Uncertainty-aware Efficient Subgraph Isomorphism using Graph Topology

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Abstract
Subgraph isomorphism or subgraph matching is generally considered as an NP-complete problem, made more complex in practical applications where the edge weights take real values and are subject to measurement noise and possible anomalies. To the best of our knowledge, almost all subgraph matching methods utilize node labels to perform node-node matching. In the absence of such labels (in applications such as image matching and map matching among others), these subgraph matching methods do not work. We propose a method for identifying the node correspondence between a subgraph and a full graph in the inexact case without node labels in two steps - (a) extract the minimal unique topology preserving subset from the subgraph and find its feasible matching in the full graph, and (b) implement a consensus-based algorithm to expand the matched node set by pairing unique paths based on boundary commutativity. Going beyond the existing subgraph matching approaches, the proposed method is shown to have realistically sub-linear computational efficiency, robustness to random measurement noise, and good statistical properties. Our method is also readily applicable to the exact matching case without loss of generality. To demonstrate the effectiveness of the proposed method, a simulation and a case study is performed on the Erdos-Renyi random graphs and the image-based affine covariant features dataset respectively.

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1 Introduction

In recent years, the number of applications employing graphs have increased exponentially, with the scientific community using graphs to denote relationships between the features of interest (Goyal and Ferrara 2018). A fundamental problem arising in these applications is the subgraph isomorphism problem, also known as subgraph matching, whereby an optimal correspondence is sought between nodes of two given graphs, where one graph is derived from the other. We note here that graph matching is a specialized case of the subgraph matching problem when two graphs are of the same size. Optimality differs according to problem description and domain, but generally refers to the alignment of global graph structures, along with other node features when available.

Ullman in his seminal paper (Ullman 1976) showed that isomorphism can always be estimated using brute-force enumeration as a default strategy which amounts to a depth-first search. The backtracking strategy devised in the paper is used to significantly reduce the size of the search space. Cordella et al. (2004) proposed an improvement of Ullman’s algorithm, the VF2 algorithm, by utilizing a data structure during exploration to significantly reduce memory requirements along with five feasibility rules for pruning the search tree. Both the above approaches solve the exact matching problem where the corresponding nodes and edges between the two graphs share same weights. Conversely, in many practical applications, the nodes can be corrupted by measurement noise and edges can be absent which renders exact matching ineffective. In this case, the practitioners rely not on the exact correspondence but rather some similarity measures. The first set of inexact matching algorithms perform a series of editing operations such as node and edge insertion, deletion or substitution, in order to attain an exact matching (Cordella et al. 1998; Tsai and Fu 1983; Shapiro and Haralick 1985). As is understood, in the case of subgraphs having a much lesser nodes than the full graphs, these methods are really inefficient in solving the matching.

The second set of inexact matching algorithms formulate and solve an optimization algorithm to obtain the node correspondence. Graduated assignment algorithm (Gold and Rangarajan 1996) combines graduated nonconvexity, two-way (assignment) constraints, and sparsity to match graphs even in the presence of noise. Egozi et al. (2012) provides a probabilistic approach to spectral matching which provides a computationally efficient approach towards graph matching. Suh et al. (2015) augments the integer quadratic problem (IQP) objective with a compactness prior to reduce the number of outliers matched. They utilize a Markov chain Monte Carlo (MCMC) to solve the optimization problem. They show that using these modifications can help improve the matches. These approaches
require construction of a weight matrix between the vertices of the two graphs and are thus,
constrained by small graph sizes and pairwise interactions.

There have been some recent work in geometry preserving linear node assignments. Zaslavskiy et al. (2008) proposed an approximate method as a quadratic assignment problem over the set of permutation matrices, where a permutation matrix is a binary matrix describing whether the particular nodes are matched or not. There have been other approaches involving constructing permutation matrices under specific real-valued approximations (Cho et al., 2010; Zhou and De la Torre, 2012) but they have problems where there are poor geometric alignments with high deformations. Byrne (2013) proposed a graph matching technique which preserves the global topological structure by finding an optimal simplicial chain map. Although the author provides an explanation of how this technique can be extended for higher topologies, the formulation shows a matching between the nodes and the edges between the nodes to constrain the homology. For these approaches, even though the topology is constrained as a result of the optimization, the topology constraint is not inherently employed in the matching.

