CS57300
PURDUE UNIVERSITY

APR 7, 2025

DATA MINING

DESCRIPTIVE MODELING

DATA MINING COMPONENTS

- Task specification: **Description**
- Knowledge representation
- Learning technique
- Evaluation and interpretation

DESCRIPTIVE MODELS

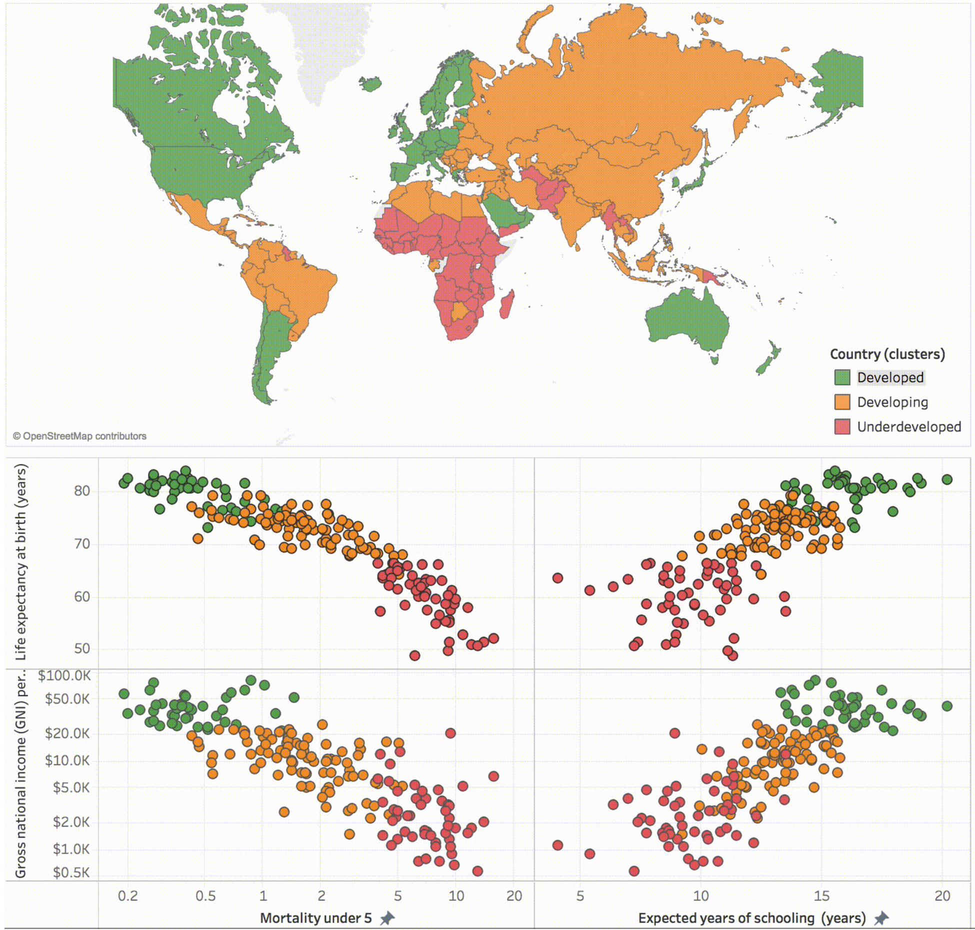
- Descriptive models **summarize** the data
  - Provide a global summary of the data which gives insights into the domain
  - May be used for prediction, but prediction is not the primary goal
- Also known as **unsupervised learning**
  - No predefined “class” labels for each data instance

DESCRIPTIVE MODELING

- Data representation: data instances represented as attribute vectors $\boldsymbol{x}(i)$, often in the form of $n \times p$ tabular data (i.e., p attributes)
- Task—depends on approach
  - Clustering: summarize the data by characterizing groups of similar instances
  - Structure learning and density estimation: determine a compact representation of the full joint distribution $P(\mathbf{X})=P(X_1,X_2,\ldots,X_p)$

CLUSTER ANALYSIS

- Decompose or partition instances into groups s.t.:
    - **Intra**-group similarity is ***high***
    - **Inter**-group similarity is ***low***
- Measure of distance/similarity is crucial

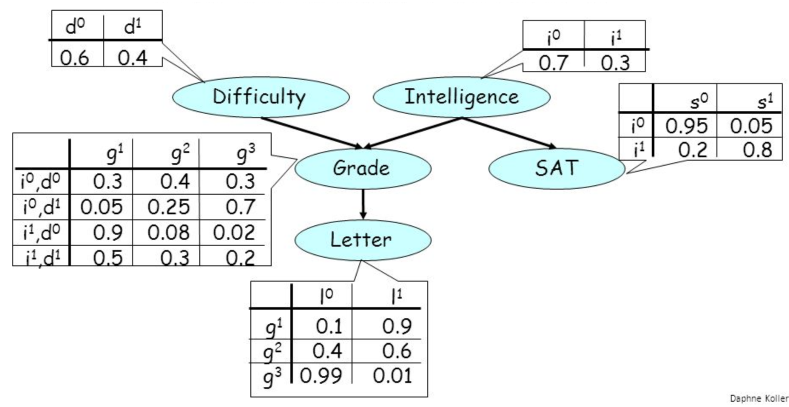


APPLICATION EXAMPLES

- **Marketing**: discover distinct groups in customer base to develop targeted marketing programs
- **Land use**: identify areas of similar use in an earth observation database to understand geographic similarities
- **City-planning**: group houses according to house type, value, and location to identify “neighborhoods”
- **Earth-quake studies**: Group observed earthquakes to see if they cluster along continent faults

