

# On the Editing Distance between Undirected Acyclic Graphs\*

Kaizhong Zhang<sup>†</sup>   Jason T. L. Wang<sup>‡</sup>   Dennis Shasha<sup>§</sup>

May 4, 1995

## Abstract

We consider the problem of comparing *CUAL* graphs (*C*onected, *U*ndirected, *A*cylic graphs with nodes being *L*abeled). This problem is motivated by the study of information retrieval for bio-chemical and molecular databases. Suppose we define the distance between two *CUAL* graphs  $G_1$  and  $G_2$  to be the weighted number of edit operations (insert node, delete node and relabel node) to transform  $G_1$  to  $G_2$ . By reduction from exact cover by 3-sets, one can show that finding the distance between two *CUAL* graphs is NP-complete. In view of the hardness of the problem, we propose a constrained distance metric, called the degree-2 distance, by requiring that any node to be inserted (deleted) have no more than 2 neighbors. With this metric, we present an efficient algorithm to solve the problem. The algorithm runs in time  $O(N_1 N_2 D^2)$  for general weighting edit operations and in time  $O(N_1 N_2 D \sqrt{D} \log D)$  for integral weighting edit operations, where  $N_i$ ,  $i = 1, 2$ , is the number of nodes in  $G_i$ ,  $D = \min\{d_1, d_2\}$  and  $d_i$  is the maximum degree of  $G_i$ .

**Key words:** Approximate pattern matching, chemical compounds, dynamic programming, editing distance, NP-completeness

---

\*This work was supported, in part, by the National Science Foundation under Grants IRI-9224601 and IRI-9224602, by the Office of Naval Research under Grant N00014-92-J-1719, by the Natural Sciences and Engineering Research Council of Canada under Grant OGP0046373, and by a grant from the AT&T Foundation.

<sup>†</sup>Department of Computer Science, The University of Western Ontario, London, Ontario, Canada N6A 5B7 (kzhang@csd.uwo.ca).

<sup>‡</sup>Department of Computer and Information Science, New Jersey Institute of Technology, University Heights, Newark, New Jersey 07102 (jason@vienna.njit.edu).

<sup>§</sup>Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012 (shasha@cs.nyu.edu).

# 1 Introduction

In this paper we study the problem of comparing two labeled undirected acyclic graphs (abbreviated as CUAL graphs).<sup>1</sup> Our specific interest in this problem comes from its applicability in bio-chemical information systems [1, 2]. Undirected labeled graphs have been used to represent two-dimensional (2-D) compounds and molecules. For example, Figure 1(a) shows two graph representations of 2-D compounds; each node in the graphs represents an atom and each edge represents a bond. The compounds can be represented alternatively as two CUAL graphs (Figure 1(b)).

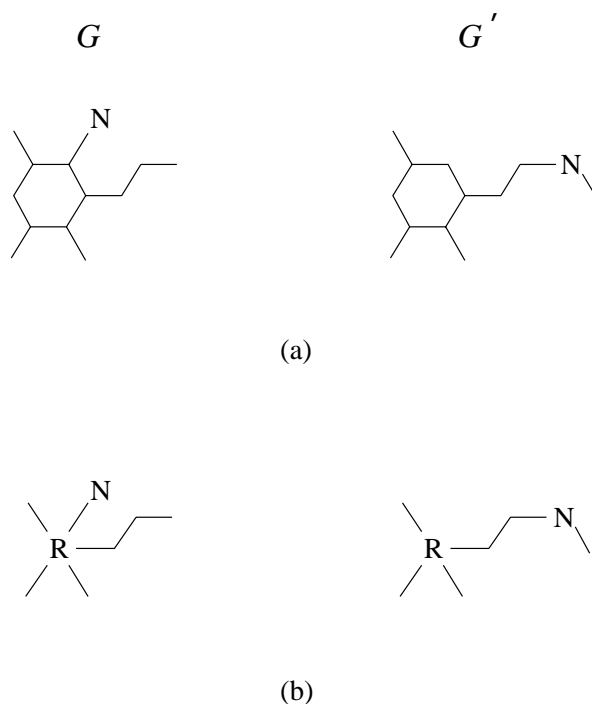


Figure 1. (a) Two examples of chemical compounds [7]. N represents a nitrogen atom. Omitted node labels are carbon atoms (C). Hydrogen atoms (H) are not included in the graph representations since their presence or absence can be deduced from the other information. (b) The same compounds can be represented as CUAL graphs, with each ring being represented by a special node label R.

One common use of the bio-chemical information systems is to perform a *similarity search*, i.e., to find database compounds that are similar to a query structure [6, 13, 14]. Many similarity measures have been devised; they are usually calculated by considering

---

<sup>1</sup>Such graphs are also known as labeled free trees. When the context is clear, we refer to CUAL graphs simply as graphs. Note that, in practice, edges of a graph may have labels. In that case, one can transform a labeled edge between two nodes  $u$  and  $v$  to a labeled node connecting  $u$  and  $v$ .

the atom, bond, or ring-centered substructural fragments found in common in the query and in a compound.<sup>2</sup> While these measures are often useful, they don’t capture many of the interesting topological differences between two compounds, which play a key role in identifying the difference in the compounds’ functionalities.

This paper presents a new (dis)similarity measure for graphs. We define the distance between two graphs  $G_1$  and  $G_2$  to be the weighted number of edit operations (insert node, delete node and relabel node) to transform  $G_1$  to  $G_2$ . By reduction from exact cover by 3-sets, one can show that finding the distance between two graphs is NP-complete. In view of the hardness of the problem, we propose a constrained distance metric, called the *degree-2 distance*, by requiring that any node to be inserted (deleted) have no more than two neighbors. This metric is a natural extension of the edit distance for strings [11] and Selkow’s distance for trees [9]. As our next example shows, it is also a practically useful metric for graphs.

**Example 1.** Consider the atom-centered fragment  $f$  and the three compounds  $G_1, G_2, G_3$  in Figure 2. According to the aforementioned fragment weighting scheme,  $G_1$  is closer to  $G_3$  than to  $G_2$  because  $f$  occurs twice in both of the  $G_1$  and  $G_3$ , whereas it occurs only once in  $G_1$  and  $G_2$ . On the other hand, according to the proposed degree-2 distance metric,  $G_1$  is closer to  $G_2$  than to  $G_3$ .<sup>3</sup> Visually,  $G_1$  is closer to  $G_2$ , consistent with the degree-2 metric; therefore we argue that this is a plausible metric.  $\square$

Thus our work provides a complementary measure capable of reflecting the structural differences between chemical compounds (except that our graphs must be acyclic, so rings must be reduced to single nodes). We believe the presented techniques can also contribute to comparison and search of 2-D and 3-D (macro)molecules in protein and DNA structures [8].

