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Polynomial Time Matching Algorithms for Tree Structured Patterns

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1 Introduction

Graph-structured data occurs in many domains, such as biomolecular database, chemical database, the World Wide Web, or semistructured data. Many researchers try to find hidden knowledge from structures of such data by using data mining techniques. The formalization of expressing graph-structured data is quite important for finding useful knowledge [10].

A term graph, which is one of expressions of graph-structured data, is a hypergraph whose hyperedges are regarded as variables. By expressing structures of data in database with term graphs, we can design tools for discovering hidden knowledge or background knowledge from graph-structured data. In Fig. 1, for example, we can obtain each tree T_1 , T_2 and T_3 from the term tree t by replacing hyperedges in t with arbitrary trees. That is, the term tree t shows common structures between them. The first-order language is much better suited for expressing background knowledge and graph structures [3]. Then, inductive logic programming (ILP) systems in knowledge discovery have been proposed [1, 2, 4]. In [8], we designed and implemented the knowledge discovery system KD-FGS for graph-structured data, which employs Formal Graph System (FGS,[11]) as a knowledge representation language and a refutably inductive inference as an ILP mechanism [9]. FGS is a kind of logic programming system which uses term graphs instead of terms in first-order logic. Therefore FGS can directly deal with graphs and is suited for expressing background knowledge obtained from graph-structured data. By using a term graph, we can design tools based on a graph pattern matching method for finding new knowledge represented by term graphs obtained from graph-structured data.

Such tools are useful for finding association rules over term graphs, producing decision trees having term graphs as vertex labels, and finding the minimum term graph by using the minimum description length principle.

In this paper, we consider a matching problem for a term graph and a standard graph. Informally, the matching problem for a term graph g and a graph G is to decide whether or not there exists a graph G' such that G' is isomorphic to G and G' is obtained by replacing each variable in g with an arbitrary graph. This problem is important for many knowledge discovery systems over term graphs for graph-structured data. Graphs have enough richness and flexibility to express unknown structures, but many elementary graph problems, e.g., subgraph isomorphism and largest common subgraph, are known to be NP-complete [5]. Due to this fact, it is difficult to solve the matching problem for a term graph in polynomial time. Then it is hard to design and implement a discovery system finding efficiently new knowledge from graph-structured data in practice. We consider interesting subclasses of term graphs, called regular term trees, such that their matching problems are solvable efficiently.

Let Σ and Λ be finite alphabets, and let X be an alphabet. An element in Σ , Λ and X is called a *vertex label*, *edge label* and *variable label*, respectively. Assume that $(\Sigma \cup \Lambda) \cap X = \emptyset$. A *term graph* $g = (V, E, H)$ consists of a vertex set V , an edge set E and a multi-set H . Each element in H is a list of distinct vertices in V and is called a *variable*. An item in a variable is called a *port*. And a term graph g has a vertex labeling $\varphi_g : V \rightarrow \Sigma$, an edge labeling $\psi_g : E \rightarrow \Lambda$ and a variable labeling $\lambda_g : H \rightarrow X$. For a set or a list S , the number of elements in S is denoted by $|S|$. The *dimension* of a variable h is the number of vertices which are

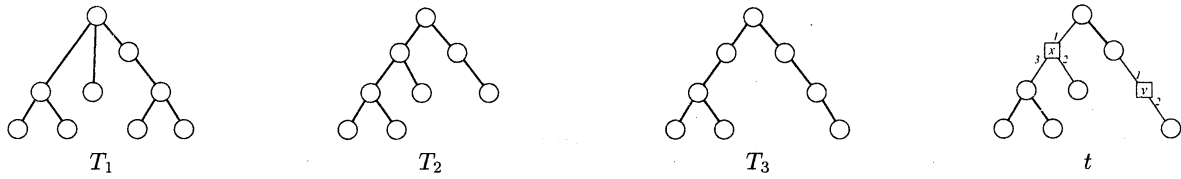


Fig. 1. A term tree t as a tree-like structured pattern which matches trees T_1 , T_2 and T_3 .

