Fast Inexact Graph Matching with Applications in Statistical Connectomics

Joshua T. Vogelstein, John M. Conroy, Louis J. Podrazik, Steven G. Kratzer, Donniell E. Fishkind, R. Jacob Vogelstein, and Carey E. Priebe

Abstract—It is becoming increasingly popular to represent myriad and diverse data sets as graphs. When the labels of vertices of these graphs are unavailable, graph matching (GM)—the process of determining which permutation assigns vertices of one graph to those of another, maintaining the adjacency structure—is a computationally daunting problem. This work presents an inexact strategy for GM. Specifically, we frame QM as a quadratic assignment problem (QAP), and then relax the feasible region to its convex hull. Our relaxed optimization function (rQAP) has the same solution as the original problem, but has the advantage of being continuously differentiable. We apply a well known and efficient nonlinear programming algorithm, Frank-Wolfe, to solve rQAP. Though this relaxation is quadratic, the optimization function is not necessarily convex. We therefore consider a number of initializations based on the geometry of the convex hull. Multiple restarts of this algorithm lead to performance that exceeds the previous state-of-the-art in *all* of 16 benchmark tests. Moreover, this approach is fast, scaling cubically with the number of vertices, requiring only about a minute on standard modern laptops for graphs with up to a few hundred vertices. We illustrate this approach via a brain-graph ("connectome") application in which vertices represent neurons in a small nematode brain (the *Caenorhabditis elegans* worm), and edges represent either chemical or electrical synapses. For every permutation of the chemical connectome and several permutations of the electrical connectome, this approach found the optimal solution. Although this strategy already natively operates on unweighted and weighted graphs, either directed or undirected, we propose a number of possible extensions, and make all code available.

Index Terms—statistical inference, graph theory, network theory, structural pattern recognition, connectome.

1 Introduction

A graph matching (GM) algorithm is any algorithm whose goal is to "align" any pair of graphs such that each vertex in one graph can be "assigned" to its corresponding vertex in the other graph. Perhaps due to its complex computational properties (it is $\mathcal{NP}$-hard [1]), GM has received widespread attention in both the mathematical graph theory and computer science communities [2]. Moreover, the potential span of applications of graph matching algorithms is vast, ranging from neural coding [3] to machine vision [4].

Our motivation for this work includes the bourgeoning field called "connectomics": the study of brain-graphs. In brain-graphs, vertices represent (collections of) neurons and edges represent either functional dependencies or structural connections [5]. In some scenarios, vertices are labeled. For example, when vertices represent single neurons in invertebrates [6] or macro-anatomical gyral regions in vertebrates [7], [8]. However, in other scenarios, even whether vertices can be labeled is questionable. For example, if one desired to compare brain-(sub)graphs from parts of brains across species or within vertebrate organisms, there is no known vertex assignment. In these scenarios GM might be an important element of any statistical analysis of these brain-graphs [9], [10].

We therefore propose a novel inexact graph matching algorithm based on the quadratic assignment problem (QAP). The intuition is relatively simple: GM is computationally difficult because the underlying feasible region is non-differentiable and the implied objective function is multimodal. A common approach to approximating difficult nonlinear programming problems is to relax the constraints on the feasible region. By relaxing the non-differentiable constraint, any gradient based algorithm may be applied to the problem [11]. Importantly, our relaxed version of the optimization problem (rQAP) yields an identical solution to the original QAP problem whenever the two graphs are simple and isomorphic. Unfortunately, the multimodality of the solution space implies that the initialization will, in general, be important. Multiple "principled" restarts can potentially facilitate an efficient stochastic search strategy.