STRUCTURE LEARNING AND DENSITY ESTIMATION

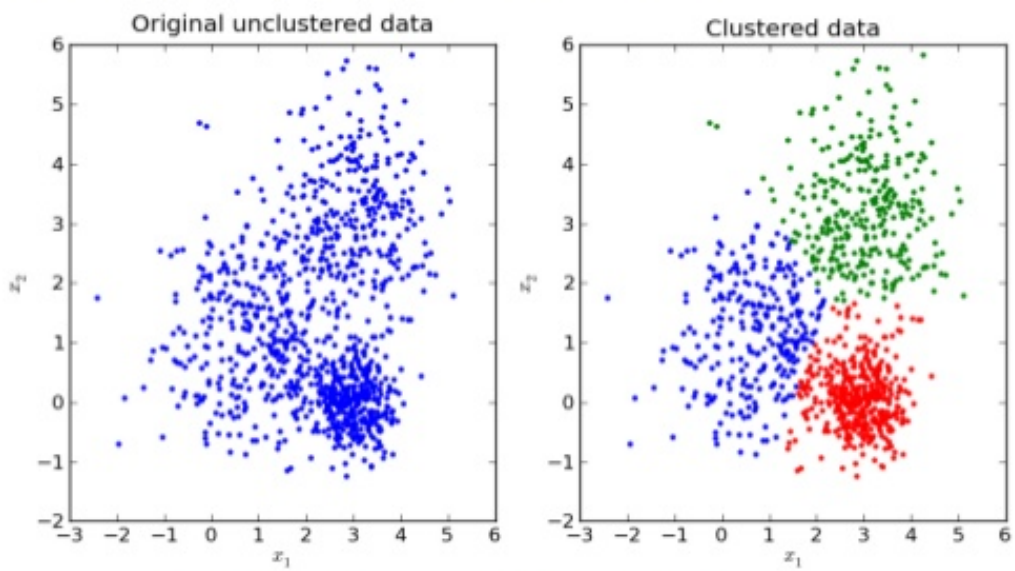
- Estimate the structure and parameters for the model that generates the observed data such that:
  - Likelihood of observing the data is high
  - Assumption: data is sampled independently from the same distribution (i.i.d)
- Example
  - Observed data: (student's IQ, student's SAT score, midterm exam difficulty, midterm exam grade, letter quality from the instructor)



DATA MINING COMPONENTS

- Task specification
- **Knowledge representation**
- Learning technique
- Evaluation and interpretation

PARTITION-BASED CLUSTERING



- Partition data instances into a fixed number of groups
- Representative algorithm: K-means

Model space:
all possible assignments of data instance to group

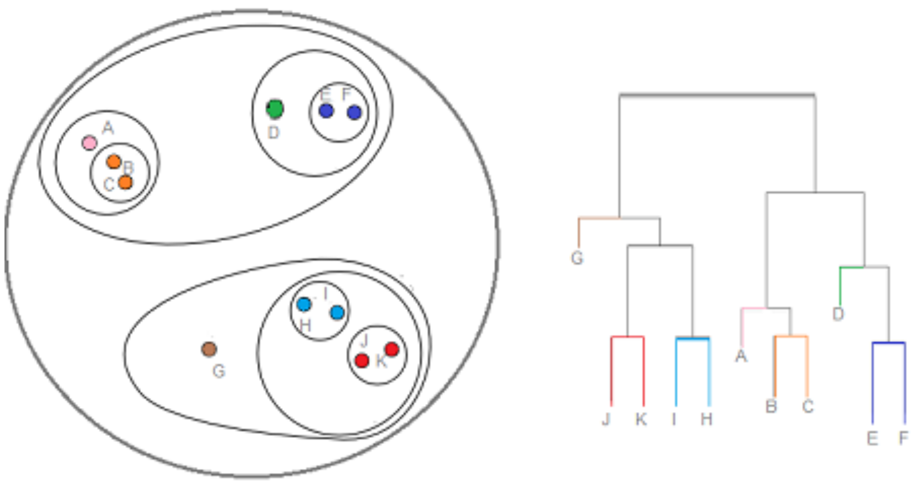
HIERARCHICAL METHODS

- Construct a hierarchy of nested clusters rather than picking K beforehand
- Approaches:
  - Agglomerative: merge clusters successively
  - Divisive: divided clusters successively