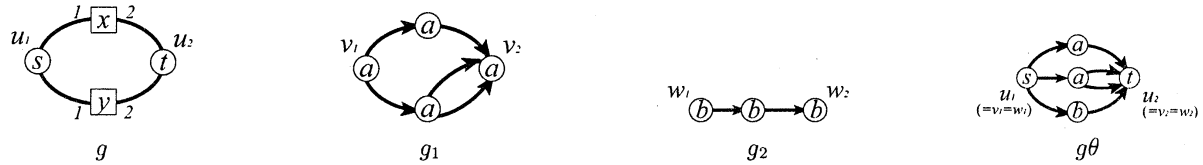


Fig. 2. A term graph $g = (V, E, H)$ is defined by $V = \{u_1, u_2\}$, $E = \emptyset$, $H = \{e_1 = (u_1, u_2), e_2 = (u_1, u_2)\}$, $\varphi_g(u_1) = s$, $\varphi_g(u_2) = t$, $\lambda_g(e_1) = x$, and $\lambda_g(e_2) = y$. $g\theta$ is obtained by applying a substitution $\theta = \{x := [g_1, (v_1, v_2)], y := [g_2, (w_1, w_2)]\}$ to g . A variable is represented by a box with lines to its elements and the order of its items is indicated by the numbers at these lines.

contained in h . The *dimension* of a term graph g is the maximum dimension over all variables in g . The *degree* of a vertex u in a term graph is the sum of the number of edges and variables containing u . The *degree* of a term graph g is the maximum degree over all vertices in g . For example, a term graph $g = (V, E, H)$ is shown in Fig. 2.

In [7], for a regular term tree t and a tree T such that the dimension of each variable in t is exactly 2 and the degree of T is unbounded, we presented a polynomial time algorithm solving the matching problem for t and T . In this paper, we show that, in general, the matching problem for a regular term tree t and a tree T is NP-complete even if the dimension of t is only 4. But, if the dimension of t is bounded by some constant greater than 1 and also the degree of T is bounded by some constant, we can give a polynomial time algorithm solving the matching problem. These show that a term tree is a quite useful expression of knowledge obtained from tree-like structured data. Our algorithms lead us to develop new knowledge discovery tools employing term graphs directly which express knowledge obtained from tree-like structured data.

2 Matching Algorithms for Tree Structured Patterns

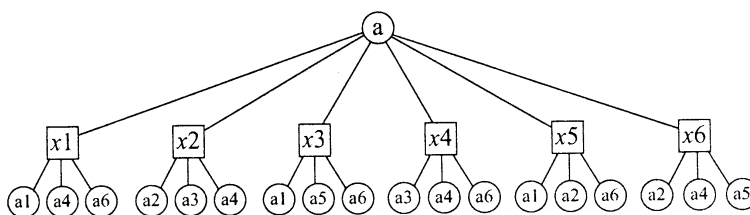
Let g be a term graph and σ a list of distinct vertices in g . We call the form $x := [g, \sigma]$ a *binding* for a variable label $x \in X$. Let g_1, \dots, g_n be term graphs. A *substitution* θ is a finite collection

of bindings $\{x_1 := [g_1, \sigma_1], \dots, x_n := [g_n, \sigma_n]\}$, where x_i 's are mutually distinct variable labels in X and each g_i has no variable labeled with an element in $\{x_1, \dots, x_n\}$. We obtain a new term graph f by applying a substitution $\theta = \{x_1 := [g_1, \sigma_1], \dots, x_n := [g_n, \sigma_n]\}$ to a term graph $g = (V, E, H)$ in the following way. For each binding $x_i := [g_i, \sigma_i] \in \theta$ ($1 \leq i \leq n$) in parallel, we attach g_i to g by removing all variables t_1, \dots, t_k labeled with x_i from H , and by identifying the m -th vertex t_j^m of t_j and the m -th vertex σ_i^m of σ_i for each $1 \leq j \leq k$ and each $1 \leq m \leq |t_j| = |\sigma_i|$. We remark that the label of each vertex t_j^m of g is used for the resulting term graph which is denoted by $g\theta$. Namely, the label of σ_i^m is ignored in $g\theta$.

A substitution $\theta = \{x_1 := [g_1, \sigma_1], \dots, x_n := [g_n, \sigma_n]\}$ is called a *tree substitution* if all of the g_i are trees. A term graph t is called a *term tree* if for any tree substitution θ which contains all variable labels in t , $t\theta$ is also a tree. When one of the vertices in t is specified as the root of the term tree, t is called a *term rooted tree*. A term tree t is said to be *regular* if each variable label in t occurs exactly once [6] (e.g. Fig. 3,4). We say that T matches t if there exists a tree substitution θ such that $t\theta$ and T are isomorphic.