In this work, we specifically focus on graph matching problems with considering measurement noise on edge weights without the presence of node labels, which are demanded in a variety of applications (Bunke, 2000) such as character recognition (Lu et al., 1991; Rocha and Pavlidis, 1994), shape analysis (Cantoni et al., 1998; Lourens, 1998), chemical structure analysis (Balaban, 1985), etc. The idea of matching topology between subgraph and full graph is inspired by the random sample consensus (RANSAC) literature (Fischler and Bolles, 1981; Derpanis, 2010). Graph topology provides a description of graph connectivity as the basic structure of a graph. Our intuition is that matching the unique minimal unit that preserves a pre-specified graph topology between the subgraph and full graph improves the matching efficiency and robustness. Post to the topology-based matching, the remaining unmatched edges in the subgraph are further matched to the corresponding edges in the full graph. However, there are three fundamental questions that arise - (a) what is the minimal topology-preserving unit? (b) how do we guarantee the matching uniqueness? (c) how do we match the remaining edges after the initial match has occurred?

The primary contributions of this work are:

- **Inexact matching in absence of node labels** Almost all of the subgraph matching methods rely on node labels to provide some information regarding the nodes. In absence of such information, these methods fail to find feasible subgraph matches. Our method therefore, fills this gap and provides a matching method which does not need to incorporate labels for matching.
• **Globally consistent matching in the presence of large amounts of outliers/deformation.** Almost all subgraph matching algorithms rely on a single optimization step to search for the node correspondence minimizing the matching loss, which may lead to invalid matching since the true matching may not result in the minimal matching loss under measurement noises. Our proposed approach provides robust global matching under large noise by defining a graph-topology-based structure in the subgraph and searching for feasible matches of nodes sharing the same graph-topology-based structure between the full graph and subgraph. Given the feasible initial match, the consensus based searching expands the search for new matched nodes in a breadth-first tree approach to collect the number of nodes which can be matched uniquely. This formulation takes into account the noise in the edges by statistically modeling them and proving theoretically that this can converge to the true matching.

• **Providing efficiency in subgraph matching.** Using a hypothesis based searching leads to a fast convergence whereby a wrong initial matching leads to a weaker final match set. Parallelizing the consensus based searching step can yield further efficiencies without sacrificing accuracy.

The rest of the paper is organized as follows: Section 2 presents the mathematical formulation of the graph matching problem and our proposed approach. Section 3 provides a robust simulation study to compare the strengths of our algorithm and in section 4 we evaluate performance on homology preserving subgraph matching for image registration applications. Section 5 provides the conclusions.

2 **Method**

2.1 **Problem formulation**

We start with a formal definition of graphs. A graph is denoted by $G = (V, E, w)$, where $V$, $E$ and $w$ represent the set of nodes, the set of edges and edge weights respectively. Let $|\cdot|$ denote the number of elements in a set. Each node is denoted by a node index $v \in \{1,\ldots,|V|\}$. Each edge is expressed as $e = (i, j)$ indicating that nodes $i$ and $j$ are connected by an edge. The edge weight $w : (i, j) \rightarrow \mathbb{R}$ is a function mapping an edge to the real-valued weight.

In our problem setting, let $G_f = (V_f, E_f, w)$ and $G_s = (V_s, E_s, w)$ denote the full graph and subgraph of interest, respectively. Here the subscript “f” represents “full” while the
subscript “s” represents “sub”. The objective of the subgraph matching problem is to seek a matching policy \( \phi \), that projects each node \( v \in V_s \) to the corresponding node \( \phi(v) \in V_f \). In some graph matching literature, the policy function can be also expressed as a \( |V_f| \times |V_s| \) permutation matrix \( X \), whose \((i, j)\)-th element equals to 1 if \( \phi(j) = i \). Without ambiguity, for any \( e = (i, j) \in E_s \), we define \( \phi(e) = (\phi(i), \phi(j)) \in E_f \) as the matched edge of \( e \). In this paper, we consider the situations where weights in the full graph are the ground truth, and the weights in the subgraph are noisy observations from the full graph, that is to assume:

\[
w(e_s) = w(\phi(e_s)) + \epsilon, \tag{1}\]

where \( \epsilon \) is the random noise following normal distribution \( N(0, \sigma^2) \) with unknown variance \( \sigma^2 \). We assume \( \epsilon \)'s are independent among different pairs of matched edges.