AGGLOMERATIVE

- For i = 1 to n:
  - Let $C_i = \{x(i)\}$
- While |C|>1:
  - Let C_i and C_j be the pair of clusters with min $D(C_i,C_j)$
  - $C_i=C_i \cup C_j$
  - Remove C_j

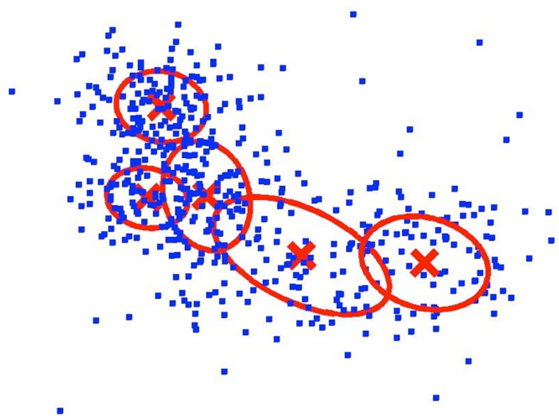
HIERARCHICAL CLUSTERING



- Build a hierarchy of clusters given the data
- Can be agglomerative (“bottom-up”) or divisive (“top-down”)

Model space:
all possible hierarchies

PROBABILISTIC MODEL-BASED CLUSTERING



$$f(x) = \sum_{k=1}^{K} w_k f_k(x; \theta)$$

probability of observing x

likelihood of x being generated from cluster k

likelihood of point belonging to cluster k

Model space:
w_k and $f_k(x; \theta)$

DATA MINING COMPONENTS

- Task specification
- Knowledge representation
- **Learning technique**
- Evaluation and interpretation

LEARNING DESCRIPTIVE MODELS

- Select a **knowledge representation** (a "model")
  - Defines a **space** of possible models $M=\{M_1, M_2, \ldots, M_k\}$
- Define **scoring functions** to "score" different models
- Use **search** to identify "best" model(s)
  - Search the space of models
  - Evaluate possible models with **scoring function** to determine the model which best fits the data

DESCRIPTIVE SCORING FUNCTIONS

- Clustering: What makes a good cluster?
  - High intra-group similarity, low inter-group similarity
  - Scoring function is often a function of within-cluster similarity and between-cluster similarity
- Example scoring functions

cluster centroid:
$$r_k = \frac{1}{n_k} \sum_{x(i) \in C_k} x(i)$$

between-cluster distance:
$$bc(C) = \sum_{1 \leq j < k \leq K} d(r_j, r_k)^2$$

within-cluster distance:
$$wc(C) = \sum_{k=1}^{K} wc(C_k) = \sum_{k=1}^{K} \sum_{x(i) \in C_k} d(x(i), r_k)^2$$

DESCRIPTIVE SCORING FUNCTIONS

- Structure learning and density estimation: Does the model representation capture the observed data well?
  - Likelihood of the observed data is often used as the scoring function
  - Also applicable to probabilistic model-based clustering

SEARCHING OVER MODELS

- Search over the model space to find the model structure / parameters that optimize the scoring function
- Discrete model space example: partition-based clustering
  - Find k clusters among n data instances: k^n possible allocations
  - Exhaustive search is intractable
  - Most approaches use iterative improvement algorithms to search the model space heuristically

SEARCHING OVER MODELS

- Continuous model space example: probabilistic model-based clustering
  - Searching for the cluster weight (i.e., w_k) and cluster parameters (i.e., $f_k(x, \theta)$) that gives the highest likelihood of observing the current data
  - Solution: **Expectation-maximization** to iteratively infer cluster member and estimate cluster parameters

DATA MINING COMPONENTS

- Task specification
- Knowledge representation
- Learning technique
- **Evaluation and interpretation**

DESCRIPTIVE MODEL EVALUATION

- Clustering evaluation
  - **Supervised**: Measures the extent to which clusters match external class label values, e.g., how likely a cluster contains only data instances of a particular class?
  - **Unsupervised**: Measures goodness of fit without class labels, e.g., how closely related instances within each cluster are and distinct instances across different clusters are?

