CS57300
PURDUE UNIVERSITY

NOVEMBER 8, 2021

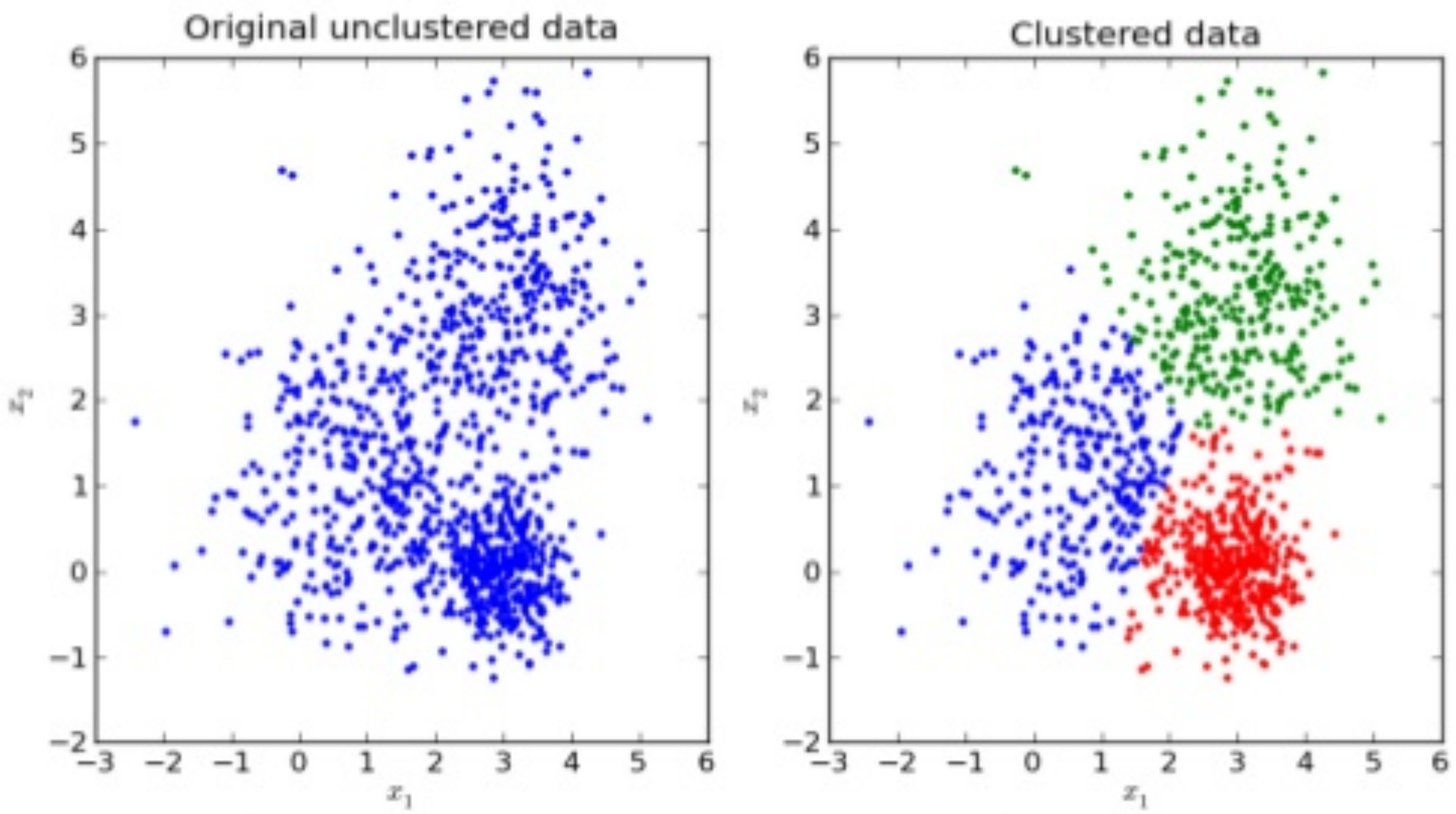
DATA MINING

DESCRIPTIVE MODELING

DATA MINING COMPONENTS

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

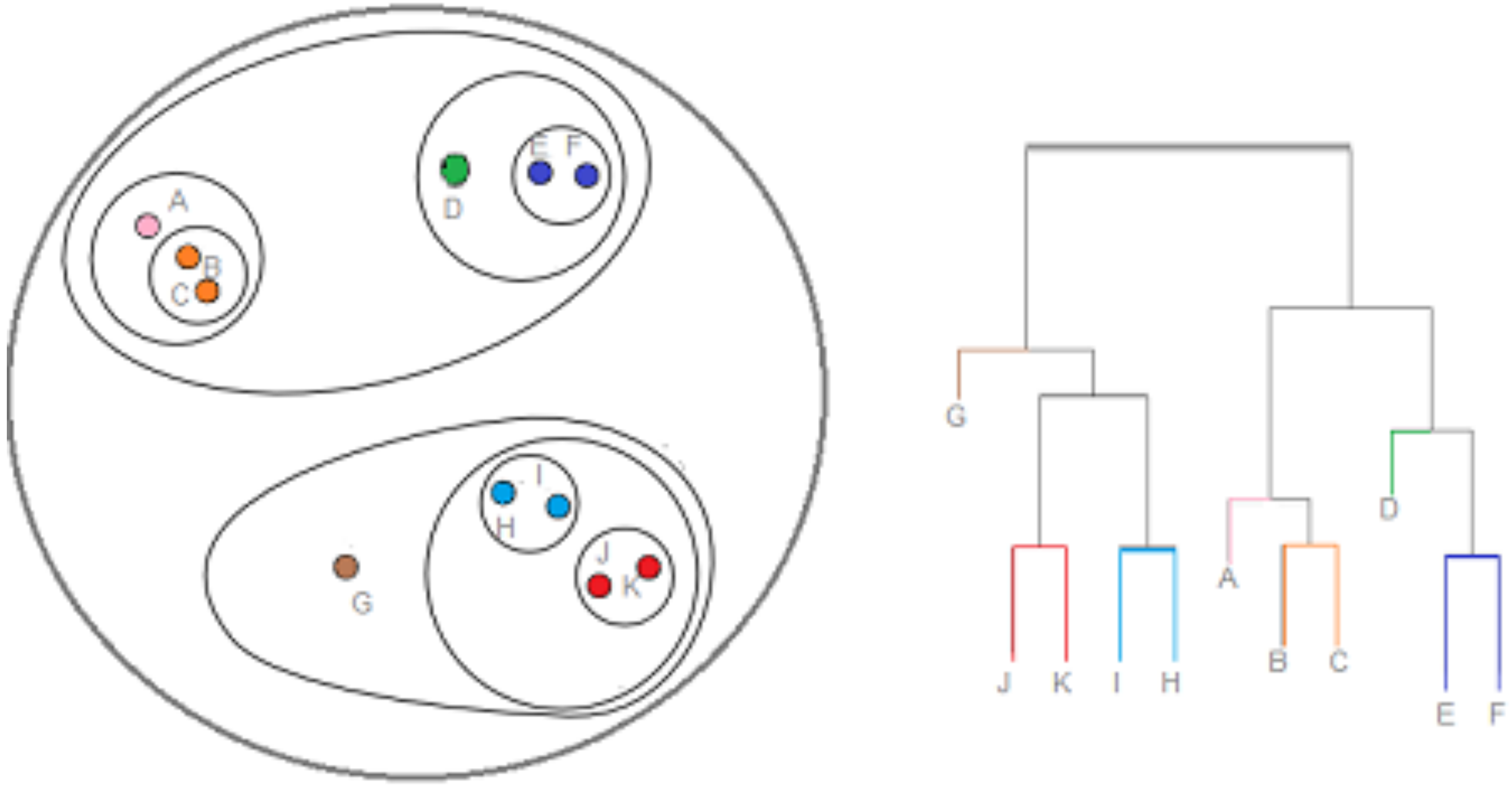
PARTITION-BASED CLUSTERING



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

