# A First Step Towards Exact Graph Edit Distance Using Bipartite Graph Matching

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**Abstract.** In recent years, a powerful approximation framework for graph edit distance computation has been introduced. This particular approximation is based on an optimal assignment of local graph structures which can be established in polynomial time. However, as this approach considers the local structural properties of the graphs only, it yields suboptimal solutions that overestimate the true edit distance in general. Recently, several attempts for reducing this overestimation have been made. The present paper is a starting point towards the study of sophisticated heuristics that can be integrated in these reduction strategies. These heuristics aim at further improving the overall distance quality while keeping the low computation time of the approximation framework. We propose an iterative version of one of the existing improvement strategies. An experimental evaluation clearly shows that there is large space for further substantial reductions of the overestimation in the existing approximation framework.

### 1 Introduction

Graph edit distance [1, 2] is one of the most flexible and versatile approaches to error-tolerant graph matching. In particular, graph edit distance is able to cope with directed and undirected, as well as with labeled and unlabeled graphs. In addition, no constraints have to be considered on the alphabets for node and/or edge labels. Moreover, through the concept of cost functions graph edit distance can be adapted and tailored to diverse applications [3, 4]. An extensive survey about graph edit distance can be found in [5].

The major drawback of graph edit distance is its high computational complexity that restrict its applicability to graphs of rather small size. In fact, graph edit distance belongs to the family of *quadratic assignment problems* (QAPs), which belong to the class of  $\mathcal{NP}$ -complete problems. Therefore, exact computation of graph edit distance can be solved in exponential time complexity only.

In recent years, a number of methods addressing the high computational complexity of graph edit distance have been proposed (e.g. [6–9]). Beyond these works, an algorithmic framework based on bipartite graph matching has been introduced recently [10, 11]. The main idea behind this approach is to convert the difficult problem of graph edit distance to a *linear sum assignment problem* (LSAP). LSAPs basically constitute the problem of finding an optimal assignment between two independent sets of entities, for which a collection of polynomial algorithms exists [12]. In [10, 11] the LSAP is formulated on the sets of nodes including local edge information. The main advantage of this approach is that it allows the approximate computation of graph edit distance in a substantially faster way than traditional methods. However, during the node assignment only local instead of global structural information is taken into account. Hence, this might lead to incorrect node assignments compared with an exact matching and thus, the derived edit distance is equal to, or larger than, the exact graph edit distance.

In order to overcome this problem and reduce the overestimation of the true graph edit distance, a variation of the original framework [10] has been proposed in [13]. Given the initial assignment found by the bipartite framework, the main idea is to introduce a post-processing step such that the number of incorrect assignments is decreased (which in turn reduces the overestimation). The proposed post-processing varies the original node assignment by systematically swapping the target nodes of two node assignments. In order to search the space of assignment variations a *beam search* (i.e. a tree search with pruning) is used. One of the most important observations derived from [13] is that given an initial node assignment, one can substantially reduce the overestimation using this local search method. Yet, beam search is sub-optimal in the sense of possibly pruning the optimal solution in an early stage of the search process.

Now the crucial question arises, how the space of assignment variations could be explored such that promising parts of the search tree are not (or at least not too early) pruned. In [13] the initial assignment is systematically varied without using any kind of heuristic or additional information to keep the best potential assignment unpruned in the tree. In particular it is not taken into account that certain nodes and/or local assignments have greater impact than other on the graph edit distance approximation and should thus be considered first in the beam search process. Clearly, considering more important node assignments and/or nodes in an early stage of the beam search process might reduce the risk of pruning the optimal assignment. In this sense we argue that the introduction of procedures and heuristics that guide the order in which the assignments are varied during beam search is a rewarding line of research.

The main objective of the present paper is to start the investigation towards new heuristics that improve the overall quality of the node assignment. In particular, we propose an iterative version of [13] to derive randomized permutations of the original mapping which serve as starting point for beam search improvements. Hence, the present paper introduces a heuristic in order to answer the general question to what extent the ordering of the nodes affects the mapping quality.