---

<sup>2</sup>For example, the much used fragment weighting scheme works by considering the number of occurrences of a particular fragment type within a compound [15]. The more frequently a fragment occurs, the greater weight it gains. Thus, a pair of molecules that had several occurrences of a given fragment in common would be considered to be more similar to each other than if they had only a single occurrence in common.

<sup>3</sup>Assume all edit operations have unit cost. The degree-2 distance between  $G_1$  and  $G_2$  is 1, obtained by relabeling the leftmost C in  $G_1$  to N in  $G_2$ , whereas the distance between  $G_1$  and  $G_3$  is 7, obtained by inserting the seven Rs into  $G_3$ .

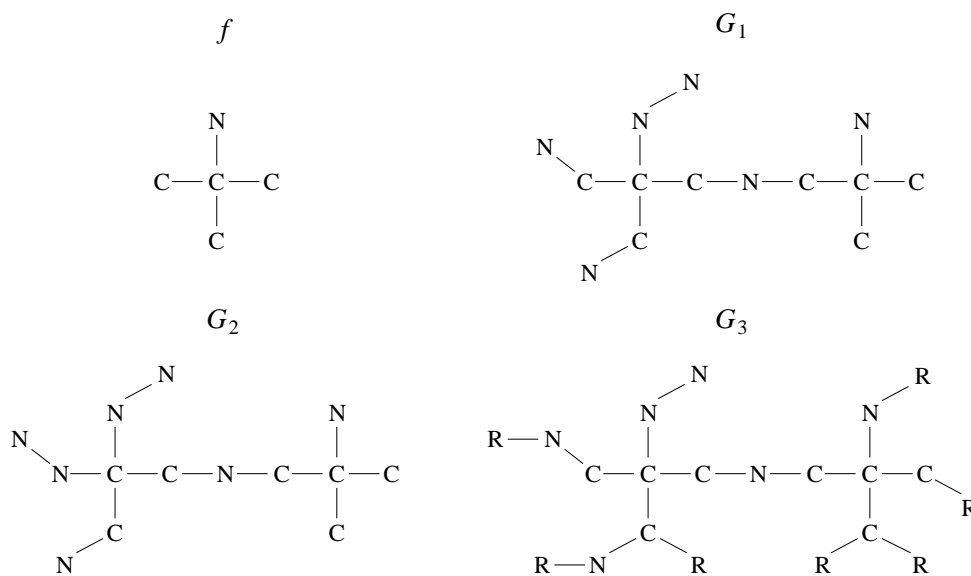


Figure 2. An augmented atom (fragment) and three chemical compounds.

## 1.1 The Main Results

Let  $G_1$  and  $G_2$  be two given graphs. We first show that finding the editing distance between  $G_1$  and  $G_2$  is NP-complete. We then develop an algorithm to find the degree-2 distance between the two graphs that runs in time  $O(N_1 N_2 D^2)$  for general weighting edit operations and in time  $O(N_1 N_2 D \sqrt{D} \log D)$  for integral weighting edit operations. Here,  $N_i$ ,  $i = 1, 2$ , represents the number of nodes in  $G_i$ ;  $deg(n)$  denotes the number of neighbors of node  $n$ ;  $d_i = \max_{n \in G_i} deg(n)$  and  $D = \min\{d_1, d_2\}$ . A subroutine of this algorithm computes the degree-2 distance between two unordered trees in time  $O(N_1 N_2 D)$  for general weighting edit operations and in time  $O(N_1 N_2 \sqrt{D} \log D)$  for integral weighting edit operations. (An unordered tree is a rooted tree in which the order among siblings is unimportant. For such trees,  $deg(n)$  is defined as the number of  $n$ 's children, excluding  $n$ 's parent).

The rest of the paper is organized as follows. Section 2 introduces some notation and definitions used in the paper and shows the NP-completeness result. Section 3 presents the algorithm for the unordered tree case. This algorithm is then used as a subroutine to compute the degree-2 distance between graphs (Section 4). We conclude the paper in Section 5.

## 2 Preliminaries

### 2.1 Edit Operations on Graphs

There are three kinds of edit operations on graphs: relabel, delete and insert a node. Relabeling node  $n$  means changing the label on  $n$ . Deleting a node  $n$  means making the neighbors of  $n$  (except an arbitrarily specified neighbor  $n'$ ) become the neighbors of  $n'$  and then removing  $n$ . (This amounts to contraction of the edge between  $n$  and  $n'$  [3] and making the resulting node have label of  $n'$ .) Insert is the complement of delete. This means that inserting  $n$  as a neighbor of  $n'$  makes a subset of the current neighbors of  $n'$  become the neighbors of  $n$ . We represent an edit operation as a pair  $(u, v) \neq (\Lambda, \Lambda)$ , sometimes written  $u \rightarrow v$ . We call  $u \rightarrow v$  a relabeling operation if  $u \neq \Lambda$  and  $v \neq \Lambda$ ; a delete operation if  $v = \Lambda$ ; and an insert operation if  $u = \Lambda$ . Let  $G_2$  be the graph that results from the application of an edit operation  $u \rightarrow v$  to graph  $G_1$ ; this is written  $G_1 \Rightarrow G_2$  via  $u \rightarrow v$ .

Let  $S$  be a sequence  $s_1, s_2, \dots, s_k$  of edit operations.  $S$  transforms graph  $G$  to graph  $G'$  if there is a sequence of graphs  $G_0, G_1, \dots, G_k$  such that  $G = G_0, G' = G_k$  and  $G_{i-1} \Rightarrow G_i$  via  $s_i$  for  $1 \leq i \leq k$ . Let  $\gamma$  be a cost function that assigns to each edit operation  $u \rightarrow v$  a nonnegative real number  $\gamma(u \rightarrow v)$ . We require  $\gamma$  to be a metric. By extension, the cost of the sequence  $S$ , denoted  $\gamma(S)$ , is simply the sum of costs of the constituent edit operations. The *distance* from  $G$  to  $G'$ , denoted  $\Delta(G, G')$ , is the minimum cost of all sequences of edit operations taking  $G$  to  $G'$ .

**Theorem 1.** *Finding  $\Delta(G, G')$  is NP-complete.*

**Proof.** The proof that this problem can be solved by a nondeterministic polynomial time algorithm is straightforward: given a distance value, just guess a sequence of edit operations for transforming  $G$  to  $G'$  and see whether the cost incurred is less than the distance value. To show the problem is NP-hard, we transform the exact cover by 3-sets problem [5] to it.

