Cluster Analysis

Discovering Natural Groupings in Data

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Today's Agenda

1. Introduction to Cluster Analysis
2. Distance and Similarity Measures
3. Hierarchical Clustering Methods
4. K-Means and Non-Hierarchical Methods
5. Determining Optimal Number of Clusters
6. Validation Techniques
7. Practical Considerations
8. Applications and Best Practices

What is Cluster Analysis?

Definition: An exploratory technique to discover natural groupings in data **without predefined categories**

What is Cluster Analysis?

Key Characteristics:

- Unsupervised learning method
- No training labels required
- Discovers hidden structure in data
- Groups similar observations together

Goal: Maximize within-cluster similarity and between-cluster dissimilarity

Cluster Analysis vs. Discriminant Analysis

Cluster Analysis	Discriminant Analysis
Unsupervised learning	Supervised learning
Discovers unknown groups	Classifies into known groups
No training labels	Requires training labels
Exploratory	Predictive
Groups observations	Creates decision boundaries

Applications: Marketing & Business

Marketing

- Customer segmentation for targeted campaigns
- Market basket analysis

Business

- Fraud detection
- Anomaly identification

Applications: Science & Healthcare

Biology & Medicine

- Disease subtype identification
- Gene expression analysis

Social Sciences

- Community detection in networks
- Document clustering

Distance and Similarity Measures

Why Distance Matters

Clustering depends on measuring how “close” observations are to each other

Common Distance Metrics

1. **Euclidean Distance** (L2 norm) - Most common
2. **Manhattan Distance** (L1 norm) - Robust to outliers
3. **Cosine Similarity** - For high-dimensional data
4. **Correlation Distance** - Pattern similarity

Euclidean Distance

Formula:

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

Euclidean Distance

Properties:

- Straight-line distance in n-dimensional space
- Sensitive to scale differences
- Assumes equal importance of all dimensions

Warning: Always standardize variables with different scales!

Manhattan Distance

Formula:

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

Manhattan Distance

When to Use:

- Data contains outliers or extreme values
- Variables represent counts
- High-dimensional spaces

Advantage: More robust than Euclidean distance

Why Standardization is Critical

Problem: Variables on different scales dominate distance calculations

Example:

- Age: 20-80 years
- Income: 20,000-200,000 dollars

Without standardization, income dominates!

Z-score Standardization

Solution: Z-score Standardization

$$z_i = \frac{x_i - \mu}{\sigma}$$

Transform to mean = 0, standard deviation = 1

Hierarchical Clustering

Builds a tree-like structure (dendrogram) showing nested clusters

Two Approaches

Agglomerative (Bottom-Up): Most common

- Start: Each observation is its own cluster
- Process: Merge closest clusters iteratively
- End: All observations in one cluster

Two Approaches

Divisive (Top-Down): Less common

- Start: All observations in one cluster
- Process: Split most heterogeneous cluster
- End: Each observation is its own cluster

Linkage Methods

How to Measure Distance Between Clusters?

Single Linkage (Nearest Neighbor)

$$d(C_1, C_2) = \min_{x \in C_1, y \in C_2} d(x, y)$$

Distance between closest points in the two clusters

Complete Linkage (Farthest Neighbor)

$$d(C_1, C_2) = \max_{x \in C_1, y \in C_2} d(x, y)$$

Distance between farthest points in the two clusters

Average Linkage

$$d(C_1, C_2) = \frac{1}{n_1 n_2} \sum_{x \in C_1} \sum_{y \in C_2} d(x, y)$$

Average distance between all pairs of points

Ward's Method

Ward's Method

Minimizes within-cluster sum of squares

Tends to produce compact, equal-sized clusters

Linkage Methods Comparison

Method	Outlier Sensitivity	Cluster Shape
Single Linkage	High	Elongated (chaining)
Complete Linkage	Low	Compact, spherical
Average Linkage	Medium	Balanced
Ward's Method	Medium	Compact, equal-sized

Linkage Methods Comparison

Recommendation: Ward's method often works best in practice

Dendrograms

Visualizing Hierarchical Structure

Reading a Dendrogram

- Horizontal axis: Observations or clusters
- Vertical axis: Distance at which clusters merge
- Height of branches: Dissimilarity between merged clusters

Determining Number of Clusters

- Look for large vertical gaps (jumps in fusion distance)
- Cut dendrogram where there's substantial increase
- Draw horizontal line: number of vertical lines crossed = k clusters

The Chaining Effect

Problem with Single Linkage:

Clusters form long, elongated chains rather than compact groups

The Chaining Effect

Why it Happens:

- Observations connect via intermediate points
- A-B-C-D form chain where each is close to neighbor
- But A and D are far apart

The Chaining Effect

Solution:

- Use complete or average linkage instead
- Or Ward's method for compact clusters

