Graph-based Data Mining: A New Approach for Data Analysis

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Abstract— The field of graph mining has drawn greater attentions in the recent times. Graph is one of the extensively studied data structures in computer science and thus there is quite a lot of research being done to extend the traditional concepts of data mining have been in graph scenario. In this paper, large data set containing medical histories of men belonging to different age groups has been taken and further divided into clusters. This data has been arranged into graphs and further into sub graphs. We have implemented the Apriori algorithm and use it to determine frequency and association between various factors influencing the fertility of men in a particular season and of a particular age group. The analysis has been done by taking into account various risk factors that influence fertility and the frequency of their occurrence.

Index Terms— graph mining, sub grpahs, medical histories, data sets, clusters, Apriori algorithm, fertility, risk factors,

1 INTRODUCTION

Graph theory is the subject that deals with graphs. Graph theory has found its applications in many areas of Computer science. Data mining is one of those fields where concepts of graph theory have been applied to a large extent. Data mining (Han et al, 2006) is the subject which deals in extraction of knowledge from the available data. Various algorithms are applied which help in the analysis and establishment of relationship between the entities. Apart from finding relationship between various entities of data, data mining algorithms have been widely used to perform cluster analysis as well. Mining large datasets with conventional algorithms is tough because of polynomial time complexities. Graph mining and management has become an important topic of research recently because of numerous applications to a wide variety of data mining problems in computational biology, chemical data analysis, drug discovery and communication networking. Traditional data mining and management algorithms such as clustering, classification, frequent pattern mining and indexing have now been extended to the graph scenario. Graph data mining has shown better results in terms of time complexities and thus is a preferred technique when handling large data sets.

2. LITERATURE BASES

Definition 1 (Graph): A graph can be defined in an abstract way using vertices or nodes, edges connecting the nodes and mapping of the edges from one vertex to the other. A weighted graph (West, Douglas B, 2005) is one in which a number is associated with each edge which is often called its weight. This measure plays a significant in indicating the relationship between the two vertices it connects. For example the graph in figure 1 has 4 vertices connected by 4 edges each of which have a weight associated with it.

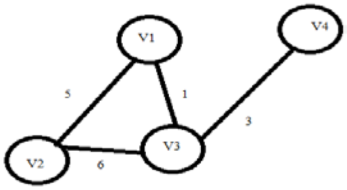


Figure 1.0

Definition 2 (Subgraph): A graph G′: {V′, E′} is said to be a subgraph of G: {V, E} if and only if it satisfies the following two conditions.

i) V′ ϵ V
ii) E′ ϵ E

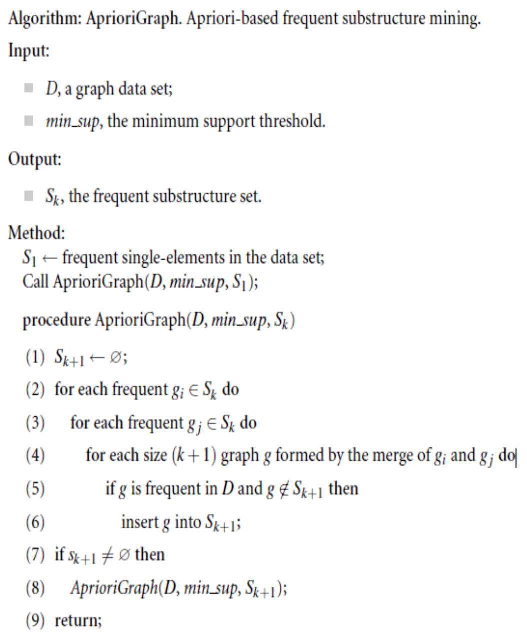
Definition 3: (Graph Transaction) A graph G is referred to as a graph transaction or simply a transaction, and a set of graph transactions GD, where GD = {G_1, G_2… Gn}, is referred to as a graph database.

Definition 4: (Support) Given a graph database GD and a graph G_s, then support of G_s is defined as

Sup (G_s): $\frac{No.of\ transactions\ involving\ Gs}{Total\ no.of\ transactions\ in\ GD}$

3. OUR APPROACH

In this paper, we have implemented the Apriori Algorithm (written below) on the procured dataset and have established various association rules which affect the men's fertility.