*Exact Cover by 3-Sets (X3C)*

Instance: A finite set  $S$  with  $|S| = 3k$  and a collection  $\mathcal{C}$  of 3-element subsets of  $S$ .

Question: Does  $\mathcal{C}$  contain an exact cover for  $S$ , that is, a subcollection  $\mathcal{C}' \subseteq \mathcal{C}$  such that every element of  $S$  occurs in exactly one member of  $\mathcal{C}'$ ?

Given an instance of the X3C problem, let the set  $S = \{s_1, s_2, \dots, s_m\}$ , where  $m = 3k$ .

Let  $\mathcal{C} = \{C_1, C_2, \dots, C_n\}$ . Here each  $C_i = \{t_{i_1}, t_{i_2}, t_{i_3}\}$  where  $t_{i_j} \in S$ ,  $1 \leq j \leq 3$ . Without loss of generality, assume  $n > k$ . We construct two graphs as shown in Figure 3. This construction can be done in polynomial time.

*Claim.* If  $\Delta(G, G') = k + 3(n - k)$ , then  $\mathcal{C}$  contains an exact cover for  $S$ .

*Proof of Claim.* Assume we use  $l_1$  deletes,  $l_2$  inserts and  $l_3$  relabels to change  $G$  to  $G'$ . Since changing node labels does not change the number of nodes in the graphs,  $|G| - l_1 + l_2 = |G'|$ . Thus,  $l_1 - l_2 = |G| - |G'| = 4n + 1 - (4(n - k) + 3k + 1) = k$ . Since only inserts and relabels can create new node labels,  $l_2 + l_3 \geq 3(n - k)$ . Thus  $l_1 + l_2 + l_3 = (l_1 - l_2) + (l_2 + l_3) + l_2 \geq k + 3(n - k) + l_2$ . So,  $\Delta(G, G') \geq k + 3(n - k) + l_2$ . If  $\Delta(G, G') = k + 3(n - k)$ , then  $l_2 = 0$ . Since  $l_1 = |G| - |G'| = k$ ,  $l_3 = 3(n - k)$ .

Now, because (i)  $G$  has  $k$  more nodes than  $G'$ , and (ii)  $G$  has  $k$  more nodes labeled *set* than  $G'$ , we have to use the  $l_1$  deletes to remove the nodes labeled *set*. On the other hand, because  $G'$  has  $3(n - k)$  nodes labeled  $\Lambda$ , we have to use the  $l_3$  relabeling operations to change the labels. Thus after applying the  $l_1$  deletes and  $l_3$  relabelings, the rest of  $G$  must be equivalent to  $G'$ . Therefore  $\mathcal{C}$  contains an exact cover for  $S$ .  $\square$

Next, given an exact cover for  $S$ , it is easy to see that  $\Delta(G, G') = k + 3(n - k)$ . Therefore  $\Delta(G, G') = k + 3(n - k)$  iff  $\mathcal{C}$  contains an exact cover for  $S$ . Thus, finding  $\Delta(G, G')$  is NP-hard.  $\square$

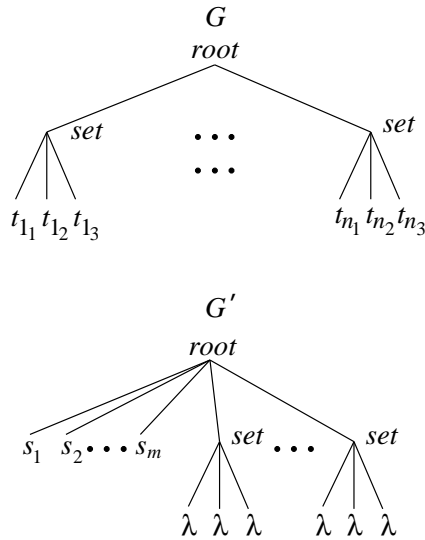


Figure 3. Two graphs  $G$  and  $G'$  constructed based on an instance of the X3C problem.

## 2.2 Degree-2 Distance

In view of the hardness of the problem, we propose to impose the following constraint on the edit operations: a node  $n$  can be deleted (inserted) only when  $\text{deg}(n) \leq 2$ .<sup>4</sup> Intuitively one can delete either a leaf or a node  $n$  with two neighbors; in the latter case, after deleting  $n$ , we simply connect its two neighbors together. When inserting  $n$  between two nodes  $n'$  and  $n''$ , we remove the edge between  $n'$  and  $n''$  and make  $n$  the neighbor of both  $n'$  and  $n''$ . These constrained edits will be referred to as the *degree-2* edit operations; they are natural in manipulating nodes and edges in the updated graphs. We define the degree-2 distance between graph  $G$  and graph  $G'$ , denoted  $\delta(G, G')$ , to be the minimum cost of all sequences of the degree-2 edit operations transforming  $G$  to  $G'$ . Clearly  $\delta$  is a metric.

## 2.3 Mappings

The degree-2 edit operations correspond to a *mapping*, which is a graphical specification of what edit operations apply to each node in the two graphs. For example, the mapping in Figure 4 shows a way to transform the CUAL graph  $G$  to the CUAL graph  $G'$  given in Figure 1. It corresponds to the sequence (delete (node with label N), insert (node with label N)).

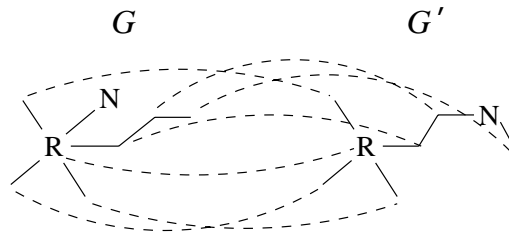


Figure 4. A mapping from  $G$  to  $G'$ . Nodes in  $G$  not touched by a mapping line are to be deleted; nodes in  $G'$  not touched by a mapping line are to be inserted. The mapping shows a way to transform  $G$  to  $G'$ .

To formalize the notion of mappings, we need some definitions. Let  $u, v, w$  be three nodes in a graph  $G$ ; let  $[u, v]$  denote the path between node  $u$  and node  $v$  inclusively. Define the *center* of the three nodes  $u, v, w$ , denoted  $\text{center}(u, v, w)$ , to be the intersection node of the three paths  $[u, v]$ ,  $[v, w]$  and  $[w, u]$ . Figure 5 illustrates the definition.