In this section, we consider the following problem for a regular term rooted tree with no label. For a regular term rooted tree with labels and a regular term unrooted tree with labels or without any label, we can also construct similar polynomial-time matching algorithms.

Regular term rooted tree t (the vertex with label "a" is the root of t).



Rooted tree T (the vertex with label "a" is the root of T).

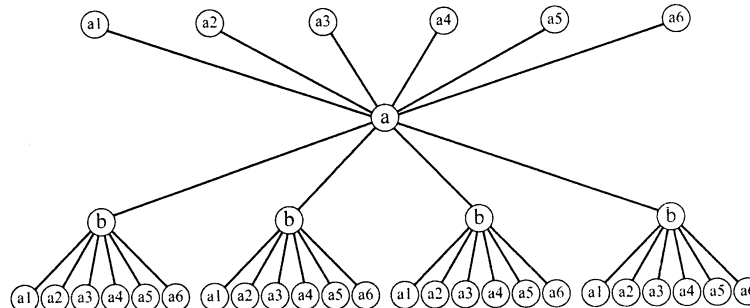


Fig. 3. A transformation from an instance (A, C) of X3C to an instance (t, T) of REGULAR TERM ROOTED TREE MATCHING. $A = \{a_1, a_2, a_3, a_4, a_5, a_6\}$, $C = \{c_1, c_2, c_3, c_4, c_5, c_6\}$, $c_1 = \{a_1, a_4, a_6\}$, $c_2 = \{a_2, a_3, a_4\}$, $c_3 = \{a_1, a_5, a_6\}$, $c_4 = \{a_3, a_4, a_6\}$, $c_5 = \{a_1, a_2, a_6\}$, $c_6 = \{a_2, a_4, a_5\}$.

REGULAR TERM ROOTED TREE MATCHING

Instance: A regular term rooted tree t and a rooted tree T .

Question: Does T match t so that the root of T corresponds to the root of t ?

First we show the following theorem.

Theorem 1. REGULAR TERM ROOTED TREE MATCHING is NP-complete even if the dimension of an input regular term rooted tree is only 4.

Membership in NP is obvious. We transform EXACT COVER BY 3-SETS (X3C) [5, page 221] to this problem (Fig. 3).

Second we explain the algorithm Matching (Fig. 5) which is a framework for deciding whether a rooted tree T matches a regular term rooted tree t .

Let $t = (V_t, E_t, H_t)$ and $T = (V_T, E_T)$ be a regular term rooted tree with root r_t and a rooted tree with root r_T , respectively. A vertex of degree one is called a *leaf* if it is not the root. A *path* from v_1 to v_i is a sequence v_1, v_2, \dots, v_i of distinct vertices such that for $1 \leq j < i$, there exists an edge or a variable which includes v_j and v_{j+1} . If there is an edge or a variable which includes v and v' such that v' lies on the path from the root r_t to v , then v' is said to be the *father* of v and v is a

child of v' . In particular for a variable h , v is said to be a *child port* of h if there is a vertex v' such that both v and v' belong to h and v is a child of v' . A *descendant* of v is any vertex on the path from v to one of the leaves of the tree.

In Matching (Fig.5), a *label* for a vertex in T is a set $\{v_1, \dots, v_k, V_1, \dots, V_\ell\}$ where $k \geq 0$, $\ell \geq 0$, v_i is a vertex in t , and V_j is a set of vertices in t . Let L_1, \dots, L_m be a collection of labels. For any $V' \subseteq V_t$, we say that L_1, \dots, L_m covers V' if there exist distinct indices $k_1, \dots, k_{m'}, \ell_1, \dots, \ell_{m''}$ among $1, \dots, m$ and also there exist $v'_i \in L_{k_i}$ and $V''_j \in L_{\ell_j}$ for each $1 \leq i \leq m'$ and $1 \leq j \leq m''$ such that $V' \subseteq \{v'_1, \dots, v'_{m'}\} \cup V''_1 \cup \dots \cup V''_{m''}$. In particular if there is no proper subcollection of L_1, \dots, L_m which covers V' then we say that L_1, \dots, L_m exactly covers V' .