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Algorithm: AprioriGraph. Apriori-based frequent substructure mining.
Input:
    ▪ D, a graph data set;
    ▪ min_sup, the minimum support threshold.
Output:
    ▪ $S_k$, the frequent substructure set.
Method:
  $S_1 \leftarrow$ frequent single-elements in the data set;
  Call AprioriGraph(D, min_sup, $S_1$);

  procedure AprioriGraph(D, min_sup, $S_k$)
    $S_{k+1} \leftarrow \varnothing$;
    for each frequent $g_i \in S_k$ do
      for each frequent $g_j \in S_k$ do
        for each size $(k+1)$ graph $g$ formed by the merge of $g_i$ and $g_j$ do
          if $g$ is frequent in $D$ and $g \notin S_{k+1}$ then
            insert $g$ into $S_{k+1}$;
    if $s_{k+1} \neq \varnothing$ then
      AprioriGraph(D, min_sup, $S_{k+1}$);
    return;
```

After applying Apriori algorithm and determining the association rules, web graphs were constructed for the data which depicts the data in weighted graph format. The research has been further extended to neural network analysis which aims at considering affect of those attributes which have values over range instead of binary values. We have also performed K means clustering which depicts the density of records in different areas. To understand the data in a better way, we converted it into a tree format.

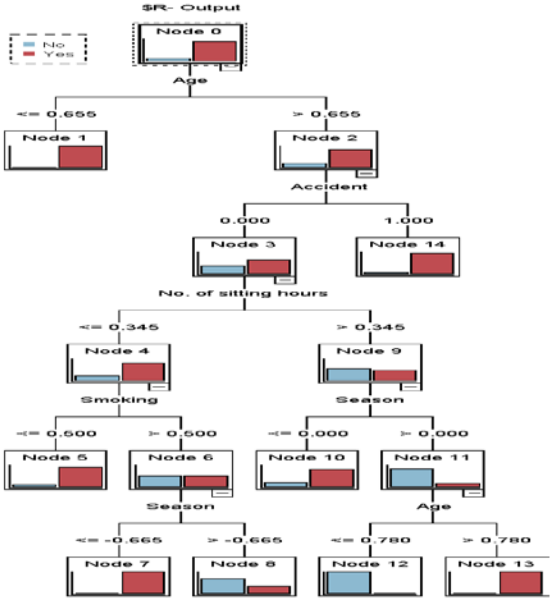


Figure 2.0

4. IMPLEMENTATION:

4.1 Description of dataset

We procured the dataset from UCI Machine learning repository which contains information about semen samples given by 100 volunteers and was analyzed according to the WHO 2010 criteria. Sperm concentrations are related to socio-demographic data, environmental factors, health status, and life habits. The data was donated to UCI repository on Jan 17, 2013.

Attribute information is tabulated below

Table 1: Attribute Information

Attribute	Value
Season in which the analysis was performed	Winter, Spring, Summer, Fall (-1,-0.33,0.33,1)
Age at the time of analysis.	18-36 (0, 1)
Childish diseases (i.e. , chicken pox, measles, mumps, polio)	1) Yes, 2) no. (0, 1)
Accident or serious trauma	1) Yes, 2) no. (0, 1)
Surgical intervention	1) Yes, 2) no. (0, 1)
High fevers in the last year	1) Less than three months ago, 2) more than three months ago, 3) no. (-1, 0, 1)

Frequency of alcohol consumption	1) several times a day, 2) every day, 3) several times a week, 4) once a week, 5) hardly ever or never (0, 1)
Number of hours spent sitting per day	(0,1)
Output	Diagnosis Normal (Yes), Altered (No)

Following are the various risk factors that have been considered in the given dataset which are believed to affect the men's fertility.

- *Childish diseases*: When infected with a disease like chicken pox, measles, mumps or polio the infection might spread to other parts of the body. This may affect the testicles and result in testicular shrinkage and infertility.
- *Accident or serious trauma*: Injury to the testicles during an accident can cause fertility. Serious trauma or depression also results in decrease in sperm count and hence causes infertility.