<sup>4</sup>Thus, to delete a node  $n$  with  $\text{deg}(n) > 2$ , one has to first delete some of its neighbors to make its degree less than or equal to 2 before removing it.



Figure 5. Illustrations of the center, which is represented by the bullet  $\bullet$ .

Let  $g[i]$  represent the  $i$ th node of graph  $G$  according to some ordering (e.g., a depth-first search order). Formally, a mapping from  $G$  to  $G'$  is a triple  $(M, G, G')$  (or simply  $M$  when the context is clear), where  $M$  is any set of pairs of integers  $(i, j)$  satisfying the following conditions:

1.  $1 \leq i \leq |G|, 1 \leq j \leq |G'|$ .
2. For any two pairs  $(i_1, j_1)$  and  $(i_2, j_2)$  in  $M$ ,  $i_1 = i_2$  iff  $j_1 = j_2$  (one-to-one).
3. For any three pairs  $(i_1, j_1), (i_2, j_2)$  and  $(i_3, j_3)$  in  $M$ ,  $(i^*, j^*)$  is also in  $M$  where  $g[i^*] = \text{center}(g[i_1], g[i_2], g[i_3])$  and  $g'[j^*] = \text{center}(g'[j_1], g'[j_2], g'[j_3])$  (center relationship preservation).

The cost of  $M$ , denoted  $\gamma(M)$ , is the cost of deleting nodes of  $G$  not touched by a mapping line plus the cost of inserting nodes of  $G'$  not touched by a mapping line plus the cost of relabeling nodes in those pairs related by mapping lines with different labels.

Mappings can be composed. Let  $M_1$  be a mapping from  $G$  to  $G'$  and let  $M_2$  be a mapping from  $G'$  to  $G''$ . Define the composition of  $M_1$  and  $M_2$ , denoted  $M_1 \circ M_2$ , as

$$M_1 \circ M_2 = \{(i, j) \mid \exists k \text{ s. t. } (i, k) \in M_1 \text{ and } (k, j) \in M_2\}.$$

The following lemmas establish the relationship between mappings and degree-2 edit operations.

**Lemma 1.** (i)  $M_1 \circ M_2$  is a mapping from  $G$  to  $G''$ . (ii)  $\gamma(M_1 \circ M_2) \leq \gamma(M_1) + \gamma(M_2)$ .

**Proof.** (i) follows from the definition of mappings. For (ii), let  $I$  be the set of nodes in  $G$  not touched by mapping lines, and let  $J$  be the set of nodes in  $G''$  not touched by mapping lines. For any  $g[i] \in G$  and  $g''[j] \in G''$ , three cases may occur:  $(i, j) \in M_1 \circ M_2$ ,  $g[i] \in I$  or  $g''[j] \in J$ . Each case corresponds to a degree-2 edit operation  $u \rightarrow v$  where  $u$  and  $v$  may be node labels or may be  $\Lambda$ . In all the cases, the triangle inequality on the distance metric  $\delta$  ensures that  $\gamma(u \rightarrow v) \leq \gamma(u \rightarrow w) + \gamma(w \rightarrow v)$ .  $\square$



**Lemma 2.** *Given  $S$ , a sequence  $s_1, s_2, \dots, s_k$  of degree-2 edit operations from  $G$  to  $G'$ , there exists a mapping  $M$  from  $G$  to  $G'$  such that  $\gamma(M) \leq \gamma(S)$ .*

**Proof.** The lemma is proved by induction on  $k$ . The base case ( $k = 1$ ) holds, since any single degree-2 edit operation preserves the center relationship in the mapping. For the general case ( $k \geq 2$ ), let  $S_1$  be the sequence  $s_1, \dots, s_{k-1}$  of degree-2 edit operations. By induction hypothesis, there exists a mapping  $M_1$  such that  $\gamma(M_1) \leq \gamma(S_1)$ . Let  $M_2$  be the mapping for  $s_k$ . By Lemma 1, we have  $\gamma(M) = \gamma(M_1 \circ M_2) \leq \gamma(M_1) + \gamma(M_2) \leq \gamma(S)$ .  $\square$

**Lemma 3.** *For any mapping  $M$  from  $G$  to  $G'$ , there exists a sequence of degree-2 edit operations  $S$  such that  $\gamma(S) = \gamma(M)$ .*

**Proof.** From the mapping conditions, if  $(i_1, j_1)$ ,  $(i_2, j_2)$  and  $(i_3, j_3)$  are in  $M$ , then  $(i^*, j^*)$  is also in  $M$  where  $g[i^*] = \text{center}(g[i_1], g[i_2], g[i_3])$  and  $g'[j^*] = \text{center}(g'[j_1], g'[j_2], g'[j_3])$ . Let  $T_1 = \{g[i] \mid \exists (i_1, j_1) \in M \text{ and } (i_2, j_2) \in M \text{ s.t. } g[i] \in [g[i_1], g[i_2]]\}$  and let  $T_2 = \{g'[j] \mid \exists (i_1, j_1) \in M \text{ and } (i_2, j_2) \in M \text{ s.t. } g'[j] \in [g'[j_1], g'[j_2]]\}$ . It's easy to see that  $T_1$  and  $T_2$  are connected. In fact, they both are trees.

From the above definitions, every node of  $G$  touched by a mapping line must be in  $T_1$ . Furthermore, any node  $u \in T_1$  not touched by a mapping line must have exactly 2 neighbors where both of the neighbors are in  $T_1$ . (Otherwise  $u$  would be the intersection node of at least three paths, each of which would contain at least one node in  $M$ , implying that  $u$  itself would be in  $M$ .) For the same reason, any node  $u \in T_1$  with  $\text{deg}(u) > 2$  must be in  $M$ .