This manuscript describes an algorithm that approximately solves a relaxed version of graph matching in cubic time (with very small leading constants). Via numerical experiments, we demonstrate that this approach outperforms several state-of-the-art algorithms on all tests in a standard benchmark library [12], indicating both its efficiency and its effectivity. We then test this approach on a brain-graph matching problem: matching the brain-graph (connectome) of a small nematode with

- *J.T. Vogelstein, D.E. Fishkind, and C.E. Priebe are with the Department of Applied Mathematics and Statistics, Johns Hopkins University, Baltimore, MD 21218. E-mail: {joshuav,def,cep}@jhu.edu, {conroyjohnm,ljpodra,sgkratz}@gmail.com, jacob.vogelstein@jhuapl.edu*
- *J.M. Conroy, L.J. Podrazik and S.G. Kratzer are with Institute for Defense Analyses, Center for Computing Sciences, Bowie, MD 20708.*
- *R.J. Vogelstein is with the Johns Hopkins University Applied Physics Laboratory, Laurel, MD, 20723.*

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302 vertices with a permuted version of itself. We are able to find the optimal solution after 3 restarts for each randomly permuted example of its chemical connectome, and typically < 30 restarts for each randomly permuted example of its electrical connectome. We are therefore optimistic that this algorithm will be useful for the massive graphs ($\mathcal{O}(10^5)$ vertices) promised to arise due to various ongoing connectome projects [13], [14].

2 Graph Matching

A labeled graph $G = (\mathcal{V}, \mathcal{E})$ consists of a vertex set s $\mathcal{V}$, where $|\mathcal{V}| = n$ is number of vertices and an edge set $\mathcal{E}$, where $|\mathcal{E}| \leq n^2$. Note that we are not restricting our formulation to be directed or exclude self-loops. Given a pair of graphs, $G_1 = (\mathcal{V}_1, \mathcal{E}_1)$ and $G_2 = (\mathcal{V}_1, \mathcal{E}_1)$, where $|\mathcal{V}_1| = |\mathcal{V}_2| = n$, let $\pi : \mathcal{V}_1 \to \mathcal{V}_2$ be a permutation function (bijection), and consider the following two closely related problems:

- **Graph Isomorphism (GI):** Does there exist a $\pi \in \Pi$ such that $(u, v) \in \mathcal{E}_1$ if and only if $(\pi(u), \pi(v)) \in \mathcal{E}_2$.
- **Graph Matching (GM):** Which π (if any) satisfies the above isomorphism criterion?

Both GI and GM are computationally difficult. GM is clearly harder than GI, since solving GM also solves GI, but not vice versa. It is not known whether GI is in complexity class $\mathcal{P}$ [15]. In fact, GI is one of the few problems for which, if $\mathcal{P} \neq \mathcal{NP}$, then GI might reside in an intermediate complexity class called $\mathcal{GI}$-complete. GM, however, is known to be in $\mathcal{NP}$-complete. Yet, for large classes of GI and GM problems, linear or polynomial time algorithms are available [16]. Moreover, at worst, it is clear that GI is only "moderately exponential," for example, $\mathcal{O}(\exp\{n^{1/2+o(1)}\})$ [17]. Unfortunately, even when linear or polynomial time GI or GM algorithms are available for special cases of graphs, the constants are typically unbearably large. For example, if all graphs have degree less than k, there is a linear time algorithm for GI. However, the hidden constant in this algorithm is $512k^3$! [18].

Because we are interested in solving GM for graphs with $\mathcal{O}(10^6)$ or more vertices, exact GM solutions will be computationally intractable. As such, we develop a fast inexact graph matching algorithm. Our approach is based on formulating GM as a quadratic assignment problem. Below, we introduce assignment problems, and reiterate their close relationship to GI and GM [19].