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Next, in Section 2, the original bipartite framework for graph edit distance approximation [10] as well as its recent extension [13], named *BP-Beam*, are summarized. In Section 3 our novel iterative version of *BP-Beam* is described. An experimental evaluation on diverse data sets is carried out in Section 4. Finally, in Section 5 we draw conclusions and outline some possible tasks and extensions for future work.

# 2 Approximate Graph Edit Distance Computation

Given two graphs,  $g_1$  and  $g_2$ , the basic idea of graph edit distance is to transform  $g_1$  into  $g_2$  using edit operations, namely, *insertions*, *deletions*, and *substitutions* of both nodes and edges. The substitution of two nodes u and v is denoted by  $(u \to v)$ , the deletion of node u by  $(u \to \epsilon)$ , and the insertion of node v by  $(\epsilon \to v)^1$ . A sequence of edit operations  $e_1, \ldots, e_k$  that transform  $g_1$  completely into  $g_2$  is called an edit path between  $g_1$  and  $g_2$ .

To find the most suitable edit path out of all possible edit paths between two graphs, a cost measuring the strength of the corresponding operation is introduced. The edit distance between two graphs  $g_1$  and  $g_2$  is then defined by the minimum cost edit path between them. Exact computation of graph edit distance is usually carried out by means of a tree search algorithm (e.g.  $A^*$ ) which explores the space of all possible mappings of the nodes and edges of the first graph to the nodes and edges of the second graph.

### 2.1 Bipartite Graph Edit Distance Approximation

The computational complexity of exact graph edit distance is exponential in the number of nodes of the involved graphs. That is considering n nodes in  $g_1$  and m nodes in  $g_2$ , the set of all possible edit paths contains  $O(n^m)$  solutions to be explored. This means that for large graphs the computation of edit distance is intractable. In order to reduce its computational complexity, in [10], the graph edit distance problem is transformed into a linear sum assignment problem (LSAP). To this end, based on the node sets  $V_1 = \{u_1, \ldots, u_n\}$  and  $V_2 = \{v_1, \ldots, v_m\}$  of  $g_1$  and  $g_2$  respectively, a cost matrix C is first established as follows:

	$c_{11}$	$c_{12}$	• • •	$c_{1m}$	$c_{1\epsilon}$	$\infty$	• • •	$\infty$
C =	$c_{21}$	$c_{22}$	• • •	$c_{2m}$	$\infty$	$c_{2\epsilon}$	• • •	$\infty$
	÷	÷	۰.	:	:	÷	۰.	÷
	$c_{n1}$	$c_{n2}$	• • •	$c_{nm}$	$\infty$	$\infty$	• • •	$c_{n\epsilon}$
0 –	$c_{\epsilon 1}$	$\infty$	• • •	$\infty$	0	0	• • •	0
0 –	$c_{\epsilon 1} \\ \infty$	$\infty$ $c_{\epsilon 2}$	· · · ·	8 8	0 0	0 0	· · · ·	0 0
0 –	$c_{\epsilon 1} \\ \infty \\ \vdots$	$\infty$ $c_{\epsilon 2}$ $\vdots$	···· ··· ·.	8 8 8	0 0 :	0 0 :	···· ··· ·	0 0 :

<sup>&</sup>lt;sup>1</sup> Similar notation is used for edges.

Entry  $c_{ij}$  denotes the cost of a node substitution  $(u_i \to v_j)$ ,  $c_{i\epsilon}$  denotes the cost of a node deletion  $(u_i \to \epsilon)$ , and  $c_{\epsilon j}$  denotes the cost of a node insertion  $(\epsilon \to v_j)$ . The left upper corner of the cost matrix represents the costs of all possible node substitutions, the diagonal of the right upper corner the costs of all possible node deletions, and the diagonal of the bottom left corner the costs of all possible node insertions. In each entry  $c_{ij}$ , not only the cost of node operation is taken into account but also the minimum sum of edge edit operation costs, implied by the corresponding node operation. That is, the matching cost of the local edge structure is encoded in the individual entries of C.

In a second step of [10], an assignment algorithm is applied to the square cost matrix  $C = (c_{ij})$  in order to find the minimum cost assignment of the nodes (and their local edge structure) of  $g_1$  to the nodes (and their local edge structure) of  $g_2$ . Note that this task exactly corresponds to an instance of an LSAP and can thus be optimally solved in polynomial time by several algorithms [12].

