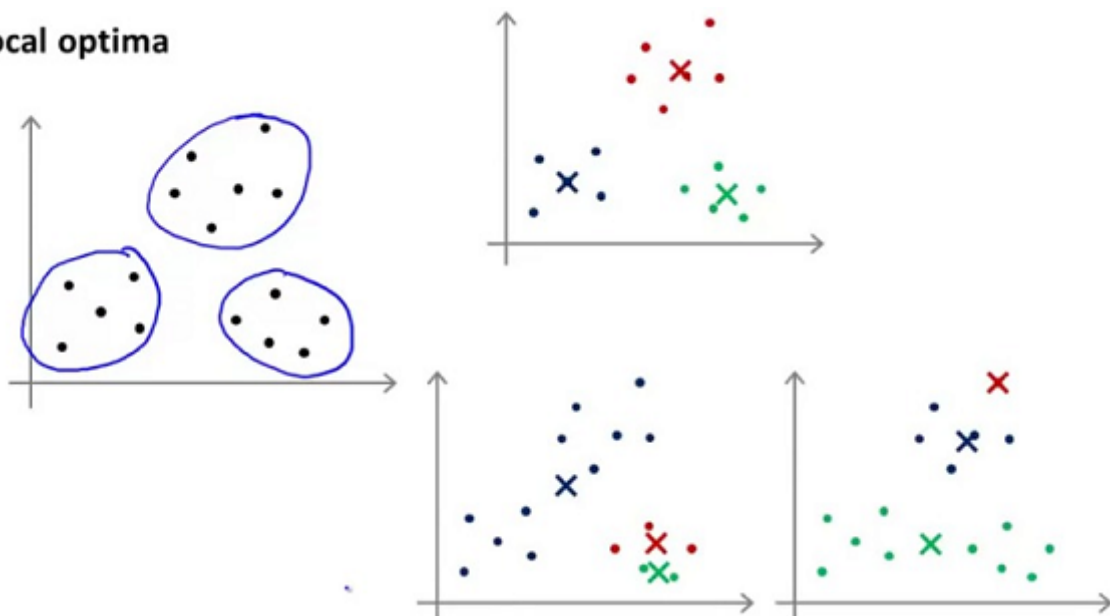
Should have $K < m$: Have number of centroids set to less than number of examples $K < m$ (It would be really weird to run K -means with a number of cluster centroids that's equal or greater than the number of examples we have).

- Randomly pick K training examples.
- Set μ_1, \dots, μ_K equal to these K examples.
 - i.e. 2 clusters ($K = 2$)
 - $\mu_1 = x^{(i)}, \mu_2 = x^{(j)}$



K -means can converge to different solutions depending on the initialization setup (risk of local optimum)

Local optima



So, if we're worried about K -means getting stuck in local optima, if we want to increase the odds of K -means finding the best possible clustering, what we can do, is try multiple, random initializations - many same results are likely to indicate a global optimum.

Algorithmically we can do this as follows:

```

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

- A typical number of times to initialize K-means is 50 - 1000
- Randomly initialize K -means
 - For each 100 random initialization run K -means
 - Then compute the distortion on the set of cluster assignments and centroids at convergent
 - End with 100 ways of cluster the data,
 - Pick clustering that gave lowest cost, the lowest distortion $J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)$
- If we're running K means with 2-10 clusters can help find better global optimum
 - If K is larger than 10, then multiple random initializations are less likely to be necessary
 - First solution is probably good enough (better granularity of clustering)

Video Question: Which of the following is the recommended way to initialize k-means?

- Pick a random integer i from $\{1, \dots, k\}$. Set $\mu_1 = \mu_2 = \dots = \mu_k = x^{(i)}$.
- Pick k distinct random integers i_1, \dots, i_k from $\{1, \dots, k\}$. Set $\mu_1 = x^{(i_1)}, \mu_2 = x^{(i_2)}, \dots, \mu_k = x^{(i_k)}$.

Pick k distinct random integers i_1, \dots, i_k from $\{1, \dots, m\}$. Set $\mu_1 = x^{(i_1)}, \mu_2 = x^{(i_2)}, \dots, \mu_k = x^{(i_k)}$.

- Set every element of $\mu_i \in \mathbb{R}^n$ to a random value between $-\epsilon$ and ϵ , for some small ϵ .