

gApprox: Mining Frequent Approximate Patterns from a Massive Network

Chen Chen[†] Xifeng Yan[‡] Feida Zhu[†] Jiawei Han[†]

[†]University of Illinois at Urbana-Champaign
{cchen37, feidazhu, hanj}@cs.uiuc.edu

[‡]IBM T. J. Watson Research Center
xifengyan@us.ibm.com

Abstract

Recently, there arise a large number of graphs with massive sizes and complex structures in many new applications, such as biological networks, social networks, and the Web, demanding powerful data mining methods. Due to inherent noise or data diversity, it is crucial to address the issue of approximation, if one wants to mine patterns that are potentially interesting with tolerable variations.

In this paper, we investigate the problem of mining frequent approximate patterns from a massive network and propose a method called gApprox. gApprox not only finds approximate network patterns, which is the key for many knowledge discovery applications on structural data, but also enriches the library of graph mining methodologies by introducing several novel techniques such as: (1) a complete and redundancy-free strategy to explore the new pattern space faced by gApprox; and (2) transform “frequent in an approximate sense” into an anti-monotonic constraint so that it can be pushed deep into the mining process. Systematic empirical studies on both real and synthetic data sets show that frequent approximate patterns mined from the worm protein-protein interaction network are biologically interesting and gApprox is both effective and efficient.

1 Introduction

In the past, there have been a set of interesting algorithms [4, 10, 6] that mine frequent patterns in a set of graphs. Recently, there arise a large number of graphs with massive sizes and complex structures in many new applications, such as biological networks, social networks, and the Web, demanding powerful data mining methods. Because of their characteristics, we are now interested in patterns that frequently appear at many different places of a single network.

Example 1 Let us consider a **Protein-Protein Interaction (PPI) network in Biology**. A PPI network is a huge graph whose vertices are individual proteins, where an edge exists between two vertices if and only if there is a significant protein-protein interaction. Due to some underlying biological process, occasionally we may observe two subnets

P_a and P_b , which are quite similar in the sense that, after proper correspondence, discernable resemblance exists between individual proteins, e.g., with regard to their amino acids, secondary structures, etc., and the interactions within P_a and P_b are nearly identical to each other¹.

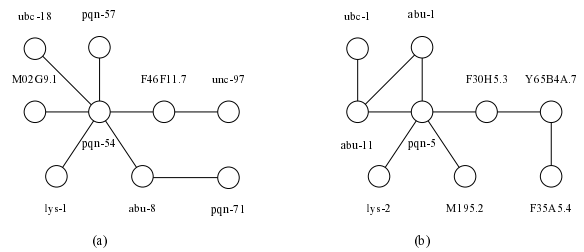


Figure 1. Two subnets extracted from the worm PPI network, where proteins at the corresponding positions of (a) and (b) are biologically quite similar, and 2 PPI deletions plus 3 PPI insertions transform (a) into (b).

There are in general two major complications to mine such massive and highly complex networks:

First, compared to algorithms targeting a set of graphs, mining frequent patterns in a single network needs to partition the network into regions, where each region contains one occurrence of the pattern. This partition changes from one pattern to another; whereas for any given partition, regions may overlap with each other as well. All these problems are not solved by existing technologies for mining a set of graphs.

Second, due to various inherent noise or data diversity, it is crucial to account for *approximations* so that all potentially interesting patterns can be captured. Cast to the PPI network we described in Example 1 (see Fig.1), as long as their similarity is above some threshold, it is ideal to detect P_b as a place where P_a approximately appears.

In retrospect, compared to the rich literature on mining frequent patterns in a set of graphs, single network based algorithms have been examined to a minor extent. [5, 7, 1]

¹In Biology, this might represent a mechanism to backup a set of proteins whose mutual interactions support a vital function of the network, so that in case of any unexpected events, the “copy” can switch in.

took an initial step toward this direction; however, they only considered the first issue and did not pay enough attention to the second, i.e., none of them mined approximate patterns. As will be manifested later, the above two issues are actually intertwined when approximation comes into play; and thus, our major challenge is to lay out a new mining paradigm that does consider approximate matching in its search space.