Let W be a set of vertices in t . The *induced term tree* of t by W is a term tree $t[W] = (W', E_t[W'], H_t[W'])$ where $W' = \{v \in V_t \mid v \text{ is in } W \text{ or there is a vertex } v' \text{ in } W \text{ such that } v \text{ is a descendant of } v'\}$, $E_t[W'] = \{\{u, v\} \in E_t \mid u \in W' \text{ and } v \in W'\}$ and $H_t[W'] = \{(v_1, \dots, v_n) \mid v_i \in W' \text{ and } (v_1, \dots, v_n) \text{ is the maximal sublist of some } h \in H_t \text{ with keeping the order of items in } h.\}$. For a single vertex $w \in V_t$, the induced term tree $t[w]$ of t by w is defined as $t[\{w\}]$. A *corresponding induced term tree* of t to $u \in V_T$ is an induced term tree by $W \subseteq V_t$ or $w \in V_t$ which

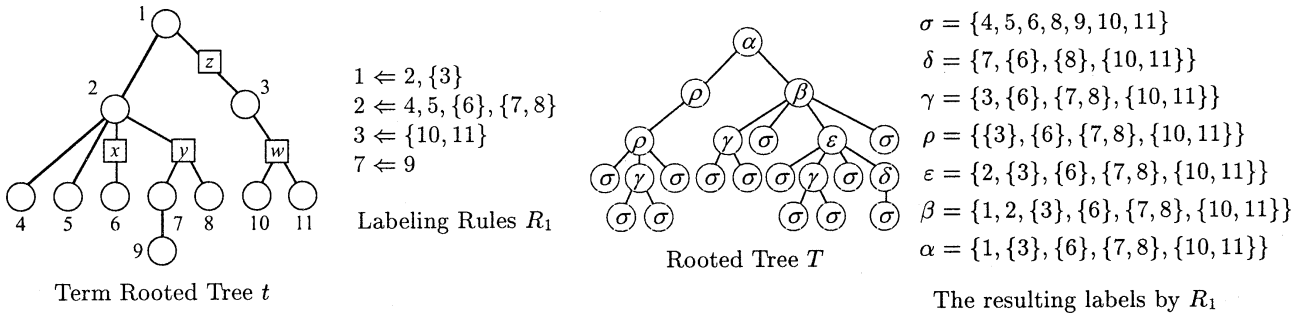


Fig. 4. An example: the labeling rule constructed from a regular term rooted tree $t = (\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11\}, \{\{1, 2\}, \{2, 4\}, \{2, 5\}, \{7, 9\}\}, \{(1, 3), (2, 6), (2, 7, 8), (3, 10, 11)\})$ with root 1 and the resulting labels of a rooted tree T after the procedure Matching terminates.

