Lecture 22: Clustering, LLoyd's algorithm (k-means), spectral clustering

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November 14, 2023

Last time: Johnson-Lindenstrauss lemma

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- Let $0 < \epsilon < 1/2$, $m > 4$. Then, there exists a linear map $A : \mathbb{R}^d \to \mathbb{R}^n$ with $n = O(\epsilon^{-2} \log m)$ such that for all $x_i, x_j \in X$, $i, j \in [m]$, $(1-\epsilon)\|x_i - x_j\|^2 \leqslant \|Ax_i - Ax_j\|^2 \leqslant (1+\epsilon)\|x_i - x_j\|^2$.

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- Informal: any set of points in high-dimensional space can be mapped to a lower-dimensional space while approximately preserving the distances between the points.

Proof

- Distortion by Gaussian random matrices: for any $x \in \mathbb{R}^d$, when the entries A_{ij} are iid standard Gaussian,

$$\mathbb{P}(n(1-\epsilon)\|x\|^2 \leqslant \|Ax\|^2 \leqslant n(1+\epsilon)\|x\|^2) \geqslant 1 - 2\exp(-(\epsilon^2 - \epsilon^3)n/4).$$

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- Then, deterministic statement of J-L lemma follows from union bound over all m^2 pairs of points.

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- Chi-squared distribution: $\rho(x) = \frac{1}{2^{n/2}\Gamma(n/2)} x^{n/2-1} e^{-x/2}, x \geqslant 0$.
- Models sum of squares of n independent standard normal random variables.

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- Let $A \in \mathbb{R}^{n \times d}$ be a random matrix with iid standard Gaussian entries. This is an example of a matrix that satisfies the RIP (restricted isometry property).

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- (Candes,Romberg, Tao 2005) If x is s-sparse, then,

$$x = \mathrm{argmin}_{z \in \mathbb{R}^d} \|z\|_1 \quad \text{s.t.} \quad Ax = Az. \tag{2}$$

Convolutional Neural Networks (source: cs231n.stanford.edu)

- Suitable for image recognition. Won the 2012 ImageNet competition and subsequent ones.
- Three types of layers: convolutional, FC, pooling
- Convolutional layer: accepts a volume of size $W_1 \times H_1 \times D_1$ and outputs a volume of size $W_2 \times H_2 \times D_2$ where $W_2 = (W_1 - F + 2P)/S + 1$ and $H_2 = (H_1 - F + 2P)/S + 1$ and $D_2 = K$.
- K is number of filters, F is filter size, S is stride, P is padding.
- Pooling layer: downsamples along width and height, and optionally along depth.
- FC layer: computes class scores, resulting in volume of size $1 \times 1 \times K$.

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- Closely related to dimensionality reduction.
- Definition of clustering depends on the definition of distance between points.
- Center-based clustering: k centers $\mu_1, \ldots, \mu_k \in \mathbb{R}^d$.

Lloyd's algorithm

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- Given centers $\mu_1, \ldots, \mu_k \in \mathbb{R}^d$, assign each point x_i to the closest center. That is,

$$C_j = \{x_i : j \in \mathrm{argmin}_l \|x_i - \mu_l\|\}.$$

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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:

$$\min_{C_1,\ldots,C_k} \sum_{j=1}^{k} \sum_{x_i \in C_j} \|x_i - \mu(C_j)\|^2.$$

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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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- $C_j^{(t)} = \{x_i : j \in \mathrm{argmin}_l \|x_i - \mu_l^{(t-1)}\|\}$.
- Since $\mu_j^{(t)} = \frac{1}{|C_j^{(t)}|} \sum_{x_i \in C_j^{(t)}} x_i = \mathrm{argmin}_{\mu \in \mathbb{R}^d} \sum_{x_i \in C_j^{(t)}} \|x_i - \mu\|^2$,

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- Thus, the ERM objective decreases at each iteration.

