k-Means Clustering and Gaussian Mixture Models

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Clustering

- Canonical unsupervised learning problem
  - Versus supervised learning
- (Draw two cluster picture)
- Given $X = \{X_1, \dots, X_n\}$, partition into sets $C_1, \dots, C_k$
  - E.g., say if $n = 5, k = 3$, then $C_1 = \{X_1, X_5\}$, $C_2 = \{X_2\}$, $C_3 = \{X_3, X_4\}$
  - k is a hyperparameter
- Goals (informally):
  - Points in a cluster are similar, points in different clusters are dissimilar

k-Means Clustering

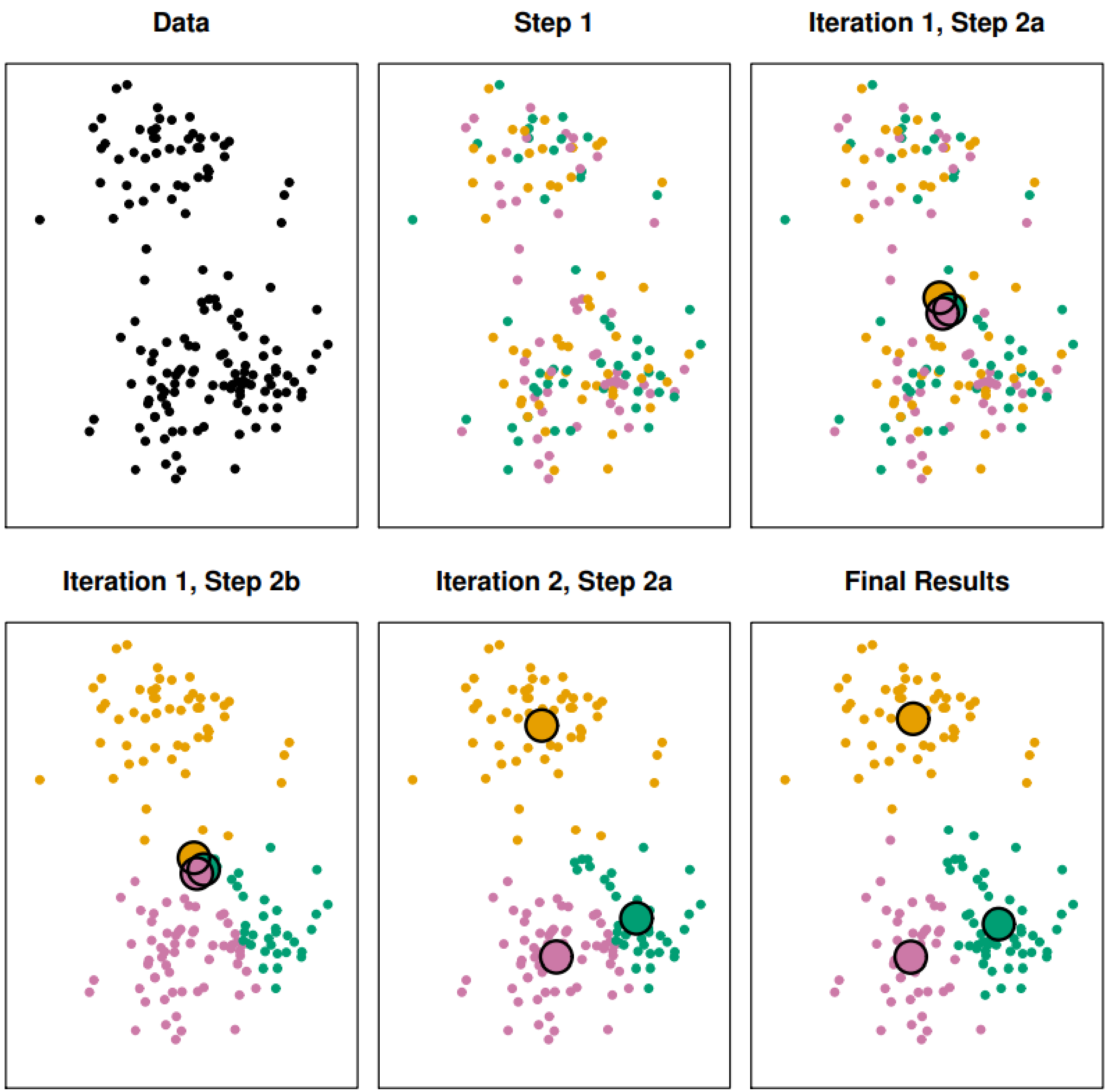
- $\min_{\text{partitions } C_1,\ldots,C_k} \sum_{j=1}^{k} W(C_j)$
  - $W(\cdot)$ is a function that measures "cost" for points in cluster j
- For k-means: $W\left(C_j\right) = \frac{1}{|C_j|} \sum_{X_i, X_i' \in C_j} \|X_i - X_i'\|_2^2$
  - Equivalently: $W\left(C_j\right) = 2 \sum_{X_i \in C_j} \left\|X_i - \mu_j\right\|_2^2$, where $\mu_j = \frac{1}{|C_j|} \sum_{X_i \in C_j} X_i$
- How to optimize?
- Slow algorithm: Try all partitions (there's a lot, roughly k^n)
- Usually: Lloyd's algorithm