To summarize, we made the following contributions:

1. We investigate the problem of *mining frequent approximate patterns from a massive network*: We give an approximation measure and show its impact on mining, i.e., how a pattern’s support should be counted based on its approximate occurrences in the network.

2. We propose a graph mining method called *gApprox* to tackle this problem: We design a novel strategy that is both complete and redundancy-free to explore the new pattern space faced by *gApprox*, and transform “frequent in an approximate sense” into an anti-monotonic constraint so that it can be pushed deep into the mining process.

3. We present systematic empirical studies on both real and synthetic data sets: The results show that frequent approximate patterns mined from the worm protein-protein interaction network are biologically interesting and *gApprox* is both effective and efficient.

4. The techniques we developed for *gApprox* are general, which can be applied to networks from other domains, e.g., social networks.

The rest of this paper is organized as follows. Section 2 presents the general model of mining frequent approximate patterns from a massive network. The mining algorithm is developed in Section 3. We report empirical studies, and give related work and discussions in Sections 4 and 5, respectively. Section 6 concludes the paper.

2 Problem Formulation

Definition 1 (Network) A network G is an edge-weighted graph, i.e., G is a 3-tuple (V_G, E_G, w_G) , where $w_G : E_G \rightarrow R^+$ is a weighting function mapping each edge $e_{uv} = (u, v) \in E_G$ to a real number $w_G[u, v] > 0$.

This setting is well-defined for many real applications, where vertices represent different entities, edges denote mutual relationship between entities, and weights indicate the tightness of such relationship (the tighter the relationship, the closer the two entities, and thus the smaller the weight).

Definition 2 (Pattern) A pattern P is a connected and induced subgraph of the network G , which can be represented by a connected vertex set $V_P \subseteq V_G$.

2.1 Approximate Pattern Occurrences

The scenario we are interested in is: P , as a fragment extracted from a particular region of G , may also appear in some other regions approximately. This is associated with

an *injective* function $m : V_P \rightarrow V_G$ mapping each vertex $v \in V_P$ to $m(v) \in V_G$. Now, to quantify the degree of approximation m incurs, we want to take into account: (1) approximation on vertices, and (2) approximation on edges.

Vertex Penalties: For a vertex $v \in V_P$, a list of matchable vertices $matchable(v) \subseteq V_G$ is provided. Let

$$dis_sim[v, m(v)] = \begin{cases} < \infty & \text{if } m(v) \in matchable(v) \\ \infty & \text{otherwise} \end{cases} \quad (0)$$

i.e., approximations can only happen within the matchable list. Usually, this is a reasonable assumption in real applications. For example, in a PPI network, though we do not want to require that two vertices are only matchable if they represent the same protein, it is also aimless to match two proteins that are very dissimilar or even irrelevant to each other. Finally, we can obtain the matchable lists by assuming a similarity cut-off δ among all pairs of vertices.

Edge Penalties: For a relationship (v_i, v_j) of P and its image $(m(v_i), m(v_j))$ under mapping m , an intuitive way to define a measure penalizing approximation is to compare the relationship tightness associated with each of them. One way of quantifying the tightness here is to plug in a *shortest path based distance*, which in essence treats the shortest path $u \rightsquigarrow v$ as a *pseudo* edge between u and v , with its weight equalling the total weight summed over $u \rightsquigarrow v$. Now, having a (pseudo) weighted edge between each pair of vertices, we can simply take an absolute difference and present the penalty function as:

$$|dist[v_i, v_j] - dist[m(v_i), m(v_j)]| \quad (1)$$

There could be other alternatives (e.g., max flow based) to define a distance between two vertices. Or, if the specific application provides us with full tightness information among all pairs of vertices, we can directly take them as input. For instance, in the case of Example 1, in order to reflect the number of PPIs that are different (i.e., present in one but missing in the other) after the pattern is embedded, we may adopt the following *dist* function for any two proteins pr_i and pr_j in the PPI network,

$$dist[pr_i, pr_j] = \begin{cases} 1 & \text{if } pr_i \text{ and } pr_j \text{ interact} \\ 2 & \text{otherwise} \end{cases} \quad (2)$$

since $|1 - 2| = 1$. In this perspective, Eq.1 and our discussions below will be built on an abstract symbol of *dist*.

