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Approximate Graph Edit Distance by Several Local Searches in Parallel

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Abstract: Solving or approximating the linear sum assignment problem (LSAP) is an important step of several constructive and local search strategies developed to approximate the graph edit distance (GED) of two attributed graphs, or more generally the solution to quadratic assignment problems. Constructive strategies find a first estimation of the GED by solving an LSAP. This estimation is then refined by a local search strategy. While these search strategies depend strongly on the initial assignment, several solutions to the linear problem usually exist. They are not taken into account to get better estimations. All the estimations of the GED based on an LSAP select randomly one solution. This paper explores the insights provided by the use of several solutions to an LSAP, refined in parallel by a local search strategy based on the relaxation of the search space, and conditional gradient descent. Other generators of initial assignments are also considered, approximate solutions to an LSAP and random assignments. Experimental evaluations on several datasets show that the proposed estimation is comparable to more global search strategies in a reduced computational time.

1 INTRODUCTION

The *graph edit distance* (GED) is a well-known measure of dissimilarity between attributed graphs, proposed in the context of error-correcting graph matching (Sanfeliu and Fu, 1983; Bunke and Allermann, 1983). A complete overview, with applications in pattern recognition and machine learning, can be found in (Neuhaus and Bunke, 2007; Riesen, 2015).

The GED captures the minimal amount of distortion needed to transform an attributed graph G_1 into an attributed graph G_2 by iteratively editing both the structure and the attributes of G_1 , until G_2 is obtained. At each iteration, one attributed node or edge is usually removed, inserted or substituted with a non-negative cost (the strength of this local distortion). The resulting sequence of *edit operations* γ , called *edit path*, transforms G_1 into G_2 . Its cost (the strength of the global distortion) is measured by $L_c(\gamma) = \sum_{o \in \gamma} c(o)$, where $c(o)$ is the cost of the edit operation o . Among all edit paths from G_1 to G_2 , denoted by the set $\Gamma(G_1, G_2)$, a *minimal-cost edit path* is a path having a minimal cost. The GED from G_1 to

G_2 is defined as the cost of a minimal-cost edit path:

$$d_c(G_1, G_2) = \min_{\gamma \in \Gamma(G_1, G_2)} L_c(\gamma). \quad (1)$$

Since $\Gamma(G_1, G_2)$ has a large, potentially infinite cardinality, edit paths are generally restricted so that each node and edge of each graph is involved in a single edit operation. With this restriction, and under some constraints on the cost $c(\cdot)$ ¹, the minimal edit path problem (Eq. 1) is equivalent to the *minimal-cost error-correcting graph matching problem* (ECGM). This graph matching problem finds optimal correspondences between the nodes of two graphs so that each node is either assigned to another node (substituted) or assigned to a dummy node (removed or inserted). Correspondences between edges (edge edit operations) are induced by these node correspondences. Like other graph matching problems, the minimal-cost error-correcting graph matching problem can be written as a *quadratic assignment problem* (QAP). Considering the general expression of QAP

¹substituting an edge e_1 by an edge e_2 is not more expensive than removing e_1 plus inserting e_2 (Bougleux et al., 2017)

(Lawler, 1963), the GED is given by (Bouglex et al., 2017):

$$d_{g,c,D}(G_1, G_2) = \min_{\mathbf{x} \in \pi_{n,m,\varepsilon}} \mathbf{c}^\top \mathbf{x} + g \mathbf{x}^\top \mathbf{D} \mathbf{x} \quad (2)$$

where $\pi_{n,m,\varepsilon} = \text{vec}[\Pi_{n,m,\varepsilon}]$ is the set of vectorized permutation matrices of size $(n+m) \times (m+n)$ (one-to-one node correspondences or assignments), n and m are the order of G_1 and G_2 respectively. The costs of editing nodes are encoded by the vector $\mathbf{c} \geq \mathbf{0}$ of size $(n+m)^2$, and the cost of editing edges by the $(n+m)^2 \times (n+m)^2$ matrix $\mathbf{D} \geq \mathbf{0}$. The parameter g is equal to 1/2 when both graphs are undirected, or 1 otherwise. Other expressions can be found in (Riesen, 2015).

Computing the GED is NP-hard (Zeng et al., 2009). Several algorithms are designed to compute an exact solution (Riesen, 2015; Lerouge et al., 2017; Blumenthal and Gamper, 2017; Abu-Aisheh et al., 2017), but they are restricted to relatively small set of graphs composed of only few nodes. Moreover, finding an approximate solution within some constant factor from the global minimum cannot be done in polynomial time (unless $P=NP$). More details on quadratic assignment problems in general can be found in (Burkard et al., 2009). In particular, good approximate solutions are obtained in short computing time by heuristic algorithms based on constructive greedy strategies, or on pure or hybrid local search strategies, *e.g.* limitation of exact algorithms (time, upper bound on the number of iterations, etc), single solution methods (simulated annealing, tabu search, greedy randomized adaptive search, relaxation-based search) or population based methods (genetic algorithms, scatter search, ant colony optimization). This paper focuses on fast methods developed for finding a good overestimation of the GED.