Any of the LSAP algorithms will return a permutation  $(\varphi_1, \ldots, \varphi_{n+m})$  of the integers  $(1, 2, \ldots, (n+m))$ , which minimizes the overall mapping cost  $\sum_{i=1}^{(n+m)} c_{i\varphi_i}$ . This permutation corresponds to the mapping

$$\psi = \{u_1 \to v_{\varphi 1}, u_2 \to v_{\varphi 2}, \dots, u_{m+n} \to v_{\varphi_{m+n}}\}$$

of the nodes of  $g_1$  to the nodes of  $g_2$ . Note that  $\psi$  does not only include node substitutions  $(u_i \to v_j)$ , but also deletions and insertions  $(u_i \to \epsilon)$ ,  $(\epsilon \to v_j)$  and thus perfectly reflects the definition of graph edit distance (mappings of the form  $(\epsilon \to \epsilon)$  can be dismissed, of course). Hence, mapping  $\psi$  can be interpreted as partial edit path between  $g_1$  and  $g_2$ , which considers operations on nodes only.

In a third step, the partial edit path  $\psi$  between  $g_1$  and  $g_2$  is completed with respect to the edges. This can be accomplished since edge edit operations are implied by edit operations on their adjacent nodes. That is, whether an edge is substituted, deleted, or inserted, depends on the edit operations performed on its adjacent nodes. The total cost  $d_{\langle\psi\rangle}(g_1, g_2)$  of the completed edit path between graphs  $g_1$  and  $g_1$  is finally returned as approximate graph edit distance. We refer to this graph edit distance approximation algorithm as  $BP(g_1, g_2)$ .

### 2.2 Improving the Approximation Using Beam Search

Several experimental evaluations indicate that the suboptimality of BP, i.e. the overestimation of the true edit distance, is very often due to a few incorrectly assigned nodes in  $\psi$  with respect to the optimal edit path. The extension presented in [13] ties in at this observation. In particular, the node assignment  $\psi$  is used as a starting point for a subsequent search in order to improve the quality of the distance approximation.

In [13], the original node assignment  $\psi$  is systematically varied by swapping the target nodes  $v_{\varphi_i}$  and  $v_{\varphi_j}$  of two node assignments  $(u_i \to v_{\varphi_i}) \in \psi$  and  $(u_j \to v_{\varphi_j}) \in \psi$ . For each swap it is verified whether (and to what extent) the derived distance approximation stagnates, increases or decreases. For a systematic variation of mapping  $\psi$  a tree search is used.

	<b>S</b> ( <i>J</i> 1, <i>J</i> 2, <i>7</i> , <i>7</i> )
1.	$d_{best} = d_{\langle \psi \rangle}(g_1, g_2)$
2.	Initialize open = { $(\psi, 0, d_{\langle \psi \rangle}(g_1, g_2))$ }
3.	while open is not empty do
4.	Remove first tree node in open: $(\psi, q, d_{\langle \psi \rangle}(g_1, g_2))$
5.	for $j = (q + 1), \dots, (m + n)$ do
6.	$\psi' = \psi \setminus \{u_{q+1} \to v_{\varphi_{q+1}}, u_j \to v_{\varphi_j}\} \cup \{u_{q+1} \to v_{\varphi_j}, u_j \to v_{\varphi_{q+1}}\}$
7.	Derive approximate edit distance $d_{\langle \psi' \rangle}(g_1, g_2)$
8.	$open = open \cup \{(\psi', q+1, d_{\langle \psi' \rangle}(g_1, g_2))\}$
9.	$ {\bf if} \ d_{\left<\psi'\right>}(g_1,g_2) < d_{best} \ {\bf then} $
10.	$d_{best} = d_{\left<\psi' ight>}(g_1,g_2)$
11.	end if
12.	end for
13.	while size of $open > b \operatorname{do}$
14.	Remove tree node with highest approximation value $d_{\langle\psi angle}$ from open
15.	end while
16.	end while
17.	return $d_{best}$