Definition 3 (Degree of Approximation) Given a pattern P and a network G , an injective mapping m embeds P in some region of G by matching a vertex $v \in V_P$ to a vertex $m(v) \in V_G$. This embedding is associated with a degree of approximation $approx(P \xrightarrow{m} G)$, which is defined as:

$$\sum_{v \in V_P} dis_sim[v, m(v)] + \sum_{v_i, v_j \in V_P} |dist[v_i, v_j] - dist[m(v_i), m(v_j)]| \quad (3)$$

Definition 4 (Approximate Occurrence) Given error tolerance Δ , the vertex set $\{m(v)|v \in V_P\}$ for an embedding m is said to be an approximate occurrence of P if and only if $\text{approx}(P \xrightarrow{m} G) \leq \Delta$.

2.2 Pattern Support with Approximation

Downward-closure is an important requirement to perform efficient mining [9], i.e., if P is a subpattern of P' ($V_P \subseteq V_{P'}$), then $\text{sup}(P) \geq \text{sup}(P')$ must hold. If this requirement is violated, for a task that asks for all patterns with support higher than min_sup , there is no way we can stop searching for even bigger patterns at any stage during the mining process, because it is always possible for a pattern to qualify min_sup after growing. This will make any algorithm suffer from *uncontrollable explosions*. Looking at Fig.2, as $\text{sup}(P_{123}) = 2 > \text{sup}(P_{12}) = 1$ if overlapping occurrences are counted, we have to follow a support definition in which overlaps are prohibited.

Definition 5 (Pattern Support with Approximation)

Two occurrences of P are said to be disjoint if and only if they do not share any vertices in common. Then, P 's pattern support with approximation is defined to be the maximal number of disjoint ones that can be chosen from the set of its approximate occurrences.

Lemma 1 $\text{sup}(P) \geq \text{sup}(P')$, if P is a sub-pattern of P' , i.e., pattern support with approximation is an anti-monotonic mining constraint.

Definition 6 (Frequent Approximate Pattern Mining)

Given a network G and two thresholds: (1) maximal degree of approximation Δ , (2) minimum support min_sup , find the pattern set \mathcal{P} such that $\forall P \in \mathcal{P}, \text{sup}(P) \geq \text{min_sup}$. Here, any $P \in \mathcal{P}$ is called a frequent approximate pattern.

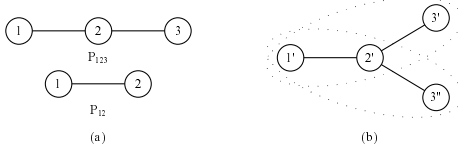


Figure 2. Embedding patterns P_{123} and P_{12} of (a) in (b), where 1 can match 1', 2 can match 2', 3 can match 3'/3''.

3 Algorithm

As a mining problem targeting all frequent approximate patterns in a network, there are two major issues we need to tackle, each of them will be discussed below.

1. Pattern Space Exploration: What is the problem's full pattern space, and how can we search through it? As we indicated in the introduction, this search space must take approximation into account.

2. Support Counting: For patterns in the search space, how can we count their support and report those frequent ones with regard to a predetermined threshold min_sup ? Based on Section 2, for each pattern, we should enumerate its approximate occurrences in the network at first, and then decide the maximal number of disjoint occurrences.

3.1 Pattern Space Exploration

As influenced by approximation, the pattern space we face here is different from that in an exact mining paradigm. Previous algorithms like [5] and [7] assume a network with vertex/edge labels, while a pattern is nothing but a labeled subgraph. By exact matching, in order to embed a pattern in some region of the network, vertices/edges at corresponding positions must have identical labels. In this sense, the pattern space there consists of "all labeled graphs", which can be organized on a lattice and explored by search strategies such as breadth-first search [4] and depth-first search with right-most extensions [10].