Subgraph matching can be formulated as an optimization problem. Under a pre-specified distance measure \( d(\cdot, \cdot) \) of edges, the overall matching loss can be quantified as a \( |V_f||V_s| \times |V_f||V_s| \) matrix \( Q \) whose \((i + |V_s|j, i' + |V_s|j')\)-th element equals to \( d((i, i'), (j, j')) \). Let \( X_v \) denote the vectorization of \( X \) by stacking its columns on top of one another. Let \( X_i \) and \( X_{(j)} \) denote the \( i \)-th row and \( j \)-th column vectors of \( X \), respectively. Let \( \mathbb{I} \) be the vector of ones. The objective function is written as:

\[
\hat{X}_v = \arg \min_{X_v} X_v^TQX_v \tag{2}
\]

subject to

\[
\mathbb{I}^T X_i = 1, \quad X_{(j)}^T \mathbb{I} = 1.
\]

The exact solution to the optimization problem in Eq.(2) can be obtained through an NP-complete non-convex integer programming. The problem can be solved via a searching algorithm (e.g. the Hungarian algorithm) or approximately solved via an integer programming solver (e.g. interior point optimizer). There are two main limitations of these existing approaches. (i) They require a computational time of \( O(|V_f|^3) \), which often exceeds the computation budget for large-scale graphs. (ii) The existing methods are designed based on the loss of edge-to-edge matching. Simply minimizing the overall matching loss in Eq.(2) may lead to erroneous results due to the measurement noise.

To overcome the above limitations, we propose a consensus-based approach that performs graph matching on a set of nodes with topological constraints, which introduces few key innovative components. First, topological constraints are employed for matching a set of
nodes. Compared to the edge weights, the connectivity between nodes imposed by the
topological constraints are invariant to the measurement noise with probability one (in the
case a positive-valued edge weight is disturbed to zero). Moreover, simultaneously matching
multiple nodes which satisfy a topological constraint can reduce computational time while
shrinking the probability of mismatching due to the measurement noise. Second, instead
of searching for the unique solution to Eq.(2) in a single step, we would like to bind the
feasible matching policies in a feasible set based on the revised version of Eq.(2) subject
to some topological constraints and then shrink the feasible set with accumulating more
nodes to the topology structure until a unique matching policy is reached. In this way, the
proposed method will be able to cover the true matching policy in the feasible region with a
high probability and identify it as the unique solution when a sufficient number of nodes are
introduced to the topology structure. It is required to define the topological constraint and
feasible set to complete the proposed method. While we do not formally show the proof,
the exact matching case can be easily shown to be a special case of our inexact matching
algorithm. We will elaborate the technical details in the following subsections.

2.2 Topology-based matching

In the first step, we aim to match a subset of $V_s$ to $V_f$, which is defined as a topology-
preserving unit. Different from the node-to-node matching in Eq.(2), the graph matching is
conducted based on multiple mutually exclusive subsets of $V_s$ following a topology concept
- p-simplex, which is defined as the convex hull of $p + 1$ affinely independent nodes. For
example, a 2-simplex represents a triangle, and a 3-simplex represents a tetrahedron in a
graph. The topology-preserving unit in the initial matching is defined as a pair of connected
p-simplexes in the graph along with the connecting path. To guarantee the validity of the
topology-preserving unit, two basic assumptions are made while formulating our approach.

- $G_s$ is a connected graph i.e. there do not exist two or more separate clusters of nodes
  without edges in between, and

- there exists more than two p-simplexes in $G_s$.

An illustrative example of a topology-preserving unit is displayed in Figure 1 where the two
2-simplexes in the subgraph on the left panel (nodes {3, 8, 9} and nodes {6, 11, 12}) and
the shortest path in between (nodes {8, 13, 12}) are considered as the topology-preserving
unit and matched with the corresponding nodes in the full graph. Let $\delta_{s,c}$ denote the
topology-preserving unit consisting of $c$ nodes, the next step is to seek a matching policy $\phi$
or equivalently a vectorized matching matrix giving the $c$ matching nodes in $G_f$. 

\[ \delta_{s,c} \]
Here we define a general feasible set of matching policies for any given subset of $V_s$, which can be naturally applied to $\delta_{a,c}$. Let $V_c$ denote any subset of $V_s$ with $c$ nodes. Let $Q(V_c)$ denote the distance measures between $V_c$ and the subsets in $V_f$ with the same node size. The feasible set of vectorized matching matrix $\tilde{X}_{v,V_c}$ is defined by revising Eq.(2) as:

$$\tilde{X}_{v,V_c} = \{X_{v,V_c} \mid X_{v,V_c}^T Q(V_c) X_{v,V_c} \leq \tau_c \}, \quad (3)$$

where $\tau_c$ is a pre-specified threshold determined by the set size $c$. Note that $Q(V_c)$ is a vector matching the subset $V_c$ towards all the subsets of the same node size in $V_f$. Revising the optimization problem into a feasible set searching problem enhances the robustness of the matching under measurement noise. Under the statistical property developed in the
later subsection, the number of elements in \( \tilde{X}_v(V_c) \) will shrink as the set size \( c \) increases. For a \( c \) large enough, a unique element will be eventually identified.