DESCRIPTIVE MODEL EVALUATION

- How to choose k ? Describe the current data precisely vs. Generalize to new data
- Example: in partition-based clustering, the model captures the data the best when k=n
- Strike a balance between between how well the model fits and the data and the simplicity of the model

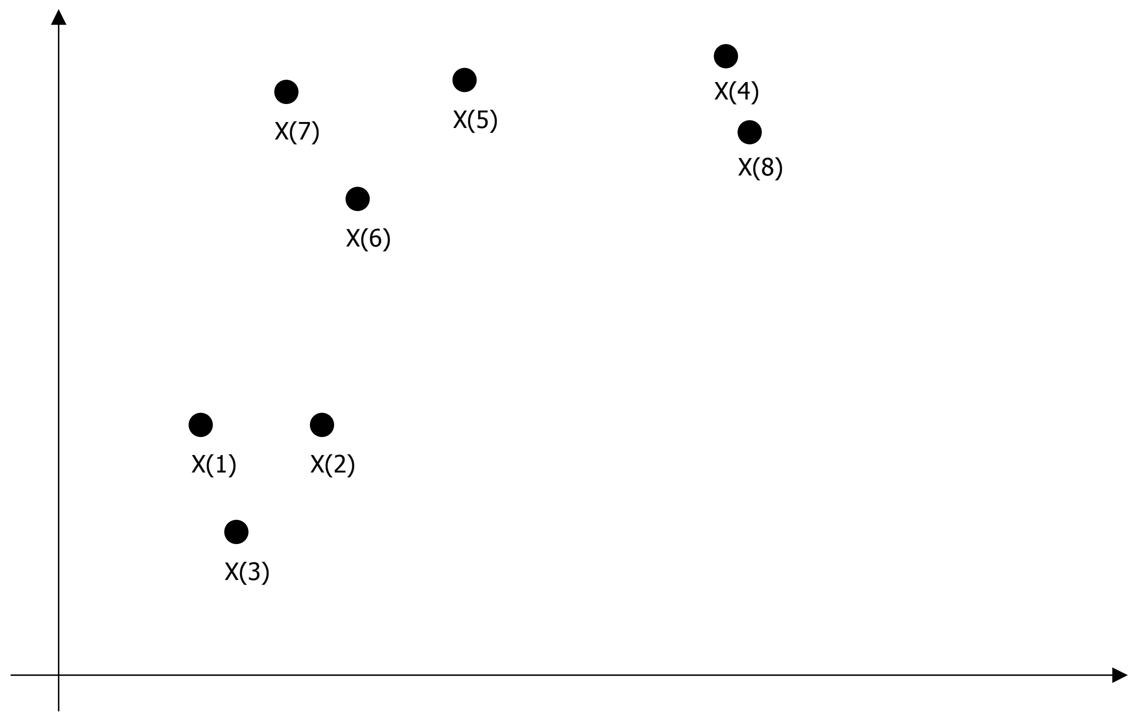
PARTITION-BASED CLUSTERING

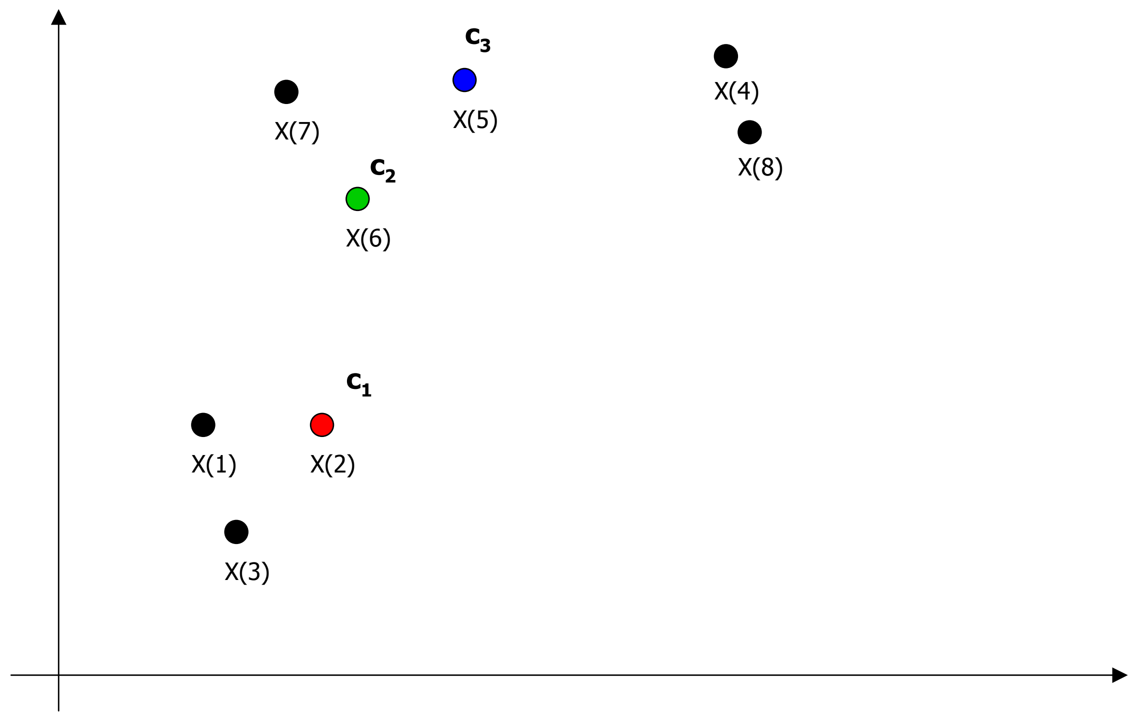
PARTITION-BASED

- Input: data D={**x**(1),**x**(2),...,**x**(n)}
- Output: k clusters C={C_1,...,C_k} such that each **x**(i) is assigned to a unique C_j
- Evaluation: Score(C,D) is maximized/minimized
    - Combinatorial optimization: search among k^n allocations of n objects into k classes to maximize score function
    - Exhaustive search is intractable
    - Most approaches use iterative improvement algorithms