As a result, we can construct the desired sequence  $S$  of degree-2 edit operations as follows. First, delete the nodes  $u \in G$  and  $u \notin T_1$ , starting from nodes with degree 1. After performing these deletes,  $G$  becomes  $T_1$ . Then, delete the nodes of  $G$  that are in  $T_1$  but not in  $M$ . These deletes are valid since all the deleted nodes have degree 2. Then, perform all the relabelings indicated by the mapping  $M$ . Then, insert the nodes of  $G'$  that are in  $T_2$  but not in  $M$ , resulting in the tree  $T_2$ . Again the inserts are valid since all the inserted nodes have degree 2. Finally insert all the other nodes of  $G'$ . Obviously  $\gamma(S) = \gamma(M)$ , which completes the proof.  $\square$

From Lemmas 2 and 3, we obtain

**Theorem 2.**  $\delta(G, G') = \min\{\gamma(M) \mid M \text{ is a mapping from } G \text{ to } G'\}$ .

**Example 2.** Consider again the graphs  $G$  and  $G'$  in Figure 4. The mapping in the figure is a minimum cost mapping and  $\delta(G, G') = 2$ .  $\square$

### 3 The Algorithm for Unordered Trees

For notational convenience, in this subsection we use  $T$  rather than  $G$  to represent a rooted unordered tree. Let  $t[i]$  denote the  $i$ th node of  $T$  according to the depth-first search order.  $T[i]$  represents the subtree rooted at  $t[i]$  and  $F[i]$  represents the forest obtained by deleting  $t[i]$  from  $T[i]$ . Let  $T_1$  and  $T_2$  be two rooted unordered trees. We use  $t_1[i_1], t_1[i_2], \dots, t_1[i_{n_i}]$  to represent the children of  $t_1[i]$  in  $T_1[i]$  and use  $t_2[j_1], t_2[j_2], \dots, t_2[j_{n_j}]$  to represent the children of  $t_2[j]$  in  $T_2[j]$ . When applied to the rooted unordered trees  $T_1$  and  $T_2$ , the mapping  $M$  defined in § 2.3 is exactly the same as the edit distance mapping between the unordered trees with the following constraint: for any two pairs  $(i_1, j_1)$  and  $(i_2, j_2)$  in  $M$ ,  $(i^*, j^*)$  is also in  $M$  where  $t_1[i^*] = lca(t_1[i_1], t_1[i_2])$ ,  $t_2[j^*] = lca(t_2[j_1], t_2[j_2])$  and  $lca(\cdot)$  represents the least common ancestor of the indicated nodes.<sup>5</sup> With this notion in mind, it's easy to develop a dynamic programming algorithm for rooted unordered trees. We now present several lemmas, which will be the basis of our algorithm.

**Lemma 4.** For all  $1 \leq i \leq N_1$  and  $1 \leq j \leq N_2$ ,

- (i)  $\delta(\emptyset, \emptyset) = 0$ ;
- (ii)  $\delta(T_1[i], \emptyset) = \delta(F_1[i], \emptyset) + \gamma(t_1[i] \rightarrow \Lambda)$ ;
- (iii)  $\delta(F_1[i], \emptyset) = \sum_{k=1}^{n_i} \delta(T_1[i_k], \emptyset)$ ;
- (iv)  $\delta(\emptyset, T_2[j]) = \delta(\emptyset, F_2[j]) + \gamma(\Lambda \rightarrow t_2[j])$ ;
- (v)  $\delta(\emptyset, F_2[j]) = \sum_{k=1}^{n_j} \delta(\emptyset, T_2[j_k])$ .

**Proof.** Immediate from definitions.  $\square$

**Lemma 5.** For all  $1 \leq i \leq N_1$  and  $1 \leq j \leq N_2$ ,

$$\delta(T_1[i], T_2[j]) = \mathbf{min} \begin{cases} \delta(T_1[i], \emptyset) + \min_{1 \leq s \leq n_i} \{\delta(T_1[i_s], T_2[j]) - \delta(T_1[i_s], \emptyset)\} \\ \delta(\emptyset, T_2[j]) + \min_{1 \leq t \leq n_j} \{\delta(T_1[i], T_2[j_t]) - \delta(\emptyset, T_2[j_t])\} \\ \delta(F_1[i], F_2[j]) + \gamma(t_1[i] \rightarrow t_2[j]) \end{cases}$$

**Proof.** Let  $M$  be a minimum-cost mapping from  $T_1[i]$  to  $T_2[j]$ . There are four cases to be

---

<sup>5</sup>An edit distance mapping  $M_e$  between two rooted unordered trees satisfies the node one-to-one relationship and preserves the ancestor relationship, i.e., supposing  $u$  is mapped to  $v$  and  $x$  is mapped to  $y$  in  $M_e$ ,  $u$  is an ancestor of  $x$  iff  $v$  is an ancestor of  $y$  [10, 16].

considered:

*Case 1.*  $i \notin M$  and  $j \in M$ . Let  $(z, j)$  be in  $M$ . Thus  $t_1[z]$  must be a node in  $F_1[i]$ . Let  $t_1[i_s]$  be the child of  $t_1[i]$  on the path from  $t_1[z]$  to  $t_1[i]$ . Thus  $\delta(T_1[i], T_2[j]) = \delta(T_1[i_s], T_2[j]) + \delta(T_1[i_1], \emptyset) + \dots + \delta(T_1[i_{s-1}], \emptyset) + \delta(T_1[i_{s+1}], \emptyset) + \dots + \delta(T_1[i_{n_i}], \emptyset) + \gamma(t_1[i] \rightarrow \Lambda)$ . Since  $\delta(T_1[i], \emptyset) = \gamma(t_1[i] \rightarrow \Lambda) + \sum_{k=1}^{n_i} \delta(T_1[i_k], \emptyset)$ , we can rewrite the right hand side of the formula as  $\delta(T_1[i], \emptyset) + \delta(T_1[i_s], T_2[j]) - \delta(T_1[i_s], \emptyset)$ . The range of  $s$  is from 1 to  $n_i$ ; therefore we take the minimum of the corresponding costs.

*Case 2.*  $i \in M$  and  $j \notin M$ . This is analogous to Case 1.

*Case 3.*  $i \in M$  and  $j \in M$ . By the mapping conditions,  $(i, j)$  must be in  $M$ . Thus  $\delta(T_1[i], T_2[j]) = \delta(F_1[i], F_2[j]) + \gamma(t_1[i] \rightarrow t_2[j])$ .

*Case 4.*  $i \notin M$  and  $j \notin M$ . We would have  $\delta(T_1[i], T_2[j]) = \delta(F_1[i], F_2[j]) + \gamma(t_1[i] \rightarrow \Lambda) + \gamma(\Lambda \rightarrow t_2[j])$ . Since  $\gamma(t_1[i] \rightarrow t_2[j]) \leq \gamma(t_1[i] \rightarrow \Lambda) + \gamma(\Lambda \rightarrow t_2[j])$  (the triangle inequality), we need not include this case in our formula.  $\square$

In calculating  $\delta(F_1[i], F_2[j])$ , we first make the following observation.