- *Surgical intervention*: Some males go through surgical intervention to improve their fertility.

Figure 3.0

4.2 Implementation using Apriori Algorithm

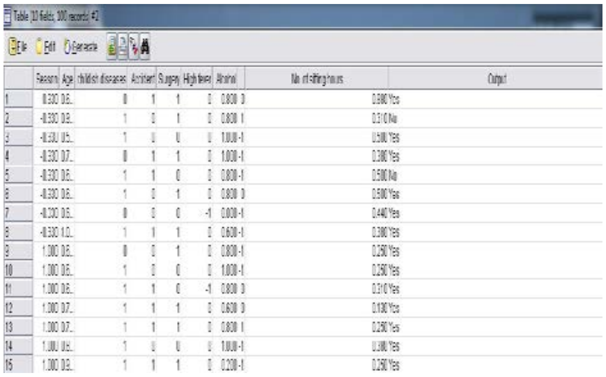
Apriori algorithm has been used for classification for datasets and establishment the association rules in between the attributes on the basis of two measures: *minimum support and minimum confidence*. For generating item sets we have used the existing Apriori algorithm and further we have extended the concept to Apriori graph mining technique.

4.2.1 Item sets:

The following item sets in Table 1.4 were generated by taking minimum support= 20%.

- *High fevers:* Fever affects the production and quality of the sperm count. This usually takes weeks to recover from.
- *Alcohol consumption:* Alcohol is considered toxic to the sperm and overuse can cause infertility.
- *Smoking habit*: Smoking results in approximately 700 chemicals entering the body. These damage the sperms and make them less likely to fertile the egg.
- *Number of hours spent sitting per day:* Sitting for long hours heats up the testicles and lack of exercise adds on to it, making the man infertile.

After procuring whole of the data we converted it into table format. Figure 3.0 shows information for 15 samples.



	Season	Age	childish diseases	Accident	Surgery	High fever	Alcohol		No of sitting hours	Output
1	0.330	0.6..	0	1	1	0	0.800	0	0.880	Yes
2	-0.330	0.9..	1	0	1	0	0.800	1	0.310	No
3	-0.330	0.5..	1	0	0	0	1.000	-1	0.500	Yes
4	-0.330	0.7..	0	1	1	0	1.000	-1	0.380	Yes
5	-0.330	0.6..	1	1	0	0	0.800	-1	0.500	No
6	-0.330	0.6..	1	0	1	0	0.800	0	0.500	Yes
7	-0.330	0.6..	0	0	0	-1	0.800	-1	0.440	Yes
8	-0.330	1.0..	1	1	1	0	0.600	-1	0.380	Yes
9	1.000	0.6..	0	0	1	0	0.800	-1	0.250	Yes
10	1.000	0.6..	1	0	0	0	1.000	-1	0.250	Yes
11	1.000	0.6..	1	1	0	-1	0.800	0	0.310	Yes
12	1.000	0.7..	1	1	1	0	0.600	0	0.130	Yes
13	1.000	0.7..	1	1	1	0	0.800	1	0.250	Yes
14	1.000	0.8..	1	0	0	0	1.000	-1	0.380	Yes
15	1.000	0.9..	1	1	1	0	0.200	-1	0.250	Yes

Table 2: Item set description

Attribute	Count of yes	Total instances	Support %
Accident	44	100	44
Childish diseases	87	100	87
Surgery	51	100	51

Since all the three attributes fulfill the minimum support criteria, we calculated the 2 item set by taking 2 attributes at a time.

Table 3: 2 frequent item set

Attribute	Count of yes	Total instances	Support %
Accident and Surgery	25	100	25

Accident and Childish Diseases	41	100	41
Surgery and Childish Diseases	42	100	42

Further we go for computation of 3 frequent item set.

Table 4: 3 frequent item set

Attribute	Count of yes	Total instances	Support%
Accident, Surgery and Childish Diseases	22	100	22

4.2.2 Generation of Association Rules:

To generate association rules we took minimum confidence as 90%. Following rules were generated.

Table 5: Association Rules

Antecedent	Consequent	Confidence
Accident, Surgery and Childish Diseases	Output	100
Accident, Surgery	Output	100
Accident	Output	93.182
Accident, Childish Disease	Output	92.683

Interpretation of Table1.7 is if e.g. for the last association rule where antecedent is accident and childish disease and the consequent is Output, it means 92.683% of the people have undergone surgery and have had childish diseases are fertile.