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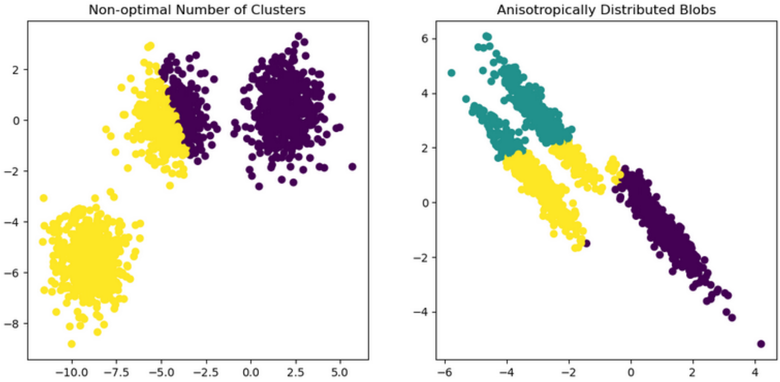
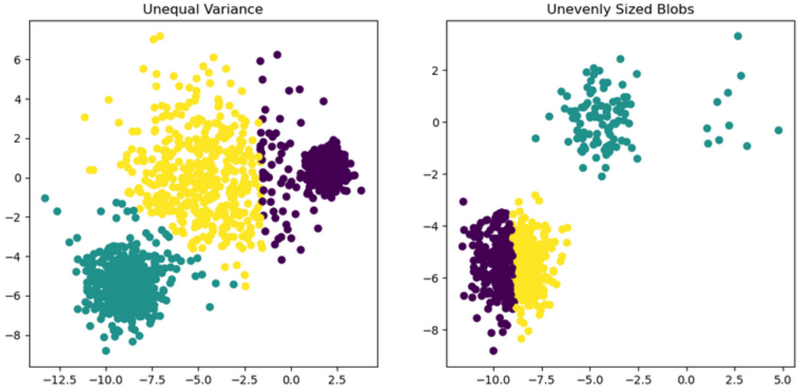
- Complexity: $O(mdk)$ per iteration, where m is the number of points, d is the dimension, and k is the number of clusters.

k-means failure modes



Source: sklearn's toy examples

k-means failure modes contd



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

RatioCut problem: spectral clustering solution

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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 $\mathrm{Tr}(H^\top LH)$.

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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.

Final project deliverables

→ Proposal 10% (2nd Nov)

→ Presentation 25%
= 1 per team 5-6 minutes

3-4 minutes

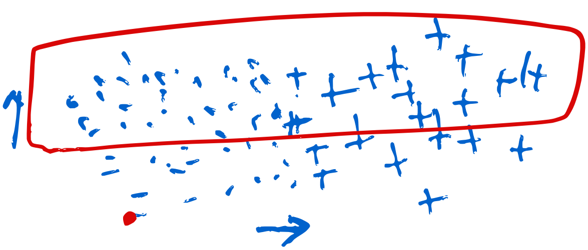
3 sessions
1 overflow session
Zoom 4-8th

7-9 pm

Finalize presentation schedules by 14th Nov

Rules for attendance (% of points for asking questions)

→ Reports (65%) : 7th Dec

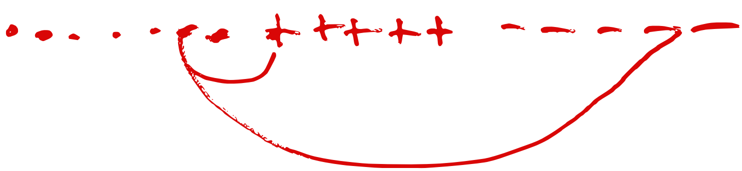


$k = 2$

$\bullet \rightarrow 1$

$+ \rightarrow 2$

Distance b/w two points



$$\rightarrow \quad w_{ij} = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$$

$$L = D - W$$

$$v^T L v = \frac{1}{2} \sum_{i,j \in [m]} w_{ij} (v_i - v_j)^2$$

$L \in \mathbb{R}^{m \times m}$ $\quad v \in \mathbb{R}^m$

Laplacian eigenmaps objective

Rayleigh quotients

$$\min_{\|v\|=1} v^T L v = \lambda_{min}(L)$$

$$\min_{\substack{V \in \mathbb{R}^{m \times k} \\ \|v_i\| = 1}} V^T L V = \min_{\substack{v_1, v_2, \ldots, v_k \\ v_i \cdot v_j = 0}} \sum_{i=1}^{k} v_i^T L v_i$$

v_i : i^{th} column of V

$$\operatorname{argmin} \sum_{i=1}^{k} v_i^T L v_i = \{\text{bottom } k \text{ eigenvectors of } L\}$$