3 Assignment Problems

Both GI and GM can be cast as assignment problems. Let $A = (a_{uv})$ and $B = (b_{uv})$ correspond to the adjacency matrix representations of graphs G_1 and G_2, respectively. That is, $a_{uv} = 1$ if and only if $(u, v) \in \mathcal{E}_1$, and zero otherwise (and similarly for B and G_2). Now, GI may be stated thusly: does there exist a $\pi \in \Pi$ such that $a_{uv} = b_{\pi(u)\pi(v)}$ for all $u, v \in [n] = \{1, \ldots, n\}$. Although assignment problems do not restrict A and B to correspond to adjacency matrices, when A and B are adjacency matrices, GM and the quadratic assignment problem (QAP) are equivalent. Our approach is based on a continuous relaxation and quadratic optimization approach, as will be described below. Because a linear assignment problem (LAP) will be a subroutine of our approach, we introduce LAP first, followed by QAP. In both cases, we will consider a matrix, $P = (p_{uv}) \in \mathcal{P}$, which is a permutation matrix if and only if it satisfies the following three constraints:

1) $P\mathbf{1} = \mathbf{1}$,
2) $P^\mathsf{T}\mathbf{1} = \mathbf{1}$,
3) $P \in \{0, 1\}^{n \times n}$.

Note that while the first two constraints are linear, the third constraint is *binary*, and decidedly *nonlinear*. This nonlinearity motivates our approach.

3.1 Linear Assignment Problems

The standard way of writing LAP is

$$\text{(LAP)} \quad \underset{\pi}{\text{minimize}} \sum_{u,v \in [n]} a_{u\pi(v)} b_{uv} \tag{1a}$$

$$\text{subject to } \pi \in \Pi, \tag{1b}$$

which can be written equivalently in a number of ways using the notion of permutation matrix introduced above:

$$\underset{P \in \mathcal{P}}{\operatorname{argmin}} \|PA - B\|_F = \tag{2a}$$

$$\underset{P \in \mathcal{P}}{\operatorname{argmin}} \, tr(PA - B)^\mathsf{T}(PA - B) = \tag{2b}$$

$$\underset{P \in \mathcal{P}}{\operatorname{argmin}} -tr(PAB^\mathsf{T}) = \tag{2c}$$

$$\underset{P \in \mathcal{P}}{\operatorname{argmin}} - \sum_{u,v \in [n]} p_{uv} a_{uv} b_{vu} = \tag{2d}$$

$$\underset{P \in \mathcal{P}}{\operatorname{argmin}} -\langle P, AB^\mathsf{T} \rangle. \tag{2e}$$

While the objective function and the first two constraints of LAP are linear, the binary constraints make solving this problem computationally tricky. Nonetheless, in the last several decades, there has been much progress in accelerating algorithms for solving LAPs, starting with exponential time, all the way down to $\mathcal{O}(n^3)$ for general LAPs, and even faster for certain special cases (e.g., sparse matrices) [19].

Consider a continuous relaxation of LAP. Specifically, let $\mathcal{D}$ be the set of doubly stochastic matrices, that is, a matrix P is doubly stochastic if and only if P satisfies the following three constraints:

1) $P\mathbf{1} = \mathbf{1}$,
2) $P^\mathsf{T}\mathbf{1} = \mathbf{1}$,
3) $P \in \mathbb{R}_+^{n \times n}$,

where the third constraint relaxes the binary constraints of the permutation matrices with a non-negativity constraint. Given this relaxation, we can state a relaxed LAP

problem:

$$\text{(rLAP)} \quad \underset{P}{\text{minimize}} \quad \sum_{u\in\mathcal{V}} -p_{uv}a_{uv}b_{vu} \tag{3a}$$

$$\text{subject to} \quad P \in \mathcal{D}. \tag{3b}$$

As it turns out, solving rLAP is equivalent to solving LAP.