Model space:
all possible assignments of data instance to group

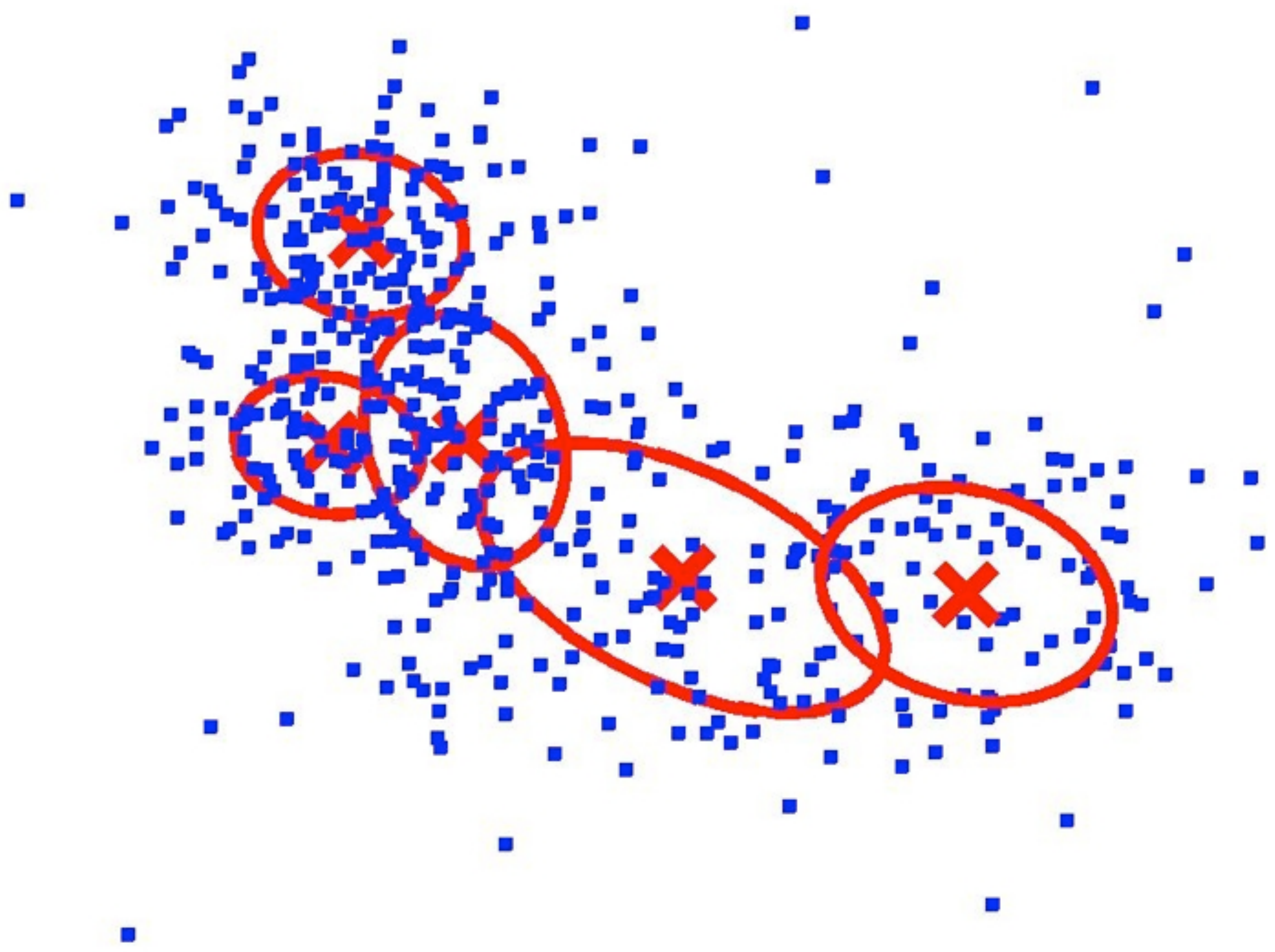
HIERARCHICAL CLUSTERING



- 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 $f_k(x;\theta)$

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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