To improve the efficiency in calculating \( \tilde{X}_v(V_c) \), we impose the topology constraints on the elements in \( \tilde{X}_v(V_c) \) to have the same topology structure as in \( V_c \). Let \( E_{V_c} \) denote the edges in \( V_c \). Let \( \phi_{X_{v,V_c}} \) denote the matching policy corresponding to \( X_{v,V_c} \). The topology constraint on \( X_{v,V_c} \) is expressed in:

\[
T_v(V_c) = \{ X_{v,V_c} \mid (\phi_{X_{v,V_c}}(v_1), \phi_{X_{v,V_c}}(v_2)) \in E_f \iff (v_1, v_2) \in E_{V_c} \}.
\]  

(4)

Combining Eq.(3) and Eq.(4) yields the feasible set:

\[
\tilde{X}_v(V_c) = \{ X_{v,V_c} \in T_v(V_c) \mid X_{v,V_c}^T Q(V_c) X_{v,V_c} \leq \tau_c \},
\]  

(5)

which can be used to search for \( \tilde{X}_v(\delta_{s,c}) \).

The feasible set is well defined once \( Q(V_c) \) and \( \tau_c \) are defined. Here \( Q(V_c) \) is calculated based on the distance measure between \( V_c \) and any given subset \( v \subset V_f \). The distance measure is defined on the differences in the averaged edge weights, that is

\[
d(V_c, v) = \left| \frac{1}{c} \sum_{i \neq j \in V_c} w_s(i,j) - \frac{1}{c} \sum_{i \neq j \in v} w_f(i,j) \right|.
\]  

(6)

The averaged edge weight is invariant to possible rotation and scaling in real graphs. Note that when all the edge weights in Eq.(6) are pairwise matched, the distance measure \( d \) is the arithmetic mean of \( c \) independent normal random variables, which shrinks to zero as \( c \) grows large according to the central limit theorem and thus guarantees the identification of the true matching policy. Under this statistical property, we propose to set the threshold \( \tau_c \) as:

\[
\tau_c = \Phi^{-1}(1 - \alpha/2) \sqrt{\frac{c \sigma}{c}}
\]  

(7)

where \( \Phi^{-1}(1 - \alpha/2) \) represents the \( 1 - \alpha/2 \) quantile of the standard normal distribution. Here \( 1 - \alpha \) is interpreted as the coverage rate of the true matching by the designed feasible set, and can be specified by the users based on the requirement on the coverage rate. An estimate of \( \sigma \) should be provided when it is not available to the user, which will be discussed in Section 3.

The first step is implemented via a depth-first searching of feasible elements based on Eq.(5), as described in Algorithm 1. The topology structure and shortest path information are used to prune the search. In particular, the following searching algorithm is designed to
find all feasible matching policies for the given topology-preserving units, which will serve as a foundation for the consensus-based searching elaborated in the next subsection.

Algorithm 1: Topology-based matching

**input**: The subgraph \( G_s \) and the full graph \( G_f \), initial parameters \( \alpha \) and \( \sigma \), number of tries \( n \)

**initialize** \( \delta_{s,c} = \{ \}, \tilde{X}_v(\delta_{s,c}) = \{ \} \)

for \( i \in 1 \ldots n \) do

Randomly draw a pair of \( p \)-simplexes \( \nu_1 \neq \nu_2 \) from \( G_s \)

Calculate the shortest path \( p(\nu_1, \nu_2) \) between \( \nu_1 \) and \( \nu_2 \)

\( V_c \leftarrow \nu_1 \cup p(\nu_1, \nu_2) \cup \nu_2 \)

\( \tilde{\nu}_{1,f} \leftarrow \) all feasible matches to \( \nu_1 \) from \( G_f \) based on Eq.(5)

\( \tilde{\nu}_{2,f} \leftarrow \) all feasible matches to \( \nu_2 \) from \( G_f \) based on Eq.(5)

for \( (\nu_{1,f}, \nu_{2,f}) \in \tilde{\nu}_{1,f} \times \tilde{\nu}_{2,f} \) do

for Path \( p(\nu_{1,f}, \nu_{2,f}) \) between \( \nu_{1,f} \) and \( \nu_{2,f} \) having the same length as \( p(\nu_1, \nu_2) \) do