Bipartite GED Fastest estimations are obtained by replacing the quadratic problem by a *linear sum assignment problem* (LSAP) (Riesen, 2015):

$$\mathbf{x}^* \in \underset{\mathbf{x} \in \pi_{n,m,\varepsilon}}{\text{argmin}} \tilde{\mathbf{c}}^\top \mathbf{x} \quad (3)$$

where the cost $\tilde{c}_{i,j}$ of assigning two nodes is defined as the optimal cost of assigning two structures, each centered at a node, with respect to the initial edit costs \mathbf{c} and \mathbf{D} . In other terms, it defines an edit distance between two structures. Several types of structures have been considered, *e.g.* star subgraphs or local neighborhoods (Riesen and Bunke, 2009; Riesen et al., 2014; Cortés et al., 2015), random walks (Gaüzère et al., 2014), or small subgraphs (Carletti et al., 2015). Using this framework the approximate GED, known as the *bipartite GED* (bGED), is

defined as the quadratic cost of a solution \mathbf{x}^* to the LSAP, *i.e.* an edit path induced by the node assignment: $\text{bGED}(G_1, G_2) = \mathbf{c}^\top \mathbf{x}^* + g \mathbf{x}^{*\top} \mathbf{D} \mathbf{x}^*$. A solution to the LSAP can be computed in cubic time with respect to the number of nodes (here $n+m$), for instance with the Hungarian algorithm. Several strategies have been proposed to reduce this time complexity, *e.g.* reformulation as a reduced LSAP (Serratos, 2014; Serratos, 2015). Alternatively, an assignment $\mathbf{x} \in \pi_{n,m,\varepsilon}$ having a low linear cost $\mathbf{x}^\top \tilde{\mathbf{c}}$ can also be computed by several greedy algorithms in quadratic time (Riesen et al., 2015; Fischer et al., 2017). The resulting *greedy bipartite GED* remains comparable to the bipartite GED on several datasets.

Greedy refinement methods To refine the bipartite GED, or its greedy version, several local search strategies have been introduced in (Riesen and Bunke, 2015; Riesen, 2015). From a solution to the LSAP defined by Eq. 3, these iterative algorithms compute one or several new assignments at each iteration by modifying the cost vector $\tilde{\mathbf{c}}$ and by eventually solving a new LSAP, or by swapping some pairs of assigned nodes. The selection of a candidate assignment depends on the quadratic function. While these methods can still compute an estimation of the GED in polynomial time, they are based on local search strategies which usually lead to a local minimum of the quadratic function. A strategy based on simulated annealing has been recently proposed in (Riesen et al., 2017) to drive the search out of a local minimum.

Relaxation-based methods Search strategies based on the relaxation of Eq. 2 have been investigated in (Bouglex et al., 2017). Initially developed for the graph matching problem (Zaslavskiy et al., 2009; Leordeanu et al., 2009; Liu and Qiao, 2014; Vogelstein et al., 2015), they relax the set of solutions to the set of doubly-stochastic matrices (values in $[0, 1]$). Then the *integer projected fixed point* (IPFP) procedure (Leordeanu et al., 2009), or the *fast approximate quadratic programming* procedure (Vogelstein et al., 2015), proceed as follows. From an initial candidate solution, they track a good local minimum of the quadratic function in the relaxed domain, by a conditional gradient descent (Frank-Wolfe algorithm (Frank and Wolfe, 1956)), and finally project the solution into the discrete domain by solving an LSAP. The quality of the estimation depends strongly on the initialization. A more global approach is proposed in (Zaslavskiy et al., 2009; Liu and Qiao, 2014). It consists to also relax the quadratic function so that it becomes more or less convex, or more or less concave. From the totally convex version to the totally concave

version, each step of the approach finds a local minimum of a relaxed version, by the Frank-Wolfe algorithm initialized by the local minimum found at the previous step. While this *path-following algorithm* does not need to be initialized, it is computationally more expensive than the previous ones.

Multistart strategy Instead of developing more complex and global strategies, local search strategies can be improved by considering several initial candidates instead of only one. Then the minimal estimation, or a corresponding assignment, is retained. While this only reduces the initialization problem, the different estimations are independent to each others and can be computed in parallel. This simple and under-estimated strategy, known as *multistart* (Burkard et al., 2009), is commonly used in non-linear approximation. For instance, for the graph matching problem, experiments presented in (Vogelstein et al., 2015) show that this strategy leads to a better estimation than the more global method based on convex-concave relaxation (Zaslavskiy et al., 2009).

Contributions In this paper, we explore the multistart strategy for improving the estimation of the GED obtained in (Bogleux et al., 2017) by the Frank-Wolfe algorithm (Sec. 2). Like for other local search strategies, the descent process is initialized with a solution to the LSAP defining the bipartite GED (Eq. 3). Depending on the cost values, several assignments may solve this LSAP. The bipartite GED selects only one of them, arbitrary. So we consider a set of solutions to the LSAP for improving both the bipartite GED and the relaxation-based approach (Sec. 3). Contrary to that, an LSAP can have only one or few solutions, and there is no guarantee that one of them is also a solution for the quadratic problem. So we consider several other types of initial assignments: approximate solutions to the LSAP by a greedy strategy, random assignments, and random doubly-stochastic matrices. The impact of the multistart strategy is analyzed empirically in Sec. 4 on several datasets. It provides comparable or better results than more global strategies, with a reduced computational time.

2 BIPARTITE GED REFINED BY FRANK-WOLFE ALGORITHM

To find an approximate GED, (Bogleux et al., 2017) proposed to refine the bipartite GED by the Frank-Wolfe algorithm. It is inspired by the IPFP procedure presented in (Leordeanu et al., 2009) for

approximate graph matching. It is a gradient-descent method based on the continuous relaxation of the binary constraints imposed on the solutions of the problem, and on first-order approximation of the quadratic functional in the relaxed domain.

Let $\pi_{n,m,\varepsilon} = \text{vec}[\Pi_{n,m,\varepsilon}]$ be the set of candidate assignments to the QAP defined by Eq. 2, where

$$\begin{aligned} \Pi_{n,m,\varepsilon} = \{ & \mathbf{X} \in \{0,1\}^{(n+m) \times (m+n)} : \\ & \mathbf{X}\mathbf{1} = \mathbf{1}, \mathbf{X}^T\mathbf{1} = \mathbf{1} \\ & \forall i = 1, \dots, n, \forall j > m, j \neq m+i, x_{i,j} = 0 \\ & \forall j = 1, \dots, m, \forall i > n, i \neq n+j, x_{i,j} = 0 \} \end{aligned}$$