K-Means Clustering

Most popular non-hierarchical method

K-Means Algorithm

1. **Initialize:** Select k random observations as centroids
2. **Assignment:** Assign each point to nearest centroid
3. **Update:** Recalculate centroids as cluster means
4. **Repeat:** Steps 2-3 until convergence

Convergence: When assignments no longer change between iterations

K-Means Objective Function

Goal: Minimize within-cluster sum of squares (WCSS)

$$\min \sum_{i=1}^{k} \sum_{x \in C_i} \|x - \mu_i\|^2$$

where μ_i is the centroid of cluster C_i

K-Means Properties

- Always converges (finite partitions, monotonically decreasing WCSS)
- Typically converges in 10-30 iterations
- Fast: O(n times k times p times iterations)

K-Means: Advantages

- Fast and scalable to large datasets
- Simple to understand and implement
- Efficient for exploratory analysis

K-Means: Limitations

- Requires specifying k in advance
- Sensitive to initialization (different starts $\longrightarrow$ different results)
- Assumes spherical clusters
- Sensitive to outliers
- Tends to create equal-sized clusters

K-Means++ Initialization

Problem: Random initialization can lead to poor results

K-Means++ Algorithm

1. Choose first centroid randomly
2. For each subsequent centroid:
   - Choose point with probability proportional to squared distance from nearest existing centroid
3. Repeat until k centroids selected

Benefit: Spreads out initial centroids, significantly improves results

K-Medoids (PAM)

Key Difference from K-Means:

- K-means: Centers are computed means (may not be actual points)
- K-medoids: Centers are actual data points (medoids)

K-Medoids (PAM)

Advantages:

- More robust to outliers
- Works with any distance metric
- Interpretable centers (actual observations)

Disadvantage: Slower than k-means (higher computational cost)

How Many Clusters?

The Fundamental Challenge:

No “ground truth” for correct number of clusters

Multiple Approaches

1. **Elbow Method** - Look for bend in WCSS plot
2. **Silhouette Analysis** - Measure cluster quality
3. **Gap Statistic** - Compare to null reference
4. **Davies-Bouldin Index** - Ratio of compactness to separation
5. **Domain Knowledge** - Business requirements

Elbow Method: Procedure

1. Run clustering for k = 1, 2, 3, …, K_max
2. Calculate WCSS for each k
3. Plot WCSS vs. k
4. Look for “elbow” - diminishing returns point

Elbow Method: Interpretation

- WCSS always decreases as k increases
- Elbow indicates where additional clusters don't help much
- Choose k at the elbow point

Limitation: Elbow not always clear - may need other methods

Silhouette Analysis

Measures how well each point fits within its cluster

Silhouette Coefficient

Silhouette Coefficient for observation i:

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

where:

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

Silhouette Interpretation

- $s(i) \approx +1$: Well-matched to cluster
- $s(i) \approx 0$: On border between clusters
- $s(i) \approx -1$: Likely in wrong cluster

Using Silhouette for Optimal k

Average Silhouette Width:

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

Silhouette Procedure

1. Run clustering for different k values
2. Calculate average silhouette width for each k
3. Choose k that maximizes $\bar{s}$

Advantage: Provides both quality measure and optimal k

Cluster Validation

Internal Validation (using data only):

- Within-Cluster Sum of Squares (WCSS) - lower is better
- Silhouette Coefficient - higher is better
- Davies-Bouldin Index - lower is better
- Dunn Index - higher is better

Cluster Validation

External Validation (when true labels available):

- Adjusted Rand Index (ARI)
- Normalized Mutual Information (NMI)

Davies-Bouldin Index

Measures ratio of within-cluster dispersion to between-cluster separation

$$\mathrm{DB} = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} \left(\frac{\sigma_i + \sigma_j}{d(c_i, c_j)} \right)$$

Davies-Bouldin Index

Interpretation:

- Lower values indicate better clustering
- Compact clusters that are far apart
- Can compare different k values or methods

Curse of Dimensionality

As dimensions (p) increase, problems arise

Curse of Dimensionality: Problems

1. Distance becomes less meaningful (all points appear equidistant)
2. Data becomes sparse (observations spread out)
3. Computational cost increases dramatically

Curse of Dimensionality: Solutions

- Use PCA or feature selection before clustering
- Select only relevant variables
- Use specialized high-dimensional algorithms

Rule: If p is large relative to n, reduce dimensions first

Handling Outliers

Impact by Method:

Method	Sensitivity
K-means	High
Ward's Method	High
Single Linkage	Medium
K-medoids	Low (Robust)

Handling Outliers: Strategies

- Pre-processing: Detect and remove outliers
- Use robust methods (k-medoids)
- Accept outlier clusters