- 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

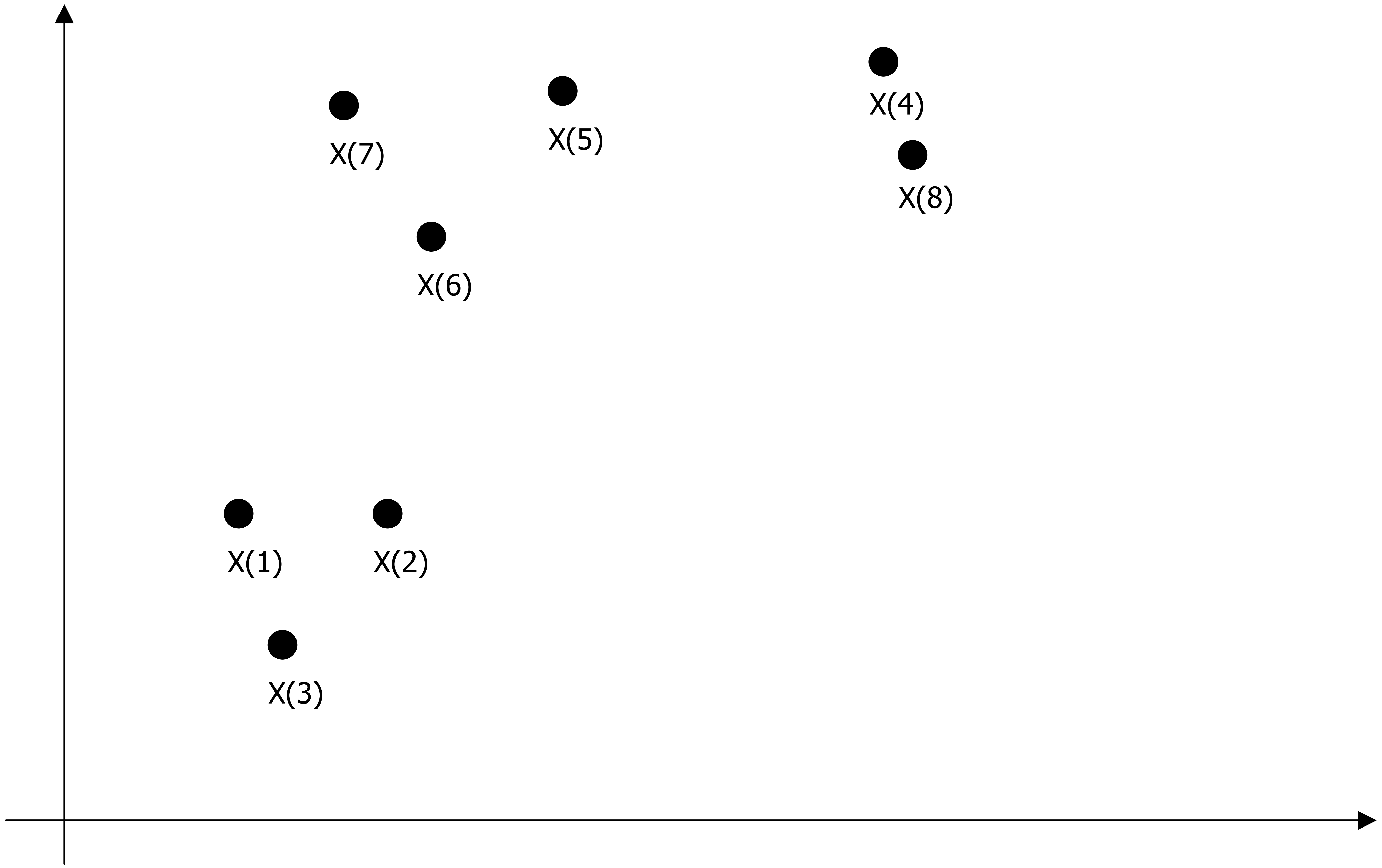
PARTITION-BASED CLUSTERING

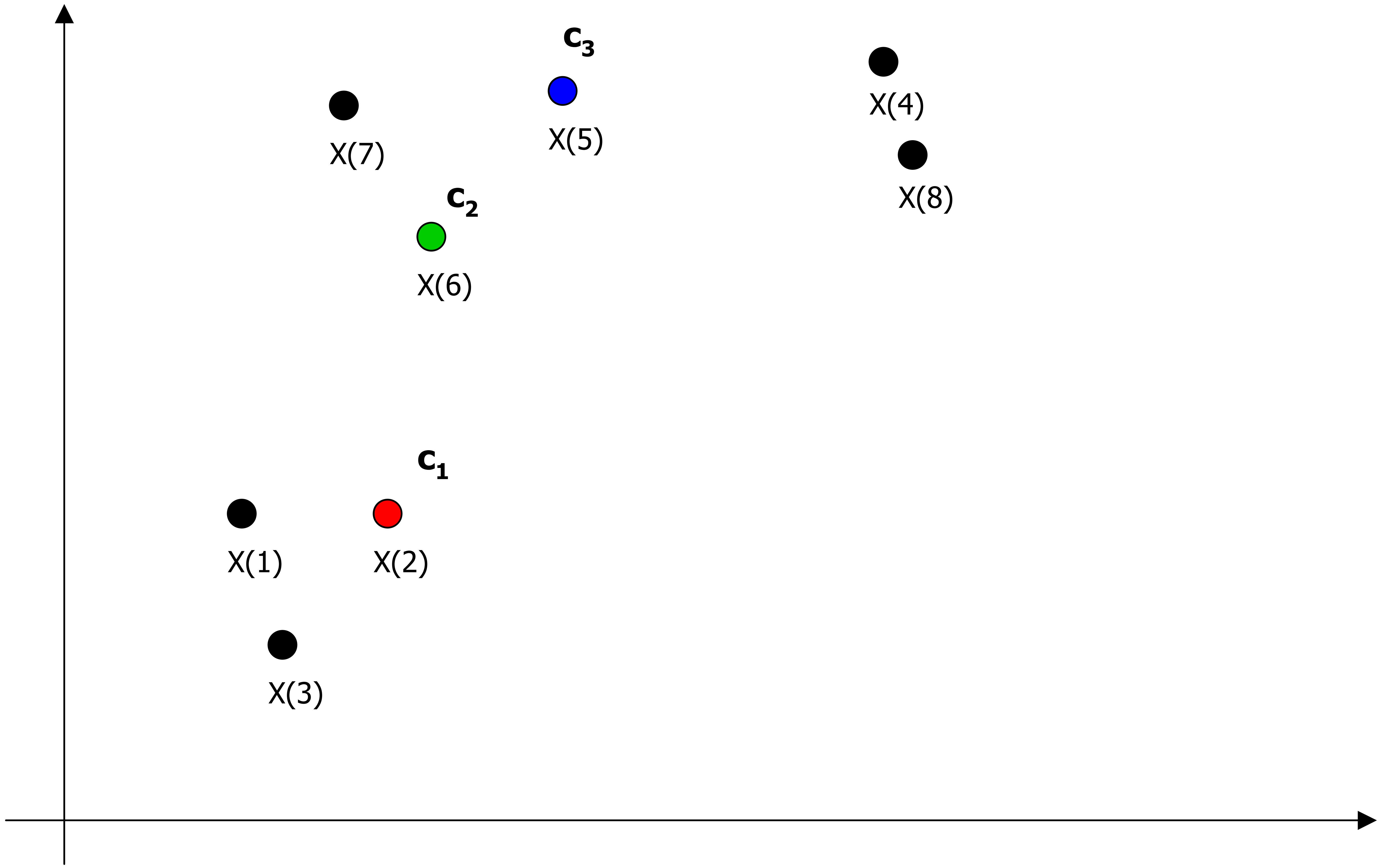