is the set of permutation matrices encoding error-correcting assignments (Bogleux et al., 2017; Riesen, 2015). Let $Q(\mathbf{x}) = \mathbf{c}^T \mathbf{x} + g \mathbf{x}^T \mathbf{D} \mathbf{x} = \mathbf{x}^T \Delta \mathbf{x}$ be the quadratic function, with $\Delta = g(\mathbf{D} + \mathbf{D}^T)/2 + \text{diag}(\mathbf{c})$. The relaxation consists in considering the set of vectorized bistochastic matrices $\text{vec}[\mathcal{D}_{n,m,\varepsilon}]$ where

$$\begin{aligned} \mathcal{D}_{n,m,\varepsilon} = \{ & \mathbf{X} \in [0,1]^{(n+m) \times (m+n)} : \\ & \mathbf{X}\mathbf{1} = \mathbf{1}, \mathbf{X}^T\mathbf{1} = \mathbf{1} \\ & \forall i = 1, \dots, n, \forall j > m, j \neq m+i, x_{i,j} = 0 \\ & \forall j = 1, \dots, m, \forall i > n, i \neq n+j, x_{i,j} = 0 \} \end{aligned}$$

Given a cost matrix Δ and an initial continuous or discrete candidate solution \mathbf{x} , the procedure IPFP(Δ, \mathbf{x}) iterates the two following steps until convergence:

1. Minimize a linear approximation of Q around the current solution \mathbf{x} in the discrete domain by solving an LSAP:

$$\mathbf{b}^* \leftarrow \underset{\mathbf{b} \in \pi_{n,m,\varepsilon}}{\text{argmin}} (\mathbf{x}^T \Delta) \mathbf{b} \quad (4)$$

2. Perform the descent by minimizing Q along the segment $[\mathbf{x}, \mathbf{b}]$ in the continuous domain:

$$\alpha^* \leftarrow \underset{\alpha \in [0,1]}{\text{argmin}} Q(\mathbf{x} + \alpha(\mathbf{b}^* - \mathbf{x})) \quad (5)$$

$$\mathbf{x} \leftarrow \mathbf{x} + \alpha^*(\mathbf{b}^* - \mathbf{x}) \quad (6)$$

The iterative process stops when

$$\mathbf{x}^T \Delta (\mathbf{x} - \mathbf{b}^*) < \beta |Q(\mathbf{x}) + \mathbf{x}^T \Delta (\mathbf{b}^* - \mathbf{x})| \quad (7)$$

holds, for a given scalar $\beta \in (0, 1)$, or if a given number of iterations is reached. Generally, the algorithm converges to a local minimum \mathbf{x} of the relaxed quadratic problem, and independently \mathbf{x} can be continuous. So a final resolution of the LSAP given by Eq. 4 is performed, and the quadratic cost $Q(\mathbf{b}^*)$ is then returned as an approximate GED.

This is a special case of Frank-Wolfe algorithm. Step 1 finds a direction of descent according to the

first-order Taylor expansion of Q around \mathbf{x} , which is given by $Q(\mathbf{y}) \approx Q(\mathbf{x}) + (\mathbf{x}^\top \Delta)(\mathbf{y} - \mathbf{x})$. The minimization of Q around \mathbf{x} is thus approximatively equivalent to the minimization of $\mathbf{x}^\top \Delta \mathbf{y}$ with \mathbf{x} fixed. Since any LSAP and its relaxed version share the same solutions, a solution to the minimization of $\mathbf{x}^\top \Delta \mathbf{y}$ in the continuous domain is reduced to solve the LSAP defined by Eq. 4. So Step 1 can be computed in cubic time in worst-case, for instance with the Hungarian algorithm. Contrary to that, Step 2 can be solved analytically in linear time.

As discussed in the introduction, the quality of the estimation returned by IPFP depends strongly on the initialization. While a random or a flat initial vector can be used, a solution to the LSAP (Eq. 3) involved in the definition of the bipartite GED leads to a better estimation of the GED (Bougheux et al., 2017). Moreover, this estimation seems to be also slightly more accurate than other local search strategies (Riesen, 2015), as evaluated in the context of ICPR GDC 2016² (Abu-Aisheh et al., 2017). IPFP is thus a good candidate for multistart local search strategies.

3 MULTISTART IPFP FOR ESTIMATING THE GED

We consider the following procedure for estimating the GED with a multistart local search strategy:

1. Generate a set $S \subseteq \mathcal{D}_{n,m,\varepsilon}$ of assignments
2. Refine the estimation $Q(\mathbf{x}, \Delta)$ of each assignment $\mathbf{x} \in S$ by the same refinement method. This provides a sequence S^* of $|S|$ assignments $\mathbf{y}_\mathbf{x} \in \pi_{n,m,\varepsilon}$ such that $Q(\mathbf{y}_\mathbf{x}, \Delta) \leq Q(\mathbf{x}, \Delta)$ is the improved estimation obtained from \mathbf{x} . Note that several assignments of S can lead to the same refined assignment, and that different refined assignments of S^* can have the same quadratic cost.
3. Return the smallest refined estimation given by $\min_{\mathbf{y} \in S^*} Q(\mathbf{y}, \Delta)$ and the set $\arg\min_{\mathbf{y} \in S^*} Q(\mathbf{y}, \Delta)$ of refined assignments reaching this minimum.

Whereas the generation of the initial set of assignments is the main difficulty of this procedure (Step 1), the refinements in Step 2 are independent to each others, hence they can be computed in parallel. This is the main advantage of this simple strategy over hybrid search strategies, which are generally not easily nor highly parallelizable. Both sequential and parallel versions of the proposed procedure are analyzed in Sec. 4 with IPFP as a refinement procedure.

²Graph Distance Contest: gdc2016.greyc.fr

The resulting estimation of the GED is denoted by *multiple IPFP* (mIPFP), i.e.

$$\text{mIPFP}(\Delta, S) = \min_{\mathbf{x} \in S} \{Q(\mathbf{y}, \Delta) : \mathbf{y} = \text{IPFP}(\Delta, \mathbf{x})\} \quad (8)$$

where S is the set of initial assignments computed in Step 1. We consider three types of initial sets:

- a. assignments solving the LSAP involved in the bipartite GED (Eq. 3), or
- b. assignments approximating this LSAP (selected by a greedy algorithm), or
- c. random assignments, or
- d. random bistochastic matrices.