**Lemma 6.** *Suppose  $(i, j) \in M$ . If two nodes  $u_1$  and  $u_2$  of  $T_1[i_s]$  are in  $M$  for some  $1 \leq s \leq n_i$ , then there must exist an integer  $t$ ,  $1 \leq t \leq n_j$ , such that the two nodes connected to  $u_1$  and  $u_2$ , respectively, by the mapping lines of  $M$  are in  $T_2[j_t]$ .*

**Proof.** Suppose not. Suppose there are  $h$  and  $k$  such that the node  $v_1$  connected to  $u_1$  by the mapping line is in  $T_2[j_h]$  and the node  $v_2$  connected to  $u_2$  by the mapping line is in  $T_2[j_k]$ . Note that  $u_3 = lca(u_1, u_2)$  is in  $T_1[i_s]$  and  $lca(v_1, v_2) = t_2[j]$ . By the mapping conditions,  $u_3$  and  $t_2[j]$  must be connected by a mapping line in  $M$ , contradicting the fact that  $(i, j) \in M$ .  $\square$

Thus, a subtree rooted at some child of  $t_1[i]$  must be mapped to a subtree rooted at some child of  $t_2[j]$ . We try to find a best mapping between the children of  $t_1[i]$  and the children of  $t_2[j]$  by constructing a weighted bipartite graph  $BG$  as follows. Let  $U = \{t_1[i_1], \dots, t_1[i_{n_i}]\}$  and  $V = \{t_2[j_1], \dots, t_2[j_{n_j}]\}$ . Assign the weight for each edge  $(t_1[i_s], t_2[j_t])$ , denoted  $\omega((t_1[i_s], t_2[j_t]))$ ,  $1 \leq s \leq n_i$  and  $1 \leq t \leq n_j$ , based on the formula

$$\omega((t_1[i_s], t_2[j_t])) = \delta(T_1[i_s], \emptyset) + \delta(\emptyset, T_2[j_t]) - \delta(T_1[i_s], T_2[j_t]).$$

Without loss of generality, assume  $n_i \leq n_j$ . To better bound the complexity of our algorithm, for each node  $u \in U$ , we only pick the top  $n_i$  highest weighted edges touching on  $u$  and store these edges as well as their end nodes in  $BG$ . Thus  $BG$  has at most  $n_i n_i$  edges and

at most  $n_i + n_i n_i$  nodes. Letting  $Ma$  be the maximum weighted matching in  $BG$ , we obtain

**Lemma 7.**

$$\delta(F_1[i], F_2[j]) = \sum_{s=1}^{n_i} \delta(T_1[i_s], \emptyset) + \sum_{t=1}^{n_j} \delta(\emptyset, T_2[j_t]) - \sum_{(u,v) \in Ma} \omega((u,v)).$$

Thus the problem of calculating  $\delta(F_1[i], F_2[j])$  becomes that of finding the maximum weighted matching in  $BG$ . One can solve the problem by using Gabow and Tarjan's algorithm in [4]. Figure 6 summarizes the algorithm.

**Algorithm A**

**Input:** Unordered trees  $T_1$  and  $T_2$ .

**Output:**  $\delta(T_1[i], T_2[j])$  where  $1 \leq i \leq N_1$  and  $1 \leq j \leq N_2$ ;

$$\delta(T_1[N_1], T_2[N_2]) = \delta(T_1, T_2).$$

$\delta(\emptyset, \emptyset) := 0$ ;

**for**  $i := 1$  **to**  $N_1$  **do**

    compute  $\delta(F_1[i], \emptyset)$  and  $\delta(T_1[i], \emptyset)$  as in Lemma 4 (ii) (iii);

**for**  $j := 1$  **to**  $N_2$  **do**

    compute  $\delta(\emptyset, F_2[j])$  and  $\delta(\emptyset, T_2[j])$  as in Lemma 4 (iv) (v);

**for**  $i := 1$  **to**  $N_1$  **do**

**for**  $j := 1$  **to**  $N_2$  **do**

        compute  $\delta(F_1[i], F_2[j])$  as in Lemma 7;

        compute  $\delta(T_1[i], T_2[j])$  as in Lemma 5;

Figure 6. Algorithm for computing  $\delta(T_1, T_2)$  for two unordered trees  $T_1$  and  $T_2$ .

**Theorem 3.** *The time complexity of Algorithm A is  $O(N_1 N_2 D)$  for general weighting edit operations and  $O(N_1 N_2 \sqrt{D} \log D)$  for integral weighting edit operations.*

**Proof.** By Lemma 5, the complexity of computing  $\delta(T_1[i], T_2[j])$  is bounded by  $O(n_i + n_j)$ . In constructing  $BG$  for calculating  $\delta(F_1[i], F_2[j])$ , for each node  $u \in U$ , it takes  $O(n_j)$  time to calculate the weights of the edges touching on  $u$  and to pick the  $n_i$  edges with the highest weights. Thus, it takes a total of  $O(n_i n_j)$  time to construct  $BG$ . Let  $V$  be the number of nodes in  $BG$  and let  $E$  be the number of edges in  $BG$ . The complexity of finding the maximum weighted matching in  $BG$  is  $O(\min\{n_i, n_j\}(E + V \log V))$  when the edges have general weights and is  $O(\sqrt{V}E \log(VW))$  when the edges have integral weights where  $W$  is the maximum weight [4]. Without loss of generality, assume  $n_i \leq n_j$ . Then  $V$  is at most  $n_i + n_i n_i$  and  $E$  is at most  $n_i n_i$ . Thus for the general weighting case, the complexity of

computing  $\delta(T_1[i], T_2[j])$  for any pair of  $i$  and  $j$  is bounded by  $O(n_i n_j + n_i(n_i n_j + V \log V))$ .  $V = \min\{n_i + n_j, n_i + n_i^2\}$ , and therefore  $\log V = \log n_i$ . Hence the complexity is bounded by

$$\begin{aligned}
& O(n_i n_j + (\min\{n_i, n_j\})^3 + ((\min\{n_i, n_j\})^2 + \min\{n_i, n_j\} \max\{n_i, n_j\}) \log n_i) \\
&= O(n_i n_j \log(\min\{n_i, n_j\}) + (\min\{n_i, n_j\})^3) \\
&= O(n_i n_j \min\{n_i, n_j\})
\end{aligned}$$

For the integral weighting case, suppose the node label alphabet for unordered trees is finite. Then the maximum edit cost is finite. As a consequence, the maximum weight  $W$  in  $BG$  is bounded by  $cV$  for some constant  $c$ . Thus, the complexity is bounded by

$$\begin{aligned}
& O(n_i n_j + \sqrt{n_i + n_j} n_i n_j \log(n_i + n_i^2)) \\
&= O(n_i n_j + \sqrt{2n_j} n_i n_j \log n_i) \\
&= O(n_i n_j + n_i n_j n_i / \sqrt{n_j} \log n_i) \\
&= O(n_i n_j + n_i n_j \sqrt{n_i} \sqrt{n_i/n_j} \log n_i) \\
&= O(n_i n_j + n_i n_j \sqrt{n_i} \log n_i) \\
&= O(n_i n_j \sqrt{\min\{n_i, n_j\}} \log(\min\{n_i, n_j\}))
\end{aligned}$$

