

University of Heidelberg  
Faculty of Mathematics and Computer Science  
Computer Vision group  
at  
Heidelberg Collaboratory for Image Processing

Master's Thesis

Application of graph matching in  
Computer Vision

Name: Ekaterina Tikhoncheva  
Matriculation number: 3237882  
Supervisor: Prof. Dr. Björn Ommer  
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### **Declaration of Authorship**

I confirm that this Master's thesis is my own work and I have documented all sources and material used. This thesis was not previously presented to another examination board and has not been published.

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**Abstract.** Graph matching is one of the fundamental problems in graph theory and computer vision. Due to its practical relevance this problem is heavily investigated and there are a lot of approximative algorithms for solving it. However a lot of algorithms are able to work efficiently only with small graphs (up to 100 nodes) and scale poorly for bigger graphs. In this thesis we introduce a novel approach for extending the usability of existing graph matching algorithms for bigger graphs. For that we introduce a two level graph matching framework. Two given graphs to match represent the lower level. To reduce the problem size we partition each of the graphs into a fix number of subgraphs and consider each subgraph as a node of a new graph (anchor graph), that is placed on the second higher level. To solve the initial matching problem we iteratively first solve the matching problem on the higher level, which gives us correspondences between nodes of the two anchor graphs. Afterwards we find in parallel correspondences between nodes of the matched subgraph pairs. To improve the initial partition before the next iteration we introduce an update rule, which allows the subgraphs to exchange nodes on their border. We demonstrate the effectiveness of our approach in matching synthetic graphs and finding correspondences between pairs of images.

**Zusammenfassung.** Graph Matching ist eines der grundlegenden Probleme in der Graphentheorie und Computer Vision. Aufgrund seiner praktischen Relevanz ist es auch ein ausgiebig erforschtes Problemfeld. Es existieren viele approximative Algorithmen, die in der Lage sind schnell eine hoch qualitative Lösung zu liefern. Allerdings sind viele der Algorithmen nur für kleine Graphen mit bis zu 100 Knoten geeignet und lassen sich schwer für größere Graphen anwenden. Aus diesem Grund haben wir uns in dieser Masterarbeit mit der Entwicklung eines neuen Ansatzes zum Graph Matching beschäftigt, der die Anwendung von existierenden Algorithmen für große Graphen mittels eines zweistufigen Ansatzes ermöglicht. Zwei gegebene Graphen sind auf der unteren Stufe platziert. Um die Schwierigkeit des Problems zu minimieren, zerlegen wir jeden einzelnen Graphen in eine fixe Anzahl von Teilgraphen, die wir mit einem Knoten eines neuen Graphen (Ankergraphen) erfassen. Die zwei Ankergraphen repräsentieren die zweite Stufe unseres Verfahrens. Zuerst finden wir die Zuordnung zwischen den Knotenmengen der beiden Ankergraphen. Um die Abbildung zwischen den Knoten der ursprünglichen Graphen zu finden lösen wir das Matchingproblem für jedes zugeordnete Paar von Teilgraphen parallel. Die Vorgehensweise wird durch eine Update-Regel erweitert und iterativ wiederholt. Wir demonstrieren die Funktionalität unseres Ansatzes mit Beispielen von künstlich generierten Graphen und der Zuordnung von Merkmalspunkten auf zwei Bildern.





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# Chapter 1

## Introduction

Graph theory is one of the oldest and widely used branches of discrete mathematics. Graphs have found an application in almost all fields of computer science, including image processing and computer vision. The reason for such a success is their simple way to model pairwise relationships between different objects. In terms of image processing and computer vision those objects can be presented by image regions, image features or even separate pixels. Such a graph representation often helps to transform an existing practical problem into a good investigated problem of graph theory. An example is image matching, which is one of the central problems in computer vision. Using a graph representation of images, which for example can be obtained by connecting selected points of images with edges, this problem can be formulated as a graph matching problem. Although the last is not easy to solve (in most cases the graph matching problem is NP-hard), there are a lot of approximative algorithms that solve it in polynomial time.

Further in this work we will see, that one distinguishes two general types of graph matching problems: exact and inexact ones. As the exact graph matching is often too strict to be applied to practical applications, such as image matching, we concentrate ourselves on the problems, that formulate the graph matching problem in an inexact way. In the most general case algorithms for solving inexact matching problems use a so-called affinity or similarity matrix of two graphs, which contains information how similar they are. However in a naive implementation such algorithms have strong limitations on the size of the graphs they are able to handle in reasonable time due to high time and memory demand. Knowing this issues the aim of this thesis is to present a novel framework that should help to extend the usability of existing graph matching algorithms to bigger graphs. The proposed framework

helps to reduce the complexity of the problem by subdividing it into smaller problems, which can be easily handled with existing algorithms. This technique can be seen as a variant of the well known divide and conquer paradigm.

This thesis is organized as follows. In chapter 2 we give a general formulation of the graph matching problem together with its possible specifications, which are determined by required properties of the matching. Additionally we show how different formulations are related to each other. We also provide an extensive overview of existing algorithms for solving graph matching problems, which contains classical widely known works as well as recently published researches in this field. Chapter 3 describes the novel two level graph matching framework based on a variation of the divide-and-conquer paradigm. In chapter 4 we report results of the application of the proposed framework to synthetic generated graphs and real images. The last chapter gives a summary of the achieved results. There we also discuss possible improvements of the developed framework and future work.

# Chapter 2

## Graph Matching

In this chapter we introduce different forms and formulations of the graph matching problem together with some algorithms for solving them. The classification we use is based on the one introduced by Conte et al. [20]. Not all algorithms, we will present, were initially mentioned in [20], but we also do not cover all of the recent ones due to their quantity. Our focus lies especially on those, that are important for further reading of this thesis.

To begin with we refresh basic definitions and notations from graph theory used in this thesis.

### 2.1 Basic definitions and notations

An *undirected graph*  $G = (V, E)$  is defined as a pair of disjoint sets  $V, E$ , where  $E \subseteq \{\{u, v\} | u, v \in V\}$  [24]. The elements of the set  $V$  are called *vertices* or *nodes*<sup>1</sup> and the elements of  $E$  are called *edges*. Where it is necessary, we will write  $V(G), E(G)$  to refer node and edge sets to the particular graph  $G$ .

The number of nodes in  $V$  defines the *size* of a graph  $G$ . Two nodes  $v_i, v_{i'} \in V$  are called *adjacent*, if there is an edge  $e = v_i v_{i'} = \{v_i, v_{i'}\} \in E$ . Each graph can be represented by its *adjacency matrix*  $A = (a_{ii'})_{n \times n}$ , where

$$a_{ii'} = \begin{cases} 1, & \text{if } \{v_i, v_{i'}\} \in E, \\ 0, & \text{otherwise} \end{cases}$$

and  $n$  is the number of nodes in the graph.

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<sup>1</sup>We use terms vertex and node further in the text as synonyms.

A *path* in a graph  $G = (V, E)$  is a sequence of nodes  $\{v_0, v_1, \dots, v_k\}$  connected by the edges  $\{v_0v_1, v_1v_2, \dots, v_{k-1}v_k\}$ , where  $v_i \in V$  and  $v_{i-1}v_i \in E$  for all  $i = 1, \dots, k$ . A path with  $v_0 = v_k$  is a *cycle*.

A graph  $G' = (V', E')$  is called a *subgraph* of a graph  $G = (V, E)$ , if  $V' \subseteq V$  and  $E' \subseteq E$ . We use the standard notation  $G' \subseteq G$  for this. A subgraph  $G'$  of  $G$  is *induced by a node subset*  $V' \subseteq V$ , if  $E' = \{e = \{v_i, v_{i'}\} | v_i, v_{i'} \in V'\}$ . Analog, a subset  $E' \subseteq E$  induces a subgraph  $G'$  of  $G$ , if  $V' = \{v \in V | v \in e \text{ and } e \in E'\}$ . For an induced subgraph we use the notation  $G' = G[V']$  and  $G' = G[E']$  [24], if it is node- or vertex-induced respectively. We also introduce a graph cut  $G \cap G' = (V \cap V', E \cap E')$  and union  $G \cup G' = (V \cup V', E \cup E')$ .

There are several special types of graphs. A graph is called *complete* if each pair of its nodes is connected by an edge. In case when each node  $v_i \in V$  of a graph  $G$  has an associated attribute  $d_i \in D$ , one speaks about an *attributed graph*  $G = (V, E, D)$ . In contrast to this, if each edge of a graph has an associated weight, the graph is called *weighted graph*. A graph is *connected*, if there is a path between each pair of its nodes. A connected, undirected graph without cycles is called a *tree*. A *hypergraph* is a graph, whose edges connect several vertices at the same time (*hyperedges*).

Let us consider two undirected attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$ . We assume the situation, where  $|V^I| = n_1$ ,  $|V^J| = n_2$  and  $n_1 \leq n_2$ . A *matching function* between  $G^I$  and  $G^J$  is a mapping  $m : V^I \rightarrow V^J$  between the sets of nodes of two graphs. It is clear, that defined in this way the mapping  $m$  is not unique. Assume, that we have some function  $S(G^I, G^J, m)$  to measure the quality of matching  $m$ . In this case, the *graph matching problem* between  $G^I$  and  $G^J$  can be defined as a problem of finding such a map  $m : V^I \rightarrow V^J$ , that maximizes the similarity score  $S(G^I, G^J, m)$  between the graphs and has some additional constraints:

$$m = \operatorname{argmax}_{\hat{m}} S(G^I, G^J, \hat{m}) \quad (2.1)$$

Based on the required properties of the mapping  $m$  one distinguishes two kinds of the graph matching problem [20]: *exact* and *inexact* ones. There are also variations inside of each group based on the definition of the similarity function between two graphs. In the following sections we will give an overview of common exact and inexact graph matching problems together with algorithms for solving them.

## 2.2 Exact graph matching

The group of exact graph matching problems is dealing with the task of finding an *edge preserving* mapping  $m$  between nodes of two graphs. With other words: if  $\{v_i, v_{i'}\} \in E^I$ , then  $\{m(v), m(v_{i'})\} \in E^J$  for all  $v_i, v_{i'} \in V^I$ . This is the class of more strict problems. The graphs, considered in this case often do not have attributes.

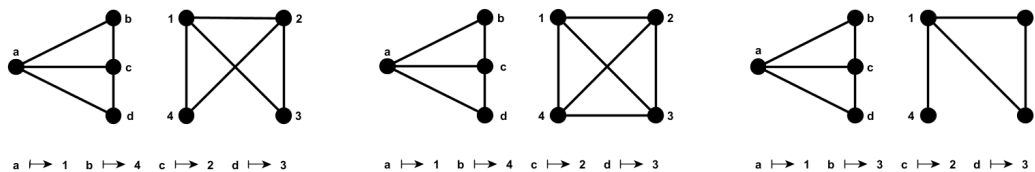
There are several forms of exact graph matching. The most known one is *graph isomorphism*: two graphs are called *isomorphic* ( $G^I \simeq G^J$ ), if a edge preserving mapping between their nodes is bijective. This implies automatically, that two graphs should have an equal number of nodes. If it is not the case, and the isomorphism holds between the one graph and a node-induced subgraph of the other graph, the problem is called *subgraph isomorphism*. Its further extension is the isomorphism between subgraphs of two graphs. The last problem can obviously have several solutions, but one is normally interested in finding a common subgraph with a maximum number of nodes or edges (*maximum common subgraphs*).