PARTITION-BASED

- 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

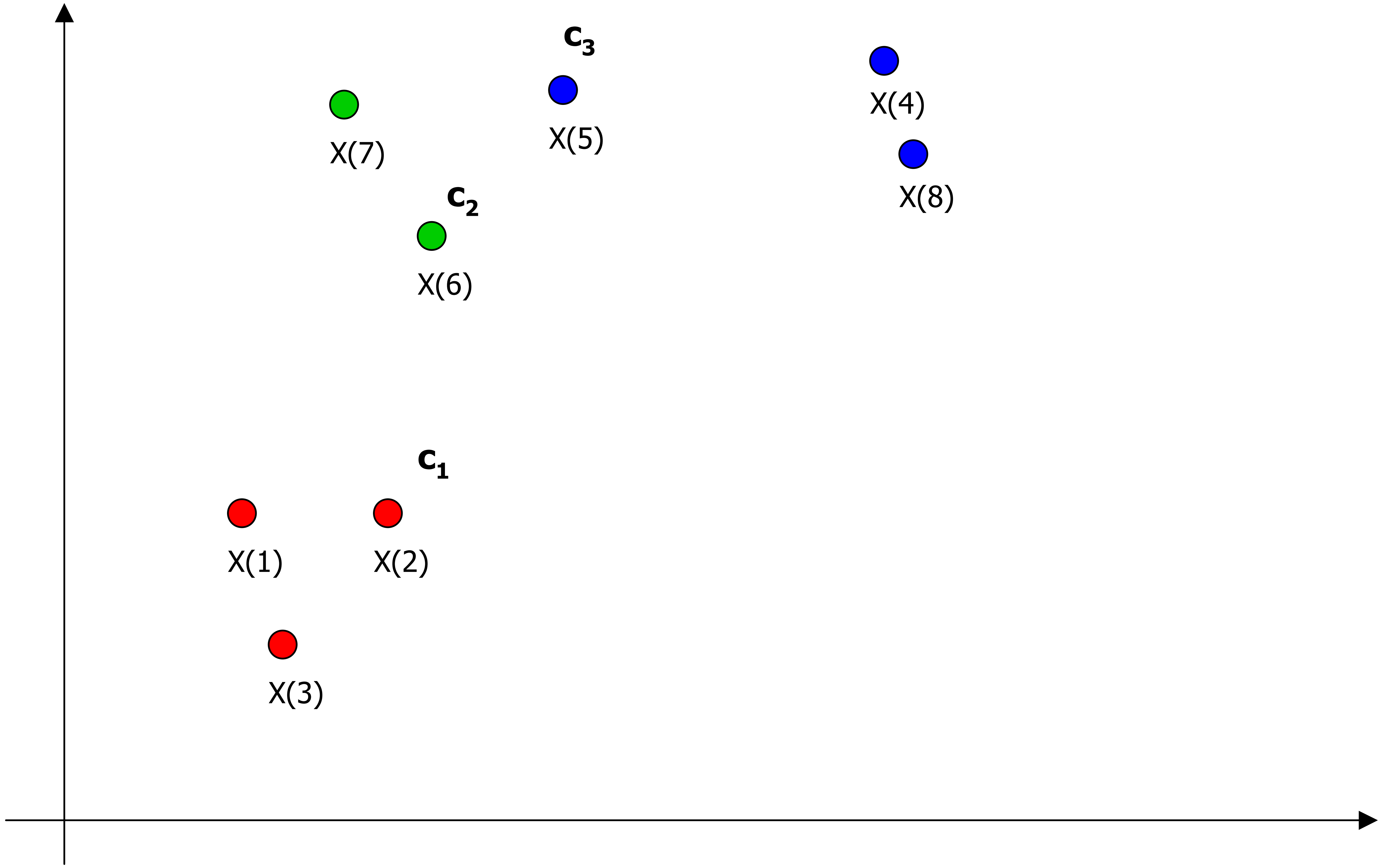
EXAMPLE: K-MEANS

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

