Lecture 23: Spectral clustering, EM algorithm

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- Given clusters $C_1, \ldots, C_k$, update centers $\mu_1, \ldots, \mu_k \in \mathbb{R}^d$ as

$$\mu_j = \frac{1}{|C_j|} \sum_{x_i \in C_j} x_i.$$

k-means algorithm (Lloyd's algorithm)

- Lloyd's algorithm is an approximate method to solve the ERM problem:

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- here, $\mu(C_j) = \frac{1}{|C_j|} \sum_{x_i \in C_j} x_i = \operatorname{argmin}_{\mu \in \mathbb{R}^d} \sum_{x_i \in C_j} \|x_i - \mu\|^2$ is the mean of the points in cluster C_j.

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- Lloyd's algorithm is a heuristic. It is not guaranteed to converge to the global optimum or even a local minimum.

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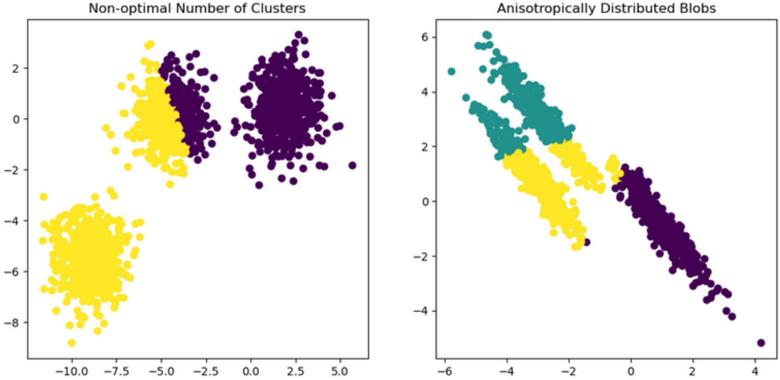
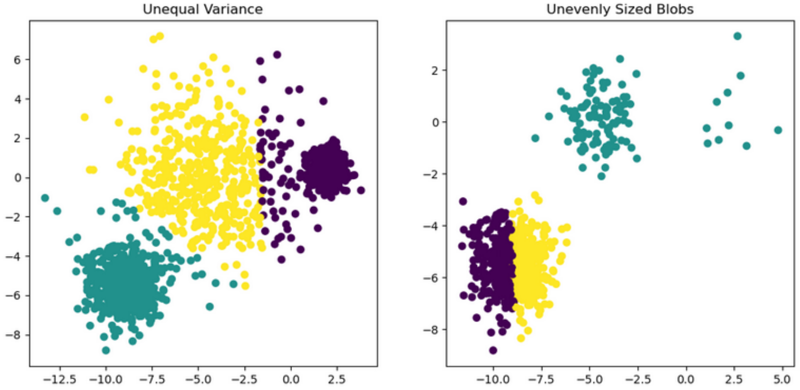
- k-means algorithm is sensitive to initialization of the centers.
- Complexity: $O(mdk)$ per iteration, where m is the number of points, d is the dimension, and k is the number of clusters.

k-means failure modes



Source: sklearn's toy examples

k-means failure modes contd



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- ERM problem: $\min_{C_1,\ldots,C_k} \sum_{j=1}^{k} \sum_{x_i \in C_j} \sum_{x_l \notin C_j} w_{il}$. Graph min-cut problem.

RatioCut problem: spectral clustering solution

- RatioCut problem: $\min_{C_1,\ldots,C_k} \sum_{j=1}^{k} \frac{\sum_{x_i \in C_j} \sum_{x_l \notin C_j} w_{il}}{|C_j|}$.

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- H has orthonormal columns.

Recall: graphical representation of X

- Choose weighting, such as, $w_{ij} = \exp(-\|x_i - x_j\|^2/2\sigma^2)$. As $\sigma \to 0$, $w_{ij} \to \mathbb{1}_{i=j}$. The $m \times m$ matrix W is the adjacency matrix of a graph.

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- Let D be the diagonal matrix with $D_{ii} = \sum_{j=1}^{m} w_{ij}$.
- Graph laplacian: $L = D - W$.
- Detects local structure / clusters in data.

