CS522 Advanced Database Systems

Cluster Analysis

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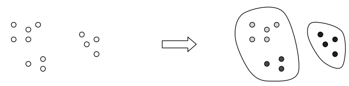
Clustering

- Group *similar* objects together
- Applications
  - Identify users who share similar interests
  - Automatically generate concept hierarchies
  - Reduce algorithmic complexity
  - ...



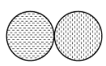
Types of Clusters

- Well separated
- Prototype based
- Contiguity based
- Density based
- Conceptual clusters

Well-separated Clusters

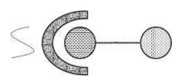
- Each point is closer to all of the points in its cluster than to any point in another cluster

Prototype-based Clusters



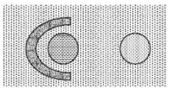
- ??

Contiguity-based Clusters



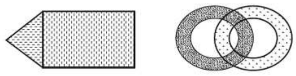
- ??
- A cluster can be considered as a *connected component* in a graph

Density-based Clusters



- A cluster is a dense region of objects surrounded by a region of low density

Conceptual Clusters



- A cluster is a set of objects that share *some property*

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Types of Clustering

- Partitional vs. Hierarchical
- Exclusive vs. Overlapping vs. Fuzzy
- Complete vs. Partial

Similarity Measure

TID	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No

- Is #1 more similar to #2 or #3?

Interval-Scaled Attributes

- Continuous-valued data measured with a linear scale (vs. exponential or logarithmic scale)

Distance Measures

- **X**=(x_1,x_2,,...,x_n) and **Y**=(y_1,y_2,...,y_n)
  - E.g. `(1,2)` and `(3,5)`

Euclidean Distance:

$$dist(\mathbf{X},\mathbf{Y}) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

Manhattan Distance:

$$dist(\mathbf{X},\mathbf{Y}) = \sum_{i=1}^{n}|x_i - y_i|$$

Minkowski Distance

$$dist(\mathbf{X},\mathbf{Y}) = \sqrt[p]{\sum_{i=1}^{n} |x_i - y_i|^p}$$

- p=1 (Manhattan Distance)
  - a.k.a. L_1 norm or L_1 distance
- p=2 (Euclidean Distance)
  - a.k.a. L_2 norm or L_2 distance

Requirements of Distance Functions

- dist(**X**,**Y**)≥0
- dist(**X**,**X**)=0
- dist(**X**,**Y**)=dist(**Y**,**X**)
- dist(**X**,**Y**)≤dist(**X**,**Z**)+dist(**Z**,**Y**)
  - *Triangular Inequality*

Problem of Units

- (10m,2km) and (5m,2.1km)?
- (10m,200lb) and (5m, 210lb)?

Standardize Interval-Scaled Attributes

- Given attribute A with values a_1, a_2, ..., a_n

Mean: $\bar{a} = \frac{1}{n}\sum_{i=1}^{n} a_i$

Mean absolute deviation: $s = \frac{1}{n}\sum_{i=1}^{n} |a_i - \bar{a}|$

Standardized measurement (*z-score*): $z_i = \frac{a_i - \bar{a}}{s}$

Binary Attributes

- Symmetric
  - E.g. gender
- Asymmetric
  - E.g. HIV test result

Contingency Table for Binary Attributes

		Record **Y**	
		1	0
Record **X**	1	q	r
	0	s	t

- Example
  - X=(1,1,0,1,0,0,0), Y=(0,1,0,1,0,1,0)

Distance Measure for Symmetric Binary Attributes

Similarity: $sim(\mathbf{X},\mathbf{Y}) = \frac{q+t}{q+r+s+t}$

Dissimilarity: $dsim(\mathbf{X},\mathbf{Y}) = \frac{r+s}{q+r+s+t}$

Distance: ??

Distance Measure for Asymmetric Binary Attributes

Similarity (Jaccard Coefficient): $sim(\mathbf{X},\mathbf{Y}) = \frac{q}{q+r+s}$

Dissimilarity: $dsim(\mathbf{X},\mathbf{Y}) = \frac{r+s}{q+r+s}$

Distance: ??

Binary Attribute Example

TID	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
1	M	Y	N	P	N	N	N
2	F	Y	N	P	N	P	N
3	M	Y	Y	N	N	N	N

- dist(1,2)?? dist(2,3)?? dist(3,1)??