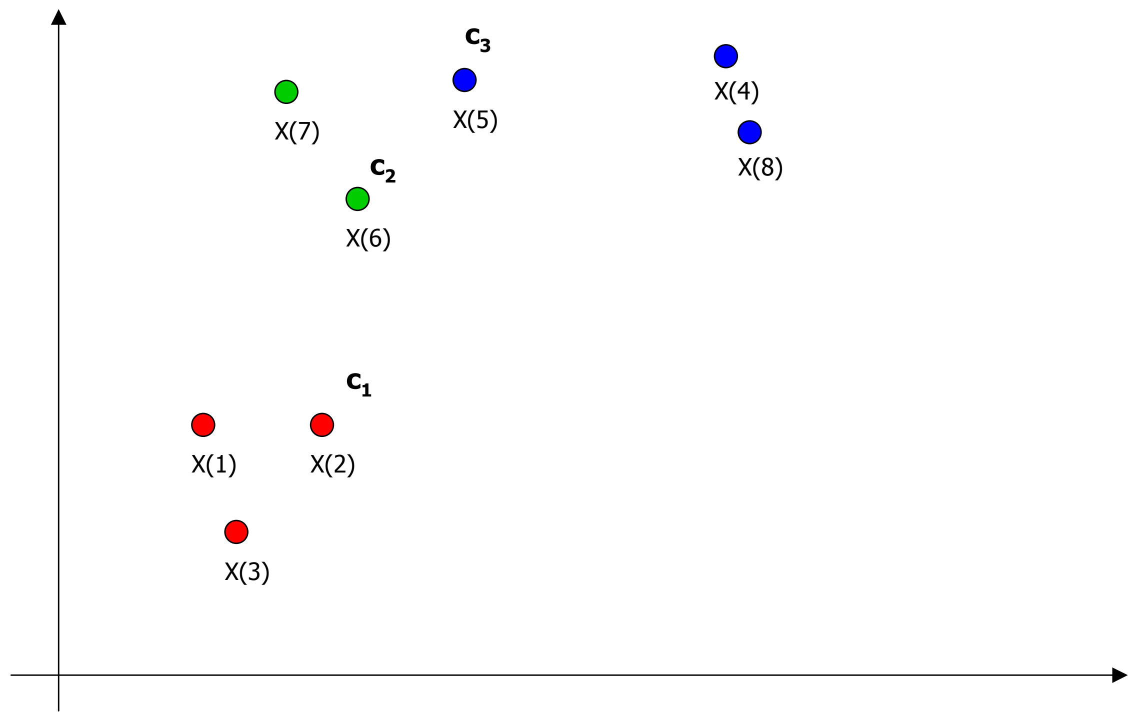
EXAMPLE: K-MEANS

- Algorithm idea:
  - Start with k randomly chosen centroids
  - Repeat until no changes in assignments
    - Assign instances to closest centroid
    - Recompute cluster centroids