Lemma proof: RatioCut objective and graph laplacian connection

- RatioCut objective$(C_1, \cdots, C_k)$

$$:= \sum_{j=1}^{k} \frac{\sum_{x_i \in C_j} \sum_{x_l \notin C_j} w_{il}}{|C_j|}.$$

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- Need to show equal to $\mathrm{Tr}(H^\top LH)$.

Laplacian eigenmaps

- Want to solve: $\min_{y_1,\cdots,y_m} \sum_{i=1}^m \sum_{j=1}^m w_{ij} \|y_i - y_j\|^2$.

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- For any vector v, $v^\top L v = (1/2) \sum_{i,j=1}^{m} w_{ij}(v_i - v_j)^2$.
- L is positive semi-definite.

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- Another interpretation: top n eigenvectors of $L^\dagger$. $L^\dagger_{ij}$ represents expected time for random walk $i \to j \to i$.
- Kernel PCA with $K = L^\dagger$ is equivalent to Laplacian eigenmaps.

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- Uses $v_i, i = 1, 2, \cdots, k$ eigenvectors of L corresponding to the k smallest eigenvalues.
- Perform k-means on rows of v_i. to obtain clusters

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- $x_i \sim \sum_{j=1}^{k} \pi_j \mathcal{N}(\mu_j, \Sigma_j)$.
- Frequentist view: there is a true (unknown) parameter $\theta = (\pi_1, \ldots, \pi_k, \mu_1, \ldots, \mu_k, \Sigma_1, \ldots, \Sigma_k)$ that generated the data.

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- Z is a latent variable, e.g., Z is the cluster assignment of X.

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- Thus, we want to solve:

$$\max_{\theta} \max_{q} \sum_{i=1}^{m} \log \sum_{j=1}^{k} q_{\theta}(z_j) p_{\theta}(x_i | z_j). \tag{1}$$

- Lemma: For fixed θ, optimal $q_{\theta} \equiv p_{\theta}(\cdot | X)$ is the conditional distribution of Z given X.

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- Use Jensen's inequality: $E \log Z \leqslant \log EZ$ for any random variable Z.
- Thus, $\ell(x, \theta) \geqslant \sum_{j=1}^{k} q_\theta(z_j) \log \frac{p_\theta(x, z_j)}{q_\theta(z_j)}$.
- This holds for any probability distribution q_θ.
- $\mathrm{ELBO}(q, \theta) = \sum_{j=1}^{k} q(z_j) \log \frac{p_\theta(x, z_j)}{q(z_j)}$.
- Thus, we have shown, $\ell(x, \theta) \geqslant \mathrm{ELBO}(q, \theta)$ for any q.

→ Presentation slots – filled
25% of grade of project

→ HW4 Nov 30^{th} / Dec 1^{st}

→ Ratio cut objective
$$= Tr(H^T L H)$$

To prove : use
for any vector $v \in \mathbb{R}^m$,
$$v^T L v = \sum_{i,j \in [m]} (v_i - v_j)^2 w_{ij}$$

$$L = D - W$$

L : Graph Laplacian

$D_{ii} = \sum_{j=1}^{m} w_{ij}$; W: weighted adjacency matrix

$$W[i,j] = w_{ij}$$

For each $i \in [k]$, put $v = h_i$
$$H = [h_1 | \cdots | h_k] \qquad H \in \mathbb{R}^{m \times k}$$

→ Ratio cut objective $= \sum_{i=1}^{k} h_i^T L h_i$

$$\rightarrow \min_{\substack{h_i \perp h_j \\ i \neq j \\ \|h_i\| = 1}} \left(\sum_{i=1}^{k} h_i^T L h_i = \sum_{i=1}^{k} r_L(h_i) \right)$$

$$\|h_i\|^2 = \sum_{j=1}^{m} h_{ij}^2 = \sum_{\{l \in [m] : x_l \in C_j\}} \frac{1}{|C_j|} = \frac{|C_j|}{|C_j|} = 1$$

$$\rightarrow \underset{H \in \mathbb{R}^{m \times k}}{\operatorname{argmin}} \sum_{i=1}^{k} r_L(h_i) = \left(\begin{array}{l} \text{orthonormal basis of eigenvectors} \\ \text{corresponding to the bottom } k \\ \text{eigenvalues of } L \end{array} \right)$$

