

## I) Important Topics to review

1. Data Exploration
  - a. Basic concepts: types of attributes, objects, etc.
  - b. Proximity measures
  - c. Basic Statistical Descriptions of Data: mean, mode, median, quartile, IQR, etc.
  - d. Data Visualization: box plot, scatter plot
2. Data Preprocessing
  - a. Basic concepts: basic tasks in data preprocessing
  - b. Data Cleaning methods
  - c. Data Integration: redundancy and correlation analysis
  - d. Data Reduction: main ideas of Principle Component Analysis (PCA), attribute subset selection
3. Finding frequent itemsets
  - a. Basic concepts: support, confidence, frequent items
  - b. Apriori algorithm
  - c. FP-tree algorithm
  - d. Comparison between the above algorithms
4. Classification
  - a. Naïve Bayes
  - b. Decision Trees: GINI index, entropy, information gain, how to build decision trees
  - c. Support Vector Machines:
  - d. KNN
  - e. Artificial Neural Networks and Backpropagation
  - f. Evaluation measures: Accuracy, Precision, Recall, F1-measure, Sensitivity, etc.
5. Clustering
  - a. Basic concepts: centroids, dendrogram,
  - b. K-means
  - c. K-medoids
  - d. Hierarchical clustering: agglomerative clustering
  - e. Gaussian Mixture Model
  - f. DBSCAN
  - g. Clustering with constraints
  - h. Biclustering
  - i. Evaluation: B-cubed precision, B-cubed recall, Silhouette coefficients, etc.
6. Outlier Detection
  - a. Basic concepts: outliers, types of outliers
  - b. Univariate outlier detection
  - c. Multivariate outlier detection
  - d. Distance-based outlier detection

## II. Exercises:

- 1) Given two objects represented by tuples (22, 1, 42, 10) and (20, 0, 36, 8)
  - a) Compute the Euclidean distance between two objects

b) Compute the Manhattan distance between two objects

2) A *partitioning* variation of Apriori subdivides the transactions of a database  $D$  into  $n$  nonoverlapping partitions. Prove that any itemset that is frequent in  $D$  with min support is  $s$  must be frequent in at least one partition of  $D$  with min support  $s$ .

3) A database has five transactions. Let  $\min sup = 60\%$  and  $\min conf = 80\%$ .

T1: {L, I, O, N}

T2: {T, I, G, E, R}

T3: {M, A, K, E}

T4: {M, U, C, K, Y}

T5: {C, O, O, K, I, E}

Find all frequent itemsets using Apriori and FP-growth, respectively.

4) (Contributed by Hang Yu Deng)

K-means algorithm: prove that given point assignments for a cluster, the mean of the points is the desired centroid that minimizes the inter-cluster variance.

5) (Contributed by Hang Yu Deng)

In DBSCAN algorithm, if  $p$  doesn't have enough neighbors, then it is marked as noise. But what if  $p$ 's neighborhood contains a core object  $q$ ? Naturally,  $p$  should be added to the cluster of the core object  $q$ . Explain whether DBSCAN can obtain this property.

6) (Contributed by Hang Yu Deng)

In Biclustering, please explain why do we choose to minimize the mean-squared residual values?

7) Suppose that the data mining task is to cluster the following eight points (with  $(x, y)$  representing location) into three clusters.

$A_1(2, 10)$ ,  $A_2(2, 5)$ ,  $A_3(8, 4)$ ,  $B_1(5, 8)$ ,  $B_2(7, 5)$ ,  $B_3(6, 4)$ ,  $C_1(1, 2)$ ,  $C_2(4, 9)$ .

The distance function is Euclidean distance. Suppose initially we assign  $A_1$ ,  $B_1$ , and  $C_1$  as the center of each cluster, respectively. Use the k-means algorithm to show only the three cluster centers after the first round of execution

### Solutions:

2) Proof by contradiction:

Suppose that there exists an itemset  $x$  that is frequent in  $D$  but not frequent in any of its partitions.

Since  $x$  is frequent in  $D$ ,  $\text{support}(x \text{ in } D) \geq s$ ; or  $\text{support\_count}(x \text{ in } D)/|D| \geq s$ .

Since  $x$  is not frequent in any of the partitions  $P_i$  of  $D$  ( $i=1, \dots, n$ ):

$\text{Support}(x \text{ in } P_i) < s$  or  $\text{support\_count}(x \text{ in } P_i)/|P_i| < s$  for all  $i=1, \dots, n$

$\rightarrow \sum_{i=1}^n \text{support\_count}(x \text{ in } P_i) / (|D|/n) < n*s$

$\rightarrow n * \text{support\_count}(x \text{ in } D) / |D| < n*s$

$\rightarrow \text{support\_count}(x \text{ in } D) / |D| < s$

This contradicts with the above hypothesis  $\rightarrow$  any itemset that is frequent in  $D$  must be frequent in one of its partitions.