In our setting, the network is not a labeled one; to accommodate approximations, what we have is a matchable list for each vertex indicating all vertices that are highly similar, treated as its "copies". Keeping this in mind, it seems necessary for us to treat every vertex as unique, which means that each induced subgraph of the network may potentially be a different pattern, i.e., "all connected vertex sets in a given network" is our new pattern space here.

In the following presentation, we are going to introduce a strategy that is both complete and redundancy-free to traverse the above search space. Fig.3 is taken as a running example. To begin with, we losslessly decompose the pattern space as follows:

1. Find all connected vertex sets in G that contain 1.
2. Remove 1 from G , and find all connected vertex sets in the new graph \tilde{G} that contain 2.
3. And so on so forth ...

where step i explores all patterns that contain vertex i but do not contain vertices $1, 2, \dots, i-1$. Now, we discuss step 1, i.e., generating all connected vertex sets starting from 1; all other steps follow the same routine.

Stage 1: After the decomposition shown in Fig.3(b), start from 1 and mark 1.

Stage 2: Expand from 1 to reach 2, 5, 6. Mark 2, 5, 6. There are totally seven connected vertex sets in this stage: $\{1,2\}, \{1,5\}, \{1,6\}, \{1,2,5\}, \{1,2,6\}, \{1,5,6\}, \{1,2,5,6\}$. Indeed, as 2, 5, 6 are all adjacent to 1, $\{1\}$ union any combination of 2, 5, 6 should be connected. Here, we can assume an order of $6 > 5 > 2$, unrepeatedly traverse the powerset of $\{2,5,6\}$ (as we do for itemsets), and finally union with $\{1\}$. The whole procedure of stage 2 is depicted in Fig.3(c).

Stage 3: Taking each of the seven connected vertex sets in stage 2 as a starting point, continue expansion. In Fig.3(d), we pick $\{1,5,6\}$ as an example and reach 4, 7. Mark 4, 7. Explore $\{1,5,6\}$ union anything in the powerset of $\{4,7\}$ in the same manner as we did in stage 2. Note that, though there is an edge between 5 and 2, we prohibit the expansion to 2, because 2 has already been marked in previous stages, in which case $\{1,5,6\} \cup \{2\} = \{1,2,5,6\}$ is just another starting point among the seven in stage 2. More

generally, only those vertices that are both adjacent and unmarked can be absorbed during expansion.

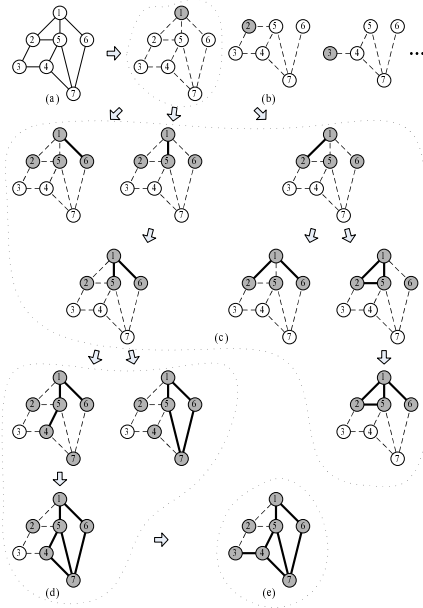


Figure 3. Exploring the Pattern Space: (a) the original graph, (b) decomposition of the problem and stage 1, (c) stage 2, (d) stage 3, (e) stage 4, where each stage is enclosed respectively within a loop. We darken marked vertices along the way, while edges are correspondingly changed from dotted to thickened as new vertices are absorbed.

Stage 4: Finally, in Fig.3(e), we pick $\{1,5,6,4,7\}$ as an example from the three connected vertex sets expanded in stage 3, for which only an unmarked 3 can be absorbed. Generate $\{1,5,6,4,7,3\}$ and stop expansion, because there are no more unmarked vertices now.