Categorical Attributes

- Example
  - Marital status: single, married, divorced
- `dist(`**`X`**`,`**`Y`**`)=(p-m)/p`
  - `m`: number of attribute matches
  - `p`: total number of attributes
- Or, encode each state with a binary attribute

Ordinal Attributes

- Example
  - Grade: F, D, C, B, A
- Given an attribute with `M` possible values `{1,2,...,M}`, map value a to the range of `[0.0,1.0]`

$$z = \frac{a-1}{M-1}$$

Records with Mixed Types of Attributes ...

$$dist(\mathbf{X},\mathbf{Y}) = \frac{\sum_{i=1}^{n} \delta_i \times dist(x_i, y_i)}{\sum_{i=1}^{n} \delta_i}$$

- δ_i is the weight of the `i`th attribute a_i's contribution toward the overall distance
  - `0` if x_i or y_i is missing, or a_i is asymmetric binary and $x_i=y_i=0$
  - `1` othewise

... Records with Mixed Types of Attributes

- $\mathrm{dist}(x_i, y_i)$
  - Interval-based: $|x_i - y_i| / (\max(a_i) - \min(a_i))$
  - Binary or categorical: 0 if $x_i = y_i$; 1 otherwise
  - Ordinal: treat as interval-based using z_i

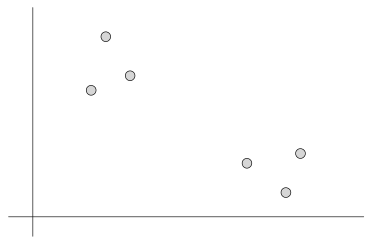
Other Distance Measures

- Cosine distance
- Tanimoto distance
- ...
- Weighted distance

K-Means

- Input: dataset D and number of clusters k
- Algorithm
  1. Randomly choose k objects as cluster centers
  2. Assign each object to the closest cluster center
  3. Update each cluster center
  4. Repeat 2 until there is no reassignment occurs

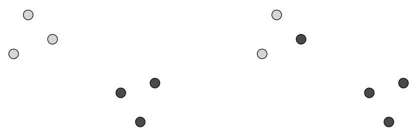
K-Means Example



Key Issues in K-Means

- Distance measure?
  - Euclidean, Manhattan, Cosine ...
- Cluster center?
  - Mean, median

Need for Objective Function



(a) (b)

- The best clustering is the one that minimize the "errors" defined by an *objective function*

Notations

D	Dataset
k	The number of clusters
C_i	ith cluster
c_i	The center of the ith cluster
x	An object

Objective Functions

Sum of the Squared Error (SSE):

$$SSE = \sum_{i=1}^{k} \sum_{x \in C_i} dist_{L_2}(x, c_i)^2$$

Sum of the Absolute Error (SAE):

$$SAE = \sum_{i=1}^{k} \sum_{x \in C_i} dist_{L_1}(x, c_i)$$

Minimize an Object Function

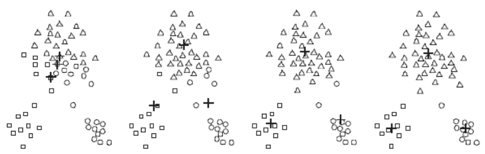
- Example:
  - One dimensional data
  - One cluster
  - SSE

$$SSE(c) = \sum_{x \in C} (c - x)^2 \quad \Rightarrow \quad \frac{\partial}{\partial c} SSE(c) = 0$$

Distances, Centroids, and Objective Functions

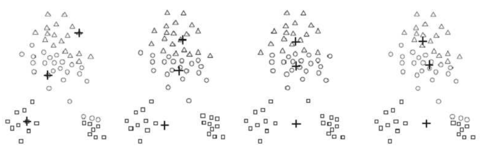
Distance Function	Centroid	Objective Function
Manhattan (L_1)	Median	Sum of L_1 distance
Squared Euclidean (L_2)	Mean	Sum of squared L_2 distance
Cosine	Mean	Sum of cosine distance
Bregman Divergence	Mean	Sum of Bregman divergence

Another K-Means Example ...



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.

... Another K-Means Example



(a) Iteration 1. (b) Iteration 2. (c) Iteration 3. (d) Iteration 4.