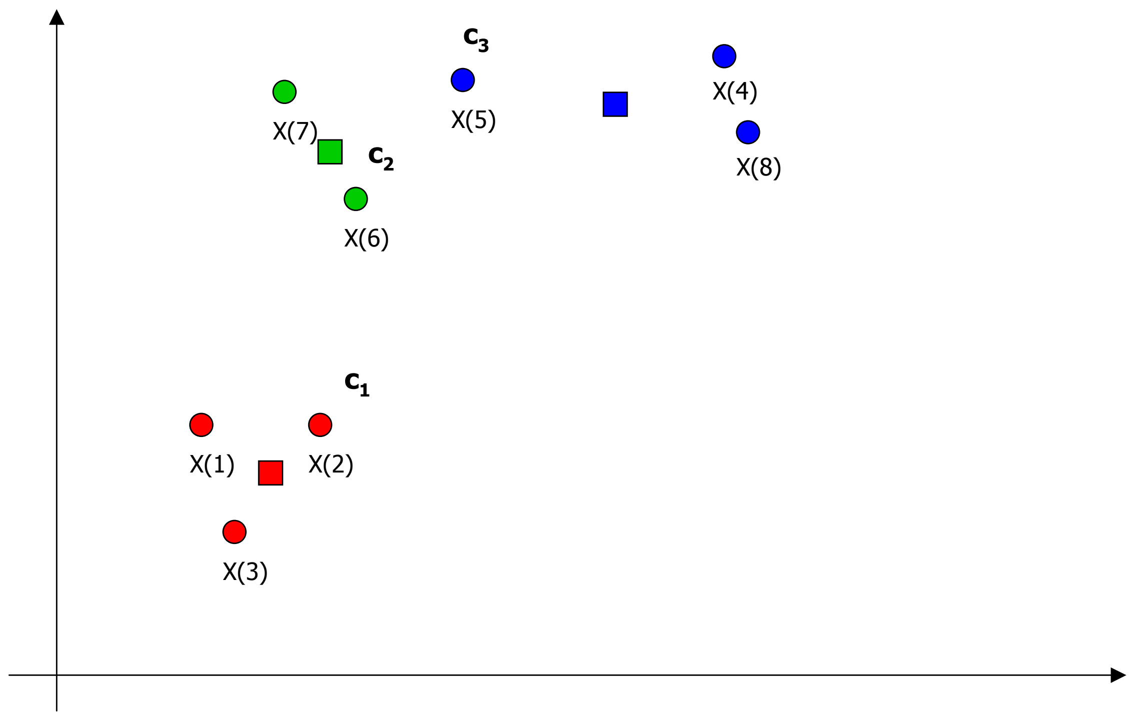

X(7)
X(5)
X(4)
X(8)
X(6)
X(1)
X(2)
X(3)



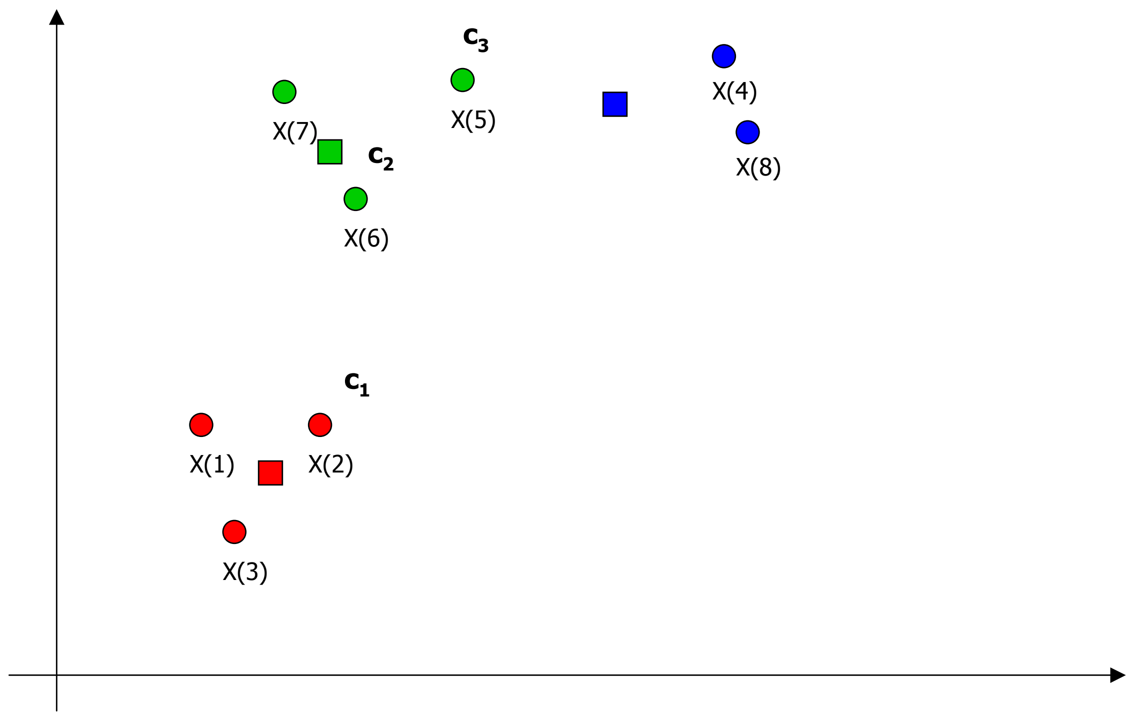
c3
X(4)
X(7)
X(5)
X(8)
c2
X(6)
c1
X(1)
X(2)
X(3)

