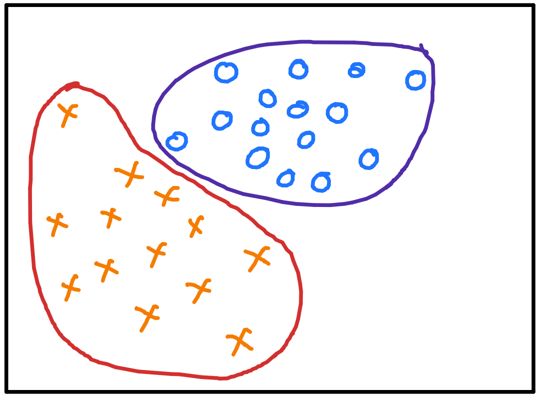
k-means Clustering



- Clustering is an unsupervised ML algorithm
- Idea in clustering
  - Samples within a cluster are similar to each other
  - Samples in different clusters are dissimilar

- We have learned about clustering with GMM using EM algorithm
  - GMM models the cluster probabilistically (soft assignments)

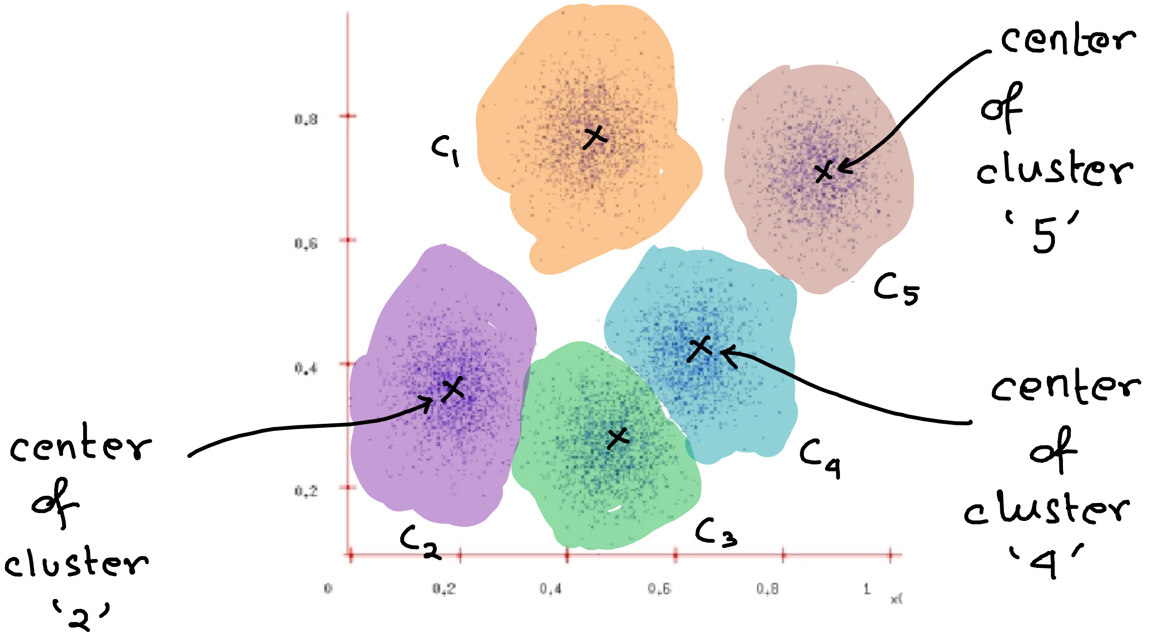
    i.e. $$\underbrace{p(\underline{x}^{(i)} \mid y = k)}_{\text{probability of data point } \underline{x}^{(i)} \text{ belonging to the 'k' th cluster}} = \pi_k \, \mathcal{N}(\underline{x}^{(i)} \mid \underline{\mu}_k, \underline{\Sigma}_k)$$

- In this lecture, we introduce the k-means clustering algorithm
  - Unlike GMM, in k-means, we do 'hard' cluster assignments and there is no probabilistic model

Intuition of k-means

- k-means assumes that there are 'K' clusters, and each point is close to its cluster center or mean (the average of points in the cluster)
  - If we knew the cluster assignment, we could easily compute the centers
  - If we knew the centers, we could easily compute which points belong to which cluster
  - Chicken and egg problem!