4) Within cluster variance:

$$E = \sum_{i=1}^k \sum_{p \in C_i} \text{dist}(p, c_i)^2$$

Suppose point assignments to clusters are available, the means of points in the clusters minimize the **within cluster variance** with those given point assignments.

To prove this, we can consider the case of one cluster  $C$  which includes points  $p_1, p_2, \dots, p_N$ , we would like to prove that the centroid  $c$  of  $C$  that minimize within-cluster-variance is indeed the mean of the points  $p_i$ . The within-cluster-variance with Euclidean distance is:

$$c = \underset{c}{\operatorname{argmin}} \sum_{i=1}^N (p_i - c)^T (p_i - c)$$

Let

$$V = \sum_{i=1}^N (p_i - c)^T (p_i - c) = n c^T c - 2 \sum_{i=1}^N p_i^T c + \sum_{i=1}^N p_i^T p_i$$

Take the derivative of  $V$  with regards to  $c$  and set it to zero, we obtain:

$$\frac{\partial V}{\partial c} = 2Nc - 2 \sum_{i=1}^N p_i = 0$$

We can find  $c$  that minimizes  $V$  is

$$c = 1/N \sum_{i=1}^N p_i$$

In other words,  $c$  is the mean point of the points  $p_1, p_2, \dots, p_N$ .

Since point assignments are fixed (clusters are defined separately), we can see that centroids that minimize the overall within-cluster-variance are mean points of those clusters.

## 5) DBScan Algorithm

**Algorithm: DBSCAN:** a density-based clustering algorithm.

**Input:**

- $D$ : a data set containing  $n$  objects,
- $\epsilon$ : the radius parameter, and
- $MinPts$ : the neighborhood density threshold.

**Output:** A set of density-based clusters.

**Method:**

- (1) mark all objects as **unvisited**;
- (2) **do**
- (3)     randomly select an unvisited object  $p$ ;
- (4)     mark  $p$  as **visited**;
- (5)     **if** the  $\epsilon$ -neighborhood of  $p$  has at least  $MinPts$  objects
- (6)         create a new cluster  $C$ , and add  $p$  to  $C$ ;
- (7)         let  $N$  be the set of objects in the  $\epsilon$ -neighborhood of  $p$ ;
- (8)         **for** each point  $p'$  in  $N$
- (9)             **if**  $p'$  is **unvisited**
- (10)                 mark  $p'$  as **visited**;
- (11)                 **if** the  $\epsilon$ -neighborhood of  $p'$  has at least  $MinPts$  points,  
                    add those points to  $N$ ;
- (12)             **if**  $p'$  is not yet a member of any cluster, add  $p'$  to  $C$ ;
- (13)         **end for**
- (14)         output  $C$ ;
- (15)     **else** mark  $p$  as **noise**;
- (16) **until** no object is **unvisited**;

Suppose that  $p$  is a border point (the epsilon-neighborhood of  $p$  doesn't contain at least  $MinPts$  points), and in the neighborhood of  $q$ , a core object.

- If  $q$  is visited before  $p$ , which forms a cluster  $C$ , then  $p$  will be added to the set  $N$  at some point following the density reachable relationships and marked as visited. The point  $p$  will be added to  $C$  at line (12). The point  $p$  will not be selected at line (3), and thus it cannot be marked as noise.

- If  $p$  is visited before  $q$  is,  $p$  is marked as noise at line (15). However, we still have chance to add  $p$  to the cluster  $C$  of  $q$  due to line (12) since a noise point doesn't belong to any cluster, and be added to cluster  $C$ .

6)

Recall: Perfect bicluster with coherent values  $e_{ij} = c + a_i + b_j$

You can prove that a perfect bicluster  $I \times J$  with coherent value will have  $H(I, J) = 0$  and  $e_{ij} = e_{iJ} + e_{Ij} - e_{IJ}$

In reality, perfect biclusters are rare. We seek to find a bicluster that is closest to "perfect", or we would like to minimize the noise.

$$\text{residue}(e_{ij}) = e_{ij} - e_{iJ} - e_{Ij} + e_{IJ}$$

Mean-squared residue limits the noise (in term of residues) from the whole submatrix.