The further simplification of the graph isomorphism is to require an injective edge-preserving mapping, instead of an bijective one. This problem is called *graph monomorphism*. Correspondences between nodes of the graphs are still one-to-one, but the second graph may contain additional nodes and edges compared to the first graph. Note, that each subgraph isomorphism defines a monomorphism of the graphs, however the opposite statement is not correct.

A even weaker form of a graph matching problem is *graph homomorphism*. It allows a many-to-one mapping between nodes of two graphs, meaning that one node can correspond to several nodes of the other graph. The only restriction on a mapping  $m$  in this case is to be total (i.e. every node  $v_i \in V^I$  has to be mapped into  $V^J$ ). In Fig. 2.1 one can see examples of different exact graph matching problems. Node correspondences are listed below each subfigure.

All problems except graph isomorphism are proofed to be *NP*-complete [30]. This can be shown through a reduction of the respective matching problem to the clique problem. The graph isomorphism is currently shown to be in the class *NP* [30, 69]. However for some special types of graphs there exist polynomial time algorithms (e.g. for trees [2, 30]).

In the following we describe several approaches for solving exact graph matching problems.



(a) Graph isomorphism      (b) Graph monomorphism      (c) Graph homomorphism

**Figure 2.1:** Exact graph matching problems. Node correspondences are listed below each subfigure.

## 2.3 Methods for solving exact graph matching problems

The most used approach to solve an exact graph matching problem is based on a tree search with backtracking. This method starts with an empty set of correspondences and tries stepwise to expand it according to provided rules until a complete solution is found. Each partial solution represent a node of a search tree and all nested solutions build a branch in this tree. If it happens, that in some step a current set of correspondences cannot be expanded further due to problem constraints, the current branch in the tree is cut. The method backtracks to the last feasible solution and tries to find another way to proceed further. The algorithms based on a tree search are very slow, if they need to traverse the whole tree. However, they can be speeded up by applying some heuristics to detect unpromising branches and exclude them from the search. The most known algorithm in this group, which uses depth-first-rule to traverse a tree, is the branch and bound algorithm [61].

One of the first algorithms, that used the described technique, is the one by Ullman [75]. Later it was extended and improved mostly by the suggestion of a new pruning heuristics. A small comparison of different algorithms in this group with diverse heuristics is reported in [42]. We also want to mention here another well known algorithm on graphs, which uses the tree search method, namely the algorithm by Bron and Kerbosch [5] for finding cliques in an undirected graphs. The last problem is closely related to the graph matching, as the maximal common subgraph problem can be reduced to the problem of finding the maximal clique [30].

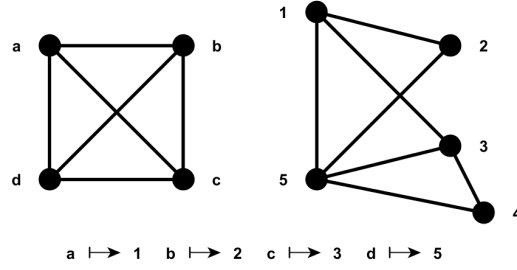
From the other techniques we want to mention the algorithm described by MacKay [52], which uses group theory to solve the graph isomorphism problem, and an



approach based on decision trees [53, 71, 72] for matching graph ((sub)graph isomorphism) against a set of graphs.

## 2.4 Inexact graph matching

As we mentioned above exact graph matching problems are often not applicable to real-world problems. There are mainly two reasons for that. On the one hand, the same object can be described by graphs with different structures. This could be a consequence of object deformations or noise influence, which can occur in some real world applications. On the other hand, solving a graph matching problem exactly can be time and/or memory consuming. As a consequence one can be interested in solving graph matching problems inexactly. In this case, a strong edge preserving mapping between the nodes of two graphs is not required.



**Figure 2.2:** Inexact graph matching

Let us recall the problem statement (2.1):

$$m = \operatorname{argmax}_{\hat{m}} S(G^I, G^J, \hat{m})$$

where  $S(G^I, G^J, \hat{m})$  defines a similarity measure between the attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$ . The mapping  $m$  is required to be total and sometimes also injective, to guarantee a one-to-one matching. We call further algorithms, that solve inexact graph matching problem, inexact.

Depending on the case, if an algorithm for solving problem (2.1) finds a global solution or not, this algorithm is called *optimal* or *suboptimal*, respectively. The choice, which algorithm to select depends on a specific problem. It should be noted, that an optimal inexact algorithm is not necessary faster than a one, which solves an exact graph matching problem. On the other hand, suboptimal inexact algorithms often do not have any performance guarantee.

There are also different ways to define a similarity function  $S(G^I, G^J, m)$ , which leads to a high number of different approaches inside the group of algorithms that solve inexact graph matching problem. In the following section we summarize the most common forms of the objective function of the problem (2.1).

### Graph matching objective function

In some of the literature (e.g. [35, 48, 50, 64, 78, 82]), instead of defining a similarity function as it is done in Eq. (2.1), one speaks about dissimilarity between two graphs. The goal in this case is to minimize the disagreement in the graph structure. Two formulations of the problem are equivalent and can be easily transformed from one into the other.

### Quadratic Optimization Problem

Let us consider two attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$ . We want to find a mapping  $m$  between the nodes of this graphs. Let the size of the graphs be  $n_1$  and  $n_2$  respectively. Generally,  $n_1$  and  $n_2$  can be different, but then we assume without losing generality, that  $n_1 \leq n_2$ . Here and further we require a mapping  $m$  in (2.1) to be total and injective, which guarantees, that each node of the first graph will be matched to exactly one node of the second graph (one-to-one matching).

We start first with an even stricter assumption, that  $n_1 = n_2 = n$  and that the matching is bijective. In this case a mapping between nodes of two graphs defines a permutation  $\sigma$  of the set  $\{1, \dots, n\}$ . Each permutation  $\sigma$  can be represented by the permutation matrix  $P = \{P_{ij}\}$ , where

$$P_{ij} = \begin{cases} 1, & \text{if } \sigma(i) = j, \\ 0, & \text{otherwise.} \end{cases}$$

We denote with  $\Pi_n$  the set of all feasible permutations:

$$\Pi_n = \{P \in \{0, 1\}^{n \times n} \mid \sum_{i=1, \dots, n} P_{ij} = \sum_{j=1, \dots, n} P_{ij} = 1 \quad \forall i, j = 1, \dots, n\}$$

Let matrices  $A^I$  and  $A^J$  be the adjacency matrices of the graphs  $G^I$  and  $G^J$  respectively. We assume, that in case of weighted graphs, the adjacency matrices contain edge weights instead of binary values. We can now formulate the graph matching problem as the following minimization problem (compare with

[35, 48, 50, 64, 76, 82]):

$$P = \operatorname{argmin}_{\hat{P} \in \Pi_n} \|A^I - \hat{P}A^J\hat{P}^T\|^2 + \|D^I - \hat{P}D^J\|_2^2 \quad (2.2)$$

where  $\|\cdot\|$  is the matrix Frobenius norm and  $\|\cdot\|_2$  is the Euclidean norm ( $L^2$  norm). Some authors (e.g. Vogelstein et al. in [78]) use slightly different, but equivalent reformulation of it, namely:

$$P = \operatorname{argmin}_{\hat{P} \in \Pi_n} \|A^I\hat{P} - \hat{P}A^J\|^2 + \|D^I - \hat{P}D^J\|^2, \quad (2.3)$$

After some transformations, the problem (2.2) can be reformulated as (see [10], Appendix A):

$$P = \operatorname{argmin}_{\hat{P} \in \Pi_n} \operatorname{vec}(\hat{P})^T (-(A^J)^T \otimes (A^I)^T) \operatorname{vec}(\hat{P}) - \operatorname{vec}(D^I(D^J))^T \operatorname{vec}(\hat{P}) \quad (2.4)$$

where  $\otimes$  denotes the Kronecker product and  $\operatorname{vec}(\hat{P})$  is a column-wise vectorization of  $\hat{P} \in \Pi_n$ .

The minimization problem (2.4) is the *quadratic assignment problem*, which is known to be *NP*-hard [10, 66].

The two formulations (2.2) and (2.4) have their advantages and disadvantages. The main benefit of (2.2) is the low space complexity  $\mathcal{O}(n^2)$ , whereas the space requirement of (2.4) estimates with  $\mathcal{O}(n^4)$ . This makes the second formulation to be tractable only for relative small graphs. The drawback of both formulations is the strict penalization function of edge disagreements, namely the squared Euclidean distance between matched edges. This follows straight forward from (2.2). In this sense the last formulation can be easily generalized in the way we present in the following.

We return back to the case where  $n_1 \neq n_2$ . Let us denote with a binary vector  $x \in \{0, 1\}^{n_1 n_2}$  the column-wise vectorization of the assignment matrix  $P$ , which is not necessarily a permutation matrix anymore. It is obviously, that  $x_{(j-1)n_1+i} = 1$ , if a node  $v_i \in V^I$  is matched to a node  $u_j \in V^J$ , and  $x_{(j-1)n_1+i} = 0$  otherwise. For simplicity we will write further  $x_{ij}$  instead of the complicated form  $x_{(j-1)n_1+i}$ .

To measure a similarity between graphs one considers two different kinds of similarities: second-order *edge similarity* and first-order *node similarity*. The first one is defined as a function of the edges  $s_E : E^I \times E^J \rightarrow \mathbb{R}$  and should penalize a disagreement in the structure of two graphs. The second one  $s_V : V^I \times V^J \rightarrow \mathbb{R}$  represents

additional constraints on the possible node correspondences (for example matched nodes should have similar attributes).

Using the introduced notation and definitions of the node and edge similarity functions the function  $S(G^I, G^J, m)$  in (2.1) can now be rewritten as follows:

$$S(G^I, G^J, m) = \sum_{\substack{x_{ij}=1 \\ x_{i'j'}=1}} s_E(e_{ii'}, e_{jj'}) + \sum_{x_{ij}=1} s_V(v_i, v_j) \quad (2.5)$$

This formula can also be expressed in matrix form. We define an *affinity* or *similarity matrix*  $S \in \mathbb{R}^{n_1 n_2 \times n_1 n_2}$ , whose diagonal elements are  $s_V(v_i, v_j)$  and non-diagonal elements are  $s_E(e_{ii'}, e_{jj'})$ . Using this matrix we obtain the following formulation of the graph matching problem as an quadratic optimization problem [14, 15, 16, 20, 31, 43, 44]:

$$\operatorname{argmax}_x x^T S x \quad (2.6)$$

$$\text{s.t. } x \in \{0, 1\}^{n_1 n_2} \quad (2.7)$$

$$\sum_{i=1 \dots n_1} x_{ij} \leq 1 \quad (2.8)$$

$$\sum_{j=1 \dots n_2} x_{ij} \leq 1 \quad (2.9)$$

We notice, that in the case where  $n_1 = n_2$ , both conditions (2.8) and (2.9) will be fulfilled with equality. We call this constraints *two-way constraints* [31], as they enforce one-to-one matching.

One can easily see, that the formulation (2.6)-(2.9) can be obtained from (2.4) by setting  $S = (A^J)^T \otimes (A^I)^T$  with diagonal elements equal to  $\text{vec}(D^I (D^J)^T)$ .

Below we list different ways to define node and edge similarities between two attributed graphs we found in the literature.