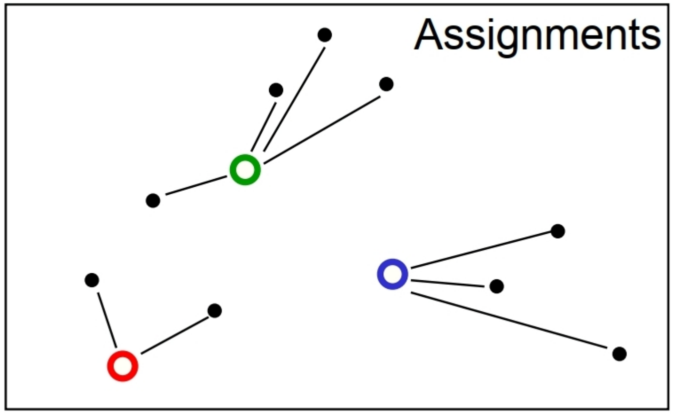
- Heuristically speaking, one could start randomly and alternate between the two!

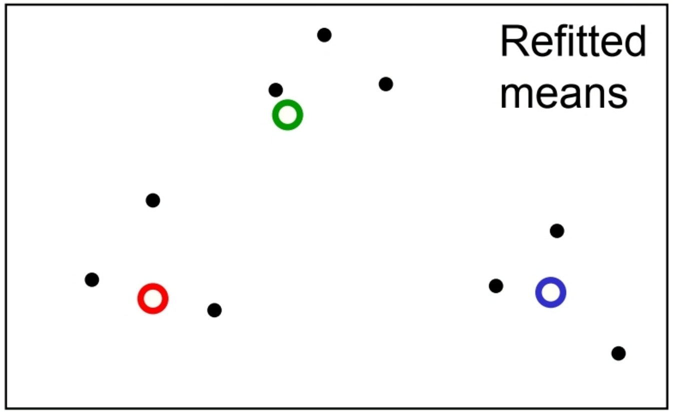


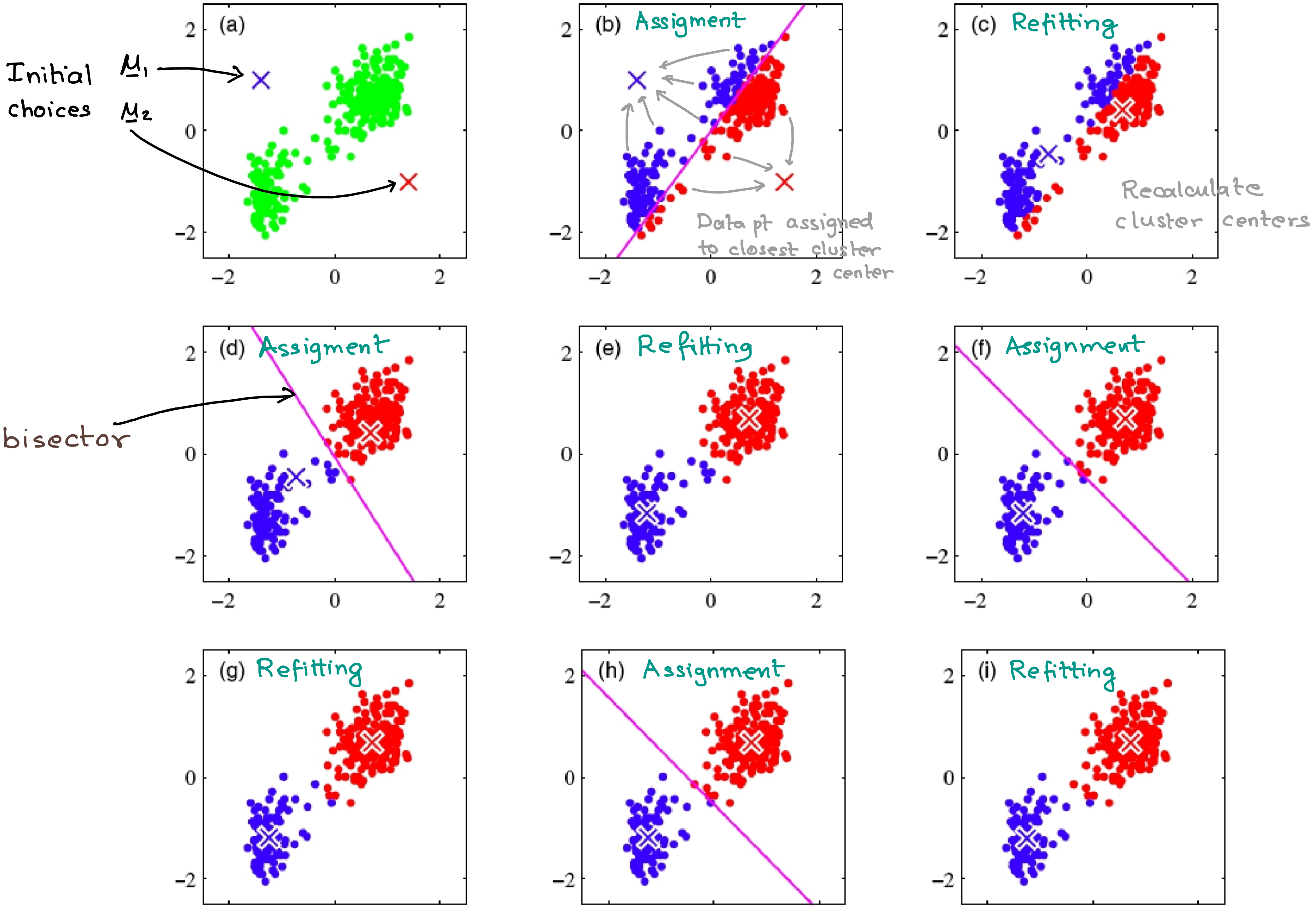
K-means

- Initialization: Randomly initialize cluster centers (or means)

- The algorithm iteratively alternates between two steps:
  - Assignment step: Assign each data point to the closest cluster
  - Refitting step: Move each cluster center to the center of gravity of the data assigned to it







(a)
Initial choices
$\underline{\mu}_1$
$\underline{\mu}_2$
(b) Assigment
Data pt assigned to closest cluster center
(c) Refitting
Recalculate cluster centers
(d) Assigment
bisector
(e) Refitting
(f) Assignment
(g) Refitting
(h) Assignment
(i) Refitting
2
0
−2
−2
0
2