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procedure Matching(regular term rooted tree  $t$  with root  $r_t$ , rooted tree  $T$  with root  $r_T$ );
begin
  Construct the set of all labeling rules  $R_{r_t}$ ;
  Label all leaves of  $T$  with the set of all leaves of  $t$ ;
  while there exists a vertex  $v$  in  $T$ 
    such that  $v$  is not labeled and all children of  $v$  are labeled do
    Labeling( $v, R_{r_t}$ );
  if the label of  $r_T$  includes  $r_t$  then  $T$  matches  $t$  else  $T$  does not match  $t$ 
end.
  
```

Fig. 5. An algorithm for deciding whether or not a rooted tree T matches a regular term rooted tree t .

matches $T[u]$, i.e., the subtree of T with the root u . In particular if the induced term tree is induced by a single vertex w , the matching between $t[w]$ and $T[u]$ has a correspondence of w to u .

First we construct the set of all labeling rules.

Basic Labeling Rules

Let v be a vertex in t which is not a leaf. Let v_1, v_2, \dots, v_k be all children of v which are connected to v with edges. Let h_1, h_2, \dots, h_ℓ be all variables which include v , and for $i = 1, \dots, \ell$, V_i be the set of all children of v which are connected to v with the variable h_i . The labeling rule for v is defined as follows. If there is no variable which includes v , then let the generating rule of v be $v \Leftarrow v_1, \dots, v_k$, otherwise $v \Leftarrow v_1, \dots, v_k, V_1, \dots, V_\ell$.

Then we obtain the following theorem.

Theorem 2. Let t be a regular term rooted tree of dimension p such that t includes no variable of dimension 1, and let T be a rooted tree of degree d . REGULAR TERM ROOTED TREE MATCHING is solvable in $O((n + N)^2 \text{TMIS}(d^{O(p)}))$ time where n and N are the numbers of vertices in

t and T respectively, and $\text{TMIS}(s)$ is the time needed to find the maximum independent set in a graph of size s .

Corollary 1. Let t be a regular term rooted tree of dimension p such that t includes no variable of dimension 1, and let T be a rooted tree of degree d . REGULAR TERM ROOTED TREE MATCHING for the inputs t and T is solvable in $O((n + N)^2)$ time where n and N are the numbers of vertices in t and T respectively.

If the dimension of each variable in t is exactly 2 and the degree of T is unbounded, the procedure Matching by using the procedure (Fig.8) instead of the procedure (Fig.7) solves REGULAR TERM ROOTED TREE MATCHING in polynomial time.

Theorem 3 (Miyahara, et al. [7]). If the dimension of each variable in t is exactly 2, there exists a polynomial-time algorithm for solving REGULAR TERM ROOTED TREE MATCHING.

Since the maximum graph matching for a bipartite graph $\mathcal{B} = (\mathcal{V}, \mathcal{V}', \mathcal{E})$ is found in $O(|\mathcal{E}| \sqrt{\max\{|\mathcal{V}|, |\mathcal{V}'|\}})$ time, by applying the procedure (Fig.8) to all labeling rules at the same

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procedure Labeling(vertex  $u \in V_T$ , set of labeling rules  $R_{r_t}$ );
begin
   $L := \emptyset$ ;
  Let  $m$  be the number of children of  $u$  and  $L_1, \dots, L_m$  be the labels of the children;
  /* Step 1 */
  foreach  $v \leftarrow v_1, \dots, v_m$  in  $R_{r_t}$  do
    if  $L_1, \dots, L_m$  exactly covers  $\{v_1, \dots, v_m\}$  then  $L := L \cup \{v\}$ ;
  /* Step 2 */
  foreach  $v \leftarrow v_1, \dots, v_k, V_1, \dots, V_\ell$  in  $R_{r_t}$  do
    if  $L_1, \dots, L_m$  covers  $\{v_1, \dots, v_k\} \cup V_1 \cup \dots \cup V_\ell$  then  $L := L \cup \{v\}$ ;
  /* Step 3 */
  foreach variable  $h$  in  $t$  do begin
    Let  $V'$  be the set of all child ports of  $h$ ;
    foreach  $V'' \subseteq V'$  with  $V'' \neq \emptyset$  do begin
      foreach  $v \in V' - V''$  do
        if  $v$  and  $V''$  satisfy either
          (1)  $v$  is a leaf and  $V''$  is a maximal subset such that  $L_1, \dots, L_m$ 
              covers  $V''$ , or
          (2)  $v$  is the head of a rule  $v \leftarrow v_1, \dots, v_k, V_1, \dots, V_\ell$  in  $R_{r_t}$ 
              and  $V''$  is a maximal subset such that  $L_1, \dots, L_m$  covers
               $\{v_1, \dots, v_k\} \cup V_1 \cup \dots \cup V_\ell \cup V''$ .
        then  $L := L \cup \{V'' \cup \{v\}\}$ ;
      if there is no vertex  $v$  which satisfies either (1) or (2) and  $V''$  is a
          maximal subset which is covered by  $L_1, \dots, L_m$ 
      then  $L := L \cup \{V''\}$ 
    end
  end;
  Attach  $L$  to  $u$  as the label
end;

```

Fig. 6. Labeling: a procedure for labeling a vertex in T with a set of vertices in t .