Lloyd's Algorithm

1. Initialize partition $C_1, \ldots, C_k$ (could be random or carefully chosen)
2. For each cluster C_j, compute centroid $\mu_j = \frac{1}{|C_j|} \sum_{X_i \in C_j} X_i$
3. For each point X_i assign it to cluster with nearest centroid
   - Assign it to cluster with index $\arg\min_{\mathrm{j}} \|X_i - \mu_j\|_2^2$
4. Go to step 2, repeat until convergence

Main idea: given clusters, compute centers. Then given centers, compute clusters. Repeat.

Example


Data
Step 1
Iteration 1, Step 2a
Iteration 1, Step 2b
Iteration 2, Step 2a
Final Results

Comments on k-Means/Lloyd's Algorithm

- Drawbacks
  - Can be slow to converge
  - May only converge to a local optimum
    - NP-hard to optimize even to a constant factor approximation
- Solutions
  - Repeat many times with different initializations, take best

k-Means with Restarts

Comments on k-Means/Lloyd's Algorithm

- Drawbacks
  - Can be slow to converge
  - May only converge to a local optimum
    - NP-hard to optimize even to a constant factor approximation
- Solutions
  - Repeat many times with different initializations, take best
  - Do better initializations (e.g., k-means++)

Generative Models

- Given $X_1, \ldots, X_n$ drawn i.i.d. from some distribution p_θ
- Goal: Output $\hat{p} \approx p_\theta$
- Try to estimate the distribution which generated the dataset
- A simple case: $X_1, \ldots, X_n \sim N(\mu, 1)$
  - $p_\mu(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2}\right)$
- MLE: $\hat{\mu} = \arg\max_\mu \sum_{i=1}^n \log p_\mu(X_i) = \arg\max_\mu \sum_{i=1}^n -(X_i - \mu)^2 = \frac{1}{n}\sum_{i=1}^n X_i$
- Output $\hat{p} = N(\hat{\mu}, 1)$

Mixture Model

- $p_\theta(x) = \sum_{j=1}^{k} \pi_j p_{\theta^{(j)}}^{(j)}(x)$
  - π_j's are *mixing weights*: $\pi_j \geq 0$ and $\sum_{j=1}^{k} \pi_j = 1$
  - $p_{\theta^{(j)}}^{(j)}(x)$ is the PDF for component j
  - Density is a convex combination of a collection of other densities
- Intuitive way is to think about the sampling procedure
  1. Draw sample $\in \{1, \dots, k\}$ according to distribution π
  2. Output a sample from $p_{\theta^{(j)}}^{(j)}(x)$
- (Draw picture of male and female human height distributions)