Dealing with the Problem of Initial Centroid Selection

- Perform several runs of K-Means and select the clustering with the smallest SSE
  - Not as effective as you would think, especially with large k (*why??*)
- Use a hierarchical clustering algorithm on a sample to get K initial clusters
- Select centroid one by one, and each one is the farthest away from previously selected ones

Postprocessing

- Escape local SSE minima by performing alternate clustering *splitting* and *merging*

Postprocessing – Splitting

- Splitting the cluster with the largest SSE on the attribute with the largest variance
- Introduce another centroid
  - The point that is farthest from current centroids
  - Randomly chosen

Postprocessing – Merging

- Disperse a cluster and reassign its objects
- Merge two clusters that are closed to each other

Bisecting K-Means

1. Initial a list of clusters with one cluster containing all the objects
2. Choose one cluster from the list
3. Split the cluster into two using basic K-Means, and add them back to the list
4. Repeat Step 2 until k clusters are reached
5. Perform one more basic K-Means using the centroids of the k clusters as initial centroids

About Bisecting K-Means

- Step 2
  - Choose the largest cluster
  - Choose the cluster with the largest SSE
- Step 3
  - Perform basic K-Means several times and choose the clustering with the smallest SSE
- Less susceptible to initialization problems
  - *Why??*

Handling Empty Clusters

◈Choose a replacement centroid
- The point that's farthest away from any current centroid
- A point from the cluster with the highest SSE

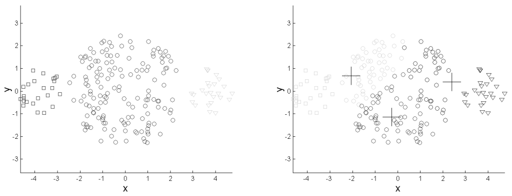
Limitations of K-Means

◈Problem with clusters of different
- Sizes
- Densities
- Non-globular shapes

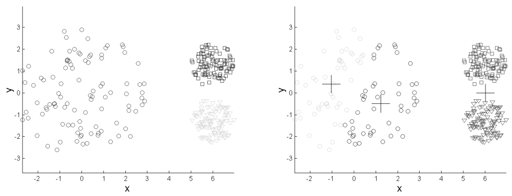
◈Problem with outliers

◈Requires the notion of *centroid*

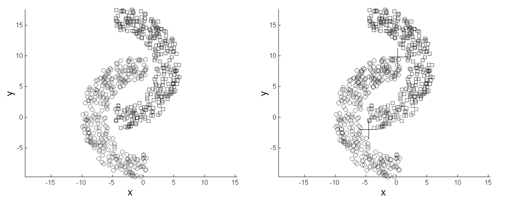
Limitations of K-Means – Differing Sizes



Limitations of K-Means – Differing Densities



Limitations of K-Means –Non-globular Shapes



K-Medoids

◈Instead of using mean/centroid, use medoid, i.e. representative object

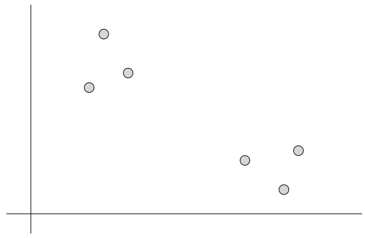
◈Objective function: sum of the distances of the objects to their medoid

◈Differs from K-Means in how the medoids are updated

PAM (Partition Around Medoids)

1. Randomly choose k objects as initial medoids
2. For each non-medoid object x
   For each medoid c_i
   calculate the reduction of the total distance if c_i is replaced by x
3. Replace the c_i with x that results in maximum total distance reduction
4. Repeat Step 2 until the total distance cannot be reduced
5. Assign each object to its closest mediod

PAM Example



K-Means vs. K-Medoids

- Requires the notion of mean/centroid
- More susceptible to outliers
- $O(kn)$ per iteration

- Works for all distance measures
- Less susceptible to outliers
- ?? per iteration

Hierarchical Clustering

- Agglomerative
  - Start with each object as a cluster
  - Recursively pick two clusters to merge
- Divisive
  - Start with all objects as a single cluster
  - Recursively pick one cluster to split

Agglomerative Hierarchical Clustering

1. Compute a *distance matrix*
2. Merge the two *closest* clusters
3. Update the distance matrix
4. Repeat Step 2 until only one cluster remains

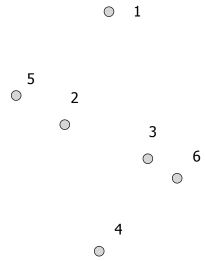
Distance Between Clusters

- Min distance
  - Distance between two closest objects
  - Min < threshold: Single-link Clustering
- Max distance
  - Distance between two farthest objects
  - Max < threshold: Complete-link Clustering
- Average distance
  - Average of all pairs of objects from the two clusters

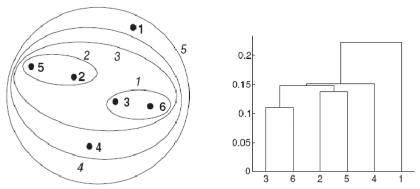
Centroid-based Distance

- ◈Mean distance
- ◈Increased SSE (Ward's Method)

Min Distance Clustering Example ...