Algorithm 1. *BP*-Beam $(a_1, a_2, \psi, b)$ 

The tree nodes in the search procedure correspond to triples  $(\psi, q, d_{\langle \psi \rangle})$ , where  $\psi$  is a certain node assignment, q denotes the depth of the tree node in the search tree and  $d_{\langle \psi \rangle}$  is the approximate distance value corresponding to  $\psi$ . The root node of the search tree refers to the optimal node assignment  $\psi$  found by BP. Hence, the root node (with depth = 0) is given by the triple  $(\psi, 0, d_{\langle \psi \rangle})$ . Subsequent tree nodes  $(\psi', q, d_{\langle \psi \rangle})$  with depth  $q = 1, \ldots, (m+n)$  contain node assignments  $\psi'$  with swapped element  $(u_q \to v_{\varphi_q})$ .

As usual in tree search based methods, a set *open* is employed that holds all of the unprocessed tree nodes. The tree nodes in *open* are kept sorted in ascending order according to their depth in the search tree (known as *breadth-first search*). As a second order criterion the approximate edit distance  $d_{\langle\psi\rangle}$  is used.

The extended framework with the tree search based improvement is given in Alg. 1. As long as *open* is not empty, we retrieve (and remove) the triple  $(\psi, q, d_{\langle \psi \rangle})$  at the first position in *open*, generate the successors of this specific tree node and add them to *open*. To this end all pairs of node assignments  $(u_{q+1} \rightarrow v_{\varphi_{q+1}})$  and  $(u_j \rightarrow v_{\varphi_j})$  with  $j = (q+1), \ldots, (n+m)$  are individually swapped resulting in two new assignments  $(u_{q+1} \rightarrow v_{\varphi_j})$  and  $(u_j \rightarrow v_{\varphi_{q+1}})$ . In order to derive node mapping  $\psi'$  from  $\psi$ , the original node assignment pair is removed from  $\psi$  and the swapped node assignment is added to  $\psi'$ . Since index jstarts at (q+1) we also allow that a certain assignment  $u_{q+1} \rightarrow v_{\varphi_{q+1}}$  remains unaltered at depth (q+1) in the search tree.

Since every tree node in our search procedure corresponds to a complete solution and the cost of these solutions neither monotonically decrease nor increase with growing depth in the search tree, we need to buffer the best possible distance approximation found during the tree search in  $d_{best}$  (which is returned as soon as *open* is empty)

As stated before, given a mapping  $\psi$  from *BP*, the derived edit distance overestimates the true edit distance in general. This overestimation is due to some incorrect node mappings in  $\psi$ . Hence, the objective of any post-processing should be to find a variation  $\psi'$  of the original mapping  $\psi$  such that  $d_{\langle \psi' \rangle} < d_{\langle \psi \rangle}$ . However, the search space of all possible permutations of  $\psi$  contains (n + m)! possibilities, making an exhaustive search (starting with  $\psi$ ) both unreasonable and intractable. Therefore, only the *b* assignments with the lowest approximate distance values are kept in *open* at all time (known as *beam search*). Note that parameter *b* can be used as trade-off parameter between run time and approximation quality. That is, it can be expected that larger values of *b* lead to both better approximations and increased run time (and vice versa). From now on we refer to this variant of the approximation framework as BP- $Beam(g_1, g_2, \psi, b)$ .

# 3 Iterative BP-Beam

Note that the successors of tree node  $(\psi, q, d_{\langle \psi \rangle})$  are generated in fixed order in *BP-Beam*. In particular, the assignments of the original node matching  $\psi$ are processed according to the depth q of the current search tree node. That is, at depth q the assignment  $(u_q \rightarrow v_{\varphi_q})$  is processed and swapped with other assignments. Note that beam search prunes quite large parts of the tree during the search process. Hence, processing correct node assignments at the top of the search tree is somewhat useless and moreover runs the risk of potentially pruning crucial parts of the tree at an early stage of the search. That is, the fixed order processing, which does not take any information about the individual node assignments into account, is a clear drawback of the procedure described in [13].

Clearly, it would be highly favorable to process important node assignments as early as possible in the tree search. Our hypothesis is that there should exist some heuristics that indicate which node assignments of  $\psi$  are the most important or critical ones and should thus be processed first. Finding such heuristics that indicate the impact of a single node assignment on the approximation quality turns out to be a highly non-trivial task. Moreover, it is not yet proven whether the order of the assignment processing actually has a great impact on the resulting distance quality.

