Clustering

Sarath Chandar

Slides borrowed from
Introduction to Data Mining, 2nd Edition
by
Tan, Steinbach, Karpatne, Kumar
What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups.
Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

- **Summarization**
  - Reduce the size of large data sets

<table>
<thead>
<tr>
<th>Discovered Clusters</th>
<th>Industry Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Technology1-DOWN</td>
</tr>
<tr>
<td>2</td>
<td>Technology2-DOWN</td>
</tr>
<tr>
<td>3</td>
<td>Financial-DOWN</td>
</tr>
<tr>
<td>4</td>
<td>Oil-UP</td>
</tr>
</tbody>
</table>

Clustering precipitation in Australia
What is not Cluster Analysis?

- **Simple segmentation**
  - Dividing students into different registration groups alphabetically, by last name

- **Results of a query**
  - Groupings are a result of an external specification
  - Clustering is a grouping of objects based on the data

- **Supervised classification**
  - Have class label information

- **Association Analysis**
  - Local vs. global connections
Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters
Types of Clusterings

- **A clustering** is a set of clusters

- Important distinction between **hierarchical** and **partitional** sets of clusters

- **Partitional Clustering**
  - A division of data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset

- **Hierarchical clustering**
  - A set of nested clusters organized as a hierarchical tree
Partitional Clustering

Original Points

A Partitional Clustering
Hierarchical Clustering

Traditional Hierarchical Clustering

Non-traditional Hierarchical Clustering

Traditional Dendrogram

Non-traditional Dendrogram
Other Distinctions Between Sets of Clusters

- **Exclusive versus non-exclusive**
  - In non-exclusive clusterings, points may belong to multiple clusters.
  - Can represent multiple classes or ‘border’ points

- **Fuzzy versus non-fuzzy**
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
  - Weights must sum to 1
  - Probabilistic clustering has similar characteristics

- **Partial versus complete**
  - In some cases, we only want to cluster some of the data

- **Heterogeneous versus homogeneous**
  - Clusters of widely different sizes, shapes, and densities
Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function
Types of Clusters: Well-Separated

- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.
Types of Clusters: Center-Based

- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the “center” of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most “representative” point of a cluster

4 center-based clusters
Types of Clusters: Contiguity-Based

- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.
Types of Clusters: Density-Based

- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.

6 density-based clusters
Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.

2 Overlapping Circles
Types of Clusters: Objective Function

- Clusters Defined by an Objective Function
  - Finds clusters that minimize or maximize an objective function.
  - Enumerate all possible ways of dividing the points into clusters and evaluate the `goodness' of each potential set of clusters by using the given objective function. (NP Hard)
  - Can have global or local objectives.
    - Hierarchical clustering algorithms typically have local objectives
    - Partitional algorithms typically have global objectives
  - A variation of the global objective function approach is to fit the data to a parameterized model.
    - Parameters for the model are determined from the data.
    - Mixture models assume that the data is a ‘mixture' of a number of statistical distributions.
Characteristics of the Input Data Are Important

- Type of proximity or density measure
  - Central to clustering
  - Depends on data and application

- Data characteristics that affect proximity and/or density are
  - Dimensionality
    - Sparseness
  - Attribute type
  - Special relationships in the data
    - For example, autocorrelation
  - Distribution of the data

- Noise and Outliers
  - Often interfere with the operation of the clustering algorithm
Clustering Algorithms

- K-means and its variants
- Hierarchical clustering
- Density-based clustering
K-means Clustering

- Partitional clustering approach
- Number of clusters, K, must be specified
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- The basic algorithm is very simple

1: Select K points as the initial centroids.
2: repeat
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: until The centroids don’t change
Example of K-means Clustering

Iteration 6
Example of K-means Clustering
K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures mentioned above.
- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to ‘Until relatively few points change clusters’
- Complexity is \( O(n \times K \times I \times d) \)
  - \( n \) = number of points, \( K \) = number of clusters, \( I \) = number of iterations, \( d \) = number of attributes
Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

\[ SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x) \]