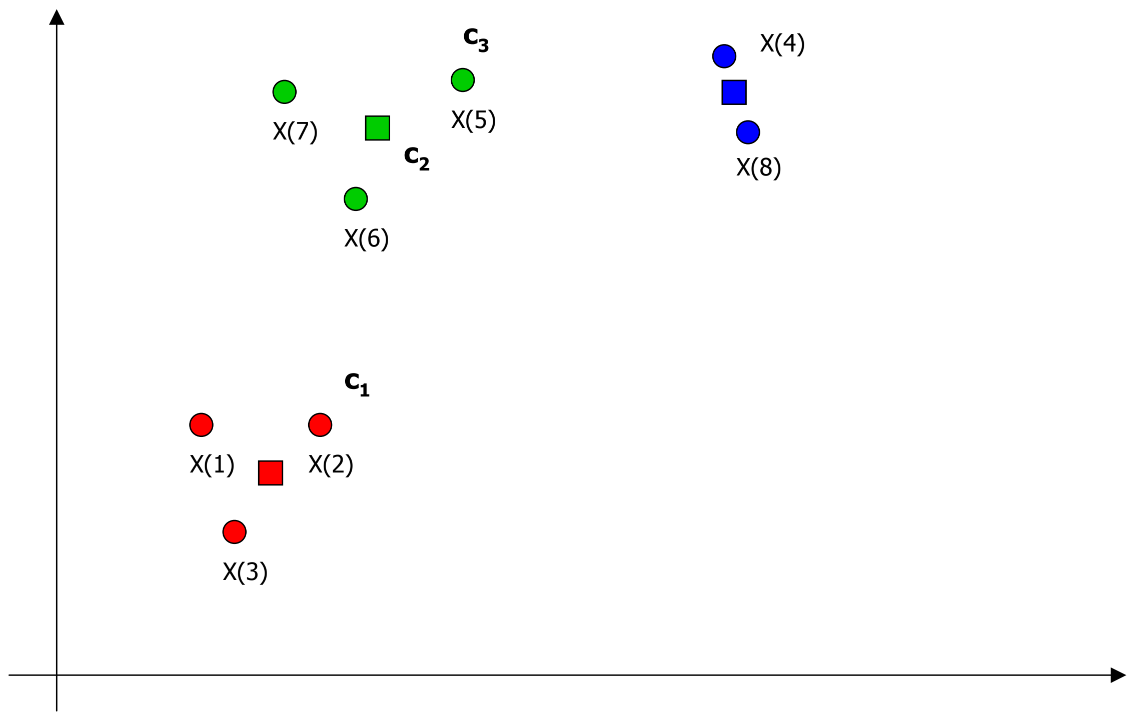


c3
X(7)
X(5)
X(4)
X(8)
c2
X(6)
c1
X(1)
X(2)
X(3)



c3
X(4)
X(7)
X(5)
c2
X(8)
X(6)
c1
X(1)
X(2)
X(3)


c3
X(4)
X(7)
X(5)
c2
X(8)
X(6)
c1
X(1)
X(2)
X(3)


c3
X(4)
X(7)
X(5)
c2
X(8)
X(6)
c1
X(1)
X(2)
X(3)

Algorithm 2.1 The `k-means` algorithm

Input: Dataset D, number clusters k

Output: Set of cluster representatives C, cluster membership vector $\mathbf{m}$

/* Initialize cluster representatives C */

Randomly choose k data points from D

Use these k points as initial set of cluster representatives C

repeat

/* Data Assignment */

Reassign points in D to closest cluster mean

Update $\mathbf{m}$ such that m_i is cluster ID of ith point in D

/* Relocation of means */

Update C such that c_j is mean of points in jth cluster

until convergence

SCORING FUNCTION OF K-MEANS

- What scoring function is K-means trying to optimize for?

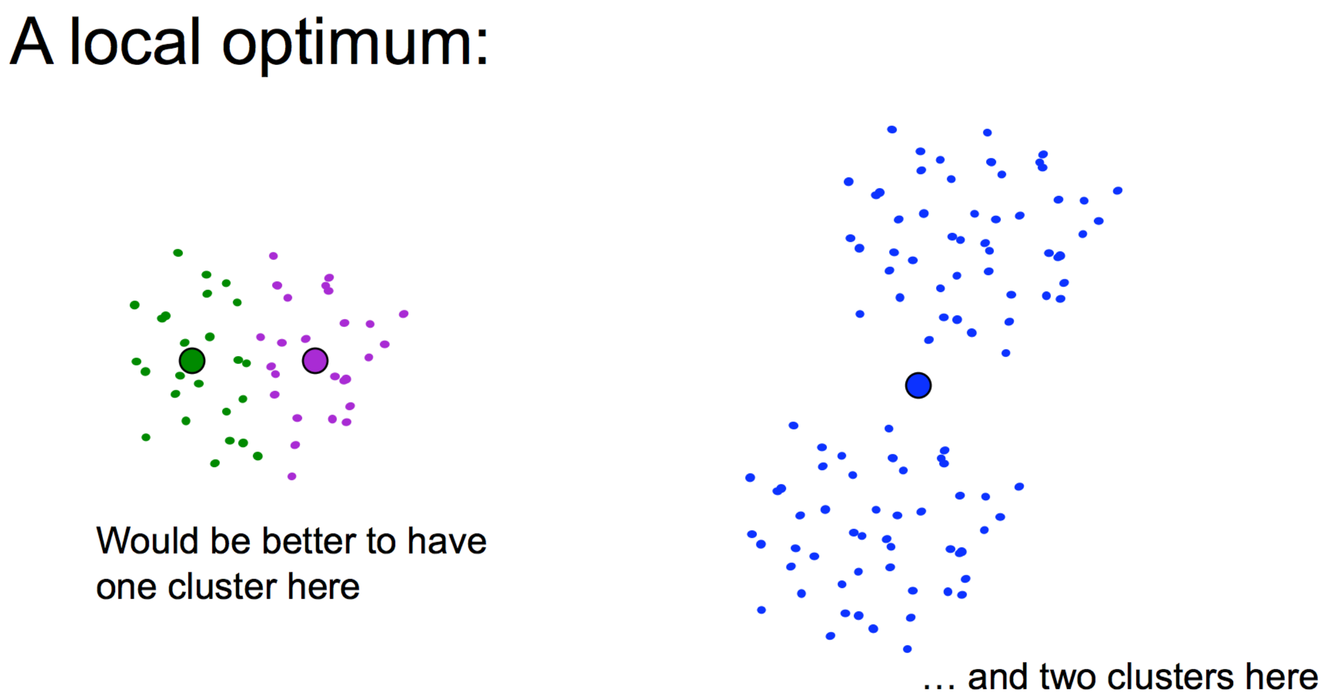
Score function: $$wc(C) = \sum_{k=1}^{K} wc(C_k) = \sum_{k=1}^{K} \sum_{x(i) \in C_k} d(x(i), r_k)^2$$

