Unsupervised Learning: Clustering

K-means, Hierarchical Clustering, DBSCAN, and Evaluation Metrics

Sarwan Ali

Department of Computer Science
Georgia State University

Understanding Clustering

Today's Learning Journey

What is Unsupervised Learning?

Definition: Learning patterns from data without labeled examples

Supervised Learning:

- Has target labels
- Goal: Predict outcomes
- Examples: Classification, Regression

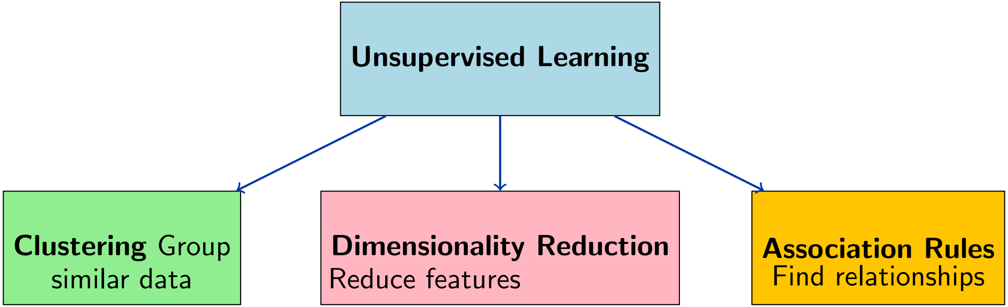
Unsupervised Learning:

- No target labels
- Goal: Discover hidden patterns
- Examples: Clustering, Dimensionality Reduction

Key Insight

Unsupervised learning helps us understand the **structure** and **relationships** within data

Types of Unsupervised Learning



Today's Focus: Clustering - grouping similar data points together

What is Clustering?

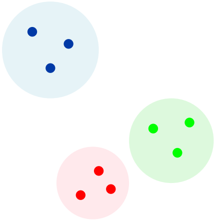
Definition: Partitioning data into groups (clusters) where:

- Points within a cluster are similar
- Points in different clusters are dissimilar

Applications:

- Customer segmentation
- Gene sequencing
- Image segmentation
- Social network analysis
- Market research

Clustered Data



How do we measure similarity? Through distance metrics!

1. **Euclidean Distance:**

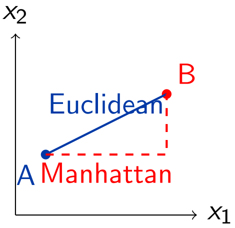
$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

2. **Manhattan Distance:**

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i|$$

3. **Cosine Similarity:** $\text{sim}(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x} \cdot \mathbf{y}}{|\mathbf{x}||\mathbf{y}|}$

Distance Visualization



Key Point

Choice of distance metric significantly affects clustering results!

K-Means Algorithm Overview

Goal: Partition n data points into k clusters

Key Idea: Minimize within-cluster sum of squares (WCSS)

$$\text{WCSS} = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} |\mathbf{x} - \boldsymbol{\mu}_i|^2$$

where C_i is cluster i and $\boldsymbol{\mu}_i$ is the centroid of cluster i.

Advantages:

- Simple and fast
- Works well with spherical clusters
- Scales well to large datasets

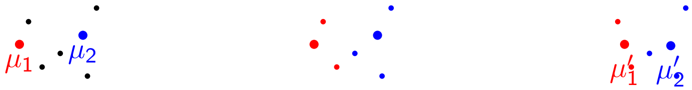
Disadvantages:

- Need to specify k
- Sensitive to initialization
- Assumes spherical clusters

K-Means Algorithm Steps

1. **Initialize:** Choose k and randomly place k centroids
2. **Assign:** Assign each point to nearest centroid
3. **Update:** Move centroids to center of assigned points
4. **Repeat:** Steps 2-3 until convergence

Step 1: Initialize **Step 2: Assign** **Step 3: Update**



K-Means: Mathematical Formulation

Objective Function:

$$J = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} |\mathbf{x} - \boldsymbol{\mu}_i|^2$$