- \( x \) is a data point in cluster \( C_i \) and \( m_i \) is the representative point for cluster \( C_i \)
  - can show that \( m_i \) corresponds to the center (mean) of the cluster
- Given two sets of clusters, we prefer the one with the smallest error
- One easy way to reduce SSE is to increase \( K \), the number of clusters
  - A good clustering with smaller \( K \) can have a lower SSE than a poor clustering with higher \( K \)
Two different K-means Clusterings

Original Points

Optimal Clustering

Sub-optimal Clustering
Limitations of K-means

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes

- K-means has problems when the data contains outliers.
Limitations of K-means: Differing Sizes

Original Points

K-means (3 Clusters)
Limitations of K-means: Differing Density

Original Points

K-means (3 Clusters)
Limitations of K-means: Non-globular Shapes

Original Points

K-means (2 Clusters)
Overcoming K-means Limitations

One solution is to use many clusters.
Find parts of clusters, but need to put together.
Overcoming K-means Limitations

Original Points

K-means Clusters
Overcoming K-means Limitations

Original Points

K-means Clusters
Importance of Choosing Initial Centroids

Iteration 6
Importance of Choosing Initial Centroids

Iteration 1

Iteration 2

Iteration 3

Iteration 4

Iteration 5

Iteration 6
Importance of Choosing Initial Centroids ...
Importance of Choosing Initial Centroids ...

Iteration 1

Iteration 2

Iteration 3

Iteration 4

Iteration 5
Problems with Selecting Initial Points

- If there are K ‘real’ clusters then the chance of selecting one centroid from each cluster is small.
  - Chance is relatively small when K is large
  - If clusters are the same size, n, then

\[
P = \frac{\text{number of ways to select one centroid from each cluster}}{\text{number of ways to select } K \text{ centroids}} = \frac{K!n^K}{(Kn)^K} = \frac{K!}{K^K}
\]

- For example, if K = 10, then probability = \(10!/10^{10} = 0.00036\)
- Sometimes the initial centroids will readjust themselves in ‘right’ way, and sometimes they don’t
- Consider an example of five pairs of clusters
10 Clusters Example

Starting with two initial centroids in one cluster of each pair of clusters
10 Clusters Example

Starting with two initial centroids in one cluster of each pair of clusters
Starting with some pairs of clusters having three initial centroids, while other have only one.
10 Clusters Example

Starting with some pairs of clusters having three initial centroids, while other have only one.
Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Generate a larger number of clusters and then perform a hierarchical clustering
- Bisecting K-means
  - Not as susceptible to initialization issues
**K-means++**

- This approach can be slower than random initialization, but very consistently produces better results in terms of SSE
  - The k-means++ algorithm guarantees an approximation ratio $O(\log k)$ in expectation, where $k$ is the number of centers

- To select a set of initial centroids, $C$, perform the following

1. Select an initial point at random to be the first centroid
2. For $k - 1$ steps
3. For each of the $N$ points, $x_i$, $1 \leq i \leq N$, find the minimum squared distance to the currently selected centroids, $C_1, \ldots, C_j$, $1 \leq j < k$, i.e., $\min_j d^2( C_j, x_i )$
4. Randomly select a new centroid by choosing a point with probability proportional to $\frac{\min_j d^2( C_j, x_i )}{\sum_i \min_j d^2( C_j, x_i )}$
5. End For
Pre-processing and Post-processing

- **Pre-processing**
  - Normalize the data
  - Eliminate outliers

- **Post-processing**
  - Eliminate small clusters that may represent outliers
  - Split ‘loose’ clusters, i.e., clusters with relatively high SSE
  - Merge clusters that are ‘close’ and that have relatively low SSE
  - Can use these steps during the clustering process
    - ISODATA
Bisecting K-means

- Bisecting K-means algorithm
  - Variant of K-means that can produce a partitional or a hierarchical clustering

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1: Initialize the list of clusters to contain the cluster containing all points.
2: repeat
3: Select a cluster from the list of clusters
4: for $i = 1$ to number_of_iterations do
5: Bisect the selected cluster using basic K-means
6: end for
7: Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: until Until the list of clusters contains $K$ clusters

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CLUTO: http://glaros.dtc.umn.edu/gkhome/cluto/cluto/overview
Bisecting K-means Example
DBSCAN is a density-based algorithm.

