

grouping into * of groups \rightarrow hyperparameter

center of cluster = the mean of samples
not necessarily a sample

* clustering is nondeterministic (not same solution always)

loss fun \rightarrow

* measure $\Rightarrow \sum$ of ^{squared} distances from center (smaller is better)

* 3 techniques of clustering:-

depends on
the initial assignment

① K-means (NP-hard)

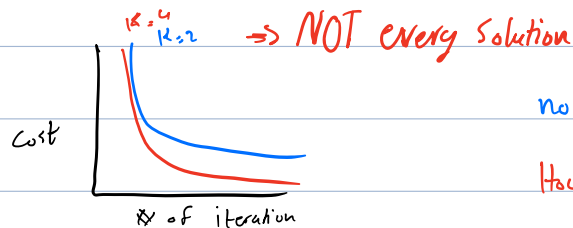
* of clusters (hyper-parameter)



① select K centers (nearest by Euclidean)

② loop { assignment to nearest K
update the center } NOT always optimal

③ converge \Rightarrow no change in step 2 always converge

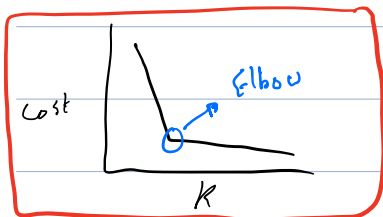


no error $\Rightarrow K =$ * of samples

How to find K?

- from your problem (* of room...)

- Elbow technique



\rightarrow more K \Rightarrow less cost

* K-means++ (Smart Initialization)

to ensure you select good centers

non-deterministic:-

Select first center randomly, then select the
farthest random

1 - multiple runs

2 - Smart run K-means++

* types of K-means

① LBG algorithm \Rightarrow Start with 2 then split them until we got K

② MacQueen algorithm

speed: update as you assign faster

good: close to normal K-means

problems:-

- K-means is spherical because we use L_2 distance
- if you have overlapping
- all clusters are equals

Expectation maximization

② EM for mixtures of Gaussian

- not sphericals

- not identified by center, identified by Gaussian PDF (mean and σ^2)

it has fixed solution (more robust)
→ Soft clustering

normal distribution

we will have 2 means in 2D plane

will be covariance

calculate the probability of a point that belongs to N_{blue}

$$P(y=b|x, N(\mu_b, \sigma_b)) = \frac{P(x|y) P(y)}{P(x)} \rightarrow \pi_j$$

w_{ij}

Probability of sample x belongs to blue cluster

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma_b} e^{-\frac{1}{2} \frac{(x-\mu_b)^2}{\sigma_b^2}}$$

the maximum Probability



more than 1D

$$\frac{1}{\sqrt{(2\pi)^d \Sigma}} e^{-\frac{1}{2} \frac{(\vec{x}-\vec{\mu})^T \Sigma^{-1} (\vec{x}-\vec{\mu})}{\Sigma}}$$

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \text{cov}_{12} \\ \text{cov}_{21} & \sigma_2^2 \end{bmatrix}$$

$$\text{Correlation} = \frac{\text{cov}}{\sigma_1 \sigma_2} = [-1, 1]$$

if cov between two features is 1 you can remove one of them

$$\text{Cov}(x, y) = \mu(xy) - \mu(x) * \mu(y)$$

How to cluster:-

① randomly select 2 samples

② $\mu = \text{sample}$, $\sigma = \text{random}$

$$\textcircled{3} P(y) = \frac{1}{2}$$

slide 40 → ④ loop

- expectation (assign) → all samples
- maximization (update the means (weights * mean))

- both may stuck in local minimal
- EM is not better than K-means in all problems

K-means

- initialize the cluster

$$c_1 = \mu_1 = x_i$$

$$c_2 = \mu_2 = x_i$$

$$\vdots$$

$$\mu_k$$

- Repeat {

- assign

$$\text{- update : } c_i = \frac{x_1 + x_2 + \dots}{n_i}$$

}

- converge = no new assign

EM

- initialize the clusters (Gaussian)

$$\mu_i, \Sigma_i (\sigma^2), \pi_i \left(\frac{1}{K} P(y=k) \right)$$

- Repeat {

- expectation:

$$\frac{P(x|y_i) P(y_i)}{\sum_{j=1}^K P(x|y_j) P(y_j)} = P(y_i|x)$$

- maximization:

$$u_j = \frac{\sum_{i=1}^n x_i w_{ij}}{\sum_{i=1}^n w_{ij}}$$

$$\pi_j = \frac{E w_{ij}}{n}$$

}

	K=1	K=2
μ_1	0.4	0.6
μ_2	0.9	0.1
μ_3	0.8	0.2

$$\mu_1 = \frac{2 \times 0.4 + 2 \times 0.9 + 0.8}{2.1}$$

	x_1	x_2	$x_1 x_2$
S_1	6	4	24
S_2	3	3	9
S_3	4	3	12

$$\text{Cov}(x_1, x_2) = E(x_1 x_2) - E(x_1) E(x_2)$$

$$= 15 - 4.3 \cdot 3.3 \approx 1.0$$

$$\mu_i = [\mu_{i1}, \mu_{i2}]$$

$$\pi_{k+1} = \frac{w_{i1}}{n_i}$$

$$\Sigma_{k+1} = \begin{bmatrix} \sigma_{ii}^{(n)} & \text{Cov}(n) \\ \text{Cov}(n) & \sigma_{jj}^{(n)} \end{bmatrix}$$

- converge when the change is small

③ Agglomerative hierarchical clustering

- no need for input K

- clustering at multiple levels

- bottom up (looking for smallest) Dendrogram (threshold is horizontal line)

should use the biggest gap

XX measuring the distance between clusters:-

- single linkage algo smallest linkage (chains)

- complete linkage algo largest linkage (homogenized)

- Ward algo average

• Measuring the distance between to clusters:

Now the question is, how do we measure the distance between two clusters? We will explain to methods:

1-Single linkage: in this method, we will take the distance between the closest two points in two clusters and we will consider it as the distance between the two cluster.

For example, suppose we have two cluster, C1 has two sample (X1 , X2) and C2 has two samples (X3 , X4). Assume the distance between them is as follow:

$$\text{Distance}(X1, X3) = 2$$

$$\text{Distance}(X1, X4) = 1.5$$

$$\text{Distance}(X2, X3) = 7$$

$$\text{Distance}(X2, X4) = 0.5$$

Since the smallest distance 0.5 then we will consider the distance between C1 and C2 is 0.5.

2- Complete linkage: in this method, we will take the distance between the furthest two points in two clusters and we will consider it as the distance between the two cluster. If we take our previous example and using the complete linkage method, then the distance between C1 and C2 will be 7.

-We can use Euclidean distance to measure the distance between two points.

-After we found all the distance between clusters, we will merge the closest two clusters as we did in our previous example.