K-means Objective

What is actually being optimized?

k-means clustering amounts to selecting the 'k' clusters such that the distances of the points to the cluster centers, summed over all data points, is minimized:

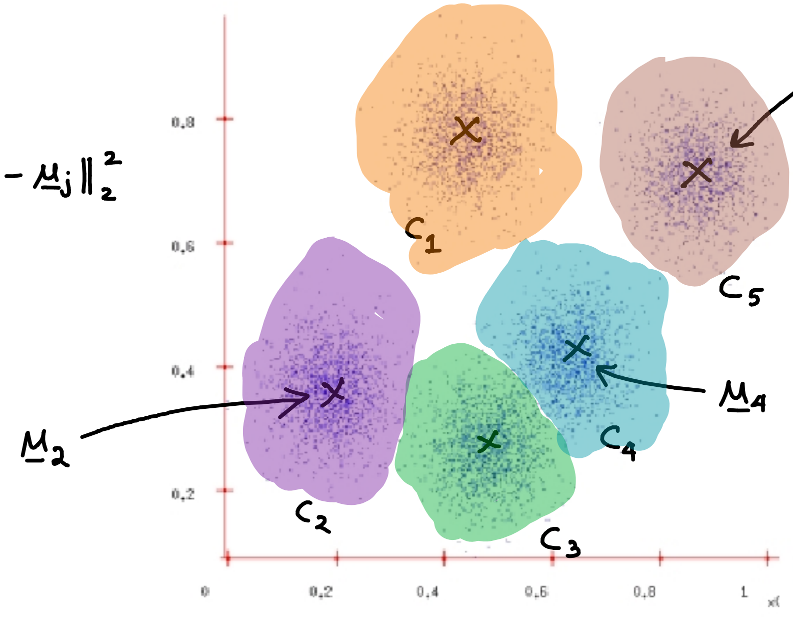
$$\{r_k^{(i)}, \underline{\mu}_k\} = \arg\min_{\{r_k^{(i)}, \underline{\mu}_k\}} \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \|\underline{x}^{(i)} - \underline{\mu}_k\|_2^2$$

mean of all data pts $\underline{x}^{(i)} \in C_m$

center of cluster m

Indicator function

$$r_k^{(i)} = \begin{cases} 1 & \text{if } k = \underset{j}{\text{argmin}} \|\underline{x}^{(j)} - \underline{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$



$$\underline{\mu}_5 = \frac{1}{|C_5|} \sum_{i=1}^{N} r_5^{(i)} \underline{x}^{(i)}$$