Algorithm 1 gives pseudo-code for the above process.

Theorem 1 *Explore()* in Algorithm 1 is both complete and redundancy-free, i.e., given a network G , (1) it only generates connected vertex sets in G ; (2) it can generate all connected vertex sets in G ; (3) it does not generate the same connected vertex set more than once.

3.2 Support Counting

Now we are ready to look at support counting, in which our first task is to enumerate the approximate occurrences of any pattern encountered during Section 3.1’s pattern space exploration. Since *Explore()* follows a depth-first fashion, which continuously absorbs new vertices and expands the current pattern P to P' until backtracking, we can incrementally obtain the occurrences of P' based on those of P , i.e., whenever we expand P to $P' = P \cup \{v\}$, the occurrences of P are also expanded by adding another vertex that is matchable with v . Occurrences with degree of approximation more than Δ and patterns with support less than min_sup are dropped immediately.

A pattern P ’s support is defined to be the maximal number of “disjoint” ones that can be chosen from P ’s approximate occurrences in the network. However, deciding this maximum turns out to be a very hard problem, which is related to the NP-Complete *maximal independent set*, as some previous works have shown [5]. If it is crucial to report the “accurate frequency” of patterns, we can always calculate it by brute-force; otherwise, an upperbound, like the one developed in Algorithm 2, is enough, which will be used to stop growing patterns based on the downward-closure property.

Algorithm 1 Complete and Non-redundant Exploration

Function: *Explore*(G)

Input: a network G .

Output: all connected vertex sets in G .

- 1: **for each** $v \in G$ **do** $mark(v) = false$;
- 2: pick a vertex u with smallest ID, $mark(u) = true$, output $\{u\}$;
- 3: *DFS_vertical*($G, \{u\}$);
- 4: remove u from G , and let the resulting graph be \tilde{G} ;
- 5: *Explore*(\tilde{G});

Function: *DFS_horizontal*(G, P, V_{expand})

Input: a network G , a set P of connected vertices in G , a vertex set V_{expand} whose powerset is to be unioned with P .

Output: all connected vertex sets in G that consist of P , a proper subset of V_{expand} , and some currently unmarked vertices.

- 1: Order the vertices in V_{expand} as $v_1 < \dots < v_k$;
- 2: **for** $i = 1$ **to** k **do**
- 3: $P' = P \cup \{v_i\}$, output P' ;
- 4: $V'_{expand} = \{v_{i+1}, \dots, v_k\}$;
- 5: *DFS_horizontal*(G, P', V'_{expand});
- 6: *DFS_vertical*(G, P');

Function: *DFS_vertical*(G, P)

Input: a network G , a set P of connected vertices in G .

Output: all connected vertex sets in G that consist of P and some currently unmarked vertices.

- 1: $V_{expand} = \{v | v \in G, v \notin P, mark(v) = false, \text{ and } P \cup \{v\} \text{ is connected in } G\}$;
 - 2: **for each** $v \in V_{expand}$ **do** $mark(v) = true$;
 - 3: *DFS_horizontal*(G, P, V_{expand});
 - 4: **for each** $v \in V_{expand}$ **do** $mark(v) = false$;
-

Algorithm 2’s idea in providing an upperbound on the maximal number of disjoint ones that can be chosen from a pattern’s occurrences is explained by the following example. Think each occurrence as a vertex set and assume there are 4 of them: $\{v_1, v_2\}, \{v_1, v_3\}, \{v_1, v_4\}, \{v_2, v_5\}$, then v_1 acts like a “bottleneck” – because it is contained in 3 sets: $\{v_1, v_2\}, \{v_1, v_3\}, \{v_1, v_4\}$, which is the most among all 5 vertices. Obviously, at most 1 set can be chosen from these