Proposition 1. *LAP and rLAP are equivalent, meaning that the argument that minimizes one also minimizes the other.*

Proof: Let P' be a solution to LAP and let $P = \sum_{i\in[k]} \alpha_i P^{(i)}$ be a solution to rLAP for some positive integer k, permutation matrices $\{P^{(i)}\}_{i\in[k]}$, and positive real numbers $\{\alpha_i\}_{i\in[k]}$ such that $\sum_{i\in[k]} \alpha_i = 1$. If

$$\begin{aligned}\langle AB^\mathsf{T}, P\rangle &= \langle AB^\mathsf{T}, \sum_{i\in[k]} \alpha_i P^{(i)}\rangle = \sum_{i\in[k]} \alpha_i \langle AB^\mathsf{T}, P^{(i)}\rangle \\ &< \langle AB^\mathsf{T}, P'\rangle,\end{aligned}$$

then we have a contradiction, because P' is a feasible solution to rLAP. □

This relaxation motivates our approach to approximating QAP.

3.2 Quadratic Assignment Problems

Koopmans and Beckman [20] introduced QAP in its original form:

$$\text{(QAP)} \quad \underset{P}{\text{minimize}} \quad \sum_{u,v\in[n]} a_{\pi(u)\pi(v)}b_{uv} \tag{4a}$$

$$\text{subject to} \quad \pi \in \Pi. \tag{4b}$$

More recently, a number of equivalent formulations have been developed:

$$\underset{P\in\mathcal{P}}{\operatorname{argmin}} \left\|PAP^\mathsf{T} - B\right\|_F = \tag{5a}$$

$$\underset{P\in\mathcal{P}}{\operatorname{argmin}} tr(PAP^\mathsf{T} - B)^\mathsf{T}(PAP^\mathsf{T} - B) = \tag{5b}$$

$$\underset{P\in\mathcal{P}}{\operatorname{argmin}} -tr(B^\mathsf{T}PAP^\mathsf{T}) = \tag{5c}$$

$$\underset{P\in\mathcal{P}}{\operatorname{argmin}} -\sum_{u\in\mathcal{V}} p_{uv}a_{uv}b_{uv}p_{vu} \tag{5d}$$

$$\underset{P\in\mathcal{P}}{\operatorname{argmin}} -\langle A, PBP^\mathsf{T}\rangle. \tag{5e}$$

Our approach follows from relaxing the binary constraint from the trace formulation of the problem, Eq. (5c). Specifically, we desire to solve the following relaxed QAP problem:

$$\text{(rQAP)} \quad \underset{P}{\text{minimize}} \quad -tr(B^\mathsf{T}PAP^\mathsf{T}) \tag{6a}$$

$$\text{subject to} \quad P \in \mathcal{D}. \tag{6b}$$

rQAP is therefore a quadratic problem with linear and boundary constraints, meaning that relatively standard solvers may be employed.

Importantly, the convex hull of permutation matrices is the set of doubly stochastic matrices, implying that this is a "natural" relaxation in a very meaningful sense. Moreover, although the objective function $f(P) = -tr(B^\mathsf{T}PAP^\mathsf{T})$ is quadratic, it is not necessarily convex. This follows from computing the Hessian of f with respect to P

$$\nabla^2_P = B \otimes A + B^\mathsf{T} \otimes A^\mathsf{T}, \tag{7}$$

which is not necessarily positive definite ($\otimes$ indicates the Kronecker product). This means that the solution space will potentially be multimodal, making initialization important. With this in mind, below, we describe an algorithm that is guaranteed to find a local optimum of rQAP.

4 Fast Inexact Graph Matching Algorithm

Our strategy has three components:

I. Choose an initial estimate.
II. Find a local solution to Eq. (6).
III. Project that solution onto the set of permutation matrices.

We refer to one run of the above three steps as `rQAP`. Upon using m restarts, we report only the best solution, and we refer to the whole procedure as $\texttt{rQAP}_m$. Below, we provide details for each component.

I: Find a suitable initial position $P^{(0)} \in \mathcal{D}$ While any doubly stochastic matrix would be a feasible initial point, two choices seem natural: (i) the "flat doubly stochastic matrix," $J = \mathbf{1}\cdot\mathbf{1}^\mathsf{T}/n$, which is the center of the feasible region, and (ii) the identity matrix, which is a permutation matrix. Therefore, if we run `rQAP` once, we always start with one of those two. If we use multiple restarts, each initial point is "near" the flat matrix. Specifically, we sample K, a random doubly stochastic matrix using 10 iterations of Sinkhorn balancing [21], and let $P^{(0)} = (J + K)/2$.