# of data pts that belong to cluster '5'

How to optimize?

Optimization problem:

$$\{r_k^{(i)}, \underline{\mu}_k\} = \underset{\{r_k^{(i)}, \underline{\mu}_k\}}{\arg\min} \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \|\underline{x}^{(i)} - \underline{\mu}_k\|_2^2$$

- This is a combinatorial optimization which is NP-hard to solve
- An alternating minimization strategy is used to solve the optimization:
  - If we fix the centers $\{\underline{\mu}_k\}$, then we can easily find the optimal assignments $r_k^{(i)}$ for each sample $\underline{x}^{(i)}$

$$\{r_k^{(i)}\} = \underset{\{r_k^{(i)}\}}{\arg\min} \sum_{k=1}^{K} r_k^{(i)} \|\underline{x}^{(i)} - \underline{\mu}_k\|_2^2$$

That is, assign each point to the cluster with the nearest center

e.g. if $\underline{x}^{(i)}$ is assigned to cluster k

$$r_1^{(i)} = 0, \quad r_2^{(i)} = 0, \quad \ldots, \quad r_k^{(i)} = 1, \ldots, \quad r_K^{(i)} = 0$$

How to optimize?

Optimization problem:

$$\min \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \| \underline{x}^{(i)} - \underline{\mu}_k \|_2^2$$

- An alternating minimization strategy is used to solve the optimization:

  - Similarly, if we fix the assignments $r_k^{(i)}$, then we can easily find optimal centers $\underline{\mu}_k$

$$\frac{\partial}{\partial \mu_\ell} \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^{(i)} \| \underline{x}^{(i)} - \underline{\mu}_k \|_2^2 = 0$$

$$\Rightarrow \quad 2 \sum_{i=1}^{N} r_\ell^{(i)} (\underline{x}^{(i)} - \underline{\mu}_\ell) = 0$$

$$\Rightarrow \quad \boxed{\underline{\mu}_\ell = \frac{\sum_{i=1}^{N} r_\ell^{(i)} \underline{x}^{(i)}}{\sum_{i=1}^{N} r_\ell^{(i)}}}$$

K-means algorithm (Lloyd's algorithm)

Data: $\{ \underline{x}^{(i)} \}_{i=1}^{N}$, number of cluster K

Procedure:

- Initialization : Set K cluster means $\underline{\mu}_1, \dots, \underline{\mu}_K$ to random values
- Repeat until convergence (until assignments do not change)
  - Assignment : Each data point $\underline{x}^{(i)}$ is assigned to nearest center

$$k^{(i)} = \arg\min_{j} \| \underline{x}^{(i)} - \underline{\mu}_j \|$$

and the responsibilities

$$r_k^{(i)} = \mathbb{I}\left[k^{(i)} = k \right] \quad \text{for } k = 1, \dots, K$$

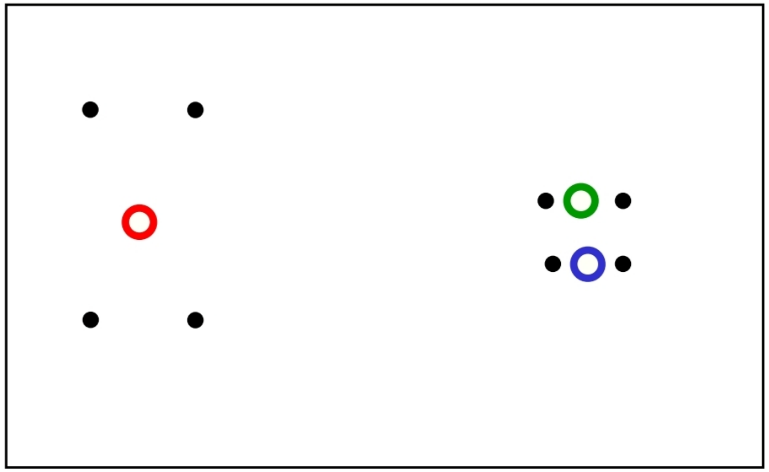
  - Refitting : Each center is set to mean of data assigned to it

$$\underline{\mu}_K = \frac{\sum_i r_k^{(i)} \underline{x}^{(i)}}{\sum_i r_k^{(i)}}$$