When to Use Hierarchical Clustering

- Small to medium datasets (n < 5,000)
- Want to explore different k values
- Need hierarchical structure
- Don’t know k in advance

When to Use K-Means

- Large datasets (n > 5,000)
- Approximately know k
- Need speed and efficiency
- Clusters roughly spherical

Cluster Analysis Workflow

1. **Define objective** - What questions to answer?
2. **Select variables** - Domain knowledge
3. **Preprocess data** - Handle missing values, outliers
4. **Standardize** - If variables on different scales
5. **Choose method** - Based on data characteristics

Cluster Analysis Workflow

6. **Determine k** - Multiple criteria
7. **Run clustering** - Multiple times for k-means
8. **Validate results** - Internal and stability checks
9. **Interpret clusters** - Profile and name clusters
10. **Refine and iterate** - Based on insights

Common Pitfalls to Avoid

1. **Not standardizing** when variables have different scales
2. **Using k-means** with non-spherical clusters
3. **Ignoring outliers** - can severely distort results
4. **Over-interpreting** - clustering always finds structure, even in random data

Common Pitfalls to Avoid

5. **Using too many variables** - curse of dimensionality
6. **Running k-means once** - try multiple initializations
7. **Choosing k without validation** - use multiple methods

Best Practices

1. **Try multiple methods** - Compare hierarchical, k-means, etc.
2. **Validate stability** - Bootstrap samples, different initializations
3. **Visualize extensively** - Scatter plots, dendrograms, parallel coordinates

Best Practices

4. **Use domain knowledge** - Statistical metrics + practical sense
5. **Document decisions** - Why certain methods, parameters chosen
6. **Check interpretability** - Can you explain and use clusters?

Key Takeaways: Fundamental Concepts

- Cluster analysis discovers natural groupings (unsupervised)
- Distance measures are crucial (Euclidean, Manhattan)
- Standardization essential for different scales

Key Takeaways: Methods

- Hierarchical: Creates tree structure, multiple k values
- K-means: Fast, scalable, requires specifying k
- K-medoids: Robust alternative to k-means

Key Takeaways: Validation

- Elbow method and silhouette analysis for optimal k
- Multiple validation measures for quality assessment

Summary: Method Selection Guide

Situation	Recommended Method
Small dataset (n < 1,000)	Hierarchical (Ward's or Average)
Large dataset (n > 10,000)	K-means with k-means++
Outliers present	K-medoids or preprocessing
Non-spherical clusters	DBSCAN or hierarchical

Summary: Method Selection Guide

Situation	Recommended Method
Don't know k	Hierarchical, then elbow/silhouette
High dimensions	PCA first, then k-means
Mixed data types	Gower distance with hierarchical

Advanced Topics (Beyond This Course)

Density-Based Methods:

- DBSCAN - finds arbitrary shapes, identifies outliers

Model-Based:

- Gaussian Mixture Models (GMM) - probabilistic approach

Advanced Topics (Beyond This Course)

Fuzzy Clustering:

- Soft assignment (membership degrees)

Subspace Clustering:

- For high-dimensional data, different subspaces

Real-World Applications: Business

Marketing & Business:

- Customer segmentation for targeted marketing
- Product recommendation systems
- Market basket analysis

Real-World Applications: Healthcare

Healthcare:

- Patient stratification for personalized medicine
- Disease subtype identification
- Medical image segmentation

Real-World Applications: Finance

Finance:

- Fraud detection and anomaly identification
- Credit risk assessment
- Portfolio diversification

Example: Customer Segmentation

Scenario: E-commerce company with 100,000 customers

Variables:

- Purchase frequency
- Average order value
- Product category preferences
- Time since last purchase
- Customer lifetime value

Example: Customer Segmentation Process

1. Standardize variables (different scales)
2. Try k-means for k = 2 to 10
3. Use elbow method and silhouette analysis
4. Identify k = 5 optimal clusters
5. Profile each segment
6. Develop targeted marketing strategies

Recommended Resources: Books

Textbooks:

- Everitt et al. (2011) - Cluster Analysis (5th ed.)
- James et al. (2021) - Introduction to Statistical Learning

Recommended Resources: Software

Software:

- Python: scikit-learn (KMeans, AgglomerativeClustering)
- R: stats package (kmeans, hclust)

Recommended Resources: Online

Online:

- StatQuest YouTube channel
- Scikit-learn documentation
- Coursera/edX courses on unsupervised learning

Questions?

Thank you for your attention!

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Next Steps: This Week

For This Week:

- Review lecture notes thoroughly
- Practice with provided examples
- Complete practice questions
- Prepare for E06 quiz

Next Steps: Preparation for Evaluation

Preparation for Evaluation:

- Understand distance measures and when to use each
- Know linkage methods and their properties
- Practice interpreting dendrograms
- Understand k-means algorithm and convergence
- Be able to explain validation methods