II: Find a local solution to Eq. (6) As mentioned above, Eq. (6) is a quadratic problem with linear equality and boundary constraints. A number of off-the-shelf algorithms are readily available for finding local optima in such problems. We utilize the Frank-Wolfe (FW) algorithm, which is both (i) a kind of projection descent algorithm and (ii) a successive linear programming algorithm. The FW algorithm was originally designed for solving quadratic problems with linear (equality and/or inequality) constraints [22]. It later became used more generally for nonlinear programming problems [23]. Specifically, it can be used to solve optimization problems of the following form:

$$\text{(FW)} \quad \underset{x}{\text{minimize}} \quad f(x) \tag{8a}$$

$$\text{subject to} \quad x \in \mathcal{S}, \tag{8b}$$

where $\mathcal{S} \subset \mathbb{R}^d$ is a polyhedral set (a set described by linear constraints) and the function $f : \mathcal{S} \to \mathbb{R}$ is continuously differentiable. Here we provide a detailed view of applying FW to rQAP. Given an initial position, $P^{(i)}$, iterate the following four steps.

Step 1: Compute the gradient $\nabla f(P^{(i)})$*:* The gradient f with respect to P is given by

$$\nabla f(P^{(i)}) = -AP^{(i)}B^\mathsf{T} - A^\mathsf{T}P^{(i)}B. \tag{9}$$

Step 2: Compute the direction $\widetilde{P}^{(i+1)}$*:* The direction is giving by that which minimizes a first order Taylor series approximation to $f(P)$ around the current estimate, $P^{(0)}$: The first order Taylor series approximation to $f(P)$ is given by

$$\widetilde{f}^{(i)}(P) := f(P^{(i)}) + \nabla f(P^{(i)})^\mathsf{T}(P - P^{(i)}) \tag{10}$$

Thus, Step 1 of FW is

$$\widetilde{P}^{(i+1)} = \operatorname*{argmin}_{P\in\mathcal{D}} f(P^{(i)}) + \nabla f(P^{(i)})^\mathsf{T}(P - P^{(i)}) = \tag{11a}$$

$$\operatorname*{argmin}_{P\in\mathcal{D}} \nabla f(P^{(i)})^\mathsf{T}P = \tag{11b}$$

$$\operatorname*{argmin}_{P\in\mathcal{D}} \langle \nabla f(P^{(i)}), P\rangle, \tag{11c}$$

which is a LAP. This can be seen by considering Eq. (2e). Let $A = \nabla_P^{(i)}$ and $B = I$ (the $n \times n$ identity matrix), and Eq. (11c) is identical to Eq. (2e).

Step 3: Compute the step size $\alpha^{(i)}$ Given $\widetilde{P}^{(i+1)}$, the new direction is given maximizing the *original* optimization problem, Eq. (6), along the line segment from $P^{(i)}$ to $\widetilde{P}^{(i+1)}$ in $\mathcal{D}$.

$$\alpha^{(i)} = \operatorname*{argmin}_{\alpha\in[0,1]} f(P^{(i)} + \alpha^{(i)}\widetilde{P}^{(i)}). \tag{12}$$

This can be performed exactly, because f is a quadratic function.

Step 4: Update $P^{(i)}$ Finally, the new estimated doubly stochastic matrix is given by

$$P^{(i+1)} = P^{(i)} + \alpha^{(i)}\widetilde{P}^{(i+1)}. \tag{13}$$

Stopping criteria Steps 1–4 are iterated until convergence, computational budget limits, or some other stopping criterion is met. These four steps collectively comprise the FW algorithm for solving Eq. (6).