### Edge similarity

One possible approach to calculate an edge similarity is to calculate *edge dissimilarity*  $d_E : E^I \times E^J \rightarrow \mathbb{R}$  first and then transform it into similarity by using, for example, one of the following functions [13, 14, 15, 16]:

$$\bullet \quad s_E(e_{ii'}, e_{jj'}) = \exp\left(-\frac{d_E(e_{ii'}, e_{jj'})^2}{\sigma_s^2}\right) \quad (2.10)$$

$$\bullet \quad s_E(e_{ii'}, e_{jj'}) = \max(\beta - d_E(e_{ii'}, e_{jj'})/\sigma_s^2, 0) \quad (2.11)$$

where  $e_{ii'} \in E^I$  and  $e_{jj'} \in E^J$ . The parameters  $\sigma_s$  and  $\beta$  define a sensibility of a graph matching algorithm to the dissimilarities between the graphs.

This leads us to the question how to calculate edge dissimilarity. The most obvious way is to compare the weights of the edges, if they are provided. An other alternative could be to use the length of the edges [13, 14, 15, 16], if coordinates of the nodes in some system (usually Cartesian coordinates) are known. It is a significant assumption, which holds however true for almost all graphs arose in practical applications.

Sometimes node attributes can be used to calculate edge dissimilarities. For example, if graph nodes are described by an ellipse with known center coordinates and orientation, one can calculate so-called geometric dissimilarity of the edges [13, 15]:

$$d_E(e_{ii'}, e_{jj'}) = \frac{1}{2}(d_{geo}(m_{i'}|m_i) + d_{geo}(m_i|m_{i'})) \quad (2.12)$$

$$d_{geo}(m_{i'}|m_i) = \frac{1}{2}(\|x_{j'} - H_i x_{i'}\| + \|x_{i'} - H_i^{-1} x_{j'}\|) \quad (2.13)$$

$$d_{geo}(m_i|m_{i'}) = \frac{1}{2}(\|x_j - H_{i'} x_i\| + \|x_i - H_{i'}^{-1} x_j\|) \quad (2.14)$$

where  $m_i$  is a correspondence between nodes  $v_i \in V^I$  and  $v_j \in V^J$  and  $H_i$  is an affine homography from  $v_i$  to  $v_j$  estimated based on elliptic regions around each node.  $x_i$  and  $x_j$  denote the centers of this elliptic regions.

Another way to calculate edge similarities could be to use directly some similarity measure, such as cosine similarity<sup>2</sup>.

### Node similarity

If a given graph has node attributes, the most natural method to measure a similarity of two nodes is to compare their attributes. In most of the seen literature, the node attributes are represented by  $r$ -dimensional real vectors:  $D^i, D^j \subset \mathbb{R}^r$ . This means, we can adopt all techniques<sup>3</sup> described in the previous paragraph to define a node similarity function. Additionally, in case when node attributes can be considered as some distribution (e.g. distribution of gray values of an image around a node), one can use metrics to measure the distance between two distributions. For example, Schellewald and Schnörr [68] used the earth mover's distance for this purpose.

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<sup>2</sup>The cosine similarity of two vectors  $x_1, x_2 \in \mathbb{R}^n$  is equal to  $s_{cos} = \frac{x_1^T x_2}{\|x_1\|_2 \|x_2\|_2}$

<sup>3</sup>with exception of the geometric dissimilarity measure

**Error correcting graph matching**

Another way to measure the similarity between two graphs is based on a *graph edit distance* [8]. The graph edit distance is defined through costs of *graph edit operations*, that transform one graph into another. Those operations are insertion, deletion and substitution of nodes and edges of a graph. An algorithm, that uses graph edit distance for graph matching, is often called *error correcting* [20].

Consider two attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$  and a matching  $m$  between subsets  $\bar{V}^I, \bar{V}^J$  of  $V^I$  and  $V^J$  respectively. The edit operations on nodes can be directly defined by the mapping  $m$  [6]:

- if  $m(v_i) = v_j$  for  $v_i \in \bar{V}^I, v_j \in \bar{V}^J$ , then a node  $v_i$  is *substituted* by a node  $v_j$
- nodes in  $V^I \setminus \bar{V}^I$  are *deleted*
- nodes in  $V^J \setminus \bar{V}^J$  are *inserted*.

An edit operation of an edge is defined based on a transformation applied to its end nodes. For example, insertion of a node  $v_j \in V^J$  implies that all edges, connected to this node, are also inserted. Alternatively, if a node  $v_i \in V^I$  is deleted, then all edges incident to this node are also deleted. We say, that an edge  $\{v_i, v_{i'}\} \in E^I$  was substituted by an edge  $\{v_j, v_{j'}\} \in E^J$ , if the nodes  $v_i, v_{i'}$  were mapped in  $v_j, v_{j'}$  respectively.

We assume that all operations can be performed simultaneously. Let  $S = \{s_1, s_2, \dots, s_k\}$  denote a set of operations needed to transform the graph  $G^I$  into the graph  $G^J$ . Each edit operation  $s_i, 1 \leq i \leq k$ , has an assigned nonnegative cost  $c(s_i)$ . The cost of the whole sequence  $S$  is defined as  $\sum_{i=1}^k c(s_i)$ . Using this and following the papers [8, 79] we define a *edit distance* between the graphs  $G^I$  and  $G^J$  as follows:

$$dist(G^I, G^J, m) = \min_{S=\{s_1, \dots, s_k\}} c(S) \quad (2.15)$$

The task of the error-corrected graph matching is to find such a mapping  $m$  between  $V^I$  and  $V^J$ , which induces the cheapest transformation between the graphs.

The cost functions of each operation are often defined as functions of edge weights and node attributes. However their exact definition depends on a specific application. Sometimes it can be helpful, when the distance measure (2.15) defines a metric, which is not automatically the case. Bunke and Allermann [8] have shown that the graph edit distance can fulfill the properties of a metric under specific conditions on the cost functions of the individual edit operations. For example, one of this

conditions is, that a single operation is always preferred to a sequence of two operations with the same result (triangular inequality of the operation cost functions). Later, Bunke and Shearer [9] have suggested a new graph edit distance that does not depend on the cost of the edit operations and is a metric.

An interesting question is, how does the error corrected graph matching problem correspond to other matching problems defined previously. It was shown in [7] that graph isomorphism, subgraph isomorphism and maximum common subgraph problems can be considered as a special case of the error correcting graph matching. The same holds true for the inexact graph matching problem formulated as in (2.2). This is easy to see, if one rewrite the objective function of (2.2)<sup>4</sup> as  $\sum_{i=1}^n \sum_{i'=1}^n (A_{ii'}^I - A_{\sigma(i)\sigma(i')}^J)^2$ . A comparison of this expression with the definition of  $c(S)$  in (2.15) leads us directly to the idea, how to set the edge insertion/deletion/substitution cost functions so that the problem formulations are equivalent:

$$c(e_{\text{subst}}) = (A_{ii'}^I - A_{\sigma(i)\sigma(i')}^J)^2 \quad c(e_{\text{insert}}) = (A_{\sigma(i)\sigma(i')}^J)^2 \quad c(e_{\text{del}}) = (A_{ii'}^I)^2$$

## 2.5 Methods for solving inexact graph matching problems

In the following we briefly describe common approaches for solving inexact graph matching problems in the field of Computer Vision and Pattern Recognition. We have subdivided them into groups based on their main idea.

### 2.5.1 Discrete optimization

#### Tree search methods

Similar to the exact graph matching problems tree based methods with backtracking were successfully applied to solve inexact graph matching problems. They were heavily used for the error-correcting graph matching. In this case a searching procedure can be efficiently guided, so that the required time is shorter than the exponential time needed by a blind searching. This can be done by defining the score of the tree nodes as a sum of two scores: a matching score of a current partial solution and a heuristically estimated score of remaining nodes. The algorithms in this group differ mainly in a suggested heuristics for calculation of future costs and in rules for tree

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<sup>4</sup>For simplicity we assume that the costs of the edit operations does not depend on the node attributes and therefore we can omit the second term in Eq. (2.2)

traversing. The mostly used strategies for tree traversing are depth-first-search [21] and  $A^*$ -Algorithm [33].

One of the first algorithms for inexact graph matching based on tree search was presented by Tsai and Fu in paper [74]. It is an optimal inexact graph matching algorithm. For further examples of tree search methods for inexact graph matching we refer to papers [8, 70, 79].

### **Simulated Annealing**

Simulated annealing is a heuristic for searching the global optimum of a given energy function [10]. It is an extension of the Metropolis Algorithm [54], that was suggested for finding an equilibrium of a physical system consisting of individual particles by heating it first and then cooling it slowly down. Speaking in terms of a graph matching problem its solutions define states of a system and corresponding objective scores its energy. The idea is to find a state with the lowest energy by performing some random changes in a system. This can be a random exchange of correspondences between two pairs of matched nodes. A change, that decreases the total dissimilarity of graphs, is always accepted. On the other side, a change, that increases the energy function, is accepted with some probability. This probability and number of changes per iteration is controlled by the temperature parameter  $T$ . The lower  $T$  the fewer changes are allowed and the lower the accepted probability is.

The application of simulated annealing to graph matching problems can be found in [35]. This heuristic can also be used to solve a quadratic assignment problem [10].

### **2.5.2 Continuous optimization**

This group of methods is one of the biggest and best investigated. The main idea is to transform the inexact graph matching problem into a continuous optimization problem. This can be done, for example by relaxing the integer constraints in the discrete optimization problems (2.2), (2.6)-(2.9). A found solution must be converted afterwards back onto the discrete domain. Depending on techniques applied to solve a continuous problem we subdivide this group into several subgroups. The list of the algorithms presented here is not complete. As we already mentioned, we selected mainly the classical approaches and/or those we investigated during the work on this thesis.



The first subgroup of algorithms contains the algorithms, that relax all constraints of a graph matching problem, find a continuous solution of the new nonlinear problem and project it back onto the discrete domain in such a way, that a final solution fulfills the problem constraints.

In 1996 Gold and Rangarajan presented a graduated assignment algorithm for graph matching (GAGM) [31]. It is an iterative algorithm, which uses the *deterministic annealing*<sup>5</sup> to solve the graph matching problem formulated as in (2.6)-(2.9). The authors use Taylor series approximation to relax the initial quadratic assignment problem to a linear assignment problem. The two-way constraints are enforced at each iteration by converting a found continuous solution onto a double stochastic matrix by applying exponentiation and Sinkhorn normalization [73]. This technique is called *soft-assign*. The deterministic annealing was also used in [60] to solve Lagrangian Relaxation of the problem (2.2) and in the robust point matching algorithm with thin-plane spline (RPM-TPS) [19]. The solution obtained by this method is however not necessary optimal and the behavior of the algorithms depends highly on the selected parameters, especially those, which control the annealing schema.

Another iterative algorithm was proposed in [44] and is called an integer projected fixed point method (IPFP). It consists of two steps, which we shortly describe below. In the first step, an initial solution has to be chosen. It can be, for example, a continuous or discrete solution obtained by some other algorithm. The second step iteratively improves this solution by applying the *Frank-Wolfe algorithm* [29] adapted to the graph matching problem. This algorithm first finds the best search direction by solving an linear assignment problem. The last arises as in GAGM by the maximization of the first-order Taylor series approximation of the objective function. The maximization is performed in the discrete domain using the Hungarian algorithm [40]. Then the initial objective function is further maximized in a continuous domain along the found direction. The authors show, that in praxis IPFP tends to converge towards discrete solutions, that are close to the optimum.

