Lecture 22: 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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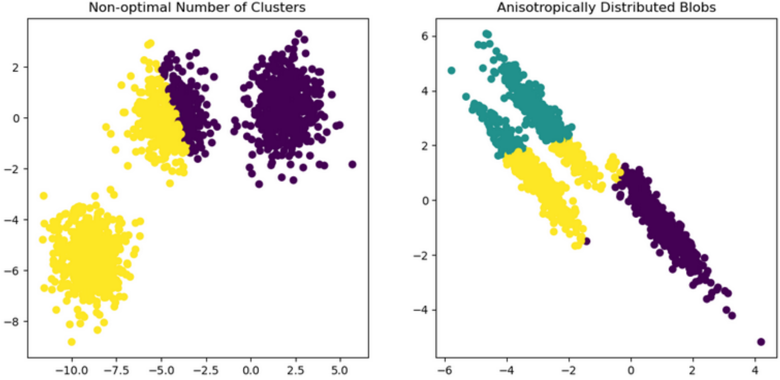
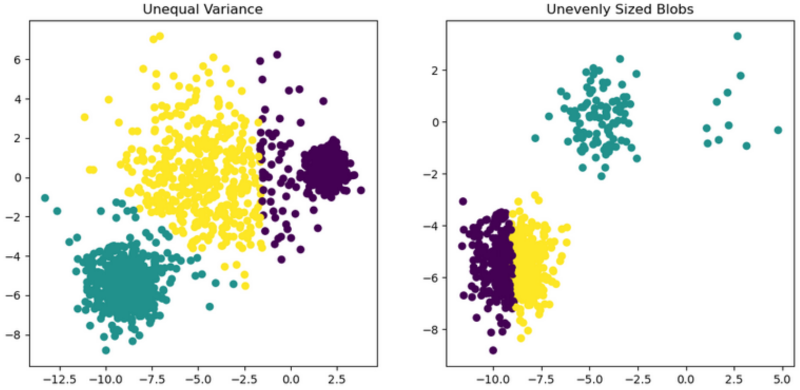
- Complexity: $O(mdk)$ per iteration, where m is the number of points, d is the dimension, and k is the number of clusters.

k-means failure modes



Source: sklearn's toy examples

k-means failure modes contd



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- W is a weighted adjacency matrix of a graph.
- 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: $\min_{C_1,\dots,C_k} \sum_{j=1}^{k} \frac{\sum_{x_i \in C_j} \sum_{x_l \notin C_j} w_{il}}{|C_j|}$.

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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$(C_1, \cdots, C_k)$

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

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- 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 $q_\theta \equiv p_\theta(X|Z)$ is the posterior 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.

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- Repeat until convergence.

EM algorithm properties

- EM algorithm decreases $\hat{R}_S(\theta) = \sum_{i=1}^{m} \ell(x_i, \theta)$ at each iteration.
- $\ell(x, \theta_{t+1}) = \mathrm{ELBO}(q_{t+2}, \theta_{t+1}) \geqslant \mathrm{ELBO}(q_{t+1}, \theta_{t+1}) \geqslant \mathrm{ELBO}(q_{t+1}, \theta_t) = \ell(x, \theta_t)$.

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- $p_\theta(x|z_j) = \mathcal{N}(\mu_j, \Sigma_j)$; $p_\theta(z_j) = \pi_j$.
- E step: $q_{t+1}(z|x) = p_{\theta_t}(z|x) = \frac{p_{\theta_t}(x|z)p_{\theta_t}(z)}{p_{\theta_t}(x)}$.
- M step: $\theta_{t+1} = \mathrm{argmax}_\theta \sum_{i=1}^{m} \sum_{j=1}^{k} q_{t+1}(z_j|x_i) \log \frac{p_\theta(x_i, z_j)}{q_{t+1}(z_j|x_i)}$.
- $\mu_{j,t+1} = \sum_{i=1}^{m} q_{t+1}(z_j|x_i) x_i$.
- $\pi_{j,t+1} = \frac{1}{m} \sum_{i=1}^{m} q_{t+1}(z_j|x_i) / Z_{j,t+1}$.

VAE revisited

- Hard to compute q_t in general. VAE solves this problem differently.
- $p_\theta(x|z) = \mathcal{N}(f_\theta(z), \sigma^2 I)$. (Decoder: f_θ)
- $q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \Sigma_\phi(x))$. (Encoder: μ_ϕ, Σ_ϕ)