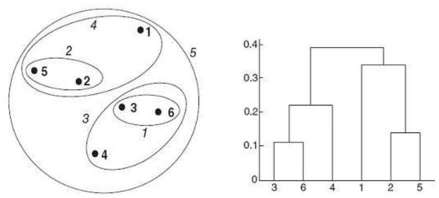


... Min Distance Clustering Example



(a) Single link clustering. (b) Single link dendrogram.

Max Distance Clustering Example



(a) Complete link clustering. (b) Complete link dendrogram.

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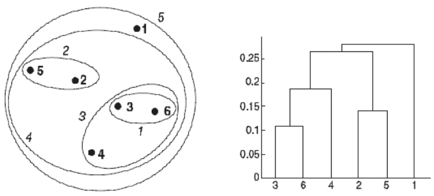
Average Distance Clustering Example



(a) Group average clustering. (b) Group average dendrogram.

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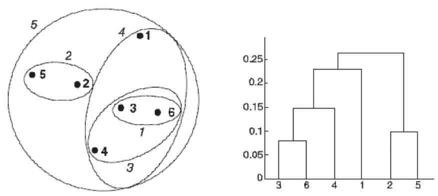
Ward's Clustering Example



(a) Ward's clustering. (b) Ward's dendrogram.

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About Hierarchical Clustering

- Produces a hierarchy of clusters
- Lack of a global objective function
- Merging decisions are final
- *Expensive*
- Often used with other clustering algorithms

BIRCH

- Balanced Iterative Reducing and Clustering using Hierarchies

Clustering Feature (CF)

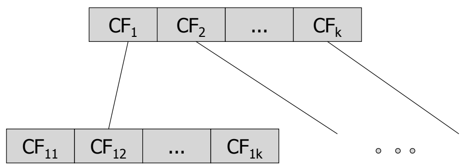
- CF=<N, **LS**, SS>

N: number of objects

LS (Linear Sum): $\mathbf{LS} = \sum_{i=1}^{N} \mathbf{x}_i$

SS (Square Sum): $SS = \sum_{i=1}^{N} \mathbf{x}_i^2 = \sum_{i=1}^{N} \mathbf{x}_i \bullet \mathbf{x}_i$

CF Tree



CF Tree Construction – Input

- Dataset
- Threshold Condition
  - `Diameter D of a cluster < d`

Centroid: $\mathbf{x}_0 = \frac{\sum_{i=1}^{N} \mathbf{x}_i}{N}$

Radius: $R = \sqrt{\frac{\sum_{i=1}^{N} (\mathbf{x}_i - \mathbf{x}_0)^2}{n}}$

Diameter: $D = \sqrt{\frac{\sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbf{x}_i - \mathbf{x}_j)^2}{N(N-1)}}$

CF Tree Construction – Insert

- Insert an object into its closest cluster in a leaf node
  - The object is inserted if the resulting cluster does not violate the threshold condition
  - Otherwise the object is inserted as a cluster of by itself
- When a node is full, split it and rebalance the tree (similar to B+ Tree Insertion)

CF Tree Howto's

- Find closest cluster
  - *Object-to-cluster distance*
- Insert object into a cluster
  - *Update CF*
  - Check threshold condition
    - *Calculate diameter*
- Split node and rebalance tree
  - Merge clusters that are close to one anther
    - *Cluster-to-cluster distance; calculate CF of the merged cluster*

Diameter Calculation

- Calculate diameter using CF

$$D = \sqrt{\frac{2N \times SS - 2\mathbf{LS}^2}{N(N-1)}}$$

Diameter Calculation Example

- A cluster with three 1-D objects
  - $\mathbf{x_1}=(x_1)$
  - $\mathbf{x_2}=(x_2)$
  - $\mathbf{x_3}=(x_3)$