4.3 Web Graph Construction

The graph in figure 4.0 was constructed using all the flag attributes. Every flag attribute was given allotted two nodes; one representing either yes or 1 and the other representing either no or 0.

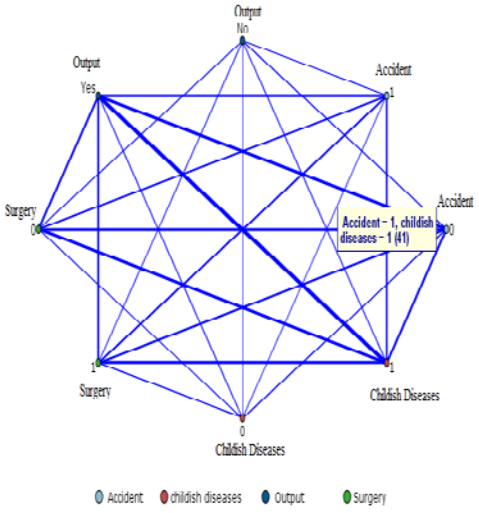
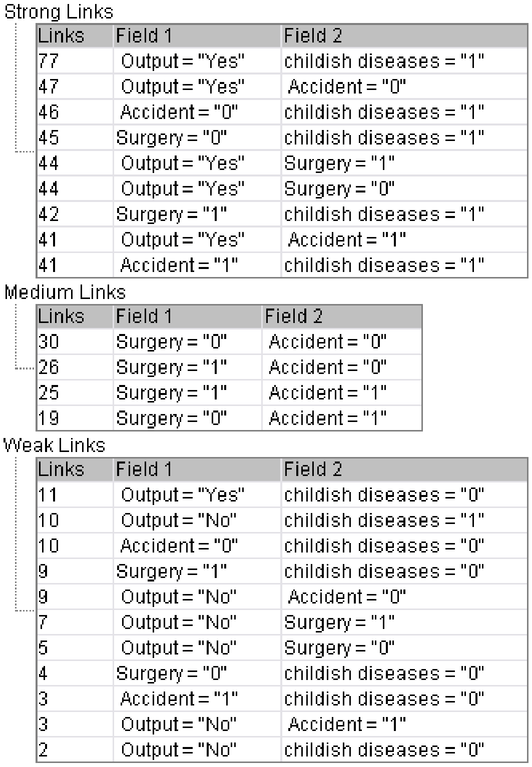


Figure 4.0

The edges in the graph can be classified into three categories: *Heavy link, medium link and weak link*. This classification was made on the basis of the count (weight) of that particular edge. It has been summarized below.

The purpose of going one step ahead of weighted graph was to create visual effect of the count and making it easier for analysis. As one can see from the graph itself, the strongest link is the edge between Output=Yes and Childish Diseases=1.



Strong Links

Links	Field 1	Field 2
77	Output = "Yes"	childish diseases = "1"
47	Output = "Yes"	Accident = "0"
46	Accident = "0"	childish diseases = "1"
45	Surgery = "0"	childish diseases = "1"
44	Output = "Yes"	Surgery = "1"
44	Output = "Yes"	Surgery = "0"
42	Surgery = "1"	childish diseases = "1"
41	Output = "Yes"	Accident = "1"
41	Accident = "1"	childish diseases = "1"

Medium Links

Links	Field 1	Field 2
30	Surgery = "0"	Accident = "0"
26	Surgery = "1"	Accident = "0"
25	Surgery = "1"	Accident = "1"
19	Surgery = "0"	Accident = "1"

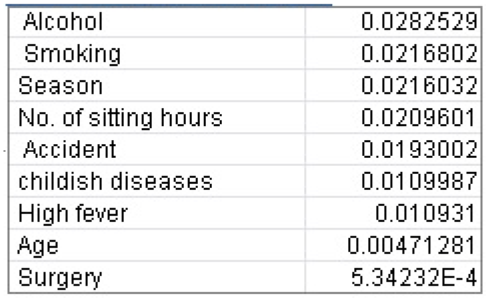
Weak Links

Links	Field 1	Field 2
11	Output = "Yes"	childish diseases = "0"
10	Output = "No"	childish diseases = "1"
10	Accident = "0"	childish diseases = "0"
9	Surgery = "1"	childish diseases = "0"
9	Output = "No"	Accident = "0"
7	Output = "No"	Surgery = "1"
5	Output = "No"	Surgery = "0"
4	Surgery = "0"	childish diseases = "0"
3	Accident = "1"	childish diseases = "0"
3	Output = "No"	Accident = "1"
2	Output = "No"	childish diseases = "0"

Table 1.2

4.4 Neural Network:

On constructing the neural network for our data set, we got the relative importance of the parameters that we used on the output (i.e., the decision whether a man has normal fertility or not. The neural net uses minimal statistical or mathematical knowledge and shows the output by the way the human mind processes the information. After running our data sets in the Neural Net it was found that Alcohol has the most importance in determining the fertility, followed by smoking and the season in which the test was taken.



Alcohol	0.0282529
Smoking	0.0216802
Season	0.0216032
No. of sitting hours	0.0209601
Accident	0.0193002
childish diseases	0.0109987
High fever	0.010931
Age	0.00471281
Surgery	5.34232E-4

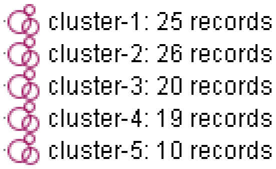
Table 1.3: Neural Net Results

The importance of neural network in this research is that it represents the effect of those attributes which have a range of values.

4.5 Clustering:

Clustering in graphs is well researched topic and many algorithms have been proposed by various authors. In graph related clustering, there are two possible approaches: 1. Determination of dense node clusters in a single large graph. 2. There are multiple graphs of modest size and one wants to cluster those graphs as objects. In this research, we followed the first approach in which we implemented K means clustering algorithm. The reason for choosing K means clustering was that it is an effective partitioning clustering algorithm. As explained by Macqueen[4,] The procedure follows a simple and easy way to classify a given data set through a certain number of clusters fixed a priori. Every cluster is defined with a centroid and each object is assigned to the group which has the closest centroid.

While implementation, we specified number of clusters to be extracted as 5.



cluster-1: 25 records
cluster-2: 26 records
cluster-3: 20 records
cluster-4: 19 records
cluster-5: 10 records

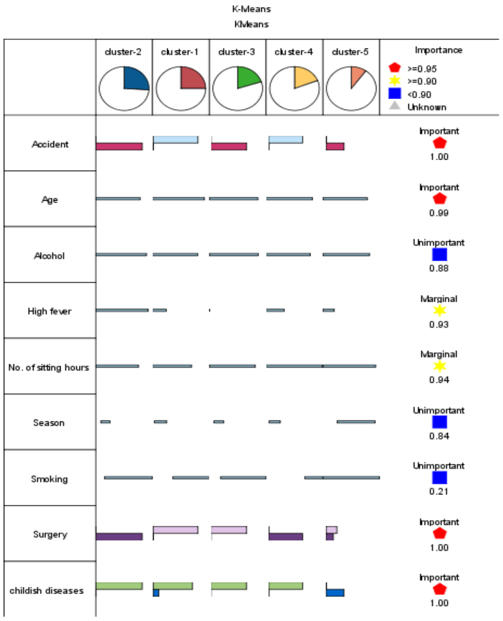


Figure 5.0

5 GRAPH DATA MINING

Approaches to Graph mining have been categorized into 5 categories (Takashi et al): *Greedy based approach, mathematical graph theory based approach, Inductive logic programming, Inductive database based approach and kernel function based approach*.

As Takashi et al have explained "Apriori Graph mining falls under mathematical graph theory based approach because this approach mines the large datasets based on support measures. One vertex is assigned to each of the graphs from the frequent graphs and then frequent graphs which are relatively larger in size are searched in bottom up approach. Let the number of vertices contained in a graph be its "size", an adjacency matrix of a graph whose size is k be X_k, the ij-element of X_k, x_{ij} and its graph, G (X_k). AGM can handle the graphs consisting of labeled vertices and labeled edges. The vertex labels are defined as Np (p=1…α) and the edge labels, Lq(q = 1…β). Labels of vertices and edges are indexed by natural numbers for computational efficiency. The AGM system can mine various types of sub graphs including general subgraph, induced subgraph, and connected subgraph, ordered sub tree, unordered subtree and subpath. The candidate generation of frequent induced subgraph is done as follows. Two frequent graphs are joined only when the following conditions are satisfied to generate a candidate of frequent graph of size k+1. Let X_k and Y_k be adjacency matrices of two frequent graphs G(X_k) and G(Y_k) of size k. If both G (X_k) and G (Y_k) have equal elements of the matrices except for the elements of the k^{th} row and the k^{th} column, then they are joined to generate Zk+1 as follows.

$$X_k = \begin{pmatrix} X_{k-1} & \boldsymbol{x}_1 \\ \boldsymbol{x}_2^T & 0 \end{pmatrix}, \quad Y_k = \begin{pmatrix} X_{k-1} & \boldsymbol{y}_1 \\ \boldsymbol{y}_2^T & 0 \end{pmatrix},$$

$$Z_{k+1} = \begin{pmatrix} X_{k-1} & \boldsymbol{x}_1 & \boldsymbol{y}_1 \\ \boldsymbol{x}_2^T & 0 & z_{k,k+1} \\ \boldsymbol{y}_2^T & z_{k+1,k} & 0 \end{pmatrix},$$