The Fast Approximative Quadratic Programming Algorithm (FAQ), presented in [78], also uses the Frank-Wolfe algorithm to solve a continuous relaxation of the problem (2.3). However FAQ performs completely in a continuous domain and has a third step, which maps a found continuous solution back onto the discrete domain.

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<sup>5</sup>Deterministic annealing is similar to the simulated annealing, but uses deterministic techniques to find a minimum of an energy function by a current value of a temperature parameter [62].

Unlike IPFP, the FAQ algorithm does not use the similarity matrix  $S$ . This gives it a big advantage as less space is required. Therefore it is possible to apply the algorithm to big size graphs<sup>6</sup>.

Another approach, that uses the Frank-Wolfe algorithm, is the PATH-Algorithm [82]. The algorithm first finds the global optimum of the Lagrangian relaxation of the minimization problem (2.3). This is done by applying the Newton method [4]. Afterwards the found solution is projected back onto the discrete domain by solving a sequence of convex and concave problems with the Frank-Wolfe algorithm.

The fast projected fixed-point algorithm (FastPFP) proposed by Lu et al. [48] is very close to IPFP. This algorithm uses the *projected fix point method* to find a solution of a continuous relaxation of the problem (2.2). Compared to IPFP the new algorithm uses projections onto a continuous domain, instead of a discrete. Furthermore the authors proofed the linear convergence rate of their algorithm, whereby the convergence rate of IPFP is unknown. The FastPFP, similar to FAQ, does not have a memory issue because it does not use a similarity matrix  $S$ . Also it is generally faster than both IPFP and FAQ, as it does not solve a linear assignment problem on each iteration.

A completely different approach to solve the graph matching problem was suggested by Schellewald and Schnörr [68]. They formulated the graph matching problem as a regularized bipartite matching problem [24], which is then relaxed to a convex semidefinite program. The last can be solved with standard algorithms, such as the interior point method [4]. A novelty of the algorithm consists in a probabilistic post-processing step, which convert a found continuous solution onto a discrete one. The suggested algorithm is easy to apply, as it has only one parameter. However the considered relaxation problem has a squared size comparing to the initial problem [22]. Consequently, the algorithm is not suitable for big graphs.

### Spectral methods

A big group of algorithms for solving graph matching problems is built by those, which use an eigenvalue decomposition [4] of the adjacency matrices of given graphs. The idea behind this is, that the eigenvalues of the adjacency matrices of two isomorphic graphs are equal, as they are invariant to the node permutation<sup>7</sup>.

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<sup>6</sup>Evaluation results in the paper include test with graphs with up to 1000 nodes

<sup>7</sup>Indeed, let  $A$  and  $B$  be adjacency matrices of two isomorphic graphs. This means, that  $B = PAP^T$ , where  $P$  is a permutation matrix. If  $\alpha$  is an eigenvalue of  $A$  ( $Av = \alpha v$ ) and  $u = Pv$ ,

One of the first algorithms, which uses spectral techniques, is the one by Umeyama [76]. He considers the case, when two graphs have the same number of nodes and matching between them is bijective. This means, that a desired correspondence matrix must be a permutation matrix. The author proves, that an orthogonal matrix, which minimizes the objective function of (2.2) without second summand, can be formulated based on the eigenvalue decomposition of the adjacency matrices of given graphs. The terms of this decompositions are used to define a linear assignment problem, whose solution is a solution of the initial problem. In case, when given graphs are sufficiently close, the obtained solution is optimal or nearly optimal.

We want to mention, that this algorithm is highly limited in its application due to its requirements. An additional drawback is that it works only with graph geometry and does not consider attributes of nodes and edges.

The more recent algorithm in this group of methods is called spectral matching (SM) [43]. The algorithm works with the general problem formulation (2.6)-(2.9). It relaxes both two-way and integer constraints (2.7)-(2.9) and obtain the optimal solution of this relaxation by taking the principal eigenvector of the matrix  $S$ . This is done by using *the power iteration method* [32]. The found continuous solution is binarized by applying a simple greedy heuristic, that enforces previously relaxed matching constraints.

A generalization of the SM algorithm is proposed in [25]. The authors suggest to consider similarities between tuples of nodes and not only pairs to improve the graph matching quality. They formulate a new problem using hyper-graphs and tensor notation. The solution strategy is however the same as it is in [43]: the solution is approximated with the principal eigenvector of the matrix  $S$  and discretized afterwards. However, the power iteration method has been adopted to the tensor based problem, because it cannot be applied directly.

Before going to the next section we want to describe shortly a max-pooling approach by Cho and Duchenne [16], which uses ideas similar to both GAGM [31] and SM [43], but replaces one of the sums in a updating step with maximum-operation. The algorithm solves the graph matching problem formulation (2.6)-(2.9) by relaxing its integer constraints and omitting sum constraints. To approximate a solution of  $\operatorname{argmax}_x x^T S x$  the max-pooling algorithm similar to GAGM uses first order Taylor

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then the following holds  $Bu = (PAP^T)u = (PA)(P^T u) = (PA)v = P(\alpha v) = \alpha u$ . So  $\alpha$  is an eigenvalue of  $B$ .

expansion of the objective function. The maximization of the Taylor approximation can be done by the power method as it is done in SM. The resulting update formula of the correspondence  $(v_i, v_j), v_i \in V^I, v_j \in V^J$  has the form:

$$(Sx)_{ij} = x_{ij}s_V(v_i, v_j) + \sum_{i' \in N_i} \sum_{j' \in N_j} x_{i'j'} s_E(e_{ii'}, e_{jj'}), \quad (2.16)$$

where  $N_i$  denotes a direct neighborhood of a node  $v_i$ , i.e. set of its adjacent nodes. The max-pooling algorithm uses a maximum function instead of the second sum in the second term, which leads to

$$(Sx)_{ij} = x_{ij}s_V(v_i, v_j) + \sum_{i' \in N_i} \max_{j' \in N_j} x_{i'j'} s_E(e_{ii'}, e_{jj'}). \quad (2.17)$$

This simple idea helps to suppress noisy entries of the outlier matches, because they have more likely low similarity values. The proposed algorithm shows very good results in presence of numerous outliers, although there is no theoretical justification of its convergence.

### Probabilistic frameworks

Another group of algorithms applies *relaxation labeling* to solve graph matching problems. The aim of the relaxation labeling is to find an optimal assignment between set of labels and set of objects. Each label has some initial probability to be assigned to certain objects. Those probabilities are set based on some informations known about the objects. In terms of graph matching problems, nodes of one graph are considered as objects and nodes of another graph as labels. The initial probabilities of assignments between the nodes are calculated based on the node and edge attributes.

Earlier works on this formulation are the one by Fischer and Elschlager [28] and Rosenfeld et al. [63]. In both cases, the proposed algorithms start with some initial label probabilities and try to reduce a labeling ambiguities at each iteration based on labels of neighboring nodes. Initial probabilities can be calculated based on the node connectivity or on the node attributes and/or edge weights, if such are provided. The process runs till convergence or some predefined number of iterations. The algorithms are heuristic, but reduce the complexity of the initial problem to polynomial [18].

A first algorithm with theoretically proofed update rule is suggested by Kittler and Handcock [38]. This was later improved by Christmas et al. [18], who suggested a

method to include provided node attributes and edge weights into the update rule of the labeling probabilities and not only in the initialization step.

Later algorithms formulate the graph matching problem as the Maximum A Posteriori probability (MAP) estimation. For example, the matching process in [80] is a process of node exclusion and insertion, so that the MAP rate monotonically increases in each iteration. This technique is suggested to effectively cope with possible outliers in the sets of graph nodes. A node is considered as an outlier, if its deletion improves the consistency in the structure of two graphs. The structural constraints hereby are defined by a dictionary of feasible mappings between local neighborhoods (super-cliques) of nodes of two graphs. The algorithm shows good results in case of big number of outliers, but is slow.

Another interesting idea is presented in paper [49]. Given are two graphs, nodes of the first graph are considered as an observed data and the nodes of the second graph as hidden random variables. In this formulation the graph matching problem is solved using the *Expectation-Maximization algorithm* (EM) [23]. A similar algorithm is presented in the recent paper [67]. However, it works with the continuous correspondences between the graph nodes and projects them in the discrete domain using the soft-assign technique described previously. It also includes structural information<sup>8</sup> into the matching process, whereby the algorithm from [49] uses only geometrical information. Both algorithms however are not applicable to big graphs due to the unlimited increasing of the formulated density function with the size of the graphs [3]. A new scalable graph matching algorithm, which also uses EM to solve the problem formulated in a maximum likelihood estimation framework, is presented recently in [3]. The scalability is achieved there by constraining the number of candidate matches between two node sets and by letting only close node neighborhoods to vote for candidate matches.

### Methods using clustering techniques

We want to special emphasize the methods, that use clustering techniques to improve the graph matching score or performance.

Minsu Cho [13] proposes to use *agglomerative clustering* on a set of candidate matches to effectively cope with outliers. The problem is formulated as in (2.6)-

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<sup>8</sup>Structural relations between nodes are given through the adjacency matrix of a graph. Geometrical relations are represented as relative position of the nodes with respect to each other [67].

(2.9). The considered graphs are attributed, so that candidate matches are selected based on the distance between node attributes. The algorithm is controlled by the dissimilarity measure between two clusters, which is defined as the average of  $k$  smallest pairwise dissimilarities between points in two clusters. This linkage model is called by the authors *adaptive partial linkage model*. Notice, that the points in clusters are pairwise correspondences between graph nodes. The dissimilarity between two nodes is defined as a linear combination of the node attribute dissimilarities and geometric dissimilarities (see Eq. (2.12)). Empirical results show, that correct correspondences tend to build bigger clusters. In contrast to that, the outliers are likely to stay in small groups, so it is possible to detect them using threshold value of the cluster size.

Another algorithm based on the hierarchical clustering is suggested by Carcassoni and Hancock [11]. Its main idea is to provide additional constraints, that can be used to improve the robustness of a graph matching algorithm against graph deformations. This was successfully achieved by performing independently spectral clustering of the given graphs and then first finding correspondences between clusters and afterwards between the nodes inside the clusters. The correspondences between clusters represent the desirable additional constraints. To perform matching the authors used a probabilistic matching algorithm.

A further benefit of using clustering methods is the potential complexity reduction. The first idea to achieve this is based on a hierarchical graph matching and appears, for example, in the work by Qui and Hancock [59]. They suggest to use a graph partition to create a new simplified graph, whose nodes represent clusters of the initial graph. After partitioning graphs are matched in a similar manner as it is suggested by Carcassoni and Hancock [11], where the derived clusters tie matching constraints. The used partition method is based on a spectral method and creates a set of non-overlapping node neighborhoods<sup>9</sup>. To build those they use Fiedler vector (eigenvector associated with the second smallest eigenvalue of a graph Laplacian matrix, see [26]). The authors provide a study, which shows that the matching with the proposed partition technique is stable under structural errors. Additionally, they show, that the simplified graphs preserve the structure of initial graphs. The last is shown by performing clustering of a group of different graphs before and after simplification.

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<sup>9</sup>A node neighborhood is defined here as a node with all its adjacent nodes.

The second idea to reduce complexity of the initial matching problem uses graph clustering to create a set of independent subproblems. The matching is then performed for each subproblem independently and due to the reduced problem size faster. A solution of the whole problem is then obtained by combining local solutions. The great benefit of such an approach is the ability to parallelize the computation process, which can lead to a significant time reduction.