- Density = number of points within a specified radius (Eps)

- A point is a **core point** if it has at least a specified number of points (MinPts) within Eps
  - These are points that are at the interior of a cluster
  - Counts the point itself

- A **border point** is not a core point, but is in the neighborhood of a core point

- A **noise point** is any point that is not a core point or a border point
DBSCAN: Core, Border, and Noise Points

MinPts = 7

noise point

border point

core point

Eps

C
B
A
DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

```python
current_cluster_label ← 1
for all core points do
    if the core point has no cluster label then
        current_cluster_label ← current_cluster_label + 1
        Label the current core point with cluster label current_cluster_label
    end if
    for all points in the Eps-neighborhood, except $i^{th}$ the point itself do
        if the point does not have a cluster label then
            Label the point with cluster label current_cluster_label
        end if
    end for
end for
```
DBSCAN: Core, Border and Noise Points

Original Points

Point types: core, border and noise

Eps = 10, MinPts = 4
When DBSCAN Works Well

- Resistant to Noise
- Can handle clusters of different shapes and sizes
When DBSCAN Does NOT Work Well

Original Points

- Varying densities
- High-dimensional data

(MinPts=4, Eps=9.75).

(MinPts=4, Eps=9.92)
DBSCAN: Determining EPS and MinPts

- Idea is that for points in a cluster, their $k^{th}$ nearest neighbors are at roughly the same distance.
- Noise points have the $k^{th}$ nearest neighbor at farther distance.
- So, plot sorted distance of every point to its $k^{th}$ nearest neighbor.

![Graph showing sorted distances of points to their 4th nearest neighbors.](image)
Cluster Validity

- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall

- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters?

- But “clusters are in the eye of the beholder”!

- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters
Clusters found in Random Data

Random Points

K-means

DBSCAN

Complete Link
Different Aspects of Cluster Validation

1. Determining the **clustering tendency** of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.

2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.

3. Evaluating how well the results of a cluster analysis fit the data **without** reference to external information.
   - Use only the data

4. Comparing the results of two different sets of cluster analyses to determine which is better.

5. Determining the ‘correct’ number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.
Measures of Cluster Validity

- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - **External Index**: Used to measure the extent to which cluster labels match externally supplied class labels.
    - Entropy
  - **Internal Index**: Used to measure the goodness of a clustering structure *without* respect to external information.
    - Sum of Squared Error (SSE)
  - **Relative Index**: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy

- Sometimes these are referred to as *criteria* instead of *indices*
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.
Measuring Cluster Validity Via Correlation

- Two matrices
  - Proximity Matrix
  - Ideal Similarity Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters

- Compute the correlation between the two matrices
  - Since the matrices are symmetric, only the correlation between \( n(n-1) / 2 \) entries needs to be calculated.

- High correlation indicates that points that belong to the same cluster are close to each other.

- Not a good measure for some density or contiguity based clusters.
Measuring Cluster Validity Via Correlation

- Correlation of ideal similarity and proximity matrices for the K-means clusterings of the following two data sets.

\[
\text{Corr} = -0.9235 \\
\text{Corr} = -0.5810
\]
Using Similarity Matrix for Cluster Validation

- Order the similarity matrix with respect to cluster labels and inspect visually.
Clustering in random data are not so crisp

DBSCAN
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp

K-means
Using Similarity Matrix for Cluster Validation

DBSCAN
Clusters in more complicated figures aren’t well separated

Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE

SSE is good for comparing two clusterings or two clusters (average SSE).