Given an integer $k \geq 1$, each generator returns a set $S_k \subseteq \mathcal{D}_{n,m,\varepsilon}$ composed of at most k assignments. In addition, in order to study the impact of each type of set on the estimation of the GED, two calls of a same generator with parameters k and l provide two sets S_k and S_l such that:

$$k < l \Rightarrow S_k \subseteq S_l \quad (9)$$

In such a case, for all $k \geq 1$, mIPFP satisfies:

$$\text{mIPFP}(\Delta, S_k) \geq \text{mIPFP}(\Delta, S_{k+1}) \geq \text{mIPFP}(\Delta, S_{k_{\max}})$$

where k_{\max} denotes the maximum number of assignments that can be computed with the generator. Hence k controls the ratio between computational time and closeness to $\text{mIPFP}(\Delta, S_{k_{\max}})$.

Minimal-cost assignments and multiple bipartite GED This generator computes a set S_k by enumerating at most k solutions to the LSAP involved in the definition of the bipartite GED (Eq. 3):

$$S_k(\tilde{\mathbf{c}}) \subseteq \arg\min_{\mathbf{x} \in \pi_{n,m,\varepsilon}} \tilde{\mathbf{c}}^\top \mathbf{x} \quad (10)$$

where the vector $\tilde{\mathbf{c}}$ encodes the transformed costs between nodes. Remark that from the set $S_k(\tilde{\mathbf{c}})$, a *multiple bipartite GED* (mbGED) is directly defined by:

$$\text{mbGED}(\Delta, S_k(\tilde{\mathbf{c}})) = \min_{\mathbf{x} \in S_k(\tilde{\mathbf{c}})} Q(\mathbf{x}, \Delta) \quad (11)$$

Since the generator fulfills the inclusion condition given by Eq. 9, mbGED satisfies:

$$\text{mbGED}(\Delta, S_k(\tilde{\mathbf{c}})) \geq \text{mbGED}(\Delta, S_{k+1}(\tilde{\mathbf{c}})), \quad \forall k \geq 1.$$

Moreover, the bipartite GED, $\text{bGED}(\Delta, \tilde{\mathbf{c}})$ defined in Section 1 may be interpreted as $\text{mbGED}(\Delta, S_1(\tilde{\mathbf{c}}))$. We have hence $\text{mbGED}(\Delta, S_k(\tilde{\mathbf{c}})) \leq \text{bGED}(\Delta, \tilde{\mathbf{c}})$, for all $k \geq 1$. This multiple bipartite GED have also been tested in our experimental evaluation. Note that by definition we have $\text{mIPFP}(\Delta, S_k(\tilde{\mathbf{c}})) \leq \text{mbGED}(\Delta, S_k(\tilde{\mathbf{c}}))$.

Enumerating k solutions to an LSAP instance is equivalent to enumerating k perfect matchings in a bipartite graph, which can be performed in polynomial-time complexity by several algorithms. Indeed, consider the LSAP defined by $\arg\min_{\mathbf{x}} \mathbf{c}^\top \mathbf{x}$. Let \mathbf{x}^* be a solution to this problem, and let (\mathbf{u}, \mathbf{v}) be the corresponding pair of solutions to its dual problem, known as the *labeling problem*. The real vectors \mathbf{u} and \mathbf{v} associate a real number to each node of the first graph and the second graph, respectively, such that $c_{ij} \leq u_i + v_j$ for all (i, j) and $\mathbf{c}^\top \mathbf{x}^* = \mathbf{1}^\top \mathbf{u} + \mathbf{1}^\top \mathbf{v}$. Then the bipartite graph composed of the edges $c_{ij} = u_i + v_j$ contains all the solutions to the LSAP. It defines the *equivalence graph* of the primal-dual problem. Both primal and dual solutions can be computed by the Hungarian algorithm (Burkard et al., 2009). So a global procedure to generate k solutions to the LSAP is given by:

1. Compute a pair $(\mathbf{x}^*, (\mathbf{u}, \mathbf{v}))$ of solutions to the LSAP and its dual problem by the Hungarian algorithm.
2. Construct the equivalence graph from \mathbf{u} , \mathbf{v} and \mathbf{c} .
3. Enumerate at most k assignments in the equivalence graph to produce the set S_k .

To enumerate the k assignments, we have chosen the recursive algorithm proposed in (Uno, 1997). It is deterministic and it fulfills the inclusion condition given by Eq. 9. It provides k solutions in $O(kN)$ time complexity for a bipartite graph with N nodes. Note that for enumerating assignments in $\pi_{n,m,\varepsilon}$ and for favoring large differences between assignments in the resulting set S_k , the algorithm needs to be slightly modified. These modifications do not change its functioning nor its complexity. They will be detailed in a future paper.

Low-cost assignments The second generator enumerates at most k assignments by a greedy algorithm that tries to approximate the solution to the LSAP defined by Eq. 10. Given the cost matrix $\tilde{\mathbf{c}}$, it is given by the following procedure:

1. Sort all the costs \tilde{c}_{ij} in ascending order. This provides a sorted vector \mathbf{s} .
2. Add an assignment $\mathbf{x} \in \pi_{n,m,\varepsilon}$ to S_k by assigning the nodes in the order determined by \mathbf{s} while maintaining assignment constraints. Let \tilde{c}_{\max} be the cost associated to the last pair of assigned elements.
3. Construct a bipartite graph, similar to the equivalence graph presented in the previous paragraph, so that (i, j) is an edge if $\tilde{c}_{i,j} \leq \tilde{c}_{\max}$.

4. Enumerate at most k low-cost assignments in the bipartite graph computed in the previous step to produce the set S_k , as before with (Uno, 1997).