The described idea is followed by Lyzinski et al. [50]. The aim of the authors is to parallelize a graph matching algorithm for matching very big graphs. However the problem, they consider, is semi-supervised, what means that correct correspondences between some nodes are known. It is obvious, that the matching results of the subdivided problem depends highly on the quality of the graph clusters and established correspondences between the clusters of two graphs. In a perfect clustering, nodes that should be matched, must lie in the corresponding subgraphs. To ensure that the clustering is sufficiently good, the authors propose a technique, that first spectrally embeds graphs and then jointly cluster them. The algorithm was successfully applied to graphs with 20000 – 30000 nodes.

## 2.6 Discussion

In this chapter we have introduced the graph matching problem and talked about different approaches for solving it. We have seen, that this problem can have many variations depending on the required properties of matching. One distinguishes often two main groups: exact and inexact graph matching problems. The first group is characterized by searching for a structure preserving mapping between two graph. This requirement is however often too strict for practical applications, where some variations in the graph structure are normal. For this reason we concentrated ourself on the inexact graph matching problems, whose aim is to find the best possible matching between two graphs. We have shown different ways to formulate inexact graph matching problems (e.g. as quadratic assignment, least squares problems or using graph edit distance) and how different formulations are connected to each other. At the end we have given an overview of existing algorithms for solving graph matching problems. We used the extensive survey by Conte et al. [20] as a baseline and extended it further with recent works in the field. Most of the existing algorithms were developed for matching relative small graphs (often only up to 100 nodes) and their direct application to bigger graphs is sometimes impossible due to

the polynomial increase of time and storage demand. In the next chapter we describe a framework, which allows an application of existing graph matching algorithms for matching bigger graphs.



# Chapter 3

## Two level graph matching

In this chapter we describe our novel approach for graph matching. Our aim however was not to develop a new matching algorithm, but to propose a framework, which would help to solve problems, where the direct application of existing matching algorithms is impossible due to memory requirements or runtime. This is often the case when a graph matching problem is formulated using a similarity matrix between graphs (see Eq. (2.6)). The main idea of our approach is based on a variation of the *divide and conquer* technique [21], which is well known for example from its application for array sorting algorithms. According to this general paradigm, a given graph matching problem, which is too difficult to be solved directly, is subdivided into smaller subproblems. Those subproblems are created in such a way, that they can be solved without great effort. A resulting solution is then combined from local solutions of single subproblems. A disadvantage of such an approach is however, that a runtime improvement is sometimes paid with a drop in the accuracy. Due to that, one want to have a trade off between speed up and accuracy. What is more important depends on the particular problem.

Several existing algorithms share similar ideas. Those which are closest to our approach were described in the previous chapter under the group of algorithms based on clustering techniques. Below we review them shortly again to point out, that none of them is completely repeated by our framework.

This chapter is organized as follows. First of all we formulate a considered graph matching problem and show some issues of this formulation. In the second part, we describe our two level graph matching framework, which should help to cope with the formulated problems.

### 3.1 Problem statement

Consider two attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$ , where  $V^{I(J)}$ ,  $E^{I(J)}$ ,  $D^{I(J)}$  denote set of nodes, set of edges and set of node attributes respectively. We assume the situation, that those graphs are undirected and do not have multiple edges between nodes. Let the size of the first graph be  $n_1$  and the second  $n_2$ . Without loss of generality, we assume that  $n_1 \leq n_2$ . Attributes of the graphs are  $r$ -dimensional real vectors:  $D^I, D^J \in \mathbb{R}^r$ .

We define a problem of matching two graphs  $G^I$ ,  $G^J$  as a quadratic assignment problem (same formulation as Eqs. (2.6)-(2.9)).

$$\operatorname{argmax}_x x^T S x \quad (3.1)$$

$$\text{s.t. } x \in \{0, 1\}^{n_1 n_2} \quad (3.2)$$

$$\sum_{i=1 \dots n_1} x_{ij} \leq 1 \quad (3.3)$$

$$\sum_{j=1 \dots n_2} x_{ij} \leq 1 \quad (3.4)$$

We denote a pair of nodes  $(v_i, v_j)$ , where  $v_i \in V^I$  and  $v_j \in V^J$ , as a correspondence between the sets  $V^I$  and  $V^J$ . Let  $M$  be a set of all possible correspondences between the nodes of the graphs  $G^I, G^J$ . Obviously  $M$  consists of  $n_1 n_2$  node pairs. Then the vector  $x \in \{0, 1\}^{n_1 n_2}$  is an indicator vector of a subset  $m = \{(v_i, v_j) | v_i \in V^I, v_j \in V^J\}$  of the set  $M$ . This means, that element  $x_k$  of this vector is equal 1 if and only if the corresponding  $k$ -th node pair  $(v_i, v_j)$  is selected into subset  $m$ . The constraints (3.3), (3.4) ensure, that each node of the graph  $G^I$  is matched to exactly one node of the second graph  $G^J$ .

The matrix  $S \in \mathbb{R}^{n_1 n_2 \times n_1 n_2}$  in Eq. (3.1) encloses the precomputed information about similarity of two graphs. Rows (columns) of this matrix correspond to the elements in the set  $M$  of all possible node correspondences. Its diagonal elements  $S_{kk}, k = 1, \dots, n_1 n_2$ , contain similarity measurements of the node pairs  $(v_i, v_j) \in M$ . The non-diagonal elements measure similarity of edges between two pairs of matched nodes. Our aim is to find maximal  $n_1$  correspondences between the nodes of the graphs  $G^I, G^J$ , which maximizes the similarity value between those graphs.

As we saw in the previous chapter, the selected formulation of a graph matching problem is widely used as the most general one. However, the size of the affinity matrix  $S$  can cause problems due to the required memory demands. For example, a

dense affinity matrix between two graphs with 200 nodes each needs approximately 12Gb memory (double precision). There are several possible ways to reduce the memory complexity of the formulated graph matching problem. Here we mention three possible approaches.

The first one is to reduce a set of candidate correspondences by selecting a subset  $M' \subset M$ . This can be done, for example, by restricting the number of candidate matches for a node  $v_i \in V^I$  to some number smaller than  $n_2$ . This method is often used, as it not only solves memory issues of the problem formulation as defined in Eqs. (3.1)-(3.4), but also reduces the algorithmic complexity of many algorithms, which highly depend on the number of possible matches (e.g. [14, 15, 16, 43]).

The second possibility is to make the matrix  $S$  sparser by excluding the comparison of some nodes or edges from the consideration. In case of big graphs this can however lead to a high loss of initially provided information and influences dramatically the quality of a resulting matching.

The third possibility is to replace the initial problem of graph matching by a set of smaller subproblems, that arise by partitioning given graphs into subgraphs and matching those subgraphs. It means, that the matrix  $S$  is divided into blocks, where each block represent a similarity matrix between two subgraphs. Thereby the similarities of edges, whose nodes belong to different subgraphs after problem splitting, will be ignored. On the one hand, this approach solves the memory problem by replacing the initial matrix  $S$  with a set of smaller affinity matrices. On the other hand, it does not necessarily reduce the time complexity of the initial problem, as selection of correspondences between subgraphs means in the worst case their pairwise matching in all possible combinations. Otherwise, further information will be lost. Despite the mentioned drawbacks, the single subgraph matching problems can be eventually parallelized, that still makes the approach attractive to be applied on big graphs.

In the framework for graph matching, that we describe in detail below, we use the third of the described techniques. We divide given initial graphs into subgraphs and iteratively search first for correspondences between the subgraphs and then for node correspondences between matched subgraphs. For subgraph matching we use an existing matching algorithm. A graph partitioning is performed only at the initialization step, but after each iteration subgraphs have a chance to exchange nodes on their borders.

To our best knowledge the described method was not published before. Especially, we haven't seen an iterative graph matching algorithm based on graph clustering so far, which updates initial partitions. At the same time there is a certain overlap in ideas between ours and existing works. The algorithm proposed by Lyzinski et al. [50] uses graph partitioning to parallelize a semi-supervised graph matching problem, where some correspondences between graph nodes are provided. The graph matching problem is formulated as a minimization problem (2.2), that does not use an affinity matrix  $S$ . The given matches between graph nodes are used to cluster two graphs jointly and to find correspondences between subgraphs. As a consequence, subgraphs of given graphs are similar enough to ensure the matching quality. However the proposed clustering method cannot be used for an unsupervised matching.

An idea similar to our one to use graph partition for graph matching in unsupervised cases was used by Carcassoni and Hancock [11], Qui and Hancock [59] and recently by Nie et al. [56]. From them only the algorithm by Nie et al. [56] considers the same maximization problem as we do. The two other algorithms formulate the graph matching problem in terms of relaxation labeling. Also the definition of the graph clusters differs between the algorithms. Qui and Hancock, as well as Nie et al., consider clusters, that are built by direct neighborhoods of nodes. The resulting partition can be overlapping [56] or not [59]. Our algorithm and the one in the paper of Carcassoni and Hancock [11] consider the more general case, where a graph partition is given by a disjoint set of arbitrary subgraphs of a graph. Finally, similar to our approach Qui and Hancock [59] use the extracted graph partitioning to create a new graph, whose nodes represent clusters of the initial graph. They call this process graph simplification. However their approach quite differs from ours, because of the special definition of clusters, another problem formulation and a different approach for solving the single matching problems, as we mentioned in the previous chapter.

We also would like to mention the progressive graph matching algorithm by Cho and Lee [15]. This is an iterative algorithm, which is built similar to our approach on top of an existing graph matching algorithm. It starts with a set of candidate matches between nodes of the initial graphs and updates this set in each iteration by replacing some candidates with better ones. The selection of new candidates is based on the estimation of a homography between features of matched nodes. In case of bigger graphs this approach reduces the problem to a smaller one by keeping fixed the number of considered candidate matches and solve the smaller

problem. As opposite to this we reduce the complexity by considering a set of smaller subproblems, which together solve the initial problem.

In the remainder of this chapter we describe in detail our graph matching framework.