\( v = \nu_{1,f} \cup p(\nu_{1,f}, \nu_{2,f}) \cup \nu_{2,f} \)

if \( d(v, V_c) \leq \tau_c \) then

\( \delta_{s,c} \leftarrow \delta_{s,c} \cup V_c \)

\( \phi_{X_v,V_c}(V_c) \leftarrow v \)

Calculate \( X_{v,V_c} \) based on \( \phi_{X_v,V_c}(V_c) \)

for \( X_v(\delta_{s,c}) \in \tilde{X}_v(\delta_{s,c}) \) do

\( X_v(\delta_{s,c}) \leftarrow X_v(\delta_{s,c}) \cup X_v,V_c \)

end

end

end

**output**: Topology-preserving unit \( \delta_{s,c} \) and the feasible matching \( \tilde{X}_v(\delta_{s,c}) \)

2.3 Consensus-based searching

After the initial matching of the topology preserving nodes in \( \delta_{s,c} \), a consensus-based algorithm is developed to sequentially match the remaining nodes in \( V_s \setminus \delta_{s,c} \). The basic concept is to seek for the feasible matching of paths whose starting nodes are in \( \delta_{s,c} \) and the rest nodes are in \( V_s \setminus \delta_{s,c} \). Instead of matching the topology-preserving unit in the previous
step, we aim to match paths of length \( q \) based on the feasible set defined in Eq. (5). The feasible set can be narrowed down as the path length \( q \) grows large. We start with an empty node set \( \eta_{s,v} \) with \( v = 0 \) and expand the set by searching for feasible matching of paths in \( V_s \setminus \delta_{s,c} \) until it contains a unique element. The algorithm is terminated when no new nodes can be matched between \( G_s \) and \( G_f \). Specifically, we propose the following consensus-based searching algorithm, Algorithm 2.

**Algorithm 2: Consensus-based searching**

**input**: Topology-preserving unit \( \delta_{s,c} \), unmatched node set \( V_s \setminus \delta_{s,c} \), initial parameters \( \alpha \) and \( \sigma \)

**initialize** \( v = 0 \), \( \eta_{s,v} = \{\} \), \( \tilde{X}_v(\eta_{s,v}) = \{\} \)

**while** \( \eta_{s,v} \neq V_s \setminus \delta_{s,c} \) **do**

- Sample an edge \( e_s \in E_s \) incidence to a node in \( \eta_{s,v} \) and a node \( a_s \in V_s \setminus \eta_{s,v} \)
- \( \eta_{s,v} \leftarrow \eta_{s,v} \cup \{v : v \in e_s\} \)
- \( v \leftarrow v + 1 \)
- \( v' \leftarrow 0 \)
- \( \tilde{\eta}_{s,v'} = \{\} \)

**while** \( \exists \) an edge \( e'_s \in E_s \) incidence to \( a_s \) and a node \( b_s \in V_s \setminus \eta_{s,v} \) **do**

- \( \tilde{\eta}_{s,v'} \leftarrow \tilde{\eta}_{s,v'} \cup e'_s \)
- \( v' \leftarrow v' + 1 \)
- \( a_s \leftarrow b_s \)
- Compute feasible matching for \( \tilde{\eta}_{s,v'} \) in \( V_f \) according to Eq. (5), store it in \( \tilde{X}_v(\tilde{\eta}_{s,v'}) \)

**if** \( \tilde{X}_v(\eta_{s,v'}) \) is unique **then**

- \( \eta_{s,v} \leftarrow \eta_{s,v} \cup \tilde{\eta}_{s,v'} \)
- \( v \leftarrow v + v' \)
- \( \tilde{X}_v(\eta_{s,v}) \leftarrow \tilde{X}_v(\eta_{s,v}) \cup \tilde{X}_v(\tilde{\eta}_{s,v'}) \)
- **break**

**end**

**end**

**output**: Node correspondence for \( \tilde{X}_v(\eta_{s,v}) \)
2.4 Theoretical Guarantees

Theorems are developed to evaluate the false positive and false negative rates in Subsection 2.4. The first theorem shows that the feasible sets in Eq.(5) will cover the true matching nodes with a pre-specified probability $1 - \alpha$, which guarantees the identification of the true matching nodes by applying the proposed method.