Step 1 and Step 2 correspond to a constructive strategy proposed in (Riesen et al., 2015) for computing the greedy bipartite GED. Note that contrary to this method, we use the classical *counting sort* algorithm for integers costs. Given integer costs in $\{0, \dots, p\}$, it sorts all the costs in $\tilde{\mathbf{c}}$ in $O(2E)$ time complexity, where E is the size of $\tilde{\mathbf{c}}$. Due to the greedy strategy, the bipartite graph computed in Step 3 necessarily includes the equivalence graph associated to the LSAP. So Step 4 is able to enumerate more and different assignments than the previous generator.

Random assignments The third generator computes a set S_k of k assignments in $\pi_{n,m,\varepsilon}$; randomly generated (uniform distribution). We will see in the following section that such sets can lead to interesting estimations of the GED compared to those obtained with the two previous generators.

Random Bistochastic matrices Similarly, we generate random matrices in $\mathcal{D}_{n,m,\varepsilon}$ according to the method prescribed in (Cappellini et al., 2009). First it constructs a random stochastic matrix so that values in each column are i.i.d. and stochastic. This matrix is then refined by Sinkhorn-Knopp algorithm (Sinkhorn and Knopp, 1967; Knight, 2008) to produce a bistochastic matrix. Its vectorization is retained as a element of S_k .

4 EXPERIMENTS

In this section, we evaluate the proposed methods through several experiments, in order to quantify the benefit that can be achieved by taking into account several optimal and suboptimal assignments. The C++ source code we used is available online³.

GED estimators. We tested in our experiments a set of bipartite approximation methods and a set of quadratic ones. Concerning the bipartite approaches, we compare two versions of bGED (Riesen and Bunke, 2009), (Gaüzère et al., 2014) differentiated by the choice of the bipartite cost matrix computation method. The procedure of (Riesen and Bunke, 2009) aims at taking into account the local neighborhood of graph nodes in the construction of the cost matrix,

³<https://github.com/bgauzere/graph-lib>

Table 1: Maximum, minimum, mean and standard deviation of the number K of optimal solutions reached by Uno’s Algorithm. The procedure has been stopped at 10,000 optimal bipartite mappings at the most, implying that these results are not representative of the whole set of optimal bipartite solutions, which is even bigger. The bipartite cost matrix computation schemes are (Riesen and Bunke, 2009) and (Gaüzère et al., 2014).

| Dataset | (Riesen and Bunke, 2009) | | | | (Gaüzère et al., 2014) | | | |
|---------|--------------------------|-----------|-----------|-------------|------------------------|-----------|-----------|-------------|
| | $\max(K)$ | $\min(K)$ | \bar{K} | $\sigma(K)$ | $\max(K)$ | $\min(K)$ | \bar{K} | $\sigma(K)$ |
| Alkane | 10000 | 1 | 6198 | 3847 | 10000 | 1 | 993 | 1977 |
| Acyclic | 10000 | 1 | 2313 | 3496 | 10000 | 1 | 182 | 857 |
| MAO | 10000 | 48 | 7695 | 3711 | 10000 | 1 | 948 | 2714 |
| PAH | 10000 | 10000 | 10000 | 0 | 10000 | 128 | 9894 | 879 |
| CMU | 16 | 1 | 1.6 | 1.5 | - | | | |

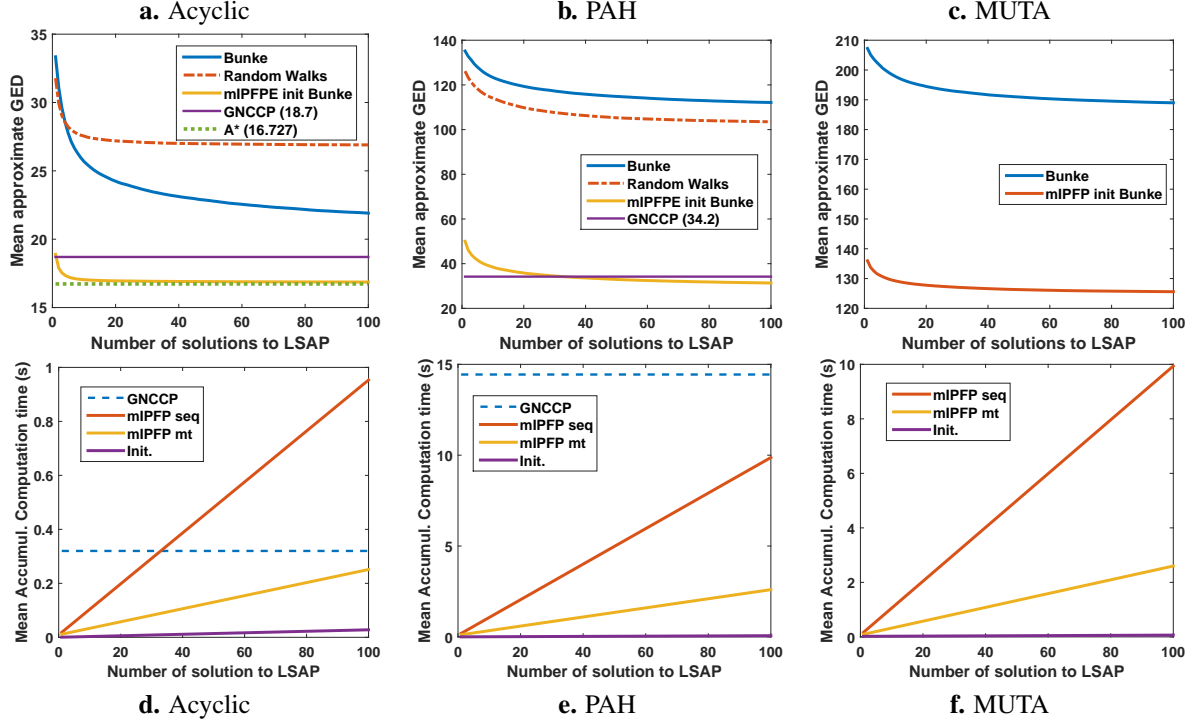


Figure 1: Approximate GED (a., b. and c.) and computation times of IPFP against GNCCP (d., e. and f.) sequential (seq) and multi-threaded (mt) implementations, in accordance with the number of initial mappings. The exact GED (A^*) is known for Acyclic, and GNCCP could not be applied on MUTA because of its high time complexity.