Cluster-to-Cluster Distances

- Cluster-to-cluster distances that can be calculated using CF
  - D_0: centroid Euclidean distance
  - D_1: centroid Manhattan distance
  - D_2: average inter-cluster distance
  - D_3: average intra-cluster distance
  - D_4: variance increase distance

About BIRCH

- Single scan of data
  - CF tree is kept in memory
  - Size of the CF tree can be adjusted using the threshold value
- Cluster the leaf node clusters
  - More natural clusters
  - Sparse clusters detected as outliers
- Require the notion of centroid

DBSCAN

- Density-Based Spatial Clustering of Applications with Noise
- A density-based clustering algorithm

Classification of Points

- Given a radius ε and the minimum number of points `MinPts` within a radius of ε (ε-neighborhood)
  - Core point
    - Has more points in its ε-neighborhood than `MinPts`
  - Border points
    - Within the ε-neighborhood of a core point
  - Noise points

Point Examples

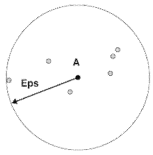


Figure 8.20. Center-based density.

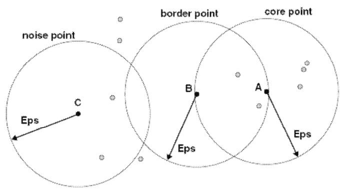
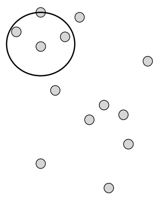


Figure 8.21. Core, border, and noise points.

The DBSCAN Algorithm

- Label all points as core, border, or noise
- Remove all noise points
- Put an edge between all core points that are with ε of each other
- Make each connected group of core points a cluster
- Assign border points to *one of the clusters* of their associated core points

DBSCAN Example



Select DBSCAN Parameters

- k-dist: distance to the kth nearest neighbor
- k=4 is usually reasonable for most 2-D datasets

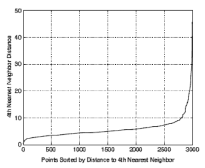


Figure 8.23. K-dist plot for sample data.

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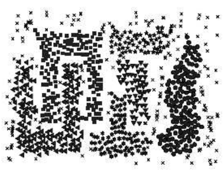
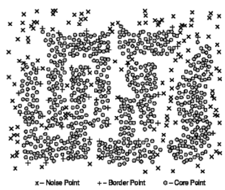
More DBSCAN Examples



(a) Clusters found by DBSCAN.



(b) Core, border, and noise points.

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About DBSCAN

- Handle clusters with arbitrary shapes and sizes
- Limitations
  - Clusters with varying densities
  - High dimensional data
- Could be expensive because of nearest neighbor computer
  - Use a spatial index structure like R tree or k-d tree

Other Clustering Algorithms

- More efficient
  - Speed
  - Scalability
- High dimensional data
- Constraint-based

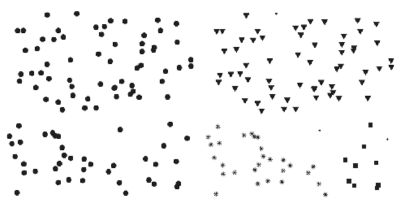
Cluster Evaluation

- a.k.a. *Cluster Validation*
- Unsupervised
  - Using no external information other than the data itself
- Supervised
  - With external information such as given class labels

Reasons Not To Evaluate

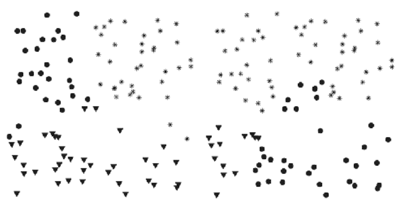
- Clustering is often used as part of exploratory data analysis
- Clustering is often used as part of other algorithms
- Clustering algorithms, in some sense, define their own types of clusters

Reasons To Evaluate ...



(a) Original points. (b) Three clusters found by DBSCAN.

... Reasons To Evaluate



(c) Three clusters found by K-means. (d) Three clusters found by complete link.