Algorithm 2 Providing a Support Upperbound

Function: Upperbound(M_P)Input: the set of occurrences M_P for a pattern P .Output: an upperbound on the maximal number of disjoint vertex sets that can be chosen from M_P .

```
1: sup_bound= 0;
2: while  $M_P \neq \emptyset$  do
3:   let  $v$  be the one that appears in the greatest number
   of vertex sets in  $M_P$ ;
4:   sup_bound=sup_bound+1;
5:   for each  $m \in M_P$  do
6:     if  $m$  contains  $v$  then remove  $m$  from  $M_P$ ;
```

3 in order to ensure disjointness. Keep iterating the same procedure, we go on to consider the remaining set $\{v_2, v_5\}$ after all sets containing v_1 are removed: As we can get only 1 disjoint set here, the total number of disjoint occurrences that can be chosen is at most $1 + 1 = 2$.

Lemma 2 Given a pattern P , its support must be less than or equal to the Upperbound(M_P) provided by Algorithm 2.

Now we are ready to combine all above together and deliver **gApprox**. The main skeleton of gApprox is Algorithm 1’s pattern space exploration: When examining each pattern encountered, i.e., on the 3rd line of DFS_horizontal(), we expand the occurrences of P (i.e., M_P) to obtain those of P' (let them be $M_{P'}$), and then based on $M_{P'}$, Upperbound() is called to decide whether P' should be grown further: If not, we terminate early. In summary, gApprox is formed by simply inserting occurrence enumeration, support upperbound calculation, and a conditional branch on the 3rd line of Algorithm 1’s DFS_horizontal() function.

4 Experiments

We performed empirical study on both real and synthetic graph data sets. The real graph dataset is a worm PPI network, obtained from the DIP database (Database of Interacting Proteins: <http://dip.doe-mbi.ucla.edu>). The synthetic data generator is provided by Kuramochi et al. [4]. All experiments are done on a Windows machine with 3GHz Pentium IV CPU and 1GB MEM; programs are written in C++.

4.1 Worm PPI Network

The worm PPI network contains 2,637 proteins and 4,030 PPIs. There are 12,902 pairs of matchable proteins having BLAST similarity score higher than $\delta = 10^{-7}$. The most “frequent” protein has 74 “copies”, while on average a protein is similar to $\frac{12902}{2637} \approx 4.9$ counterparts, which suggests that we must set min_sup low in order to capture frequent patterns.

We want to discover protein subnet patterns that approximately occur in more than min_sup locations of the PPI

network. As introduced in Section 2.1, Eq.1 is used to quantify the distance between any two vertices in the network. In order to focus solely on the interactions of proteins, within δ , we treat the “vertex (protein) mismatch” penalty dis_sim as 0. Fig.1(a) is one of the patterns discovered, while Fig.1(b) gives its occurrence whose degree of approximation is 5 (2 edge deletions plus 3 edge insertions). In addition to similar interconnecting topologies, the two subnetworks are composed of proteins with similar functions and are often from the same protein family. Pairs of functionally similar proteins are located in similar locations in the network, indicating that these two protein networks may be responsible for similar biological mechanisms. For example, proteins pqn-54 and pqn-5 have the highest degree in each network and are both Prion-like-(Q/N-rich)-domain-bearing proteins. The proteins adjacent to these two proteins also share similar function such as lys-1 and lys-2 which are both lysozyme proteins.

Apart from pattern interestingness, we further examine the computational characteristics of gApprox. Fig.4 and Fig.5 illustrate the number of frequent approximate patterns and performance (i.e., running time) with varying minimum support (min_sup) and maximal approximation (Δ).

It can be seen that when Δ increases, both the running time and the number of frequent approximate patterns increase; while a reverse situation exists for min_sup . These phenomena are well expected. Note that, in Fig.4 and Fig.5, $\Delta = 4$ is the maximal approximation marked on the plots; although 4 seems to be a relatively small number, it is not small indeed: From Fig.1, we can see that patterns here are in general not very “dense” networks – approximation on 4 PPIs means 50% error tolerance for a pattern with 8 PPIs, which is already a quite significant amount. Even though, our algorithm can still finish in about 6 minutes, which clearly demonstrates the efficiency of gApprox.