with costs which correspond to the matchings of local stars. In contrast, the bipartite cost matrix given by (Gaüzère et al., 2014) represents costs of matching local random walks. These two versions are extended with mbGED by enumerating optimal bipartite assignments as described in section 3. We consider also random assignments *i.e.* random permutations, generated following a uniform distribution by the use of the `std::random_shuffle` procedure of the C++ standard library, as well as low-cost, sub-optimal, bipartite assignments which approximate the ones of (Riesen and Bunke, 2009), obtained via a greedy algorithm. These bipartite methods correspond to the three kinds of initialization described in section 3 and their results are given in the first part of Table 2.

The quadratic approaches (second part of this table) present a set of versions of IPFP and their extended mIPFP versions along with a convex-concave procedure, GNCCP (Liu and Qiao, 2014), described for GED estimation in (Bougleux et al., 2017) since it uses a global search strategy which iterates instances of IPFP algorithm. We complete this set of experiments with the method of (Neuhaus and Bunke, 2007) which aims at resolving a relaxed version of the quadratic assignment problem with classical optimization tools.

The IPFP versions differ by their initializations or sets of initial mappings. These sets are those described in section 3. In addition, we also consider the continuous initial vector \mathbf{j} of same structure as matrix

Table 2: Mean approximate graph edit distance (d), error (e) and computation time in seconds (t), with a number of initial assignments $k = 40$ on GREYC’s chemistry datasets. Nomenclature : bipartite estimation (bGED), IPFP quadratic estimation (IPFP), m stands for *multiple version*, and r stands for *recentered version*

| Algorithm | Alkane | | | Acyclic | | | MAO | | PAH | | |
|--|---|---|-------------|-------------------|--------------|-------------------------------|-------------------|--------------|-------------------|--------------|-------------------|
| | d | e | t | d | e | t | d | t | d | t | |
| A* | 15.3 | | | 16.7 | | | | | | | |
| Bipartite | bGED Rie. and Bun. (2009) | 37.8 | 22.5 | $\approx 10^{-4}$ | 33.3 | 16.6 | $\approx 10^{-4}$ | 95.7 | 10^{-3} | 135.2 | 10^{-3} |
| | bGED Gai. et al (2014) | 36.0 | 20.7 | 0.02 | 31.8 | 15.0 | 0.02 | 85.1 | 1.48 | 125.8 | 2.60 |
| | mbGED Rie. and Bun. (2009) | 25.5 | 10.2 | 0.01 | 23.1 | 6.4 | 0.01 | 75.1 | 0.05 | 116.0 | 0.02 |
| | mbGED Gai. et al (2014) | 26.0 | 10.6 | 0.03 | 27.0 | 10.3 | 0.02 | 76.0 | 1.50 | 105.8 | 2.65 |
| | mbGED Random | 60.2 | 44.9 | $\approx 10^{-4}$ | 52.6 | 35.8 | $\approx 10^{-4}$ | 164.3 | $\approx 10^{-4}$ | 194.1 | $\approx 10^{-4}$ |
| | mbGED Greedy | 39.0 | 23.6 | $\approx 10^{-4}$ | 38.1 | 20.7 | $\approx 10^{-4}$ | 99.6 | $< 10^{-3}$ | 135.7 | $< 10^{-3}$ |
| Frank-Wolfe | IPFP _{Flat} uniform init. | 18.6 | 3.2 | 0.02 | 20.0 | 3.3 | 0.01 | 45.8 | 0.1 | 50.7 | 0.25 |
| | IPFP _{Init.} Rie. and Bun. (2009) | 18.1 | 2.7 | 0.02 | 18.9 | 2.1 | 0.009 | 38.4 | 0.04 | 50.0 | 0.09 |
| | IPFP _{Init.} Gai. et al (2014) | 18.0 | 2.7 | 0.04 | 18.7 | 2.1 | 0.02 | 38.7 | 1.53 | 46.8 | 2.68 |
| | IPFP _{Random} init. | 19.9 | 4.6 | 0.02 | 22.2 | 5.4 | 0.01 | 56.3 | 0.07 | 53.2 | 0.10 |
| | IPFP _{Random} bistoch. init. | 19.3 | 3.9 | 0.03 | 19.8 | 3.1 | 0.04 | 51.9 | 0.32 | 51.8 | 0.48 |
| | IPFP _{Greedy} init. | 18.1 | 2.8 | 0.02 | 18.8 | 2.1 | 0.01 | 38.8 | 0.02 | 50.3 | 0.03 |
| | mIPFP _{Init.} Rie. and Bun. (2009) | 15.4 | 0.07 | 0.20 | 16.9 | 0.2 | 0.10 | 31.4 | 0.48 | 33.6 | 1.10 |
| | mIPFP _{Init.} Gai. et al (2014) | 15.6 | 0.20 | 0.18 | 17.4 | 0.7 | 0.08 | 33.4 | 1.75 | 30.5 | 3.58 |
| | mIPFP _{Random} init. | 15.3 | 0.01 | 0.22 | 16.74 | < 0.01 | 0.13 | 33.3 | 0.81 | 36.6 | 1.17 |
| | mIPFP _{Random} bistoch. init. | 15.3 | 0.01 | 0.20 | 16.73 | < 0.01 | 0.13 | 31.6 | 1.60 | 34.8 | 2.94 |
| | mIPFP _{Greedy} init. | 15.4 | 0.06 | 0.17 | 16.8 | 0.03 | 0.11 | 31.8 | 0.46 | 35.4 | 1.01 |
| | Frank-Wolfe recentered | rIPFP _{Init.} Rie. and Bun. (2009) | 17.9 | 2.5 | 0.03 | 18.7 | 2.0 | 0.03 | 38.5 | 0.14 | 48.3 |
| rIPFP _{Init.} Gai. et al (2014) | | 17.7 | 2.4 | 0.07 | 18.7 | 2.0 | 0.05 | 35.8 | 1.63 | 45.3 | 2.73 |
| rIPFP _{Random} init. | | 18.2 | 2.9 | 0.04 | 19.1 | 2.4 | 0.03 | 45.9 | 0.15 | 50.6 | 0.19 |
| rIPFP _{Random} bistoch. init. | | 18.2 | 2.9 | 0.03 | 19.0 | 2.3 | 0.03 | 45.0 | 0.15 | 50.7 | 0.19 |
| rIPFP _{Greedy} init. | | 17.8 | 2.5 | 0.04 | 18.6 | 1.9 | 0.03 | 38.7 | 0.14 | 48.0 | 0.18 |
| rmIPFP _{Init.} Rie. and Bun. (2009) | | 15.4 | 0.12 | 0.09 | 16.8 | 0.1 | 0.07 | 31.37 | 0.40 | 31.5 | 0.70 |
| rmIPFP _{Init.} Gai. et al (2014) | | 15.5 | 0.21 | 0.15 | 17.2 | 0.4 | 0.09 | 32.40 | 1.75 | 29.8 | 2.96 |
| rmIPFP _{Random} init. | | 15.3 | 0.03 | 0.10 | 16.74 | 0.02 | 0.07 | 31.40 | 0.48 | 32.8 | 0.75 |
| rmIPFP _{Random} bistoch. init. | | 15.3 | 0.04 | 0.10 | 16.75 | 0.03 | 0.07 | 31.42 | 0.44 | 32.8 | 0.74 |
| rmIPFP _{Greedy} init. | | 15.4 | 0.08 | 0.10 | 16.75 | 0.03 | 0.08 | 31.39 | 0.48 | 32.4 | 0.75 |
| GNCCP | | 16.6 | 1.2 | 0.58 | 18.7 | 1.3 | 0.32 | 34.3 | 9.23 | 34.2 | 14.44 |
| Neuhaus and Bunke (2007) | 20.5 | - | 0.07 | 25.7 | - | 0.04 | 59.1 | 7.0 | 52.9 | 8.2 | |