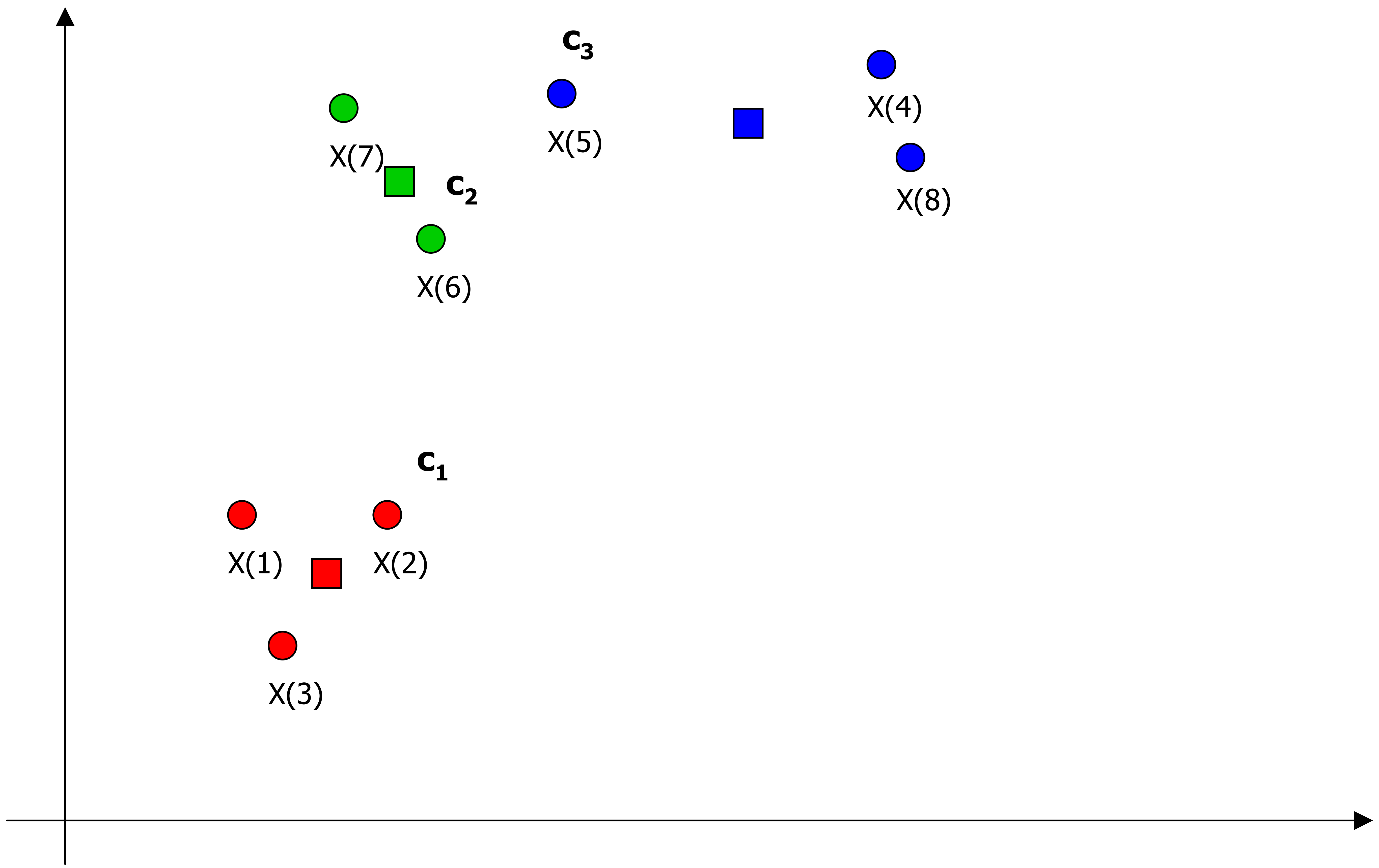

X(4)
X(7)
X(5)
X(8)
X(6)
X(1)
X(2)
X(3)



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



c_3