As a starting point towards the question of whether or not the ordering of the assignment processing in *BP-Beam* has great influence on the quality of the distance approximation, we propose a procedure with random re-orderings of the individual assignments. Thus, given a mapping  $\psi$  obtained from *BP*, we propose to perform several iterations over *BP-Beam*. In every iteration the original mapping  $\psi$  is randomly reordered and fed into *BP-Beam*. This leads to an iterative version of *BP-Beam* called *IBP-Beam* from now on. *IBP-Beam* takes two parameters, namely the number of iterations k and the beam size b.

The algorithm *IBP-Beam* is given in Alg. 2. The first three lines correspond to the three major steps of the original approximation. Then, the main loop is carried out k times. In each iteration a newly ordered assignment  $\psi'$  is generated by randomly permuting the original assignment  $\psi$  derived from *BP*. Then, the assignment and the corresponding distance are possibly improved using *BP-Beam* taking  $\psi'$  as starting point for the tree search. Whenever the *BP-Beam* 

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Algorithm 2. IBP-Beam $(g_1, g_2, k, b)$				
$\frac{1}{2}$ .	Build cost matrix $C = (c_{ij})$ according to the input graphs $g_1$ and $g_2$ Compute optimal node assignment $\psi = \{u_1 \rightarrow v_{\varphi_1}, \dots, u_{m+n} \rightarrow v_{\varphi_{m+n}}\}$ on $C$			
3.	$d_{best} = d_{\langle \psi \rangle}(g_1, g_2)$			
4.	i = 1			
5.	while $i \leq k$ do			
6.	$\psi' = RandomPermutation(\psi)$			
7.	$d_{beam} = BP\text{-}Beam(g_1, g_2, \psi', b)$			
8.	$d_{best} = \min\{d_{best}, d_{beam}\}$			
9.	i + +			
10.	end while			
11.	return $d_{best}$			

is able to further decrease the distance approximation, the best solution  $d_{hest}$  is replaced by the novel approximation.

Clearly, further reductions of the overestimation with this random iterative procedure, would highly encourage the hypothesis that there might be heuristics that would solve the same task of reordering in a deterministic manner (in particular when the number of iterations k needed remains small).

#### 4 **Experimental Evaluation**

The goal of the experimental evaluation is to verify whether the proposed extension is able to reduce the overestimation of graph edit distance approximation returned by BP and in particular BP-Beam, and how the iterative process affects the computation time. Three data sets from the IAM graph database repository involving molecular compounds (AIDS), fingerprint images (Fingerprint), and symbols from architectural and electronic drawings (GREC) are used to carry out this experimental part. For further details about these data sets we refer to [14]. For all data sets, subsets of 100 graphs are randomly selected on which 10,000 pairwise graph edit distance computations are performed.

#### 4.1 Impact of Meta Parameter b and k

In this first experiment we aim at researching the impact of the two parameters b and k on *IBP-Beam*. To this end we perform several executions of the *IBP-Beam* with  $b, k \in \{1, 5, 10, 15, 20\}$ , leading to 25 different distance approximations. We compute the sum of the difference between the exact distance  $(A^*)$  and the distance obtained by *IBP-Beam*. Figure 1 shows such sum of differences as a function of the number of iterations k (x-axis) and the beam size b (y-axis).

First, we observe that the sum of differences is monotonically reduced as long as k and b are increased. We can also observe that we are able to obtain distance values very close to the exact distance on all data sets. Finally (and probably most importantly), we note that the major part of the reduction in the sum of differences is already obtained with values of k and b of 5. Further increases of both parameters lead to relatively small further reductions of the overestimation.



**Fig. 1.** Sum of difference between  $A^*$  and IBP-Beam(k,b) as a function of the number of iterations k (x-axis) and the beam size b (y-axis)

### 4.2 Relative Overestimation and Computation Time

Next we measure the mean relative overestimation  $\phi o$  [%] and the mean computation time  $\phi t$  [ms] for all algorithms (see Table 1). The mean relative overestimation  $\phi o$  of a certain approximation is computed as the relative difference to the sum of distances returned by  $A^*$ . The relative overestimation of  $A^*$  is thus zero and the value of  $\phi o$  for BP is taken as reference value and corresponds to 100%. The computation times  $\phi t$  measures the average matching time for a pair of graphs. Note that for both BP-Beam and IBP-Beam the beam size b is fixed to 5 (thus this parameter is not shown in the Table 1, but only k).