ces in $\mathcal{D}_{n,m,\varepsilon}$, so that each coefficient unconstrained to be null is defined by:

$$j_{k,l} = \frac{2}{n+m+2} \quad (12)$$

Flat initial vectors are used as an initialization of the Frank-Wolfe algorithm in several works to begin with a centered candidate solution. In Table 2, IPFP_{INIT} refers to the IPFP method (section 2) initialized with a discrete or continuous solution $\mathbf{x} \in S^{\text{INIT}} = S_{k=1}^{\text{INIT}}$, where S_k^{INIT} is a set of k solutions corresponding to INIT. mIPFP then refers to mIPFP($\Delta, S_k^{\text{INIT}}$), the multistart version of IPFP that is, IPFP_{INIT} stands for mIPFP($\Delta, S_1^{\text{INIT}}$). Finally, we consider initializations re-centered in the continuous space from an initial $\mathbf{x}_0 \in S_k^{\text{INIT}}$:

$$\mathbf{x} = \frac{1}{2}(\mathbf{x}_0 + \mathbf{j}) \quad (13)$$

These re-centered versions are denoted by rIPFP and rmIPFP in Table 2. The sequential and parallel versions of mIPFP are both implemented, but the times

given in the tables refer to the multi-threaded variant with at most 4 threads.

Datasets. We performed our experiments on 5 chemoinformatics datasets⁴ and a geometric one. The chemistry data are symbolic graphs representing molecules. Nodes correspond to atoms and edges are valence bounds. There are four different types of graphs : acyclic unlabeled (Alkane), acyclic labeled (Acyclic), unlabeled (PAH) and labeled (MAO). The fifth chemistry dataset MUTA (Riesen and Bunke, 2008), is originally separated into seven subsets by molecule size, from 10 to 70 atoms. In our experiments, we randomly selected a subset of 100 graphs over all the molecule sizes in MUTA, to let insertions and deletions play an appreciable role, which is not the case when the graph size is fixed

⁴Available at <https://iapr-tc15.greyc.fr/links.html>

Table 3: Mean approximate graph edit distance (d), error (e) and computation time (t), with a number of initial assignments $k = 40$. Datasets MUTA and CMU.

| Algorithm | MUTA | | CMU $k = 16$ | |
|----------------------------------|------------|-------------|--------------|-------------|
| | d | t | d | t |
| bGED R. and B. | 209 | 0.02 | 1810 | 0.01 |
| mbGED R. and B. | 196 | 0.9 | 1791 | 0.10 |
| mbGED Random | 276 | $< 10^{-3}$ | $> 10^6$ | $< 10^{-3}$ |
| mbGED Greedy | 210 | 0.005 | 4418 | 0.02 |
| IPFP _{Init.} R. and B. | 136 | 0.07 | 410 | 0.07 |
| IPFP _{Random init.} | 142 | 0.1 | 6532 | 0.90 |
| IPFP _{Init.} Greedy | 136 | 0.09 | 414 | 0.02 |
| mIPFP _{Init.} R. and B. | 127 | 3.25 | 410 | 1.35 |
| mIPFP _{Random init.} | 128 | 5.20 | 472 | 13.64 |
| mIPFP _{Init.} Greedy | 133 | 3.58 | 415 | 0.7 |
| GNCCP | - | - | 408 | 6.66 |

The Geometric graphs of CMU (Riesen and Bunke, 2008) represent 30 points of interest manually picked up over a series of images depicting a toy house captured from different viewpoints. Nodes are labeled according to the coordinates of the points (precision of 10^{-6}) and edge labels are the euclidean distance between them. Note that the GED-estimation method of (Gaüzère et al., 2016) needs the data to be integer typed, hence it could not be applied to the CMU datasets in our experiments. The graph pairs we tested on this dataset are the same as in (Abu-Aisheh et al., 2015).