X(4)
X(7)
X(5)
X(8)
c_2
X(6)
c_1
X(1)
X(2)
X(3)



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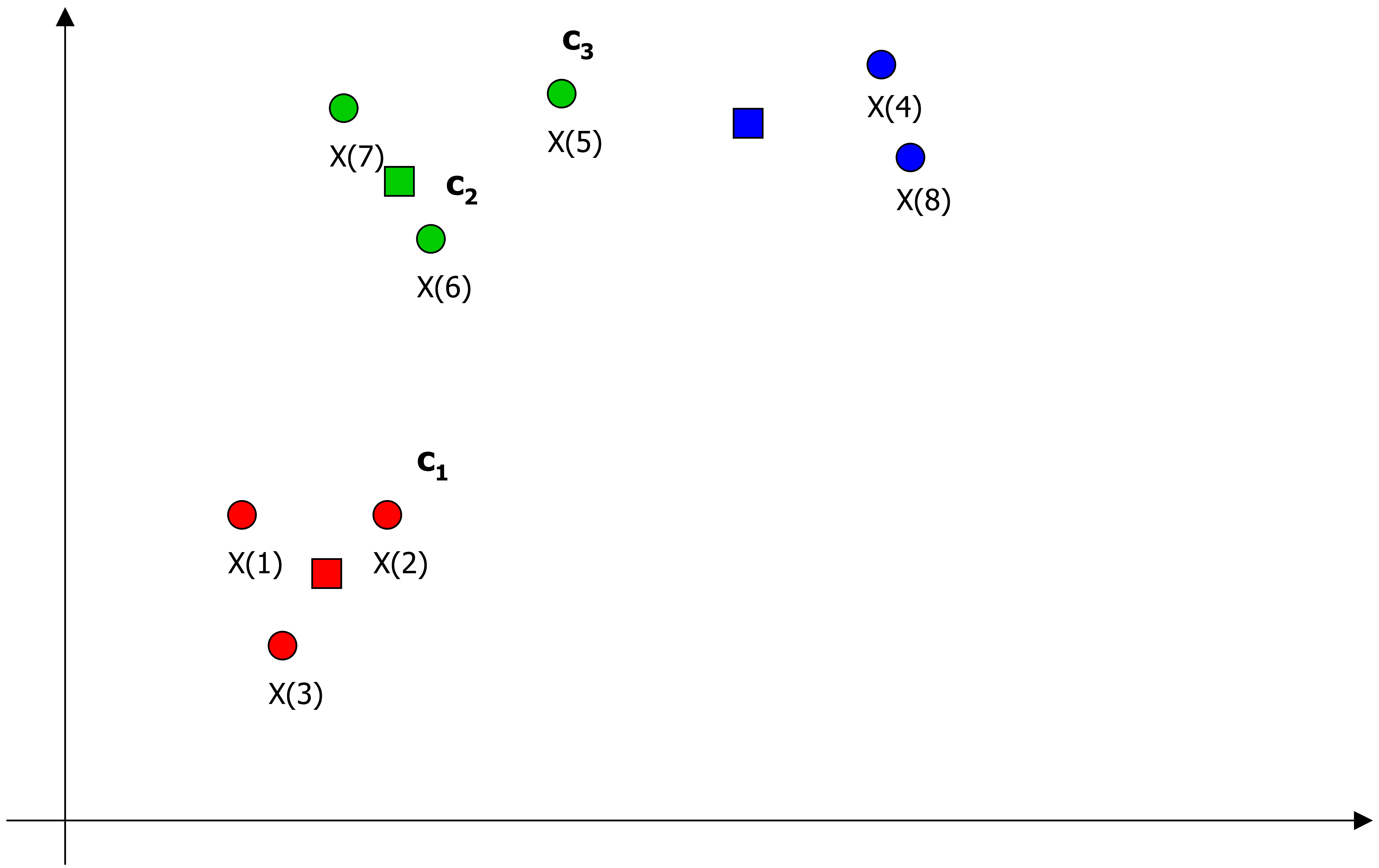
c1
X(1)
X(2)
X(3)