III: Projecting onto the set of permutation matrices Let $P^{(I)}$ be the doubly stochastic matrix resulting from the final iteration. We project $P^{(I)}$ onto the set of permutation matrices, yielding

$$\hat{P} = \operatorname*{argmin}_{P\in\mathcal{P}} -\langle P^{(I)}, P\rangle, \tag{14}$$

which is a LAP. Thus, this completes one restart of `rQAP`.

5 Theoretical Results

5.1 LAP vs. QAP

At surface, LAP and QAP are quite similar. In fact, the gradient of the LAP objective function is $2AB^\mathsf{T}$. Comparing this gradient to the gradient of the QAP objective function—Eq. (9)—one can see that when (i) $P^{(i)}$ is the identity matrix and (ii) both A and B are symmetric (for example, for undirected graphs), the two gradients are identical. Thus, if QAP is initialized at the identity matrix and the graphs are undirected, the first permutation matrix—the output of *Step 2* in our `rQAP` algorithm—is identical to the LAP solution; although the line search will make $P^{(1)}$ not equal the LAP solution in general.

5.2 rQAP solves QAP in certain special cases

Although, rLAP and LAP are always equivalent, in general, it is not the case that rQAP and QAP are equivalent. However, in a certain important special case, rQAP and QAP are equivalent.

Theorem 1. *If A and B are the adjacency matrices of simple graphs (symmetric, hollow, and binary) that are isomorphic to one another, then the optimal solution to rQAP is equal to the optimal solution to QAP.*

Proof:

□

6 Numerical Results

6.1 QAP benchmarks

To assess numerical properties or $\texttt{rQAP}_m$, we compare its performance with recent state-of-the-art approaches on the QAP benchmark library [12]. Specifically, [24] reported improved performance in all but two cases, in which the QPB method of Cremers et al. [25] achieved a lower minimum. In *all* cases, $\texttt{rQAP}_3$ outperforms the previous best result, often by orders of magnitude in terms of relative error. In three cases, $\texttt{rQAP}_{100}$ achieves the absolute minimum. In 12 out of 16 cases, the simple $\texttt{rQAP}_1$ algorithm outperforms the others (starting with the flat doubly stochastic matrix). See Figure 1 for quantitative comparisons.

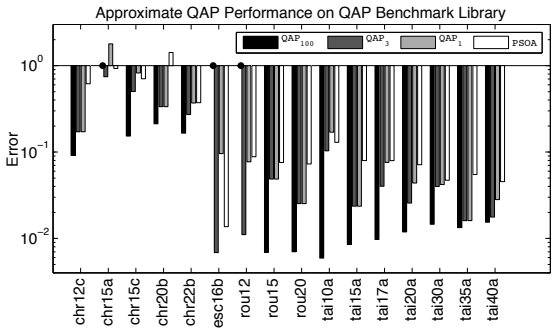

Fig. 1: $\texttt{rQAP}_3$ outperforms the previous state-of-the-art (PSOA) on all 16 benchmark graph matching problems. Moreover, $\texttt{rQAP}_1$ outperforms PSOA on 12 of 16 tests. For 3 of 16 tests, $\texttt{rQAP}_{100}$ achieves the minimum (none of the other algorithms ever find the absolute minimum), as indicated by a black dot. Let f_* be the minimum and $\hat{f}_x$ be the minimum achieved by algorithm x. Error is $\hat{f}_x/f_* - 1$.

6.2 Algorithm Complexity and leading constants

As mentioned above, GM is computationally difficult; even those special cases for which polynomial time algorithms are available, the leading constants are intractably large for all but the simplest cases. We therefore determined the average complexity of our algorithm *and* the leading constants. Figure 2 suggests that our algorithm is not just cubic in time, but also has very small leading constants ($\approx 10^{-7}$ seconds), making using this algorithm feasible for even reasonably large graphs.