**Theorem 1.** Let $X^*_v(V_c)$ denote the true vectorized matching matrix corresponding for the node set $V_c$. The feasible set covers the true matching nodes with probability $1 - \alpha$, i.e.,

$$
\mathbb{P} \left[ X^*_v(V_c) \in \tilde{X}_v(V_c) \right] = 1 - \alpha.
$$

**Proof:** Let $V^*_{c,f}$ denote the true matching node set for $V_c$ according to Eq.(5),

$$
\mathbb{P} \left[ X^*_v(V_c) \in \tilde{X}_v(V_c) \right] = \mathbb{P} \left[ d(V_c, V^*_{c,f}) \leq \tau_c \right]
$$

$$
= \mathbb{P} \left[ \frac{1}{c} \sum_{i \neq j}^{c} w_s(i, j) - \frac{1}{c} \sum_{i \neq j}^{c} w_f(i, j) \leq \tau_c \right]
$$

$$
= \mathbb{P} \left[ \frac{1}{c} \sum_{j=1}^{c} \epsilon_j \leq \tau_c \right],
$$

where $\epsilon_j$’s are $c$ independent and normally distributed random variables defined in Eq.(1). Note that $\frac{1}{c} \sum_{j=1}^{c} \epsilon_j$ also follows a normal distribution $N(0, \sigma^2/c)$. Thus we have

$$
\mathbb{P} \left[ X^*_v(V_c) \in \tilde{X}_v(V_c) \right] = 2\Phi(\sqrt{c\tau_c}/\sigma) - 1
$$

$$
= 2(1 - \alpha/2) - 1
$$

$$
= 1 - \alpha.
$$

On the other hand, we would like the proposed feasible set to exclude any irrelevant node set, especially when the number of nodes $c$ grows large. The theorem is formally established as follows.

**Theorem 2.** Let $\mu = \inf_{(e_s, e_f) \in E_s \times E_f} |\mathbb{E}[w(e_s)] - \mathbb{E}[w(e_f)]| / \sigma > 0$, where $e_s$ and $e_f$ are not matched. The probability of excluding an irrelevant vectorized matching matrix $X_v$ from $\tilde{X}_v(V_c),$

$$
\mathbb{P} \left[ X_v \notin \tilde{X}_v(V_c) \right] > \Phi \left( \frac{-\Phi^{-1}(1 - \alpha/2) - \mu \sqrt{c}}{\sqrt{2c}} \right) + 1 - \Phi \left( \frac{\Phi^{-1}(1 - \alpha/2) - \mu \sqrt{c}}{\sqrt{2c}} \right),
$$
**Proof:** given $X_v$ is not a true vectorized matching matrix for $V_c$, there exists at least a pair of edges that are not matched. Let $(e_1, e_2)$ denote the unmatched pair of edges, then we have

$$
\mathbb{P}
\left[
X_v \notin \tilde{X}_v(V_c)
\right]
\geq
\mathbb{P}
\left[
|w(e_1) - w(e_2)| > \tau_c
\right]
\geq
\mathbb{P}
\left[
|Z_{1,2}| > \tau_c
\right],
$$

where $Z_{1,2}$ is a normally distributed random variable with mean $\mu \sigma$ and variance $2\sigma^2$. Therefore we have

$$
\mathbb{P}
\left[
|Z_{1,2}| > \tau_c
\right] = \Phi\left(-\frac{-\tau_c - \mu \sigma}{\sqrt{2\sigma}}\right) + 1 - \Phi\left(\frac{\tau_c - \mu \sigma}{\sqrt{2\sigma}}\right)
= \Phi\left(-\frac{-\Phi^{-1}(1 - \alpha/2) - \mu \sqrt{c}}{\sqrt{2c}}\right) + 1 - \Phi\left(\frac{\Phi^{-1}(1 - \alpha/2) - \mu \sqrt{c}}{\sqrt{2c}}\right).
$$

Note that $\mathbb{P}
\left[
|Z_{1,2}| > \tau_c
\right]$ is a monotonic increasing function with $c$, implying that the proposed feasible can exclude the irrelevant nodes when $c$ grows large.

### 2.5 Computational complexity

The computational complexity of the proposed method can be estimated as follows. Suppose $k$ $p$-simplexes are initially matched. Let $\bar{c}$ denote the average number of nodes in each $\delta_{s,c}$, $m_f$ denote the total number of $p$ simplexes in $G_f$, and $\bar{d}_f$ denote the average degree in $G_f$. The computational cost in the initial matching step is $\mathcal{O}(m_fk\bar{d}_f(\bar{c} - 2(p + 1)))$, where the multiplication of the first two terms evaluates the computation time for matching the $p$-simplexes while the last two terms quantifies the computation time for matching the shortest path in between. The computation time for the consensus step is dominated by the efforts in path-wise matching of the remaining nodes after the initial matching, which is $\mathcal{O}\left((n_s - k(p + \bar{c} - 1))\bar{d}_f\right)$.