Gaussian Mixture Model

- $p_\theta(x) = \sum_{j=1}^{k} \pi_j N(\mu_j, \Sigma_j, x)$
  - Note: $N(\mu_j, \Sigma_j, x)$ is the PDF of $N(\mu_j, \Sigma_j)$ at the point x
- (Draw picture of 3-GMM)
- Different from clustering
  - Clustering is a non-stochastic setting
  - Goal is a bit different: identify clusters vs estimate parameters

Gaussian Mixture Models

- Problem would be easy if we knew which component each came from
- Let Z_i be the component that X_i was sampled from, $Z_i \in \{1, \dots, k\}$
- If we knew then

$$\hat{\theta} = \arg\max_{\theta} \sum_{i=1}^{n} \log p_\theta(x_i) = \arg \max_{\theta=\{(\pi_j, \mu_j, \Sigma_j)\}} \sum_{i=1}^{n} \log \left(\sum_{j=1}^{k} \mathbf{1}_{\{Z_i=j\}} \pi_j N(\mu_j, \Sigma_j, x) \right)$$

$$\hat{\pi}_j = \frac{1}{n} \sum_{Z_i=j} 1 \,, \hat{\mu}_j = \frac{1}{\sum_{Z_i=j} 1} \sum_{Z_i=j} X_i \,, \hat{\Sigma}_j = \frac{1}{\sum_{Z_i=j} 1} \sum_{Z_i=j} (X_i - \hat{\mu}_j)(X_i - \hat{\mu}_j)^T$$

- If we knew the components, then just take empirical estimates… but we don’t.

Expectation Maximization (EM)

- Problem would have been easy if we knew which component each point came from
  - May be impossible to tell in some cases (draw point between two Gaussians)
  - Instead, say it came from multiple components fractionally (50-50 drawing)
- Expectation Maximization: a “soft” version of k-means
  - A point belongs to *multiple* components instead of just one

1. Given θ, fractionally assign points X_i to mixture components
2. Given fractional assignment of X_i to clusters, compute best θ

Deriving the EM Updates, starting at $\arg\max_\theta \sum_i \log p_\theta(X_i)$

$$\log p_\theta(X_i)$$

$$= \log \sum_{j=1}^{k} p_\theta(X_i, Z_i = j)$$

$$= \log \sum_{j=1}^{k} \frac{q_i(Z_i = j)}{q_i(Z_i = j)} p_\theta(X_i, Z_i = j)$$

(think q_i as a “guess” for the distribution of Z_i)

$$= \log \sum_{j=1}^{k} q_i(Z_i = j) \frac{p_\theta(X_i, Z_i = j)}{q_i(Z_i = j)}$$

$$= \log \mathrm{E}_{Z_i \sim q_i} \left[\frac{p_\theta(X_i, Z_i)}{q_i(Z_i)} \right]$$

$$\geq \mathrm{E}_{Z_i \sim q_i} \log \left[\frac{p_\theta(X_i, Z_i)}{q_i(Z_i)} \right]$$

(by Jensen’s inequality)

$$= \sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j) - \sum_{j=1}^{k} q_i(Z_i = j) \log q_i(Z_i = j)$$

In summary

$$\arg\max_{\theta} \sum_i \log p_\theta(X_i)$$

$$\geq \arg\max_{\theta,\{q_i\}} \sum_i \left(\sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j) - \sum_{j=1}^{k} q_i(Z_i = j) \log q_i(Z_i = j) \right)$$

E Step (Expectation Step)

$$\arg\max_{\theta,\{q_i\}} \sum_i \left(\sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j) - \sum_{j=1}^{k} q_i(Z_i = j) \log q_i(Z_i = j) \right)$$