Where X_{k-1} is the adjacency matrix representing the graph whose size is k-1, xi and yi(i = 1, 2) are (k-1)*1 column vectors. The elements $z_{k,k+1}$ and $z_{k+1,k}$ represent an edge label between kth vertices of X_k and Y_k. Their values are mutually identical because of the diagonal symmetry of the undirected graph. Here, the elements $z_{k,k+1}$ and $z_{k+1,k}$ of the adjacency matrix Z_{k+1} are not determined by X_k and Y_k. In case of an undirected graph, two possible cases are considered in which 1) there is an edge labeled Lq between the kth vertex and the k+ 1th vertex of G(Z_{k+1}) and 2) there is no edge among them. Accordingly β+1 adjacency matrices whose (k, k+1) element and (k + 1, k)-element are "0" and "Lq" are generated. X_k and Y_k are called the first matrix and the second matrix to generate Z_{k+1} respectively. Because the labels of the kth nodes of X_k and Y_k are the same, switching X_k and Y_k, i.e., taking Yk as the first matrix and X_k as the second matrix, produces redundant adjacency matrices. In order to avoid this redundancy, the two adjacency matrices are joined only when the following condition is satisfied.

code(the first matrix) ≤ code(the second matrix)

The adjacency matrix generated under these constraints is a "normal form". The graph G of size k+1 is a candidate frequent graph only when adjacency matrices of all induced subgraphs whose size are k are confirmed to be frequent graphs. If any of the induced subgraphs of G(Z_{k+1}) is not frequent, Z_{k+1} is not a candidate frequent graph, because any induced subgraph of a frequent graph must be a frequent graph due to the anti-monotonicity of the support. This check to use only the former result of the frequent graph mining is done without accessing the graph data set. After the generation of candidate subgraphs, their support is counted by accessing the data set. To save computation for the counting, the graphs in the data set are represented in normal form matrices, and each subgraph matching is made between their normal forms. This technique significantly increases the matching efficiency. The process continues in level-wise manner until no new frequent induced subgraph is discovered."

6 CONCLUSION AND FUTURE WORK

In this research, we analyzed various factors that affect the men's fertility. Various association rules were established which can help can help the doctors identify multiple cause to infertility. As the concept of basket analysis was further extended to Apriori Graph Mining, it makes the data mining of large datasets highly effective by making use of adjacency matrixes as explained. This research can be very helpful in the field of ontology and medical sciences. It can be extended to study of various cancers, liver problems with risk factors as alcohol and fats. It can also be extended to the study of genetic diseases and determining the probability of occurrence of those diseases in the child. Also, we plan to implement it on the datasets containing information of various districts with their population and diseases which can help the Ministry of Health to determine the prevalent diseases in particular areas and take appropriate steps.

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8 ACKNOWLEDGEMENTS

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