Therefore for the general weighting case, the complexity of Algorithm A is

$$\begin{aligned}
& \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} O(n_i n_j \min\{n_i, n_j\}) \\
&\leq \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} O(n_i n_j \min\{d_1, d_2\}) \\
&\leq O(\min\{d_1, d_2\} \sum_{i=1}^{N_1} n_i \sum_{j=1}^{N_2} n_j) \\
&\leq O(N_1 N_2 \min\{d_1, d_2\}) \\
&= O(N_1 N_2 D)
\end{aligned}$$

Likewise, for the integral weighting case, the complexity of Algorithm A is  $O(N_1 N_2 \sqrt{\min\{d_1, d_2\}} \log(\min\{d_1, d_2\})) = O(N_1 N_2 \sqrt{D} \log D)$ .  $\square$

## 4 The Algorithm for CUAL Graphs

Let  $G_1$  and  $G_2$  be two CUAL graphs. By definitions, if  $(i, j)$  is in a minimum cost mapping from  $G_1$  to  $G_2$ , then we can assign  $g_1[i]$  as the root of  $G_1$  and assign  $g_2[j]$  as the root of

$G_2$ , resulting in two rooted unordered trees. By applying Algorithm A to the two trees, we can find  $\delta(G_1, G_2)$ . This naive algorithm runs in time  $O(N_1^2 N_2^2 \min\{d_1, d_2\})$  when the edit operations have general cost, and in time  $O(N_1^2 N_2^2 \sqrt{\min\{d_1, d_2\}} \log(\min\{d_1, d_2\}))$  when the edit operations have integral cost.

A more careful analysis leads to a faster algorithm, referred to as Algorithm B. Let us choose an arbitrary node, say  $r$ , in  $G_1$  and assign  $r$  as the root of  $G_1$ . Thus the graph  $G_1$  can be considered as a rooted unordered tree, denoted as  $T_1^r$ . For any node  $u$  in  $G_1$ , we use  $T_1^r[u]$  to represent the unordered tree rooted at  $u$  with respect to  $G_1$ 's root  $r$ . Let  $M$  be a minimum cost mapping from  $G_1$  to  $G_2$ . There are two cases to be considered: in the rooted  $G_1$ , (i) there exists a node  $x$  such that  $x$  is touched by a line of  $M$  and all nodes touched by lines of  $M$  are in the tree  $T_1^r[x]$ ; (ii) there exist two nodes  $x_1$  and  $x_2$  such that both  $x_1$  and  $x_2$  are touched by lines of  $M$  and all nodes touched by lines of  $M$  are either in the tree  $T_1^r[x_1]$  or in the tree  $T_1^r[x_2]$ .<sup>6</sup>

*Case 1.* In this case, we choose an arbitrary node  $v$  in  $G_2$  and assign  $v$  as the root of  $G_2$ . Call the resulting tree  $T_2^v$ . Compute  $\delta(T_1^r[r], T_2^v[v])$  using Algorithm A and keep all the intermediate results. Let the neighbors of  $v$  be  $y_1, y_2, \dots, y_n$ . Then compute  $\delta(T_1^r[u], T_2^{y_j}[v])$  for all  $u \in T_1^r$  and for  $1 \leq j \leq n$ . Next we assign  $y_1$  as the new root of  $G_2$  and repeat the above computation. The order in which we assign the nodes in  $G_2$  as its root is based on the preorder traversal of  $T_2^v$ .

*Case 2.* Let  $y_1, y_2$  be in  $G_2$  such that  $(x_1, y_1) \in M$  and  $(x_2, y_2) \in M$ . Then we can find an arbitrary edge  $(v_1, v_2)$  on the path connecting  $y_1$  and  $y_2$  and split  $G_2$  at the edge into two rooted unordered trees  $T_2^{v_2}[v_1]$  and  $T_2^{v_1}[v_2]$ . Each of  $T_1^r[x_1]$ ,  $T_1^r[x_2]$ ,  $T_2^{v_2}[y_1]$ ,  $T_2^{v_1}[y_2]$  is a rooted unordered tree (see Figure 7). The best mapping from  $T_1^r[x_1]$  to  $T_2^{v_2}[y_1]$  and the best mapping from  $T_1^r[x_2]$  to  $T_2^{v_1}[y_2]$  can be obtained during the computation of Case 1.

The above enumerates all possible situations and therefore the distance is the minimum of the two cases.

**Theorem 4.** *The time complexity of Algorithm B is  $O(N_1 N_2 D^2)$  for general weighting edit operations and  $O(N_1 N_2 D \sqrt{D} \log D)$  for integral weighting edit operations.*

**Proof.** The computation of  $\delta(T_1^r[u], T_2^{y_j}[v])$  for all  $u \in T_1^r$  and for  $1 \leq j \leq n$  in Case 1 is dominated by the computation of  $\delta(F_1^r[u], F_2^{y_j}[v])$ , which in turn is bounded by the

---

<sup>6</sup>Note that there cannot be more than two nodes. If that were true (say there were three nodes  $x_1, x_2, x_3$ ), the center of the three nodes would be their least common ancestor. By the mapping conditions, this ancestor would also be in the mapping, contradicting the fact that all the nodes touched by mapping lines are in the trees rooted at  $x_1, x_2, x_3$ .

computation of the maximum weighted bipartite matching. Let the neighbors of  $u$  be  $x_1, x_2, \dots, x_m$ . ( $y_1, y_2, \dots, y_n$  are neighbors of  $v$ .) If  $\deg(v) < \deg(u)$  (i.e.,  $n < m$ ), then we can just apply Gabow and Tarjan's algorithm  $\deg(v)$  times. On the other hand, if  $\deg(v) \geq \deg(u)$ , then in the maximum weighted matching  $Ma$  between  $x_1, x_2, \dots, x_m$  and  $y_1, y_2, \dots, y_n$ , there exist  $\deg(v) - \deg(u)$  subtrees (among  $T_2^v[y_1], T_2^v[y_2], \dots, T_2^v[y_n]$ ) that are not in the matching  $Ma$ . Suppose  $y_j$  is not in  $Ma$  for some  $1 \leq j \leq n$ . Then we do not need to compute the maximum weighted matching for  $F_2^{y_j}[v]$ . (If  $y_j$  is in  $Ma$ , we have to compute the maximum weighted matching.) The number of such computations is therefore  $\deg(u)$ . Thus, we only need to apply Gabow and Tarjan's algorithm  $\min(\deg(u), \deg(v))$  times. Therefore for the general weighting case, the time complexity is

$$\begin{aligned}
& \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} O(n_i n_j \min\{n_i, n_j\}) \min\{n_i, n_j\} \\
& \leq \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} O(n_i n_j (\min\{d_1, d_2\})^2) \\
& \leq O(N_1 N_2 (\min\{d_1, d_2\})^2) \\
& = O(N_1 N_2 D^2)
\end{aligned}$$

Likewise, for the integral weighting case, the complexity is  $O(N_1 N_2 (\min\{d_1, d_2\}) \sqrt{\min\{d_1, d_2\}} \log(\min\{d_1, d_2\})) = O(N_1 N_2 D \sqrt{D} \log D)$ .