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Quality (Validity) of Clusters

- Cohesion
  - Compactness of a cluster
- Separation

Validity of Graph-based Clusters

$$cohesion(C_i) = \sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_i}} dist(\mathbf{x}, \mathbf{y})$$

$$separation(C_i, C_j) = \sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_j}} dist(\mathbf{x}, \mathbf{y})$$

Validity of Prototype-based Clusters

$$cohesion(C_i) = \sum_{\mathbf{x} \in C_i} dist(\mathbf{x}, \mathbf{c_i})$$

$$separation(C_i, C_j) = dist(\mathbf{c}_i, \mathbf{c}_j)$$

$$separation(C_i) = dist(\mathbf{c}_i, \mathbf{c})$$

Validity of A Clustering

$$validity(C) = \sum_{i=1}^{k} w_i \times validity(C_i)$$

Cluster Weights

Validity Measures	Weights
$\sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_i}} dist(\mathbf{x}, \mathbf{y})$	$1/\lvert C_i \rvert$
$\sum_{\mathbf{x} \in C_i} dist(\mathbf{x}, \mathbf{c_i})$	1
$dist(\mathbf{c}_i, \mathbf{c})$	$\lvert C_i \rvert$

Silhouette Coefficient

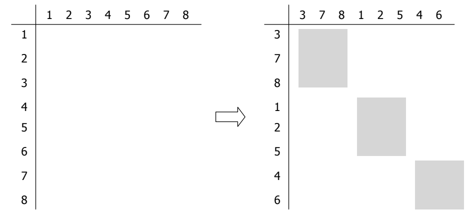
- For the `ith` object in a cluster
  - a_i: average distance to all other objects in the cluster
  - b_i: max of the average distance to the objects in a cluster that does not contain this object

$$s_i = (b_i - a_i) / \max(a_i, b_i)$$

About Silhouette Coefficient

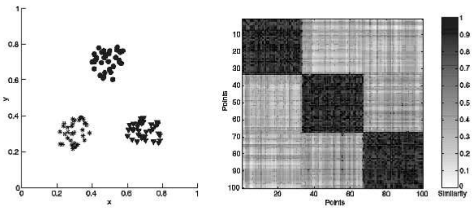
- *Range of s_i??*
- *What is a "good" value of s_i??*
- Quality of a cluster: average s_i
- Quality of a clustering: average s_i

Similarity Matrix



- 8 objects, 3 clusters: {3,7,8}, {1,2,5}, {4,6}

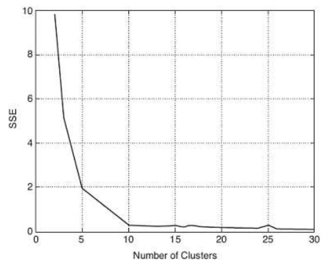
Similarity Matrix Example



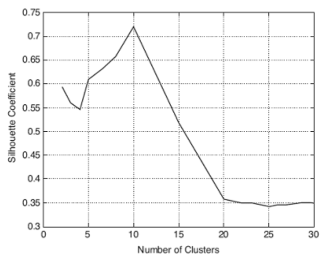
(a) Well-separated clusters.

(b) Similarity matrix sorted by K-means cluster labels.

Determine The Correct Number of Clusters ...



... Determine The Correct Number of Clusters



Clustering Tendency

- Do clusters exist in the first place?
- Determine clustering tendency
  - Cluster first, then evaluate the quality of the clustering
    - Need to try several different types of clustering algorithms
  - Statistical tests for spatial randomness

Hopkins Statistic

- Generate p random points in the data space
  - u_i: distance of a randomly generated point to its nearest neighbor in the original dataset
- Select p random points from the original dataset
  - w_i: distance of a randomly selected point to it nearest neighbor in the original dataset
- *Interpretation of Hopkins Statistic??*

$$H = \frac{\sum_{i=1}^{p} w_i}{\sum_{i=1}^{p} u_i + \sum_{i=1}^{p} w_i}$$

Supervised Measures of Cluster Validity

- Classification-oriented measures
  - Evaluate the extent to which a cluster contains the objects of a single class
- Similarity-oriented measures
  - Evaluate the extent to which two objects of the same class (or cluster) belong to the same cluster (or class)

Classification-oriented Measures

- Entropy
- Purity
- Precision, recall, F-measure

Similarity-oriented Measures ...

	Same class	Different class
Same class	f_{11}	f_{10}
Different class	f_{01}	f_{00}

... Similarity-oriented Measures

Rand Statistic: $$R = \frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

Jaccard Coefficient: $$J = \frac{f_{11}}{f_{01} + f_{10} + f_{11}}$$

Summary

- Types of clusters
- Types of clustering
- Similarity measures
- Clustering algorithms
  - Partitional: K-Means, K-Mediods
  - Hierarchical: Agglomerative, BIRCH
  - Density-based: DBSCAN
- Clustering evaluation
  - Unsupervised and supervised