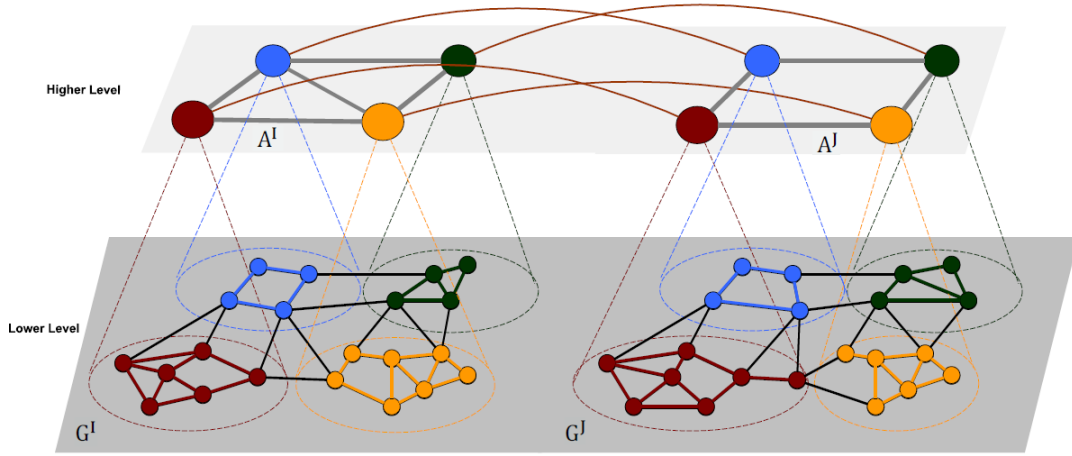
## 3.2 Two level graph matching algorithm

For simplicity we consider at the beginning only one graph  $G^I = (V^I, E^I, D^I)$  of size  $n_1$ . Assume, that we know a partition of the node set  $V^I$  of this graph into  $m_1$  non-overlapping clusters based on some rule:  $V^I = \cup_{k=1}^{m_1} V_k^I$ , where  $V_{k_1}^I \cap V_{k_2}^I = \emptyset$  for  $k_1 \neq k_2$ . Based on this partition the initial graph  $G^I$  is subdivided into a set of node induced subgraphs  $\{G[V_k^I]\}_{k=1}^{m_1}$ . Note, that it holds  $G[V^I] \cup \dots \cup G[V^{m_1}] \subset G^I$ , because edges between different subgraphs are not presented in the left union. Further, we define a mapping  $U$  between the set of graph nodes  $V^I$  and another set of nodes  $V^{Ia} = \{a_k\}_{k=1}^{m_1}$ , where a single node  $a_k$  represents a subgraph  $G[V_k^I]$ . This mapping can be expressed as an matrix  $U^{Ia} \in \{0, 1\}^{n_1 \times m_1}$  with elements

$$U_{ik}^{Ia} = \begin{cases} 1, & \text{if node } v_i \in V_k^I, \\ 0, & \text{otherwise.} \end{cases} \quad (3.5)$$

The new set  $V^{Ia}$  defines a node set of a new graph built on top of the other one. A pair of new nodes  $a_{k_1}, a_{k_2} \in V^{Ia}$  is connected with an edge if and only if there is at least one edge in the initial graph  $G^I$  between the corresponding clusters  $V_{k_1}^I$  and  $V_{k_2}^I$ . The set  $V^{Ia}$  together with the set of edges between its elements and correspondence matrix  $U^{Ia}$  builds a new graph  $A^I = (V^{Ia}, E^{Ia}, U^{Ia})$ . We will call the graph  $A^I$  an *anchor graph* of the graph  $G^I$  and its nodes *anchor nodes* or just *anchors*. The graph  $G^I$  together with its anchor graph  $A^I$  builds a two level system: the graph  $G^I$  is located on the lower (finer) level and the graph  $A^I$  on the higher (coarser) level (see Fig. 3.1).

We return now back to the case of two graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$ , which we want to match. For each of them we build an anchor graph  $A^I = (V^{Ia}, E^{Ia}, U^{Ia})$  and  $A^J = (V^{Ja}, E^{Ja}, U^{Ja})$  respectively. Now instead of matching graphs  $G^I$  and  $G^J$  directly on the lower level, we want to match first the corresponding anchor graphs. Matches between anchor nodes give us correspondences between underlying subgraphs. After that, we can perform graph matching for each pair of matched subgraphs independently. A union of local solutions from the single subgraph matching problems gives us a solution of the initial problem.



**Figure 3.1:** Two level framework for graph matching

More formally, we replace the objective function of the initial matching problem (see Eq. (3.1), (2.5)) with the new function:

$$S(G^I, G^J, m|m^a) = \sum_{\substack{v_i, v_{i'} \in V_k^I \\ v_j, v_{j'} \in V_p^J \\ m(v_i)=v_j, m(v_{i'})=v_{j'} \\ m^a(a_k)=a_p}} s_E(e_{ii'}, e_{jj'}) + \sum_{\substack{v_i \in V_k^I \\ v_j \in V_p^J \\ m(v_i)=v_j \\ m^a(a_k)=a_p}} s_V(v_i, v_j), \quad (3.6)$$

where  $S(G^I, G^J, m|m^a)$  denotes the similarity of the initial graphs given the matching  $m^a = \{(a_k, a_p) | a_k \in A^I, a_p \in A^J\}$  of the corresponding anchor graphs or, which is the same, the correspondences  $\{(V_k^I, V_p^J) | V_k^I \subset G^I, V_p^J \subset G^J\}$  between the subgraphs of the initial graphs.

Why can this approach be better than the direct one? As we can see from the previous section the time and space complexity of the considered graph matching problem depends highly on the size of initial graphs. Constructed anchor graphs are however several time smaller than the initial graphs, which means, the matching algorithm on the anchor level can be performed much faster and without high memory demand compared to the lower level. The same holds true for matching between the subgraphs. Obviously, the accuracy of such an two level matching approach depends heavily on the partition of the initial graphs into subgraphs and on the quality of a graph matching algorithm on both the higher and lower levels. We concentrate ourself on the first of this two critical moments and use an existing algorithm for graph matching. To make the described two level approach more robust against graph partitioning we suggest to use an obtained matching between two graphs to correct

their partitions. The overall procedure (matching on the higher level, matching on the lower level and partition updating) is then repeated iteratively till convergence of the objective function (3.1). We call our algorithm 2LevelGM and summarize it below in Alg.1.

---

**Algorithm 1:** 2LevelGM( $G^I, G^J, N, R, \epsilon$ )
 

---

**Input:** initial graphs  $G^I, G^J$

maximal number of iterations  $N$

convergence parameters  $R$  and  $\epsilon$

**Output:** set  $m$  of correspondences between the nodes in  $V(G^I)$  and  $V(G^J)$

```

1 construct anchor graph  $A^I$  of the graph  $G^I$ 
2 construct anchor graph  $A^J$  of the graph  $G^J$ 
3  $i=0, r=0, score_i=0$ 
4 while  $r < R$  AND  $i \leq N$  do
5      $i = i + 1$ 
6     if  $i \geq 2$  then
7          $\lfloor$  update subgraphs  $G[V_k^I], G[V_p^J], k = 1 \dots, m_1, p = 1 \dots, m_2$ 
8         match anchor graphs  $A^I, A^J$ 
9          $m_i = \emptyset$ 
10        foreach pair of matched anchors  $(a_k, a_p), a_k \in V(A^I), a_p \in V(A^J)$  do
11            match subgraphs  $G[V_k^I], G[V_p^J]$ 
12             $m_i = m_i \cup \{m_i^{kp}\}$  /*  $m_i^{kp}$  set of local correspondences */
13             $score_i = x^T S x$  /*  $x$  the indicator vector of the subset  $m_i \subseteq M$  */
14            if  $|score_i - score_{i-1}| < \epsilon$  then
15                 $r = r + 1$ 
16            else
17                 $r = 0$ 
18 return  $m_i$ 
    
```

---

In the following we describe in detail the single steps of our approach: graph partitioning (lines 1,2), graph matching algorithm on both levels (lines 8,11), as well as the update rule for current graph partitions (line 7).

### 3.2.1 Anchor graph construction

The problem of anchor graph construction for an initially given graph  $G^I = (V^I, E^I, D^I)$  turns straight forward into a problem of partitioning the graph  $G^I$ . During our work on this thesis we tried out different strategies for clustering nodes of a given graph.

Here we present those, which were more suitable for our matching framework, however generally an arbitrary algorithm for graph partitioning can be used.

Here and further we assume that the nodes of the given fine graph  $G^I$  are located on a plane. That means, for each node we have additionally to its attribute an associated pair of coordinates and therefore can define the length of an edge as the  $L^2$ -distance between its endpoints. The reason for this assumption is given by practical applications such as image or object recognition.

### Using grid

The first algorithm we describe is the most simple one. It uses a grid with fixed number of rows  $r$ , columns  $c$  and a cell width  $w$ . The grid is placed over the graph  $G^I$ . Nodes that are captured by a same grid cell belong to one cluster. Obviously, the number of clusters is equal to  $r \times c$ . We place anchor nodes in the middle of the grid cells. Two anchors are connected by an edge, if the cells they belong to have a common edge.

### Algorithms based on node merge

The next considered approach creates an anchor graph  $A^I$  with a predefined number  $m_1$  of anchors. For that we adopted a coarsening phase from multi-level graph partition algorithms [12, 34, 37, 65]. Such algorithms have generally three phases:

1. graph coarsening phase, where one creates a hierarchy of graphs by successive merging of nodes in graph on previous stage starting with the initial graph;
2. graph partition phase, where the partition problem is solved exact on the coarsest level;
3. refinement phase, where solution of the coarsest level is interpolated through all levels of the hierarchy until the initial graph.

There are several types of graph coarsening algorithms. In our work we used so-called strict aggregation scheme (SAG) [12], which groups nodes of  $G^I$  in disjoint subsets based on the strength of the edges between them. We implemented two SAG based algorithms: Heavy Edge Matching (HEM) and Light Edge Matching (LEM) [12]. Both algorithms visit nodes of the graph  $G^I$  in random order and construct an independent set of edges  $E'$  of the graph. The edge selection is based



on the edge weights<sup>1</sup>. The HEM algorithm picks and adds into  $E'$  the strongest edge adjacent to a current node  $v$ , that does not belong to the set of end nodes of edges in  $E'$  (see Alg. 2). As opposed to this, the LEM algorithm selects the weakest edge incident to a current node. The edges in  $E'$  will be contracted, i.e. their endpoints will be replaced with a new node, that lies in the middle of a contracted edge and is connected to all neighbors of its endpoints.

---

**Algorithm 2:** HEM( $G^I, m_1, N$ )
 

---

```

1  $i = 0, E' = \emptyset$ 
2 while  $|V^I| > m_1$  AND  $i \leq N$  do
3   select a random node  $v \in V^I \setminus V(E')$ 
4   if  $\exists v' = \operatorname{argmax}_{u \in V^I \setminus V(E')} w(v, u)$  then
5      $E' = E' \cup vv'$ 
6      $i = 0$ 
7   else
8      $i = i + 1$ 
9 contract edges in  $E'$ 
10 return coarsened  $G^I$ 
    
```

---

In our case, the graph  $G^I$  is not initially weighted. To use the described coarsening methods we need to define a strength of graph edges. In case of LEM-Algorithm we set the length of an edge as its strength:  $w(v, v') = \|v - v'\|_2$ . If we use HEM-Algorithm the strength of an edge is equal to  $w(v, v') = \exp(-\frac{\|v - v'\|_2}{\sigma_s^2})$  with a constant  $\sigma_s^2$ .

It is clear, that one iteration of HEM or LEM reduces the number of nodes in  $G$  at most by  $\lfloor \frac{n}{2} \rfloor$  nodes. To get an coarse graph with  $m_1$  nodes the coarsening algorithm should be repeated several times.

### 3.2.2 Anchor graph matching

In the previous section we described how to construct anchor graphs  $A^I = (V^{Ia}, E^{Ia}, U^{Ia})$  and  $A^J = (V^{Ja}, E^{Ja}, U^{Ja})$  of given graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$  respectively. Now, we focus our attention on the problem of matching two anchor graphs. For that, according to our problem formulation (see Eqs. (3.1)-(3.4)), we need to define a similarity matrix  $S^A \in \mathbb{R}^{m_1 m_2 \times m_1 m_2}$  between the graphs

---

<sup>1</sup>We denote weight of an edge  $vv' \in E^I$  with  $w(v, v')$

$A^I$  and  $A^J$ , where  $m_1 = |V^{Ia}|$  and  $m_2 = |V^{Ja}|$ . This matrix contains two types of similarities: edge similarities (non-diagonal elements) and node similarities (diagonal elements).