Input: labels L_1, \dots, L_m , vertices v_1, \dots, v_k , and sets of vertices V_1, \dots, V_ℓ ;

Note that each V_i ($i = 1, \dots, \ell$) is the set of all child ports of a certain variable and each label L_j ($j = 1, \dots, m$) contains at most one subset of V_i . If the input term rooted tree t is of bounded dimension and the input rooted tree T is of bounded degree, the size of the graph \mathcal{G} constructed below is bounded because both k and ℓ are bounded by some constants and the size of each L_i is also bounded.

begin

Construct a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ in the following way:

$\mathcal{V}_i := \{(v_i, \{j\}) \mid v_i \in L_j \ (1 \leq j \leq m)\}$,

Let \mathcal{E}_i be the complete graph constructed by \mathcal{V}_i ,

/* In the following statement, because a subset of V_i appears at most once in each L_j , it is easy to decide

whether or not $L_{j_1}, \dots, L_{j_{m'}}$ covers V_i . */

$\mathcal{V}'_i := \{(V_i, \{j_1, \dots, j_{m'}\}) \mid \{j_1, \dots, j_{m'}\}$ is a subset of $\{1, \dots, m\}$ such that $L_{j_1}, \dots, L_{j_{m'}}$ covers $V_i\}$.

Let \mathcal{E}'_i be the complete graph constructed by \mathcal{V}'_i ,

$\mathcal{V} := \bigcup_{i=1}^k \mathcal{V}_i \cup \bigcup_{i=1}^{\ell} \mathcal{V}'_i$,

$\mathcal{E} := \{(X, Y), (X', Y')\} \mid (X, Y), (X', Y') \in \mathcal{V}, X \neq X' \text{ and } Y \cap Y' \neq \emptyset\} \cup \bigcup_{i=1}^k \mathcal{E}_i \cup \bigcup_{i=1}^{\ell} \mathcal{E}'_i$.

if there is an independent set of size $k + \ell$ for the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ **then**

L_1, \dots, L_m covers $\{v_1, \dots, v_k\} \cup V_1 \cup \dots \cup V_\ell$

end;

Fig. 7. A procedure for determining whether or not L_1, \dots, L_m covers $\{v_1, \dots, v_k\} \cup V_1 \cup \dots \cup V_\ell$ (Step 2 and Step 3 (2)).

Input: labels L_1, \dots, L_m , vertices v_1, \dots, v_k , and sets of vertices $\{v'_1\}, \dots, \{v'_\ell\}$;
begin

Construct a bipartite graph $B = (\mathcal{V}, \mathcal{V}', \mathcal{E})$ in the following way:

$\mathcal{V} := \{v_1, \dots, v_k, v'_1, \dots, v'_\ell\}$, $\mathcal{V}' := \{1, \dots, m\}$,

$\mathcal{E}_i := \{\{v_i, j\} \mid v_i \in L_j \ (1 \leq j \leq m)\}$ $(i = 1, \dots, k)$,

$\mathcal{E}'_i := \{\{v'_i, j\} \mid v'_i \in L_j \text{ or } \{v'_i\} \in L_j \ (1 \leq j \leq m)\}$ $(i = 1, \dots, \ell)$,

$\mathcal{E} := \bigcup_{i=1}^k \mathcal{E}_i \cup \bigcup_{i=1}^{\ell} \mathcal{E}'_i$.

if for the bipartite graph $(\mathcal{V}, \mathcal{V}', \mathcal{E})$, there exists a graph matching which contains all vertices in \mathcal{V}

then L_1, \dots, L_m covers $\{v_1, \dots, v_k\} \cup \{v'_1\} \cup \dots \cup \{v'_\ell\}$

end;

Fig. 8. A procedure for determining whether or not L_1, \dots, L_m covers $\{v_1, \dots, v_k\} \cup \{v'_1\} \cup \dots \cup \{v'_\ell\}$ (for an input regular term rooted tree such that the dimension of each variable is exactly 2).

time, the label of u can be computed in $O(n^2 \cdot \deg(u) \sqrt{n \cdot \deg(u)})$ where $\deg(u)$ is the degree of u . Then the total time for Matching used in Theorem 3 is $O(\sum_{u \in \mathcal{V}_T} n^2 \cdot \deg(u) \sqrt{n \cdot \deg(u)})$. This does not exceed $O((n + N)^4)$.

The complexity of REGULAR TERM ROOTED TREE PROBLEM is still open if the dimension of an input regular term rooted tree is 3.

3 Conclusions

We have given an algorithmic foundation of discovering knowledge from tree structured data. We have presented polynomial time matching algorithms for tree structured patterns. Computational experiments of comparing our matching algorithm and a naive matching algorithm have shown that our matching algorithm is efficient and useful. We will incorporate the matching algorithm in the KD-FGS system and other knowledge discovery systems from tree-like structured data.

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