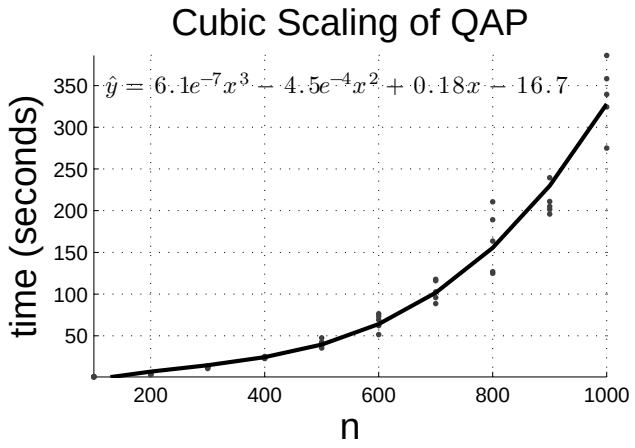

Fig. 2: Performance of `rQAP` as function of number of vertices. Data was sampled from an Erdös-Rényi model with $p = log(n)/n$. Each dot represents a single simulation. The solid line is the best fit cubic function. Note the leading constant is 10^{-7} seconds.

6.3 Brain-Graph Matching

A "connectome" is a brain-graph in which vertices correspond to (collections of) neurons, and edges correspond to connections between them. The *Caenorhabditis elegans* (*C. elegans*) is a small worm (nematode) with 302 labeled vertices. We consider the subgraph with 279 somatic neurons that form edges with other neurons [6], [26]. Two distinct kinds of edges exist between vertices: chemical and electrical "synapses" (edges). Any pair of vertices may have several edges of each type. Moreover, some of the synapses are hyperedges amongst more than two vertices. Thus, the connectome of a *C. elegans* may be thought of as a weighted multi-hypergraph, where the weights are the number of edges of each type. The $\texttt{rQAP}_m$ algorithm natively operates on weighted or unweighted graphs. We therefore conducted the following synthetic experiments. Let $A_{uvz} \in \{0, 1, 2, \ldots\}$ be the number of synapses from neuron v to neuron u of type z (either chemical or electrical), and let $A_z = \{A_{uv}\}_{u,v\in[279]}$ for $z \in \{e, c\}$ corresponding to the electrical or chemical connectome. Let $B_{iz} = Q_{iz}A_zQ_{iz}^{\mathsf{T}}$, for some Q_{iz} chosen uniformly at random from $\mathcal{Q}$ for $i = 1, \ldots, s$. For each i and z, obtain $\hat{Q}_{iz}$ using $\texttt{rQAP}_m$ as described above. Define "accuracy" as $\frac{1}{279}\sum_{uv} Q_{iz}\hat{Q}_{iz}$. Table 1 shows some summary results of applying $\texttt{rQAP}_m$ to both A_c and A_e for $s = 10$ times. Note that while the electrical connectome was more difficult, the median number of restarts was less than 30. Our stopping criteria on the number of restarts was either (i) perfect assignment or (ii) 30 restarts. Therefore, this approach achieved perfect assignment sometimes, even on this harder assignment problem.

TABLE 1: Brain-graph matching summary statistics for both the chemical and electrical connectome. The table shows the mean (standard deviation) of accuracy, number of restarts, and solution time for both connectomes. The maximum number of restarts for both was 30. The mean number of restarts for the both connectomes is less than 30, implying that our approach found the optimal solution many times, just not always for the electrical connectome. Both ran very quickly, only requiring tens of seconds.

	chemical	electrical	unit
Accuracy	100 (0)	59 (0.30)	%
Restarts	3 (0)	25 (6.7)	#
Solution Time	42 (0.42)	79 (20)	sec.

To investigate the performance of `rQAP` using an undirected graph model, we repeated the above analysis using binarized symmeterized versions of the graphs ($A_{uvz} = 1$ if and only if $A_{uvz} \geq 1$ or $A_{vuz} \geq 1$). The resulting summary statistics are nearly identical to those presented in Table 1, although speed increased by greater than a factor of two.