Let us consider a pair of anchors  $a_k, a'_k \in V^{Ia}$ . We define the length of the edge  $e_{kk'}$  between those anchors as a median of distances between nodes in the corresponding subgraphs  $G[V_k^I]$  and  $G[V_{k'}^I]$ . With other words:

$$L_{kk'} = \text{median}_{\substack{v_i \in G[V_k^I] \\ v_{i'} \in G[V_{k'}^I]}} \|v_i - v_{i'}\|_2. \quad (3.7)$$

Using this definition we calculate the similarity  $s_E^A(e_{kk'}, e_{pp'})$  between the edges  $e_{kk'} \in E^{Ia}$  and  $e_{pp'} \in E^{Ja}$  based on their length as it was done in Eq. (2.10):

$$s_E^A(e_{kk'}, e_{pp'}) = \exp\left(-\frac{(L_{kk'} - L_{pp'})^2}{\sigma_s^2}\right).$$

As we already discussed in the previous chapter, a natural way to define node similarities is to compare their attributes. However, our anchor graphs  $A^{Ia}$  and  $A^{Ja}$  do not have direct attributes in contrast to the initial graphs  $G^I, G^J$ . Further we describe two ideas, how to work around this problem.

The first idea is to assign some attributes to the anchors and proceed further in the same way, as for the initial graphs. However, if we define those attributes based only on the anchor graphs without involving the provided information about underlying initial graphs, the overall matching result can be corrupted. The reason for this is, that an anchor in one graph can get a similar attribute, as an anchor from the other graph, although those anchors represent different subgraphs in the original graphs. If they will be selected by the matching algorithm, the matching of the underlying subgraphs will have very low quality. This will have in turn an impact on the quality of the total matching of initial graphs. Consequently anchor attributes should incorporate the information about underlying subgraphs of original graphs. Consider an anchor  $a_k \in V^{Ia}$  and its underlying subgraph  $G[V_k^I] = (V_k^I, E_k^I, D_k^I)$ . We suggest two classes of attributes of the anchor  $a_k$ .

- The first one uses node attributes  $D_k^I$  of the underlying subgraph  $G[V_k^I]$ . For this purpose we adopted the *bag of features model* [45]. We build once a common dictionary of all provided attributes in the two fine graphs by performing *k-means clustering* of  $D^I \cup D^J$  into  $C$  clusters. The centers of the clusters represent "codewords". Each attribute of a node in  $V_k^I$  is afterwards mapped onto

the closest codeword. In this way, the anchor attribute  $d_1(a_k) \in \mathbb{R}^C$  is defined as normalized histogram of "codewords" in the corresponding subgraphs.

- The second class of attributes should capture the geometrical structure of underlying subgraphs. We define  $d_2(a_k) \in \mathbb{R}^{|V_k^I| \times b}$  as a set of  $|V_k^I|$  histograms  $\{d_2(a_k, v)\}$  with  $b$  bins. Each histogram  $d_2(a_k, v)$  represents a distribution of the length of the subgraph edges inside a small circle region around a node  $v \in V_k^I$ .

The similarity value between two anchors can now be determined based on the first or second type of anchor attributes. To calculate a distance between histograms we use  $\chi^2$  statistic test [77]:

$$s_1^A(a_k, a_p) = \sum_{b_i \in B} \frac{(d_1(a_k, b_i) - d_1(a_p, b_i))^2}{(d_1(a_k, b_i) + d_1(a_p, b_i))}, \quad (3.8)$$

$$s_2^A(a_k, a_p) = \frac{1}{|V_k^I|} \frac{1}{|V_p^J|} \sum_{v \in V_k^I} \sum_{u \in V_p^J} \left( \sum_{b_i \in B} \frac{(d_2(a_k, v, b_i) - d_2(a_p, u, b_i))^2}{(d_2(a_k, v, b_i) + d_2(a_p, u, b_i))} \right), \quad (3.9)$$

where  $a_k \in A^I, a_p \in A^J$  and notation  $d_1(a_k, b_i)$  and  $d_2(a_k, v, b_i)$  denote a value in the  $b_i$ -th bin of the corresponding histogram. Both defined similarities can be used separately or set together as a linear combination into one similarity function.

The second idea to determine similarity  $s^A(a_k, a_p)$  between two anchors is to perform graph matching of the underlying subgraphs  $G[V_k^I]$ ,  $G[V_p^J]$  and take its score as a similarity measure. This idea has a great drawback of high computational complexity, because we need to perform in total  $m_1 m_2$  local matches. However, in this case the objective function of the matching problem on the lower level and the one on the anchor level are closer related. For example, in case when we do not consider edge similarities between anchors and work only with anchor similarities, the objective score on the higher level represent the lower bound of the objective function (3.6) on the lower level. Indeed, this is true, because the objective function (3.6) consist in this case of two parts: the objective function on the higher level and additional summands, which correspond to the similarities of edges between clusters.

### 3.2.3 Subgraph matching

Given are two corresponding subgraphs  $G_k^I = (V_k^I, E_k^I, D_k^I)$  and  $G_p^J = (V_p^J, E_p^J, D_p^J)$ , we use cosine similarity of the node attributes to calculate node similarity between  $V_k^I$  and  $V_p^J$ . For the pairwise edge similarity we used the same formula as we used

for the anchor matching (see Eq.(2.10)), i.e.

$$s_E(e_{ii'}, e_{jj'}) = \exp\left(-\frac{(l_{ii'} - l_{jj'})^2}{\sigma_s^2}\right) \quad (3.10)$$

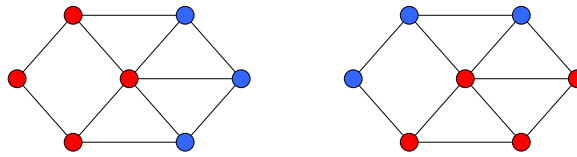
where  $l_{ii'}$ ,  $l_{jj'}$  are the lengths of edges  $e_{ii'} \in E^I$  and  $e_{jj'} \in E^J$  respectively.

### 3.2.4 Graph matching algorithm

Generally, we are not restricted to use one specific algorithm for subgraph and anchor graph matching. In this thesis we used *Reweighted Random Walks Method* (**RRWM**) [14], as it shows high matching accuracy according to results in the original paper and additionally is fast. It also shows good results in finding common subgraphs of two graphs in presence of outliers. For reasons of completeness we give an overview of this algorithm in appendix B. However, we do not provide theoretical justification of the algorithm steps and refer a reader to the original paper for that.

### 3.2.5 Graph partition update

Assume, we solved the graph matching problem on the higher and on the lower levels. That means we know pairs of correspondences between the anchor nodes  $m^a = \{(a_k, a_p) | a_k \in V^{Ia}, a_p \in V^{Ja}\}$  and between the nodes of the original graphs  $m = \{(v_i, v_j) | v_i \in V^I, v_j \in V^J\}$ . The last set is the union of the local solutions of the graph matching problem between pairs of subgraphs, as it is defined by  $m^a$ . The quality of the resulting solution  $m$  depends, as we already mentioned, in our framework not only on the quality of the graph matching algorithm, but also on the graph partitioning algorithm. Fig. 3.2 shows an example of a partition of two equal graphs, so that the matching result of subgraphs will be very pure for all possible combinations of anchors matches.



**Figure 3.2:** Example of bad partition of two equal graphs. Since clusters are very different, their matching in all possible combinations will always have low quality.

To cope with such problems, we formulated our approach as an iterative process. After each iteration the subgraphs of the initial graphs have a chance to

exchange nodes with their neighbors based on the obtained solution  $m$  and improve the matching quality of the next iteration. The proposed updating process consists of two major steps. In the first step we estimate an affine transformation between matched subgraphs based on the provided local correspondences. The next step is the actual update step, where the updating process uses the estimated transformations. We explain our approach on a pair of matched subgraphs  $G[V_k^I] = (V_k^I, E_k^I, D_k^I)$  and  $G[V_p^J] = (V_p^J, E_p^J, D_p^J)$  with the obtained local correspondence set  $m^{kp} = \{(v_i, v_j) | v_i \in V_k^I, v_j \in V_p^J\}$ .

In the first step we want to estimate two affine transformations  $T_{kp} : V_k^I \rightarrow V_p^J$  and  $T_{pk} : V_p^J \rightarrow V_k^I$  from the node set of one subgraph into the node set of another subgraph and vice versa. For that we use the state-of-the-art Coherent Point Drift (CPD) algorithm by Myronenko and Song [55]. This is a probabilistic algorithm for the point set registration problem, which finds correspondences between two set of points and a transformation that describes the mapping between the sets. We have chosen CPD, because it shows a remarkable robustness against outliers and often outperforms the other popular algorithm TPS-RPM by Chui and Rangarajan [19], which we mentioned in chapter 2. After obtaining the affine transformations  $T_{kp}$  and  $T_{pk}$  we measure a transformation error of each matched node  $v_i \in V_k^I (v_j \in V_p^J)$  as a distance between its projection into the other subgraph  $T_{kp}(v_i) (T_{pk}(v_j))$  and its matched pair  $m(v_i) = v_j \in V_p^J (m(v_j) = v_i \in V_k^I)$ :

$$\begin{aligned} err(v_i) &= \|T_{kp}(v_i) - m(v_i)\|_2 \\ err(v_j) &= \|T_{pk}(v_j) - m(v_j)\|_2 \end{aligned} \tag{3.11}$$

Based on the errors of single nodes we assign an error to the estimated transformations as a measure of their quality:

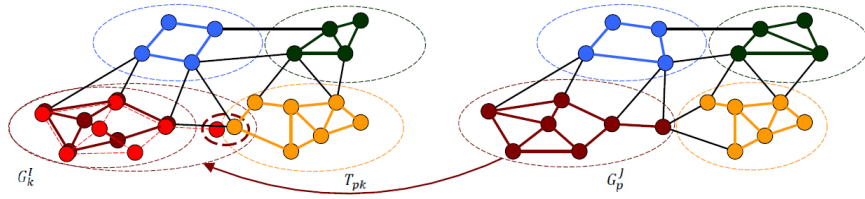
$$\begin{aligned} err(T_{kp}) &= \text{median}_{v_i \in V_k^I} err(v_i) \\ err(T_{pk}) &= \text{median}_{v_j \in V_p^J} err(v_j) \end{aligned} \tag{3.12}$$

From both transformations we select the one with the smallest error and replace the second with the inverse transformation of the selected one. For simplicity we preserve the notation  $T_{kp}$  and  $T_{pk}$  for the transformations related to the matched subgraph pair  $(a_k, a_p)$ . In this way we associate with each pair of matched subgraphs, that have at least 3 provided node correspondences<sup>2</sup>, two affine transformations between

<sup>2</sup>We need at least 3 pairs of correspondences between two sets of points to be able to estimate an affine transformation between them.

their nodes.

In the next step, we apply the estimated transformations to each subgraph of both graphs to project them onto the node space of the opposite graph (see Fig. 3.3). This means for the subgraph  $G[V_p^J]$ , that the transformation  $T_{pk}$  associated with the anchor pair  $(a_k, a_p)$  is now casted as a mapping  $T_{pk} : V_p^J \rightarrow V^I$ . For the projected points  $T_{pk}(v_j), v_j \in V_p^J$ , we find their nearest neighbors  $\bar{v}_i = NN(T_{pk}(v_j))$  in  $V^I$ . In Fig. 3.3 the projected points  $T_{pk}(v_j), v_j \in V_p^J$ , are marked with bright red color. We define a new matrix  $\bar{U}^{Ia} \in \mathbb{R}^{|V^I| \times m_1}$  and assign to its elements  $\bar{U}_{\bar{v}_i, a_k}^{Ia} = \|T_{pk}(v_j) - \bar{v}_i\|_2$  the distance between the projections  $T_{pk}(v_j)$  of  $v_j \in V_p^J$  and their nearest neighbor  $NN(T_{pk}(v_j))$  in  $V^I$ .