Can also be used to estimate the number of clusters
Internal Measures: SSE

- SSE curve for a more complicated data set

SSE of clusters found using K-means
Internal Measures: Cohesion and Separation

- **Cluster Cohesion**: Measures how closely related are objects in a cluster
  - Example: SSE

- **Cluster Separation**: Measure how distinct or well-separated a cluster is from other clusters

- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)
    \[
    SSE = WSS = \sum_{i} \sum_{x \in C_i} (x - m_i)^2
    \]
  - Separation is measured by the between cluster sum of squares
    \[
    BSS = \sum_{i} |C_i|(m - m_i)^2
    \]
  - Where \(|C_i|\) is the size of cluster \(i\)
Internal Measures: Cohesion and Separation

- Example: SSE
  - \( BSS + WSS = \text{constant} \)

\[
\begin{align*}
\text{K=1 cluster:} & & \text{SSE} = \text{WSS} = (1 - 3)^2 + (2 - 3)^2 + (4 - 3)^2 + (5 - 3)^2 = 10 \\
& & \text{BSS} = 4 \times (3 - 3)^2 = 0 \\
& & \text{Total} = 10 + 0 = 10
\end{align*}
\]

\[
\begin{align*}
\text{K=2 clusters:} & & \text{SSE} = \text{WSS} = (1 - 1.5)^2 + (2 - 1.5)^2 + (4 - 4.5)^2 + (5 - 4.5)^2 = 1 \\
& & \text{BSS} = 2 \times (3 - 1.5)^2 + 2 \times (4.5 - 3)^2 = 9 \\
& & \text{Total} = 1 + 9 = 10
\end{align*}
\]
Internal Measures: Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.
Internal Measures: Silhouette Coefficient

- Silhouette coefficient combines ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings.

- For an individual point, $i$
  - Calculate $a =$ average distance of $i$ to the points in its cluster.
  - Calculate $b =$ min (average distance of $i$ to points in another cluster).
  - The silhouette coefficient for a point is then given by

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

  - Typically between 0 and 1.
  - The closer to 1 the better.

- Can calculate the average silhouette coefficient for a cluster or a clustering.
## External Measures of Cluster Validity: Entropy and Purity

### Table 5.9. K-means Clustering Results for LA Document Data Set

<table>
<thead>
<tr>
<th>Cluster</th>
<th>Entertainment</th>
<th>Financial</th>
<th>Foreign</th>
<th>Metro</th>
<th>National</th>
<th>Sports</th>
<th>Entropy</th>
<th>Purity</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>5</td>
<td>40</td>
<td>506</td>
<td>96</td>
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<td>943</td>
<td>273</td>
<td>738</td>
<td>1.1450</td>
<td>0.7203</td>
</tr>
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</table>

**Entropy** For each cluster, the class distribution of the data is calculated first, i.e., for cluster $j$ we compute $p_{ij}$, the ‘probability’ that a member of cluster $j$ belongs to class $i$ as follows: $p_{ij} = m_{ij}/m_j$, where $m_j$ is the number of values in cluster $j$ and $m_{ij}$ is the number of values of class $i$ in cluster $j$. Then using this class distribution, the entropy of each cluster $j$ is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the $L$ is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{j=1}^{K} \frac{m_j}{m} e_j$, where $m_j$ is the size of cluster $j$, $K$ is the number of clusters, and $m$ is the total number of data points.

**Purity** Using the terminology derived for entropy, the purity of cluster $j$, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{j=1}^{K} \frac{m_j}{m} purity_j$. 

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*02/14/2018 Introduction to Data Mining, 2nd Edition 69*
Final Comment on Cluster Validity

“The validation of clustering structures is the most difficult and frustrating part of cluster analysis. Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage.”

Algorithms for Clustering Data, Jain and Dubes