c3
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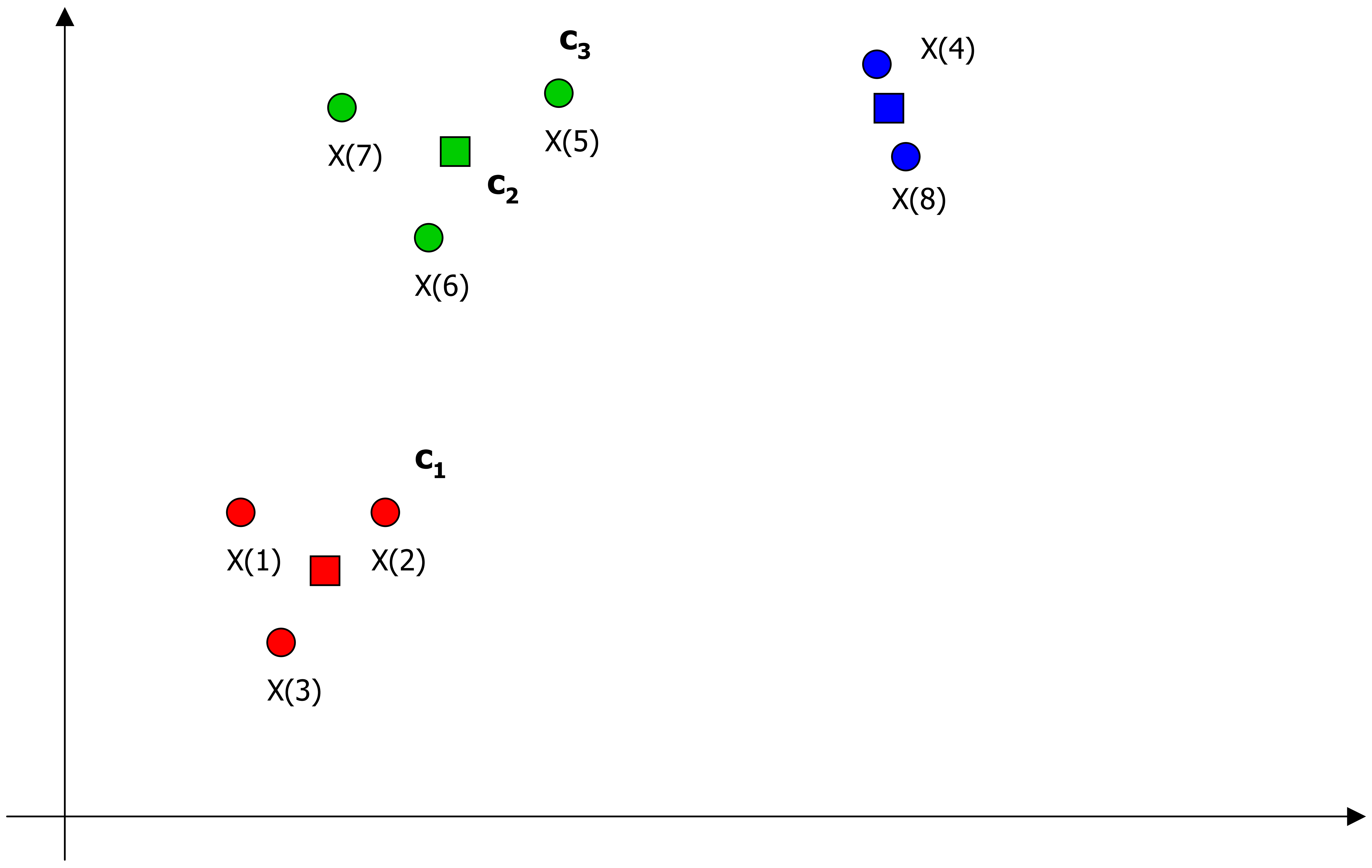

c3
X(4)
X(7)
X(5)
c2
X(8)
X(6)
c1
X(1)
X(2)
X(3)