Centroid Update Rule:

$$\boldsymbol{\mu}_i = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \mathbf{x}$$

Assignment Rule:

$$C_i = \{\mathbf{x} : |\mathbf{x} - \boldsymbol{\mu}_i| \leq |\mathbf{x} - \boldsymbol{\mu}_j| \text{ for all } j\}$$

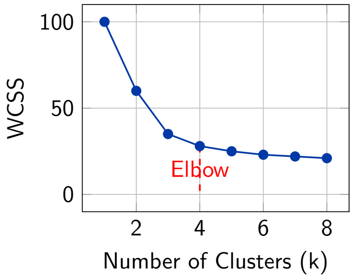
Convergence

Algorithm converges when centroids stop moving or maximum iterations reached

Choosing the Right K

The Elbow Method:

1. Run K-means for different values of k
2. Plot WCSS vs k
3. Look for the "elbow" point
4. Choose k at the elbow



Other Methods:

- Silhouette analysis
- Gap statistic
- Domain knowledge

Hierarchical Clustering Overview

Builds a hierarchy of clusters without specifying k in advance

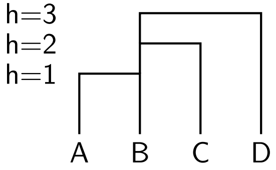
Agglomerative (Bottom-up):

- Start: Each point is a cluster
- Iteratively merge closest clusters
- End: One big cluster

Divisive (Top-down):

- Start: All points in one cluster
- Iteratively split clusters
- End: Each point is a cluster

Dendrogram



Key Advantage

Produces a complete clustering hierarchy - can choose any number of clusters

Linkage Criteria

How do we measure distance between clusters?

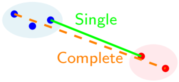
1. **Single Linkage (MIN):**

$$d(C_i, C_j) = \min_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

2. **Complete Linkage (MAX):**

$$d(C_i, C_j) = \max_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

Linkage Types



3. **Average Linkage:**

$$d(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{\mathbf{x} \in C_i} \sum_{\mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$

- **Single:** Tends to create elongated clusters (chaining effect)
- **Complete:** Creates compact, spherical clusters
- **Average:** Balanced approach

Hierarchical Clustering Algorithm

Agglomerative Clustering Steps:

1. Start with n clusters (each point is a cluster)
2. Compute distance matrix between all pairs of clusters
3. Merge the two closest clusters
4. Update distance matrix
5. Repeat until one cluster remains

Time Complexity: $O(n^3)$ - expensive for large datasets

Example: Distance Matrix Update

When merging clusters C_i and C_j into C_{ij}:

$$d(C_{ij}, C_k) = \alpha_i d(C_i, C_k) + \alpha_j d(C_j, C_k) + \beta d(C_i, C_j) + \gamma |d(C_i, C_k) - d(C_j, C_k)|$$

Different linkage criteria use different values of $\alpha_i, \alpha_j, \beta, \gamma$

Density-Based Spatial Clustering of Applications with Noise

Key Idea: Clusters are dense regions separated by sparse regions

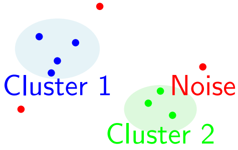
Parameters:

- ϵ (eps): Maximum distance for neighborhood
- MinPts: Minimum points to form dense region

Advantages:

- Finds arbitrary shaped clusters
- Handles noise and outliers
- No need to specify number of clusters

DBSCAN Result

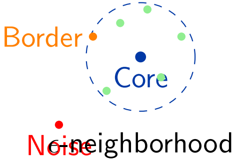


DBSCAN: Point Classifications

Three types of points:

1. **Core Points:**
    - Have at least MinPts points in ϵ-neighborhood
    - Form the "interior" of clusters
2. **Border Points:**
    - Have fewer than MinPts neighbors
    - But are in neighborhood of core point
3. **Noise Points:**
    - Neither core nor border points
    - Considered outliers

Point Types



Density Connectivity

Two points belong to same cluster if there's a path of core points between them

DBSCAN Algorithm

Algorithm Steps:

1. For each unvisited point p:
   1. Mark p as visited
   2. Find all points in ϵ-neighborhood of p
   3. If neighborhood has $\geq$ MinPts points:
      1. Mark p as core point
      2. Create new cluster with p
      3. Add all density-reachable points to cluster
   4. Else if p is in neighborhood of core point: mark as border
   5. Else: mark p as noise

Time Complexity: $O(n \log n)$ with spatial indexing, $O(n^2)$ without

Parameter Selection

- MinPts: Usually set to $2 \times$ dimensions
- ϵ: Use k-distance graph (elbow method)

Why Evaluate Clustering?

Challenge: No ground truth labels in unsupervised learning

Two Types of Evaluation:

Internal Measures:

- Use only the data itself
- Measure cluster cohesion and separation
- Examples: Silhouette, Davies-Bouldin

External Measures:

- Compare with ground truth (if available)
- Measure agreement with true clusters
- Examples: ARI, NMI, Purity

Goal

Find clustering that maximizes intra-cluster similarity and minimizes inter-cluster similarity

Silhouette Analysis

Most popular internal clustering evaluation metric

For each point i:

- $a(i)$ = average distance to points in same cluster
- $b(i)$ = average distance to points in nearest cluster

Silhouette coefficient:

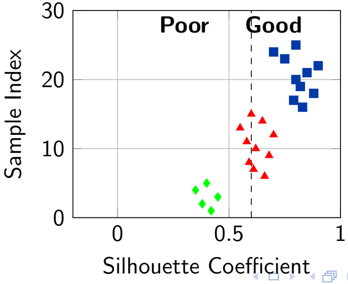
$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

Interpretation:

- $s(i) \approx 1$: Well clustered
- $s(i) \approx 0$: On cluster boundary
- $s(i) \approx -1$: Poorly clustered

Overall Score:

$$\text{Silhouette} = \frac{1}{n}\sum_{i=1}^{n} s(i)$$



Davies-Bouldin Index

Measures average similarity between clusters

For clusters i and j:

$$R_{ij} = \frac{S_i + S_j}{M_{ij}}$$

where:

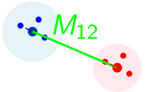
- S_i = average distance from points in cluster i to centroid
- M_{ij} = distance between centroids of clusters i and j

Davies-Bouldin Index:

$$DB = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} R_{ij}$$

Properties:

- Lower values indicate better clustering
- Range: $[0, \infty)$
- Considers both cohesion and separation



DB Components

External Evaluation Metrics

When ground truth labels are available

1. **Adjusted Rand Index (ARI):**

$$ARI = \frac{\text{RI} - E[\text{RI}]}{\max(\text{RI}) - E[\text{RI}]}$$

   - Range: $[-1, 1]$, higher is better
   - Adjusts for chance agreement

2. **Normalized Mutual Information (NMI):**

$$NMI = \frac{2 \times MI(C, T)}{H(C) + H(T)}$$

   - Range: $[0, 1]$, higher is better
   - Based on information theory

3. **Purity:** $\text{Purity} = \frac{1}{n} \sum_{i=1}^{k} \max_j |C_i \cap T_j|$
   - Range: $[0, 1]$, higher is better
   - Simple but biased toward many clusters

Algorithm Comparison

Algorithm	Advantages	Disadvantages	Time	Clusters	Best For
K-Means	Simple, Fast, Scalable	Need to specify k, Spherical clusters	$O(nkt)$	Spherical	Large datasets
Hierarchical	No k needed, Hierarchy	Expensive, Sensitive to noise	$O(n^3)$	Any shape	Small datasets, Hierarchy
DBSCAN	Arbitrary shapes, Handles noise	Parameter sensitive	$O(n \log n)$	Any shape	Irregular clusters

Selection Guidelines:

- **Dataset size:** K-means for large, Hierarchical for small
- **Cluster shape:** K-means for spherical, DBSCAN for irregular
- **Noise tolerance:** DBSCAN best, K-means worst
- **Parameter sensitivity:** Hierarchical least, DBSCAN most