Convergence of k-means algorithm

- Similar to the EM algorithm, Lloyd's algorithm converges to a stationary point of the objective function, but is not guaranteed to find the global optimum

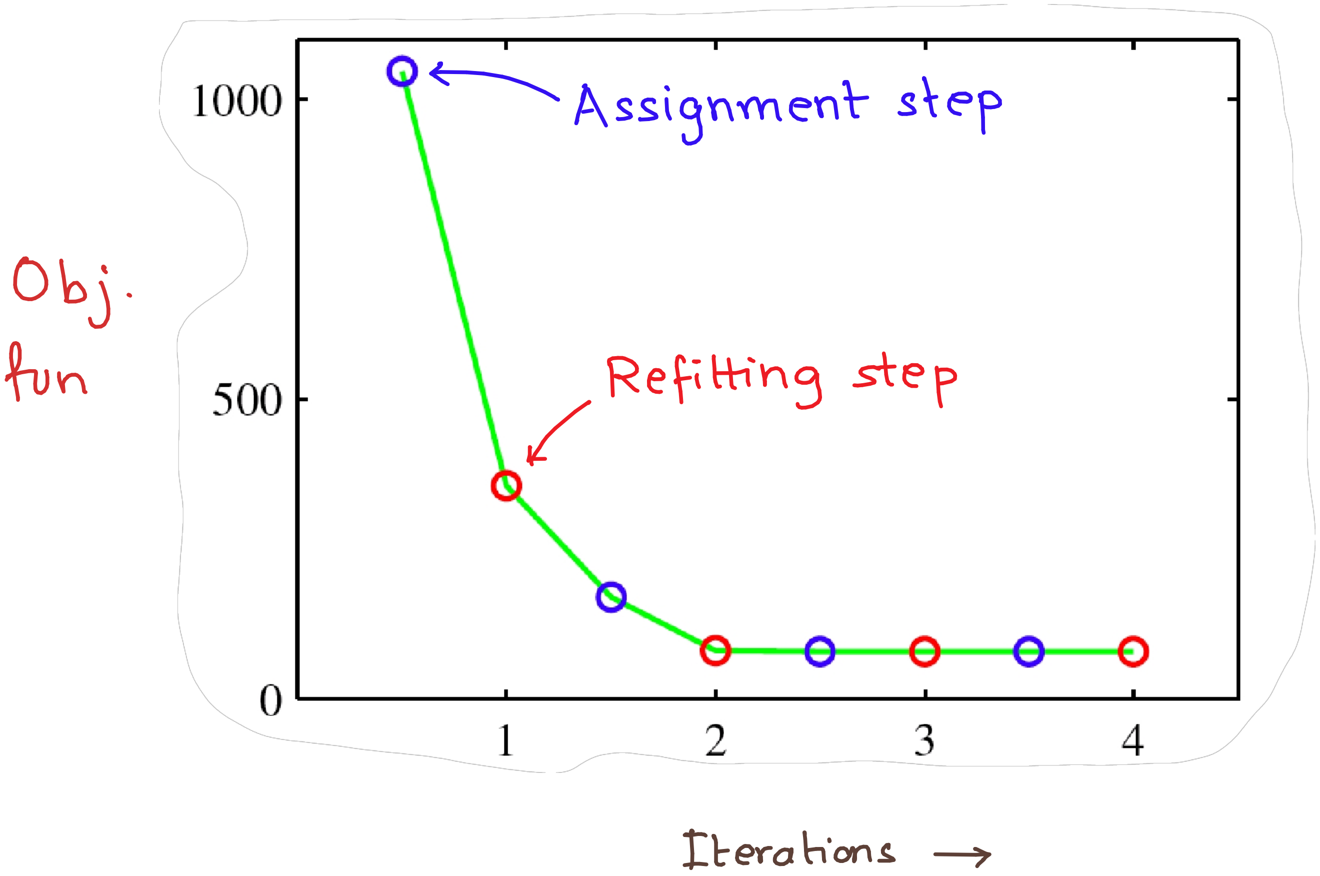
A bad local optimum



  - In practice, run it multiple times, each time with a different initialization and pick the result of the run with smallest objective function value