For Case 2, since the best mapping from  $T_1^r[x_1]$  to  $T_2^{v_2}[y_1]$  and the best mapping from  $T_1^r[x_2]$  to  $T_2^{v_1}[y_2]$  can be obtained during the computation of Case 1, this case requires at most  $O(N_1 N_2)$  time. Therefore the total time required by Algorithm B is as asserted in the theorem.  $\square$

Note that the gap between the running times of Algorithm A and Algorithm B is  $\min\{d_1, d_2\}$ . If one of the CUAL graphs has a bounded degree, then the running time of both algorithms is  $O(N_1 N_2)$ .

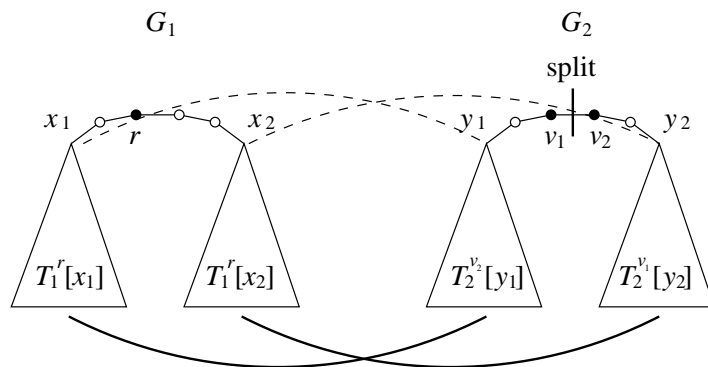


Figure 7. Illustration of Case 2 in computing  $\delta(G_1, G_2)$  for two CUAL graphs  $G_1$  and  $G_2$ .

## 5 Conclusion

Using this simple, efficient algorithm, a user can submit a query graph and obtain those data graphs approximately matching the query. To our knowledge, this work gives the first polynomial time algorithm ever presented to solve the edit distance problem between undirected acyclic graphs. We are currently implementing the algorithm and integrating it into our pattern matching toolkit [12].

## Acknowledgements

The authors thank Professor Dave Kristol and Dawn Luo for inspirational discussions. We also thank our industrial collaborators Jim Kaminski and Karen Pysniak (Schering-Plough Corporation) and Anthony Noriega (FMC, Princeton) for their constructive suggestions on an early version of this paper.

## References

- [1] J. E. Ash, P. A. Chubb, S. E. Ward, S. M. Welford, and P. Willett. *Communication, Storage and Retrieval of Chemical Information*. Ellis Horwood, Chichester, England, 1985.
- [2] J. E. Ash and E. Hyde, editors. *Chemical Information Systems*. Ellis Horwood, Chichester, England, 1975.



- [3] H. N. Gabow, Z. Galil, and T. H. Spencer. Efficient implementation of graph algorithms using contraction. In *Proceedings of the 25th Annual IEEE Symposium on Foundations of Computer Science*, pages 347–357, 1984.
- [4] H. N. Gabow and R. E. Tarjan. Faster scaling algorithms for network problems. *SIAM J. Comput.*, 18(5):1013–1036, 1989.
- [5] M. R. Garey and D. S. Johnson. *Computers and Intractability: A Guide to the Theory of NP-Completeness*. W. H. Freeman and Company, New York, 1979.
- [6] M. A. Johnson and G. M. Maggiora, editors. *Concepts and Applications of Molecular Similarity*. Wiley, New York, 1990.
- [7] J. Kaminski, B. Wallmark, C. Briving, and B.-M. Andersson. Antiulcer agents. 5. inhibition of gastric  $H^+/K^+$ -ATPase by substituted imidazo[1,2-*a*]pyridines and related analogues and its implication in modeling the high affinity potassium ion binding site of the gastric proton pump enzyme. *Journal of Medicinal Chemistry*, 34:533–541, 1991.
- [8] E. M. Mitchell, P. J. Artymiuk, D. W. Rice, and P. Willett. Use of techniques derived from graph theory to compare secondary structure motifs in proteins. *Journal of Molecular Biology*, 212:151–166, 1989.
- [9] A. S. Noetzel and S. M. Selkow. An analysis of the general tree-editing problem. In D. Sankoff and J. B. Kruskal, editors, *Time Warps, String Edits, and Macromolecules: The Theory and Practice of Sequence Comparison*, pages 237–252. Addison-Wesley, Reading, MA, 1983.
- [10] D. Shasha, J. T. L. Wang, K. Zhang, and F. Y. Shih. Exact and approximate algorithms for unordered tree matching. *IEEE Transactions on Systems, Man and Cybernetics*, 24(4):668–678, April 1994.
- [11] R. A. Wagner and M. J. Fischer. The string-to-string correction problem. *J. ACM*, 21(1):168–173, Jan. 1974.
- [12] J. T. L. Wang, K. Zhang, K. Jeong, and D. Shasha. A system for approximate tree matching. *IEEE Transactions on Knowledge and Data Engineering*, 6(4):559–571, August 1994.
- [13] W. E. Warr. *Chemical Structures*. Springer-Verlag, Berlin, 1988.

- [14] P. Willett. *Similarity and Clustering Methods in Chemical Information Systems*. Research Studies Press, Letchworth, 1987.
- [15] P. Willett. Algorithms for the calculation of similarity in chemical structure databases. In M. A. Johnson and G. M. Maggiora, editors, *Concepts and Applications of Molecular Similarity*, pages 43–61. John Wiley & Sons, Inc., 1990.
- [16] K. Zhang, R. Statman, and D. Shasha. On the editing distance between unordered labeled trees. *Information Processing Letters*, 42:133–139, 1992.