- E step: fix θ, optimize q_i's (let's focus on a single q_i for simplicity)

$$\arg\max_{q_i} \sum_{j=1}^{k} q_i(Z_i = j)(\log p_\theta(X_i, Z_i = j) - \log q_i(Z_i = j))$$

$$= \arg\max_{q_i} \sum_{j=1}^{k} q_i(Z_i = j)(\log p_\theta(Z_i = j | X_i) + \log p_\theta(X_i) - \log q_i(Z_i = j))$$

(Drop constant $\log p_\theta(X_i)$*)*

$$= \arg\min_{q_i} \mathrm{E}_{Z_i \sim q_i} \left[\log \frac{q_i(Z_i)}{p_\theta(Z_i | X_i)} \right]$$

This is the KL Divergence between distributions q_i and $p_\theta(\cdot\,|X_i)$. It is always non-negative, and minimized when $q_i(Z_i) = p_\theta(Z_i|X_i)$, so choose q_i in this way.

M Step (Maximization Step)

$$\arg\max_{\theta,\{q_i\}} \sum_i \left(\sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j) - \sum_{j=1}^{k} q_i(Z_i = j) \log q_i(X_i, Z_i = j) \right)$$

- M step: Fix q_i's, optimize θ

$$\arg\max_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j)$$

- Often solvable in closed form

The Algorithm

1. Initialize θ parameters
2. Run E step
3. Run M step
4. Repeat 2, 3

EM for GMMs

- E step: $q_i(Z_i = j) = p_\theta(Z_i = j|X_i) = \frac{p_\theta(Z_i=j,X_i)}{p_\theta(X_i)} = \frac{\pi_j N(\mu_j,\Sigma_j,X_i)}{\sum_{\ell=1}^{k} \pi_\ell N(\mu_\ell,\Sigma_\ell,X_i)}$
  - Compute for all X_i, for all $j \in \{1, \dots, k\}$
- M step (for simplicity, 1D, variance = 1. $p_\theta(x) = \sum \pi_j N(\mu_j, 1, x)$):

$$\arg\max_\theta \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \log p_\theta(X_i, Z_i = j)$$

$$= \arg\max_\theta \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \log\left(\pi_j \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\left(X_i - \mu_j\right)^2}{2}\right)\right)$$

$$= \arg\max_\theta \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \left(\log \pi_j - \frac{\left(X_i - \mu_j\right)^2}{2}\right)$$

Focus on optimizing μ_j

$$\arg\max_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \left(-\frac{\left(X_i - \mu_j\right)^2}{2} \right)$$

Optimize by taking derivative wrt μ_j and setting $= 0$

$$\sum_{i=1}^{n} -q_i(Z_i = j)\left(X_i - \mu_j\right) = 0$$

Rearranging…

$$\mu_j = \frac{\sum_i q_i(Z_i = j)\, X_i}{\sum_i q_i(Z_i = j)}$$

Focus on optimizing π_j

$$\arg\max_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \log \pi_j \qquad \left(\text{s.t.} \sum_{\ell=1}^{k} \pi_\ell = 1 \right)$$

$$\arg\max_{\theta} \sum_{i=1}^{n} \sum_{j=1}^{k} q_i(Z_i = j) \log \pi_j + \lambda \left(\sum_{j=1}^{k} \pi_j - 1 \right)$$

Differentiate wrt π_j, set equal to 0

$$\sum_{i=1}^{n} \frac{q_i(Z_i = j)}{\pi_j} + \lambda = 0$$

$$\pi_j = -\frac{1}{\lambda} \sum_{i=1}^{n} q_i(Z_i = j)$$

Focus on optimizing π_j

$$\pi_j = -\frac{1}{\lambda}\sum_{i=1}^{n} q_i(Z_i = j)$$

But what is λ? Note

$$1 = \sum_{j=1}^{k} \pi_j = -\frac{1}{\lambda}\sum_{i=1}^{n}\sum_{j=1}^{k} q_i(Z_i = j) = -\frac{n}{\lambda}$$

So $\lambda = -n$.

Therefore

$$\pi_j = \frac{1}{n}\sum_{i=1}^{n} q_i(Z_i = j)$$

Example