↓ with cols h_i

Recall Laplacian_eigenmaps

$X =$

$\rightarrow \{x_i\}_{i=1}^{m} \in \mathbb{R}^d$

$\rightarrow \quad E(x_i) \in \mathbb{R}^k$ $\qquad$ k: reduced dimension

Dim red. objective $\quad E^*(X) =$

$\rightarrow \arg\min_{\substack{H \in \mathbb{R}^{m \times k} \\ \text{with orthonormal} \\ \text{cols } h_i}} \; r_L(h_i)$

Laplacian of data $\{x_i\}_{i=1}^{m}$

$$\rightarrow \quad E^*(x_i) = [v_1(i), v_2(i), \ldots, v_k(i)]^T \in \mathbb{R}^k$$

where

$v_i \in \mathbb{R}^m$ is the i^{th} smallest eigenvector

ML

Probability distribution of X

$$l(x, \theta) = -\log P_\theta(x)$$

log likelihood

$$x_1, x_2, \ldots, x_m \overset{iid}{\sim} \mathcal{D}$$

(iid assumption)

$$\log P_\theta(x_1, \ldots, x_m) = \log \prod_{j=1}^{m} P_\theta(x_i)$$

Joint Prob dist of $X_1, \ldots, X_m$

$$= \sum_{i=1}^{m} \log P_\theta(x_i)$$

Latent variable Z is discrete and takes k diff values

$$\log P_\theta(x) = \log \sum_{j=1}^{k} q_\theta(z_j)\, P_\theta(x/z_j)$$

$$= \log \sum_{j=1}^{k} P_\theta(x, z_j)$$

q_θ : prob dist of Z

$P_\theta(X/Z)$: cond prob dis of X/Z

$P_\theta(X, Z)$: joint dist of X, Z.

ML estimation

$$\theta^*, q^* = \underset{\theta}{\arg\max}\ \underset{q}{\arg\max} \sum_{i=1}^{m} \sum_{j=1}^{k} \log\left(q(z_j) P_\theta(x_i|z_j)\right)$$

Show that:

$$P_\theta(\cdot|x) = \underset{q}{\arg\max} \sum_{j=1}^{k} \log\left(q(z_j) P_\theta(x|z_j)\right)$$

$$l(x, \theta, q) = \sum_{j=1}^{k} \log\left(q(z_j) P_\theta(x|z_j)\right)$$

$\rightarrow$ $ELBO(q, \theta, x)$

$$= \sum_{j=1}^{k} q(z_j) \log \frac{p(x, z_j)}{q(z_j)}$$

$$= - \sum_{j=1}^{k} q(z_j) \log \frac{q(z_j)}{p(x, z_j)}$$

$$= - \sum_{j=1}^{k} q(z_j) \log \frac{q(z_j)}{p(x)\, p(z_j|x)}$$

$$= \underline{- \sum_{j=1}^{k} q(z_j) \log \frac{q(z_j)}{p(z_j|x)}} + \boxed{\sum_{j=1}^{k} q(z_j)} \log p(x)$$

$$= \log p(x) - D_{KL}\left(q \| p(\ |x)\right)$$

$$\rightarrow \quad l(x, \theta) \geq ELBO(q, \theta) = \sum_{j=1}^{k} q(z_j) \log \frac{P_\theta(x, z_j)}{q(z_j)}$$

$$\rightarrow \quad q^*(z|X) = P_\theta(z|X)$$

$\rightarrow$ $ELBO\left(P_\theta(z|x), \theta\right)$

$$= \sum_{j=1}^{k} P_\theta(z_j|x) \log \frac{P_\theta(x, z_j)}{P_\theta(z_j|x)}$$

$$= \sum_{j=1}^{k} P_\theta(z_j|x) \log \frac{P_\theta(\cancel{z_j|x})\, p(x)}{P_\theta(\cancel{z_j|x})}$$

$$= \log p(x) = l(x, \theta)$$