The total computation complexity of the proposed algorithm is expressed in

$$
\mathcal{O}\left(m_fk\bar{d}_f(\bar{c} - 2(p + 1)) + (n_s - k(p + \bar{c} - 1))\bar{d}_f\right).
$$

It is worth noting that Eq(14) is upper bounded by $\mathcal{O}\left((n_f + m_f)\bar{d}_f\right) = \mathcal{O}(n_f^p)$ in the worst case scenario where the subgraph and full graph have the same size and both of them are fully connected. In this case, the number of $p$-simplexes is $m_f = \mathcal{O}(n_f^p)$, which greatly increase the computational load. However, this case is not commonly seen in real applications where the graphs are relatively sparse. For a sparsely connected graph with a smaller $m_f$ and $\bar{d}_f$ and $n_s \ll n_f$, the computational time is sub-linear with respect to $n_f$. 

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3 Simulation study

The proposed algorithm is evaluated in a simulation dataset generated from the Erdős-Rényi model (Erdős et al., 1960). Specifically, the full graph is generated as an Erdős-Rényi graph with 100 nodes. Edges are connected between each pair of nodes with a probability of 0.1 to simulate graphs in real applications where edges are sparsely presented. Each edge in the full graph is assigned with a random weight sampled from the uniform distribution $U(0, 1)$. The subgraph is consisted of 20 nodes randomly sampled from the full graph. To ensure some edge connectivity in the subgraph, neighboring nodes whose pair-wise distance is smaller than 0.5 are included. Each edge in the subgraph is then assigned with a normally distributed noise with zero mean and standard deviation of $\sigma$. The algorithm performance will be tested under different noise level $\sigma$.

A Monte-Carlo simulation study of 100 iterations is conducted for each given $\sigma \in \{0.001, 0.002, \ldots, 0.01\}$. In each iteration, both a full graph and a subgraph is generated according to the procedure described above. The standard deviation $\sigma$ is presumed to be known, and $\alpha$ is set as 0.025. The proposed algorithm takes the full graph and subgraph as the input, and returns the node correspondence. When implementing the proposed method, we set $p = 2$ to focus the topology matching on triangles. This is because a smaller $p$ provides a small searching space for all the feasible $p$–simplex and hence improves the algorithm efficiency. A discussion on the trade-off between the robustness of the method and the algorithm efficiency can be found in Section 5.

The resultant node correspondence is compared with the true node correspondence, and the percentage of the correctly matched nodes is reported to evaluate the algorithm accuracy. The computational time in each iteration is also recorded to evaluate the algorithm efficiency. The distributions of the accuracy and computational time under the Monte-Carlo simulation are summarized in Figure 2. We observe an decreasing trend of the matching accuracy as the noise level increases as expected. The averaged accuracy is above 95% when the signal-to-noise ratio is above 20 (corresponding to $\sigma = 0.05$). Regarding the computational time, it takes 4 seconds on average to seek a node correspondence between a full graph of 100 nodes and a subgraph of 20 nodes, implying the relatively high efficiency of the proposed method. We would like to mention that we tested four different subgraph matching algorithms provided in the OpenGraphMatching toolbox (Tianchang, 2021) (GraphQL (He and Singh, 2008), CECI (Bhattarai et al., 2019), Neural (Liu et al., 2020), QuickSI (Shang et al., 2008)) which yielded no results without labels. Also VF2++ (Jüttner and Madarasi, 2018), a modification of VF2, provided no results with the addition of noise.
4 Case study

We investigate the performance of the proposed algorithm for image correspondence using sampled images from the affine covariant features dataset (Mikolajczyk and Schmid, 2005). This dataset has been used as a traditional dataset for local feature detector evaluation e.g. Scale Invariant Feature Transform (SIFT) (Lowe, 1999), Gradient location-orientation histogram (GLOH) (Mikolajczyk and Schmid, 2005) etc. Image correspondence or homography is used to infer the relationship between features of two or more images of the same planar object. As the first example, we create a subset of a given image by cropping part of the original image as shown in Fig 3. Emulating other image graph extraction literature, we extracted keypoints from the images using the SIFT feature extraction. SIFT is known to be robust to changes in image scale, noise and illumination and thus can provide nodes which have same relative positions for the same object irrespective of changes in camera orientations. We utilize constrained Delaunay triangulations to connect nodes in order to form the graphs. The edge weights are given by the Euclidean distances between the nodes. Constraining the triangulations removes spurious triangles which increase computational load without adding new information. We show the graphs superimposed on the original and cropped image in Fig. 3(a). Fig. 3(b) shows the true matches between the nodes in the original and cropped image. We estimate the node correspondence by getting the coordinates of the keypoints in the cropped image and then offsetting them by the cropped origin coordinates. We then search for keypoints in the original image which lie within certain bounds and are not matched by any other keypoints.