4.2 Synthetic Data

We then test gApprox on a series of synthetic data sets, showing its efficiency.

The data set we take is D1T3kL200I10V60E1 [4], i.e., 1 (D) network with 3,000 (T) vertices (and 4,976 edges), which is generated by 200 (L) seed patterns of size 10 (I); the number of possible vertex and edge labels are set to 60 (V) and 1 (E), respectively. Here, two vertices are matchable (with $dis_sim = 0$ since they are “identical”) if the same label is assigned to them. Furthermore, we randomly pick a real number from $[0.5, 1]$ to be the weight on each edge: Since we do not want two separate vertices to have a distance close to 0, 0.5 is fixed as a lowerbound. We adopt the shortest path based distance and make a connectivity cut-off based on it. If the shortest path distance is less than 1.5, then the two vertices are considered to be connected, i.e., during pattern exploration, they are “adjacent”, and the pattern expansion from one vertex to the other is enabled.

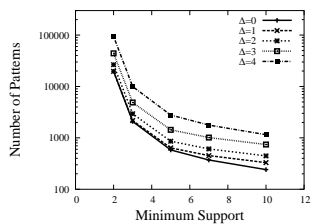


Figure 4. Pattern Number w.r.t min_sup and Maximal Approximation Δ , the worm PPI network

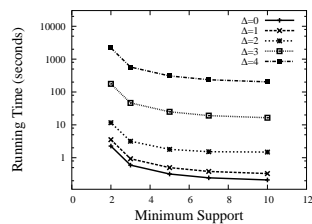


Figure 5. Running Time w.r.t min_sup and Maximal Approximation Δ , the worm PPI network

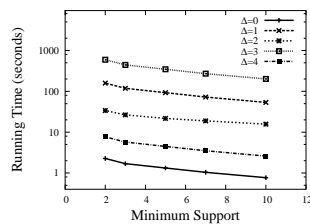


Figure 6. Running Time w.r.t min_sup and Maximal Approximation Δ , the synthetic dataset

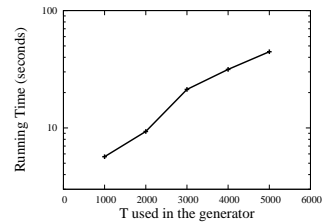


Figure 7. Running Time w.r.t the Number of Vertices in the Network, the synthetic dataset

Fig.6 shows the algorithm’s performance (i.e., running time) w.r.t min_sup and maximal approximation Δ ; the trends are similar as those depicted in Fig.5. We then change the size of the generated network, and show how gApprox reacts (Fig.7 varies the number of vertices (T) in a network from 1000 to 5000).

5 Related Work and Discussions

Quite a few algorithms have been developed to mine frequent patterns over graph data [4, 10, 6]. Most of them worked on a set of graphs, which do not apply to the single graph mining scenario here. Only a few [5, 7, 1] studied the pattern mining problem in a single network.

Some studies formulate the problem as a *searching* procedure: Given a query Q , searching asks for those places where Q exactly/approximately appears in the network. Exact search is often referred to as graph matching, which has been actively pursued for decades [2]. Recently, a few approximate search methods have also been developed to align the query path/substructure with the subject network [3, 8], with the help of pre-built indices. However, mining is still quite different from searching in that we never know what the patterns are before discovering them. Thus, there are no pre-defined queries that can be leveraged as axes for the algorithms to search around.

6 Conclusions

In this paper, we investigate the problem of mining frequent approximate patterns from a massive network: We give an approximation measure and show its impact on mining, i.e., how a pattern’s support should be counted based on its approximate occurrences in the network. An algorithm called gApprox is presented. Empirical studies show that patterns mined from real protein-protein interaction networks are biologically interesting and gApprox is both effective and efficient.

The techniques we developed for gApprox is general, which can be applied to networks from other domains as well. As a promising topic, it would be interesting to systematically study how gApprox can be modified to reach

bigger, thus more interesting patterns even faster, with some sacrifice on the completeness of mining results.

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