- An alternating optimization approach
  - Fix r_k, optimize for membership of C(x(i)): $min \sum_{i=1}^{N} (x(i) - r_{C(x(i))})^2$
  - Fix C(x(i)), optimize for r_k: $min_{r_k} \sum_{i=1}^{N} (x(i) - r_{C(x(i))})^2 = \sum_{k=1}^{K} \sum_{x \in C_k} (x - r_k)^2$
    - Take derivative with respect to r_k and set to 0 leads to $r_k = \frac{1}{|C_k|} \sum_{x \in C_k} x$

ALGORITHM DETAILS

- Does it terminate?
  - Yes, the objective function decreases on each iteration. It usually converges quickly.
- Does it converge to an optimal solution?
  - No, the algorithm terminates at a local optima which depends on the starting seeds.

K-MEANS IS SENSITIVE TO INITIAL SEEDS



K-MEANS

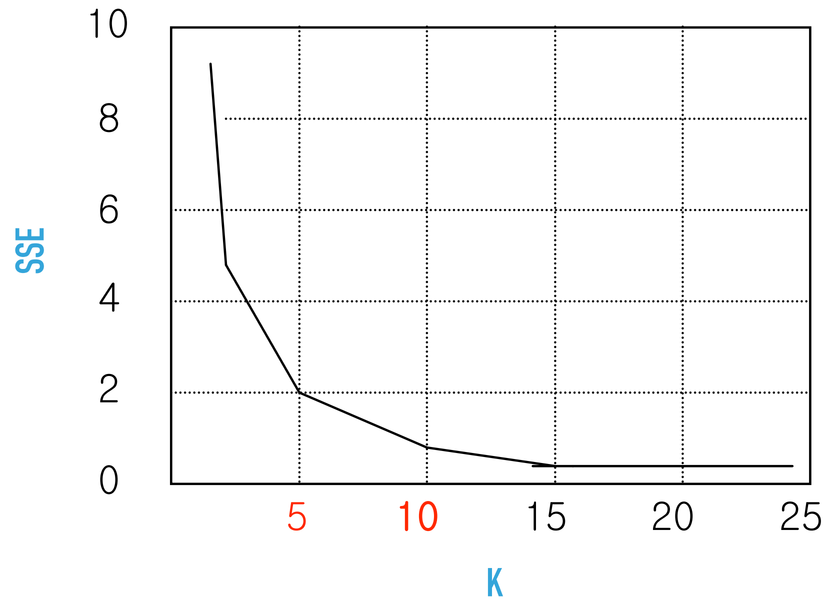
- Strengths:
  - Relatively efficient (time complexity is O(K·N·i), where i is the number of iterations)
  - Finds spherical clusters
- Weaknesses:
  - Terminates at local optimum (sensitive to initial seeds)
  - Need to specify K
  - Susceptible to outliers/noise

VARIATIONS

- Selection of initial centroids
  - Select first seed randomly and then pick successive points that are farthest away
  - Run with multiple random selections, pick result with best score
  - Use hierarchical clustering to identify likely clusters and pick seeds from distinct groups
- When mean is undefined
  - K-medoids: use one of the data points as cluster center
  - K-modes: uses categorical distance measure and frequency-based update method

HOW TO SELECT K?

- Plot objective function (i.e., within cluster error) as a function of K, and look for "elbow" in plot



K-MEANS SUMMARY

- Knowledge representation
  - K clusters are defined by canonical members (e.g., centroids)
- Model space the algorithm searches over?
  - All possible partitions of the examples into k groups
- Scoring function?
  - Minimize within-cluster Euclidean distance
- Search procedure?
  - Iterative refinement correspond to greedy hill-climbing