Fig. 3(c) gives the estimated correspondences using the proposed method. We choose a small set of triangles randomly in the subgraph which have paths connecting them. Based on the matching performance in the initial matching step, we tune the hyperparameter \( \sigma \) and find that \( \sigma = 1 \) pixel results in the optimal matching performance. The feasible sets are then constructed based on the constraints with the tuned \( \sigma \). Given there exists a feasible set, we move to the consensus step to sequentially find nodes which are connected to the matched nodes and can be uniquely matched to nodes in the full graph. From a visual inspection, we see that even in presence of errors in SIFT keypoints, our method can robustly match nodes in a topologically consistent manner. There are couple of node matches at the top of the images which are missed due to the errors being outside our bounds. In Fig. 3(d), we rotate the cropped image by 30° clockwise and estimate the matching. Given the rotational invariance in weights of the 2-simplex, we see that the proposed method can match the nodes even in this scenario. In this case though, some nodes in the right side of the cropped image are unmatched due to keypoints being absent.
and thus the connectivity assumption of the graph not being met completely. Fig. 3(e) shows the second matched set for the rotated image. In order to perform comparison with established algorithms, we choose OpenCV library (?) which has a template matching module. The template matching module computes the match between the pixels of the template and the pixels of the image with the template being slid over the image and the loss calculated. Fig. 3(f) and Fig. 3(g) provides the result of the matches between the cropped image and the rotated cropped image with the original image respectively. In both the cases, we find that template matching fails to provide an optimal solution.

5 Conclusions

We have presented a subgraph matching algorithm, providing theoretical guarantees about the accuracy of the method while looking at matching graph topology as a way to reduce the search space. Through experiments, both in simulation and real image datasets, we have presented the robustness and accuracy of the algorithm while showcasing the efficiency in simulation. The algorithm can deal with large graphs without any inherent assumptions other than weak assumptions about connectivity of the graph and presence of adequate number of simplexes. A distinctive feature of our algorithm is the concept of feasibility where an edge match is informed by the statistical threshold value found as a function of the path that the edge is part of. This can lead to substantial efficiency gains. A second distinctive feature is in the choice of the p-simplexes with the shortest path in between them as the minimum topology-preserving unit which again reduces the search space substantially. A combination of these two features leads to an algorithm that can solve an inexact subgraph matching problem with large outliers and/or deformation in sub-linear time (realistically), a large improvement over previous algorithms which are polynomial complexity, which restricts these algorithms from matching large scale graphs.

However, our approach suffers from limitations which plague all randomized algorithms. The initial p-simplex chosen in sub-graph might not be present in the full graph due to a missing edge or might be deformed beyond the thresholding level set which can lead to wrongful initial matches. Our future work would be in understanding how to utilize topology to further remove inaccurate matches - particularly, moving away from the current technique of assuming that the initial match is the truth and constantly checking the previous matches according to global topology. Furthermore, there is a known trade-off between the algorithm’s robustness and efficiency under different choices of p. Specifically, A large p improves the algorithm robustness by comparing more edges in each topology unit.
However, it sacrifices the algorithm efficiency by allowing for more feasible $p$–simplex. In this paper, the method is implemented with $p = 2$ (triangles) to improve the efficiency. For more noisy graph matching problems, it is recommended to increase $p$ for better matching performances, which will be done in the future work.

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Figure 2: Performance of the proposed method under Monte-Carlo simulation. Top panel: box plot of the matching accuracy under different noise levels. Bottom panel: box plot of the computational time under different noise levels. The upper and lower bounds of the boxes depict the 75% and 25% quantiles, respectively. The top and bottom horizontal lines represent the 95% and 5% quantiles, respectively. The scattered dots illustrate the outliers.
Figure 3: (a) The sampled graffiti image in affine covariant features dataset and cropped image. The green lines depict the constrained Delaunay triangulations of SIFT features. (b) The true image correspondence between the two images. The red lines highlight the node correspondence. (c) The estimated image correspondences from the proposed method. (d) The estimated image correspondences between the original image and rotated cropped image from the proposed method. (e) Another possible match between original image and rotated cropped image from the proposed method. (f) Failed template matching using OpenCV package for cropped image - result shown in third frame. (g) Failed template matching using OpenCV package for rotated cropped image - result shown in third frame.