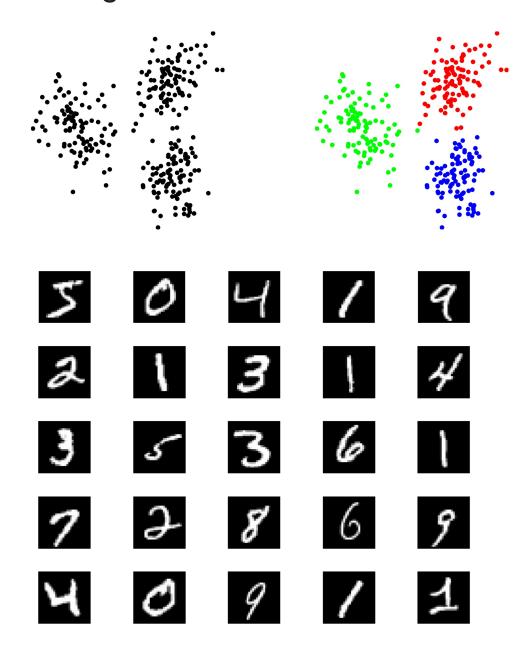
04 Clustering



Unit 1: Vectors, Book ILA Ch. 1-5

- 01 Vectors
- 02 Linear Functions
- 03 Norms and Distances
- 04 Clustering
- 05 Linear Independence

Unit 2: Matrices, Book ILA Ch. 6-11 + Book IMC Ch. 2

Unit 3: Least Squares, Book ILA Ch. 12-14 + Book IMC Ch. 8

Unit 4: Eigen-decomposition, Book IMC Ch. 10, 12, 19

Outline: 04 Clustering

- Clustering
- Algorithm
- Examples
- Applications

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Clustering in Machine Learning

Artificial Intelligence (AI): Techniques that enable machines to mimic human intelligence.

Machine Learning (ML): Techniques that enable machines to learn from data.

Supervised Learning: Task of learning a function that maps an input to an output based on example input-output pairs.

Examples:

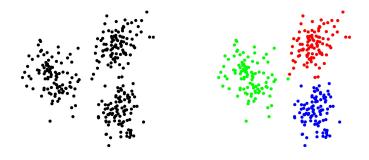
- **Regression:** maps an input to a quantitative value.
- Classification: maps an input to a categorical value.

Unsupervised Learning: Task of discovering any naturally occurring patterns in a data set. Examples:

- Clustering: discover groups (clusters) within the data: today.
- Dimension reduction: later in this class.

Clustering: Goal (Intuition)

- Given: (i) dataset of N n-vectors x_1, \ldots, x_N , (ii) integer k,
- Goal (Intuition):
 - Partition/Group/Cluster N vectors into k groups/clusters...
 - ... such that: vectors in the same group are "close".



Exercise: What is k in the figure above? What is n? What is N?

Clustering in ECE

- topic discovery and document clustering
 - x_i is word count vector for document i
- · patient clustering
 - $lacktriangleq x_i$ are patient attributes, test results, symptoms for patient i
- customer market "segmentation"
 - $lacktriangledown x_i$ is purchase history and other attributes of customer i
- financial sectors
 - x_i are n-vectors of financial attributes of company i

Clustering: Goal (Math)

- Notations:
 - Group G_j for $j=1,\ldots,k$: Set of indices in $1,\ldots,N$ representing which vectors belong to the group.
 - lacksquare Assignment c_i for $i=1,\ldots,k$: Group that x_i is in: $i\in G_{c_i}$
 - Group representative z_j for $j=1,\ldots,k$: n-vector that represents a typical element of the group G_j .
- Goal (Math): Find c_i and z_j to minimize $J^{clust} = \frac{1}{N} \sum_{i=1}^N ||x_i z_{c_i}||^2$, i.e. the mean square distance from vectors to their representatives.

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K-means algorithm

- Alternate between:
 - (i) update the groups, i.e the group assignments c_1, \ldots, c_N ,
 - (ii) update the representatives z_1, \ldots, z_k .
- Such that the objective J^{clust} decreases at each step.

(i) Update the groups

- Given: representatives z_1, \ldots, z_k
- Goal for (i): Assign vectors to groups, i.e. choose c_1, \ldots, c_N
 - We assign each vector to its nearest representative. Justification:
 - \circ Observe: c_i only appears in term $||x_i-z_{c_i}||^2$ in J^{clust}
 - \circ Conclude: to minimize over c_i , choose c_i so $\left\|x_i-z_{c_i}
 ight\|^2=min_{j\in\{1,...,k\}}\left\|x_i-z_j
 ight\|^2.$

(ii) Update the representatives

- Given the partition G_1, \ldots, G_k
- Goal for (ii): Choose representatives z_1, \ldots, z_k
 - Choose z_i = mean of the points in group j. Justification:
 - \circ Observe: J^{clust} splits into a sum of k sums:

$$J^{clust} = J_1 + \cdots + J_k, \quad J_j = rac{1}{N} \sum_{i \in G_i} \left\| x_i - z_j
ight\|^2.$$

 \circ Conclude: Choose z_j to minimize its J_j : $z_j=rac{1}{|G_j|}\sum_{i\in G_j}x_i=$ mean/center/centroid.