Analysis. Table 1 presents statistical information about the number of optimal solutions of the LSAP reached by Uno’s algorithm for each dataset. In order to keep a reasonable computation time, we bounded the algorithm by $K_{max} = 10^4$ mappings. One can see that the number of these optimal assignments can be huge for symbolic graphs. These graphs, and in particular unlabeled graphs, lead indeed to relatively flat linear cost matrices. The corresponding LSAP have then a large number of optima. In contrast, the geometric dataset CMU presents not much optimal solutions with at most 16 ones, and generally 1 to 2 optimal assignments per graph pair. These results shows that on symbolic graphs, the strategy of taking an arbitrary optimal bipartite solution to approximate the GED can legitimately be questioned, as there can be thousands of them.

Among the one-shot approaches, the bipartite approximation (Riesen and Bunke, 2009) gives estimations which are far higher than the quadratic approaches (IPFP, GNCCP and Neuhaus and Bunke). The gap deepens when the graph’s size increases, but even small graphs of Alkane and Acyclic give error rates 6 to 7 times higher than the refined assignments.

The extended version mbGED allows the estimation to decrease rapidly depending on the number of considered optimal assignments (see figure 1 **a. b. c.**). We made this observation over all the considered datasets, especially for symbolic labeled data. We can deduce that there are indeed better optimal bipartite assignments than the arbitrary ones, and moreover, the gain in term of precision considering them is significant, up to halve the error on some datasets as shown in table 2. This highlights that in the context of bipartite approximation, it is needed to search not only for an optimal assignment, but also a relevant one to estimate the GED. However, even considering 100 assignments, the bipartite estimations are still above the quadratic ones.

While the Random-Walk based method to design the bipartite cost matrix (Gaüzère et al., 2014) tends to give better approximations with $k = 1$, it stabilizes quicker when considering several assignments on small sized graphs. Our interpretation of this is that the downsized set of optimal solutions available leads to less good ones in the context of GED estimation, thus a faster convergence. More, the length of the walks, here set to 3, is large in comparison to the diameter of the small graphs, so they don’t allow to represent well the neighborhoods, hence this method is more relevant on larger graphs. Notice that the high computation time required here comes from the determination of the cost matrix, and not from the computation of the $k - 1$ remaining optimal mappings.

Compared to LSAP approaches, IPFP improves dramatically the accuracy of GED estimations. However, as stated in subsection 2, this algorithm needs to be initialized, and the initialization choice impacts a lot on the obtained approximation. This is illustrated in tables 2 and 3. Apart from the random initializations, all discrete initial vectors we tested lead to better estimations than the trivial flat uniform continuous vector \mathbf{j} . Indeed, initial vectors which are close to low local minima of the quadratic function $Q(\mathbf{x}, \Delta)$ will lead to lower results in a smaller number of iterations. In term of time complexity, IPFP will need more iterations to converge from an initial value farther from a local minimum, as we can remark in the case of random initializations. This behavior deepens with the multistart version mIPFP, as it is about iterating several times this algorithm.

GNCCP estimation is more precise than single-start IPFP on all tested datasets, as each iteration gives a better initialization to the next. An advantage of this method is that it does not need an initial guess, because the first iteration resolves a fully convex problem. However, the amount of time needed to reach the global minimum during this first iteration could be re-

duced with a relevant initial assignment. Moreover, if the first IPFP call needs too much time to converge, it can be stopped in the implementation by reaching the maximum number of iterations, thus leading to a less relevant initialization to the next IPFP call and so on. Yet, an initialization step for GNCCP is not part of this paper and could be studied in a future work.

Such as IPFP, mIPFP is strongly impacted by its initialization set, especially in term of computation time. Considering the approximation, mIPFP is the more accurate method on all the tested datasets, CMU excepted. Still, there is no initialization method that beats the others on all the datasets. Good results have been obtained via random initial assignments, which can seem surprising while each IPFP may converge to a far-from-optimal local minimum. But considering the fact that initial assignments should lie far from each others in order to get different estimation of the GED (*i.e.* generate few collisions through the IPFP process), randomly generated initial guesses may satisfy this condition. Nevertheless, each randomly initialized IPFP needs generally more time to converge, since an initial assignment has a relatively low probability to be close to a local minimum.

mIPFP beats GNCCP over all the symbolic datasets, with several kind of initializations. We believe that this result is related to the fact that one iteration of GNCCP needs more IPFP iterations to converge, and as many more as the treated problem is convex or concave. We noticed that the total number of IPFP iteration through the GNCCP procedure is frequently far higher to the total number of IPFP iterations in the sequential mIPFP process (with $k = 40$). As the number of iterations is bounded, a GNCCP iteration may not terminate on a close-to-optimal value, in particular in the convex situation, and this has an impact on the forthcoming iterations thus restraining the convergence of GNCCP. Moreover, a higher number of IPFP iterations for GNCCP leads to a higher computation time.

Finally, the re-centering procedure enhances a little the refined solutions, in particular concerning large graphs. The gain achieved with respect to the graph size begins to be significant with the dataset PAH. We also noticed a reduction of the needed time with these graphs, and these results should be subjected to further experiments on larger graphs.

5 CONCLUSIONS AND FUTURE WORK

In this paper, we propose to refine bipartite GED with multiple-initialized IPFP. We show that this simple

idea constitutes an alternative to more sophisticated procedures like GNCCP, with the advantage to be easily parallelized. We study the impact of initialization on this method through three kinds of assignments : randomly generated, low-cost, and optimal bipartite assignments. We show that our results with these strategies are relatively close to each other, and compete with state-of-the-art methods for estimating the GED with a lower computation time.

In future work, we plan to seek how to get more relevant sets of initializations to mIPFP, considering a distance between assignments or by guiding their enumeration by the quadratic costs. Another axis of consideration is to study a possible way of initializing GNCCP to get more precise estimations, in a better time complexity.

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