Convergence of k-means algorithm

- Test of convergence: If the assignments do not change in the assignment step, then converged (to at least a local minimum)



k-means should not confused with k-NN

- k-means and k-NN are different, though they have certain similarities

- Both k-means and k-NN use Euclidean distances to define similarities in input space

- Both are sensitive to the normalization of the input values

- However, kNN is a supervised learning method, while k-means is an unsupervised learning method

- The 'k' in the two methods have different meaning

Choosing the number of clusters

- The number of clusters K has to be chosen apriori for both GMM and k-means algorithm for clustering

- Increasing K will reduce training loss (or reduce the objective function)
  - If $K = N$, then each data point will have its own cluster

- Cross-validation techniques are needed to guide selection of K
  - But they need to be adapted to unsupervised setting (There is no new data error E_{new} for clustering)

- For GMM, one can use the likelihood of the validation data to find K

Training set $\{\underline{x}^{(i)}\}_{i=1}^{N}$ Validation set $\{\underline{\tilde{x}}^{(i)}\}_{i=1}^{N_v}$

$K = 1 \longrightarrow M^{(1)}, \underline{\hat{\theta}}^{(1)}$ $P\left(\{\underline{\tilde{x}}^{(i)}\}_{i=1}^{N_v} \mid \underline{\hat{\theta}}^{(1)}, M^{(1)}\right) = 0.2$

$K = 2 \longrightarrow M^{(2)}, \underline{\hat{\theta}}^{(2)}$ $P\left(\{\underline{\tilde{x}}^{(i)}\}_{i=1}^{N_v} \mid \underline{\hat{\theta}}^{(2)}, M^{(2)}\right) = 0.45$ ✓ $\rightarrow M = 2$ optimal

$K = 3 \longrightarrow M^{(3)}, \underline{\hat{\theta}}^{(3)}$ $P\left(\{\underline{\tilde{x}}^{(i)}\}_{i=1}^{N_v} \mid \underline{\hat{\theta}}^{(3)}, M^{(3)}\right) = 0.1$

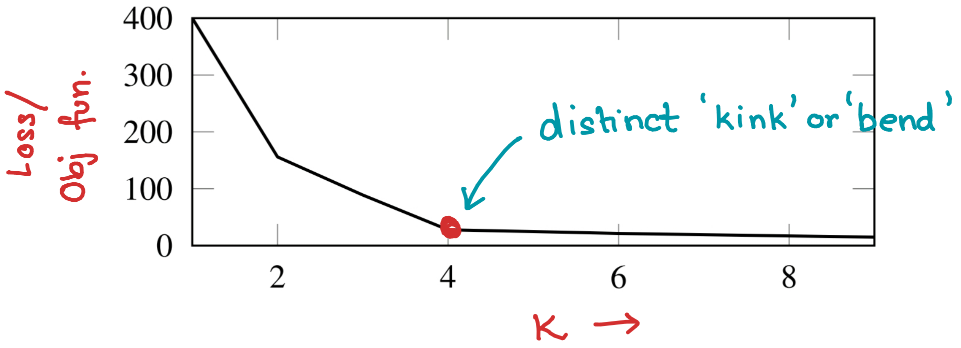
Choosing the number of clusters

- The validation methods should be handled with care

- In supervised learning, our goal is to obtain good predictions, so minimizing new data error makes sense

- In clustering, the goal is not necessarily to minimize "clustering loss" but to gain insights by finding a small number of clusters
  - So we may prefer a smaller number of clusters even if it gives not-so good validation loss

- The ELBOW method is often used for selecting K
  - plot of loss (either training, validation, or both)


Loss/
Obj fun.
K →
distinct 'kink' or 'bend'