7 Discussion

This work presents an inexact graph matching algorithm. Our key insight was to relax the binary constraint to its continuous counterpart—the doubly stochastic matrices—which is the convex hull of the original feasible region. We then demonstrate that the solution to our relaxed optimization problem, rQAP, is identical to that for QAP whenever the two graphs are simple and isomorphic to one another. These insights led to an inexact matching algorithm with a few distinct features. First, after finding a local solution to the relaxed problem, we project the resulting doubly stochastic matrix onto the set of permutation matrices. Second, we initialize the algorithm using either the identity matrix or the doubly flat matrix (the matrix where all elements are $1/n$). These choices seem to us to be the most obvious places to start if one must choose. Third, if one of those choices does not work, we restart FW with other "nearby" initial points. These modifications facilitate improved performance on *all* the benchmarks we considered. Moreover, although the algorithm scales cubically with the number of vertices, the leading constants are very small ($\mathcal{O}(10^{-7})$ seconds), so the algorithm runs quite fast on reasonably sized networks (e.g., $n \approx 100$). Indeed, on a biologically

inspired GM problem, *C. elegans* connectome mapping, this approach was both fast and effective.

Unfortunately, even with very small leading constants for this algorithm, as n increases, the computational burden gets quite high. For example, extrapolating the curve of Figure 2, this algorithm would take about 2 years to finish (on a standard laptop from 2011) when $n = 20,000$. We hope to be able to perform GM on graphs much larger than that, given that the number of neurons in even a fly brain, for example, is $\mathcal{O}(10^5)$. Therefore, more efficient implementations are of interest.

Although $\texttt{rQAP}_m$ consistently found the optimal solution for the *C. elegans* chemical connectome, connectomes for different organisms even within a species are unlikely to be identical. Even if all connectomes of a particular species were identical, measurement error will likely persist [27]. Therefore, $\texttt{rQAP}_m$'s scientific utility will largely rest on its performance under noisy conditions, which we aim to explore in future work.

Additional future work might generalize $\texttt{rQAP}_m$ in a number of ways. First, that QAP and LAP are so similar suggests that perhaps one could simply implement a single iteration of QAP starting from the identity. While not changing the order of complexity, it could reduce computational time by at least an order of magnitude, without drastically changing performance properties (because convergence typically requires around $5 - 15$ iterations for the graphs we tested). The relative performance/computational cost trade-off merits further theoretical investigations. Second, the most "costly" subroutine is LAP. Fortunately, LAP is a quadratic optimization problem with linear constraints. A number of parallelized optimization strategies could therefore potentially be brought to bear on this problem [28]. Third, our matrices have certain special properties, namely sparsity, which makes more efficient algorithms (such as "active set" algorithms) readily available for further speed increases. Fourth, for brain-graphs, we have some prior information that could easily be incorporated in the form of vertex attributes. For example, position in the brain, cell type, etc., could be used to measure "dissimilarity" between vertices. The objective function could then be modified to give

$$\widetilde{Q}_{AB} = \underset{Q \in \mathcal{D}}{\operatorname{argmin}} \left\| QAQ^{\mathsf{T}} - B \right\|_F^2 + \lambda J(Q), \qquad (15)$$

where $J(Q)$ is a dissimilarity based penalty and λ is a hyper-parameter. Finally, although this approach natively operates on both unweighted and weighted graphs, multi-graphs are a possible extension.

In conclusion, this manuscript has presented a GM algorithm that is fast, effective, and easily generalizable. To facilitate further development and applications, all the code and data used in this manuscript is available from the first author's website, http://jovo.me.

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Joshua T. Vogelstein

John C. Conroy

Lou Podrazik

Steve Kratzer

R. Jacob Vogelstein

Carey E. Priebe