**Table 1.** The mean relative overestimation of the exact distance  $(\phi o)$  in %, and the mean run time for one matcing  $(\phi t)$  in ms. for each data set and for a given algorithm. The beam size for *BP-Beam* and *IBP-Beam* algorithm is set to 5, and parameter k is varied from 5 to 20 for *IBP-Beam*.

	AIDS		Fingerprint			GR	GREC	
Algorithm	$\phi o$	$\phi t$	$\phi o$	$\phi t$		$\phi o$	$\phi t$	
A* BP	0.00 100.00	25750.22 0.28	0.00 100.00	$31645.08 \\ 0.35$		0.00 100.00	7770.81 0.27	
BP-Beam IBP-Beam(5) IBP-Beam(10) IBP-Beam(15) IBP-Beam(20)	$     15.09 \\     9.27 \\     6.11 \\     4.85 \\     4.26 $	1.82 7.81 15.27 22.79 30.41	$24.57 \\ 8.63 \\ 6.11 \\ 5.21 \\ 4.51$	$1.45 \\ 5.70 \\ 10.98 \\ 16.14 \\ 20.94$		$16.98 \\ 8.53 \\ 5.72 \\ 4.57 \\ 3.73$	2.62 12.01 23.57 35.81 47.19	

Regarding the overestimation  $\phi o$  we observe a substantial improvement of the distance quality using *BP-Beam* rather than *BP*. For instance, on the AIDS data the overestimation is reduced by 85% (similar results are obtained on the other data sets). By using *IBP-Beam* further substantial reductions of the overestimation are possible on all data sets. For instance, on the AIDS data set using *IBP-Beam* with k = 5 rather than *BP-Beam* enables a reduction from 15.09% to 9.27% (similar or even better results are obtained on the other data sets). Increasing the number of iterations further decreases the overestimation such that a distance accuracy very near to the exact edit distance is possible with our

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novel approach. These substantial reductions of the overestimation from BP to BP-Beam and from BP-Beam to IBP-Beam can also be seen in Figure 2 where for each pair of graphs the exact distance (x-axis) is plotted vs. the distance obtained by an approximation algorithm (y-axis). In fact, for IBP-Beam the line-like scatter plot along the diagonal suggests that the approximation is very near to the optimal distance.



**Fig. 2.** Exact (x-axis) vs. approximate (y-axis) edit distance on the AIDS dataset computed with (a) BP, (b) BP-Beam(5), (c) IBP-Beam(20,5)

Regarding the computation time  $\phi t$  we can report that BP provides the lowest computation time on all data sets (approximately 0.3ms per matching on all data sets). Yet, remember that this fast matching time is at the expense of the highest overestimation. BP-Beam increases the computation time to approximately 2ms per matching and IBP-Beam further increases the average run time to several milliseconds per matching. As expected, the run time of IBP-Beam linearly grows with parameter k. However, it is important to remark that in all cases the computation time is much lower than those of  $A^*$ . Overall IBP-Beam(5) seems to be a good trade-off between computation time and reduction of the overestimation.

### 5 Conclusions and Future Work

In recent years a framework based on bipartite graph matching to derive approximate solutions of the graph edit distance has been presented. In its original version it suffers from a high overestimation of the computed distance with respect to the true edit distance. In this paper, we propose an iterative extension of one of the existing bipartite-based graph edit distance approximation algorithm. The aim of the paper is to empirically investigate the influence of the order in which the assignments are explored in a post processing search process on the distance quality. The experimental evaluation on three different databases verifies that this order is actually one of the critical factors to improve the overall distance quality. Though the run times are increased when compared to our former framework (as expected), they are still far below the run times of the exact algorithm. The presented approach can be seen as a first step towards

finding determinant heuristics to guide the search through the space of possible assignment variants (starting with  $\psi$ ).

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