Data Preprocessing for Clustering

Critical preprocessing steps:

1. **Feature Scaling:**
   - Min-Max: $x' = \frac{x - \min}{\max - \min}$
   - Z-score: $x' = \frac{x - \mu}{\sigma}$
   - Robust: $x' = \frac{x - \text{median}}{IQR}$
2. **Handle Missing Values:**
   - Remove incomplete records
   - Impute with mean/median/mode
   - Use algorithms that handle missing data
3. **Dimensionality Reduction:**
   - PCA for linear relationships
   - t-SNE for visualization
   - Feature selection methods
4. **Outlier Detection:**
   - Statistical methods (Z-score, IQR)
   - Distance-based methods
   - Consider domain knowledge

Warning

Different preprocessing can lead to completely different clustering results!

Common Pitfalls and Best Practices

Common Pitfalls:

- Not scaling features
- Using wrong distance metric
- Poor parameter selection
- Ignoring domain knowledge
- Over-interpreting results
- Not validating clusters

Best Practices:

- Always scale your data
- Try multiple algorithms
- Use multiple evaluation metrics
- Visualize results when possible
- Validate with domain experts
- Document parameter choices

Validation Strategy

1. Internal metrics (Silhouette, DB Index)
2. Visual inspection (when possible)
3. Domain expert validation
4. Stability analysis (multiple runs)
5. External validation (if labels available)

Clustering Applications

Business & Marketing:

- Customer segmentation
- Market basket analysis
- Recommendation systems
- Fraud detection

Biology & Medicine:

- Gene expression analysis
- Drug discovery
- Medical image segmentation
- Disease classification

Technology:

- Image segmentation
- Social network analysis
- Web search results
- Anomaly detection

Science & Research:

- Astronomy (star classification)
- Climate modeling
- Ecology (species grouping)
- Psychology (behavioral patterns)

Key Success Factor

Understanding the domain and having clear objectives for clustering

Case Study: Customer Segmentation

Problem: E-commerce company wants to segment customers for targeted marketing

Data: Customer purchase history, demographics, website behavior

Approach:

1. **Feature Engineering:** RFM analysis (Recency, Frequency, Monetary)
2. **Preprocessing:** Scale features, handle missing values
3. **Algorithm Selection:** Try K-means, Hierarchical, DBSCAN
4. **Evaluation:** Silhouette analysis, business metrics
5. **Interpretation:** Profile each segment

Results:

- High-value customers (10%)
- Regular customers (45%)
- Occasional buyers (35%)
- At-risk customers (10%)

Business Impact:

- Personalized marketing
- Retention campaigns
- Product recommendations
- Resource allocation

Summary

What we learned today:

1. **Unsupervised Learning:** Finding patterns without labels
2. **K-Means:** Fast, simple, works well for spherical clusters
3. **Hierarchical:** Creates cluster hierarchy, expensive but flexible
4. **DBSCAN:** Handles noise and arbitrary shapes
5. **Evaluation:** Internal (Silhouette, DB) and External (ARI, NMI) metrics

Key Principles:

- No single "best" clustering algorithm
- Preprocessing is crucial
- Always validate results
- Domain knowledge is essential
- Multiple metrics provide better insight

Remember

Clustering is exploratory - the goal is to discover meaningful patterns that provide actionable insights

Next Steps

To master clustering:

Practice:

- Implement algorithms from scratch
- Work with real datasets
- Experiment with different parameters
- Compare algorithm performance

Advanced Topics:

- Spectral clustering
- Gaussian mixture models
- Fuzzy clustering
- Online clustering

Tools & Libraries:

- scikit-learn (Python)
- cluster (R)
- WEKA (Java)
- Apache Spark MLlib

Resources:

- "Pattern Recognition and Machine Learning" - Bishop
- "The Elements of Statistical Learning" - Hastie et al.
- Online courses and tutorials
- Kaggle competitions

Thank You!

Questions & Discussion

Remember: Clustering is an art as much as it is a science

sali85@student.gsu.edu