Pseudo-code

given
$$x_1, \ldots, x_N \in \mathbf{R}^n$$
 and $z_1, \ldots, z_k \in \mathbf{R}^n$
repeat
Update partition: assign i to $G_j, j = \operatorname{argmin}_{j'} \|x_i - z_{j'}\|^2$
Update centroids: $z_j = \frac{1}{|G_j|} \sum_{i \in G_j} x_i$

Convergence of K-means

until z_1, \ldots, z_k stop changing

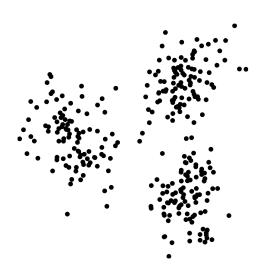
How many times do we iterate these steps?

- $\,\blacksquare\,$ Until the z_j 's stop changing: "convergence" of the algorithm.
- Remarks:
 - $lacksquare J^{clust}$ decreases at each step,
 - but in general we don't find partition that minimizes J^{clust} ,
 - the final partition depends on initial representatives.
- Recommendation:
 - lacktriangle Run k-means 10 times, with different initial representatives
 - $\ \ \, \ \ \,$ Take as final partition the one with smallest J^{clust}

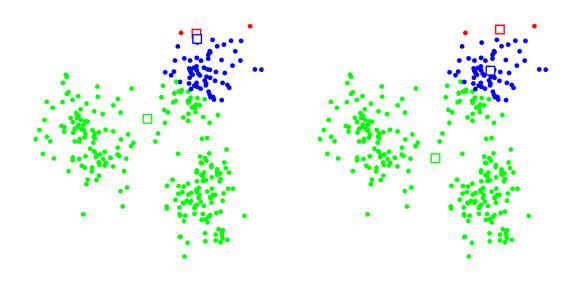
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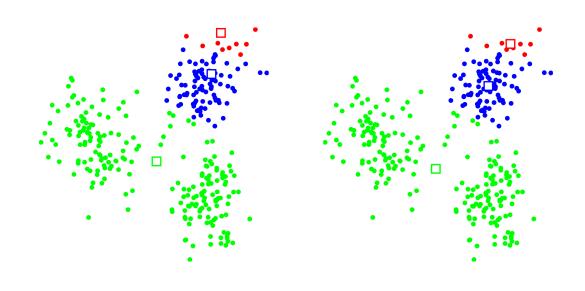
Data



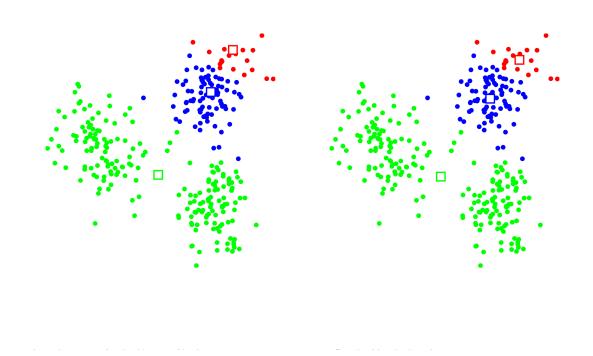
Iteration 1



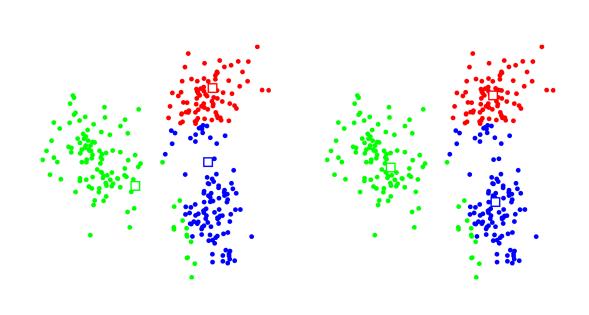
Iteration 2



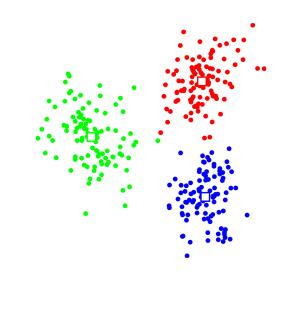
Iteration 3



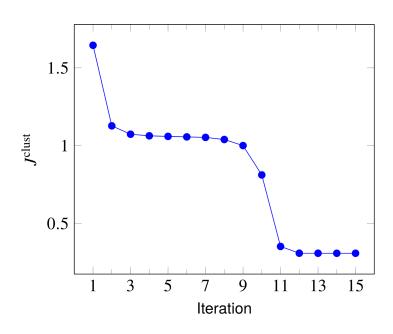
Iteration 10



Final clustering



Convergence



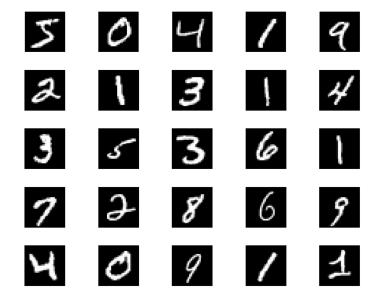
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MNIST Dataset: Find Digits

- MNIST images of handwritten digits (via Yann Lecun)
- 60,000 images of size 28 × 28, represented as 784-vectors x_i



- Goal: Group these images into groups of same digit.
- Exercice: What are k, N, n?
- Implement it practice? Will be in your next homework!

Questions?

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- Algorithm
- Examples
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Resources: Book ILA, Ch. 4