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

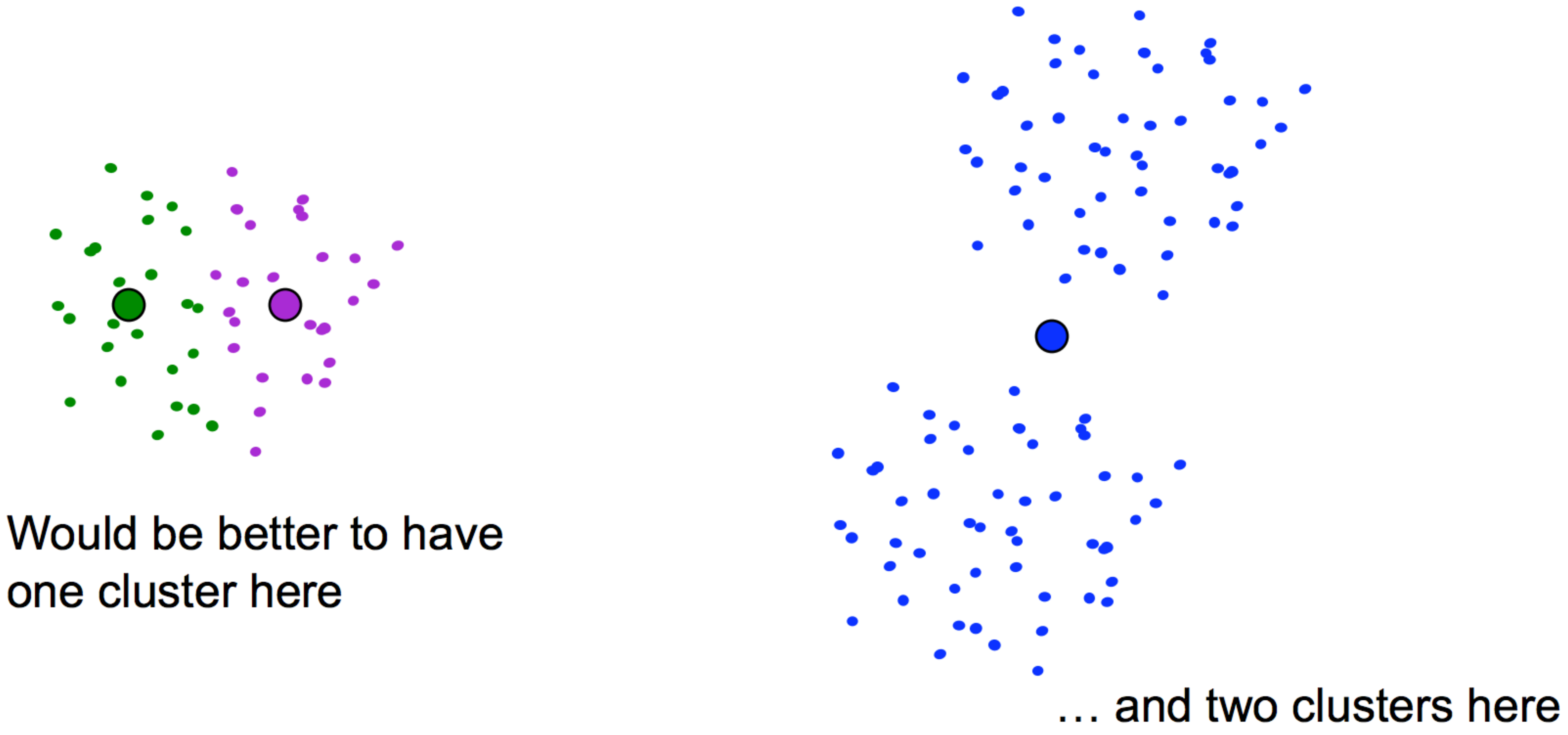
- An alternating optimization approach
  - Fix r_k, optimize for membership of C(x(i)): $min \sum_{i=1}^{N} (x(i) - r_{C(x(i))})^2$
  - Fix C(x(i)), optimize for r_k: $min_{r_k} \sum_{i=1}^{N} (x(i) - r_{C(x(i))})^2 = \sum_{k=1}^{K} \sum_{x \in C_k} (x - r_k)^2$
    - Take derivative with respect to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

A local optimum:



K-MEANS

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