**Figure 3.3:** Example of the graph partition update rule. We project the subgraph  $G_p^J$  onto the subgraph  $G_k^I$  using estimated affine transformation  $T_{pk}$ . Nodes in the graph  $G^I$ , which were overlaid by the projection of the subgraph  $G_k^J$  have a chance to be included into the subgraph  $G_k^I$ .

After performing the same procedure for all transformations  $T_{pk}$  we set all not-assigned elements of  $\bar{U}^{Ia}$  to infinite. If there are some lines in  $\bar{U}^{Ia}$  where all elements are infinite, meaning that the corresponding nodes in  $V^I$  are not selected as nearest neighbors of the projections of the nodes in  $V^J$ , then we replace those lines with the corresponding lines in the current matrix  $U^{Ia}$  (see definition (3.5)).

Our update rule for the partition of the graph  $G^I$  defined by the matrix  $U^{Ia}$  is:

$$U_{ik}^{Ia} = 1 \iff a_k = \underset{l=1, \dots, m_1}{\operatorname{argmin}} \bar{U}_{v_i, a_l}^{Ia} \quad (3.13)$$

With other words, the node  $v_i \in V^I$  is assigned to the anchor  $a_k$  if  $\bar{U}_{v_i, a_k}$  is the smallest distance between  $v_i$  and projections of the nodes in the subgraphs  $G[V_p^J]$  matched to the subgraph  $G[V_k^I]$ . Note, that unassigned nodes in  $V^I$  do not exchange their clusters. It also can happen, that one note on different iterations will be assigned to different clusters. This can often be the case on the border between two good estimated clusters. To prevent unnecessary jumps, we introduce a local memory of each node, where it saves information about clusters it belonged to and

associated value of the matrix  $\bar{U}^{Ia}$ . We assign a node to a new cluster only when a new assignment is better than the previous ones.

The partition of the second graph is updated in the same way, as it is described above for the graph  $G^I$ . The approach is summarized in Algorithm 3.

---

**Algorithm 3:** UpdateSubgraphs
 

---

**Input:**  $m^a = \{(a_k, a_p) | a_k \in V^{Ia}, a_p \in V^{Ja}\}$   
 $m = \{(v_i, v_j) | v_i \in V^I, v_j \in V^J\}$   
**Output:** updated  $U^{Ia}, U^{Ja}$

*/\* Step 1: assign affine transformations to each pair  $(a_k, a_p)$  \*/*  
**1 foreach** *matched subgraph pair  $(a_k, a_p)$  do*  
**2** $\lfloor$  calculate  $T_{kp} : V_k^I \rightarrow V_p^J$  and  $T_{pk} : V_p^J \rightarrow V_k^I$  using CPD algorithm  
*/\* Step 2: calculate new matrices  $\bar{U}^{Ia} \in \mathbb{R}^{|V^I| \times m_1}$ ,  $\bar{U}^{Ja} \in \mathbb{R}^{|V^J| \times m_2}$  \*/*  
**3 foreach** *matched subgraph pair  $(a_k, a_p)$  do*  
**4** $\lfloor \forall v_j \in V_p^J : \bar{U}_{\bar{v}_i, a_k}^{Ia} = \|T_{pk}(v_j) - \bar{v}_i\|_2$ , where  $\bar{v}_i = NN(T_{pk}(v_j)) \in V^I$   
**5** $\lfloor \forall v_i \in V_k^I : \bar{U}_{\bar{v}_j, a_p}^{Ja} = \|T_{kp}(v_i) - \bar{v}_j\|_2$ , where  $\bar{v}_j = NN(T_{kp}(v_i)) \in V^J$   
*/\* Step 3: update partitions \*/*  
**6**  $U_{ik}^{Ia} = 1 \iff a_k = \operatorname{argmin}_{l=1, \dots, m_1} \bar{U}_{v_i, a_l}^{Ia}$   
**7**  $U_{jp}^{Ja} = 1 \iff a_p = \operatorname{argmin}_{q=1, \dots, m_2} \bar{U}_{v_j, a_q}^{Ja}$   
**8 return**  $U^{Ia}, U^{Ja}$

---

The usage of the proposed graph partition strategy is illustrated in Fig. 3.3. After performing the update procedure, the most left yellow node is likely to be included in the red partition, where in fact it should belong to.

### 3.2.6 Complexity

We want to investigate the asymptotic computational complexity of our two level graph matching approach. For simplicity, we assume, that the complexity of a selected graph matching algorithm is  $\mathcal{O}(f_{GM}(n_1, n_2))$ , where  $n_1$  and  $n_2$  are the size of the graphs we want to match.

The preprocessing step of our approach consists of two stages: initial graph partitioning and creation of the codebook of the node attributes. Note that the presence of the second stage depends on the selected strategy of the anchor graph matching. The complexity of the graph partitioning is in the worst case equal to  $\mathcal{O}(n_2^2)^3$ . Indeed, for one graph with  $n$  nodes and  $m$  anchors it is equal to  $\mathcal{O}(nm)$  (using

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<sup>3</sup>We assumed  $n_1 \leq n_2$

grid approach) or  $\mathcal{O}((n - m)\Delta(G))^4$  (HEM or LEM algorithm). The complexity of the codebook creation is determined by the complexity of the clustering algorithm, which in case of Lloyd's k-means algorithm [46] comes to  $\mathcal{O}((n_1 + n_2)rC)$  per iteration, where  $r$  is the dimension of the node attribute vectors and  $C$  the number of clusters. After joining those two results we obtain that the complexity of the preprocessing step is

$$\mathcal{O}(n_2^2 + (n_1 + n_2)rCi), \quad (3.14)$$

where  $i$  is the maximum number of iterations of the k-means clustering.

The main loop of our two level graph matching approach consists of three steps. The first one is the anchor graph matching, whose complexity is  $\mathcal{O}(f_{GM}(m_1, m_2))$  plus the complexity for initialization of the similarity matrix. In case we assign attributes to the anchors to calculate node similarity between two graphs, the complexity of the initialization can be approximated by  $\mathcal{O}(m_1^2 m_2^2)$ . The complexity of the subgraph matching step afterwards results in  $\sum_{(a_k, a_p) \in m^a} \mathcal{O}(f_{GM}(|V_k^I|, |V_p^J|))$ . The complexity of the two first steps in this case is equal to

$$\mathcal{O}(m_1^2 m_2^2) + \mathcal{O}(f_{GM}(m_1, m_2)) + \sum_{(a_k, a_p) \in m^a} \mathcal{O}(f_{GM}(|V_k^I|, |V_p^J|)). \quad (3.15)$$

In case when we use graph matching to determine the similarity between anchors, the complexity of both anchor and subgraph matching is equal to

$$\sum_{(a_k, a_p) \in M^a} \mathcal{O}(f_{GM}(|V_k^I|, |V_p^J|)), \quad M^a = \{(a_k, a_p) | a_k \in V^{I^a}, a_p \in V^{J^a}\}, \quad (3.16)$$

because subgraph matching is already included in the anchor matching step.

At the end we only need to determine the complexity of our update rule. The CPD algorithm has linear complexity, which means we can estimate transformations between all matched subgraphs with demand  $\sum_{(a_k, a_p) \in M^a} \mathcal{O}(\max(|V_k^I|, |V_p^J|))$ . The actual update step afterwards has the complexity  $\mathcal{O}(n_1 m_1 + n_2 m_2)$ .

If we assume that we can completely parallelize the computation of the sum in Eq. (3.15), then the total complexity of one iteration of our two level graph matching

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<sup>4</sup>We denote with  $\Delta(G)$  the maximal degree of nodes in  $V$ , where degree of a node is equal to the number of its incident edges [24].



approach is equal to

$$\begin{aligned} & \mathcal{O}(m_1^2 m_2^2) + \mathcal{O}(f_{GM}(m_1, m_2)) + \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) \\ & + \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) + \mathcal{O}(n_1 m_1 + n_2 m_2) \end{aligned} \quad (3.17)$$

or

$$\begin{aligned} & \mathcal{O}(m_1^2 m_2^2) + \mathcal{O}(f_{GM}(m_1, m_2)) + \mathbf{m}_2 \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) \\ & + \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) + \mathcal{O}(n_1 m_1 + n_2 m_2) \end{aligned} \quad (3.18)$$

depending on the selected strategy for computing the similarity between anchor graphs. Let us notice that the constant  $m_2$  in Eq. (3.18) increases the complexity of the whole algorithm, when we use subgraph matching to calculate the similarity between anchors.

However as the complexity of the graph matching is the most expensive step (in case of RRWM  $\mathcal{O}(f_{GM}(n_1, n_2)) = \mathcal{O}(n_1^2 n_2^2)$ ), it will fully overlie the complexity of other steps and we can approximate both Eqs. (3.17) and (3.18) with

$$\mathcal{O}(f_{GM}(m_1, m_2)) + \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) \quad (3.19)$$

and

$$\mathcal{O}(f_{GM}(m_1, m_2)) + \mathbf{m}_2 \mathcal{O}(f_{GM}(\max_k |V_k^I|, \max_p |V_p^J|)) \quad (3.20)$$

respectively.

Due to this it is obvious, that the resulting complexity of our graph matching framework depends highly on the number of iterations and on the size of the anchor graphs and subgraphs.

### 3.3 Discussion

We have proposed a novel two level graph matching framework (2LevelGM) for solving a graph matching problem formulated as an quadratic assignment problem. Our framework is based on a known matching algorithm, but helps to cope with some limitations of its application, such as big space demand and high computation time. The core idea of the introduced framework is to decompose an initial graph matching problem into a set of subproblems. For that we partition graphs into subgraphs, perform matching to determine pairs of subgraphs and afterwards perform matching again for each pair of subgraphs. An obtained solution at the end is used to update

the graph partition. The whole procedure is repeated iteratively until it converges. The complexity of the proposed framework depends highly on the complexity of the used graph matching algorithm, which itself depends on the size of the anchor graph and the graph subgraphs. In the next chapter we evaluate the proposed framework on synthetic and real data examples.

# Chapter 4

## Evaluation results

In this chapter we explore the quality of the proposed two level graph matching framework (we call it further 2LevelGM) on synthetic and real examples. The quality is measured by the matching score and accuracy of an obtained solution together with the running time in seconds needed to find it. Note, that under accuracy we understand actually recall of the graph matching algorithms (i.e. number of correct detected matches divided by the number of all correct matches), as it is done in [14, 15, 16, 25, 31, 43, 44]. To rate the usefulness of 2LevelGM we provide a comparison study across different graph matching algorithms. All tests in this chapter have been executed on a computer with an Intel(R) Core(R) i5-3210M CPU 2.50GHz with 4 cores unless otherwise specified. We implemented our framework in the software package MATLAB and used 2 workers<sup>1</sup> to run 2LevelGM. The code was not optimized. The sources of additionally used libraries and algorithms for comparisons are referred directly in the text. To make the comparison fair we have measured the running time of all algorithms from the initialization step till an final discrete solution is found. We also have used the greedy assignment algorithm [43] to discretize continuous solutions, obtained by some algorithms.

### 4.1 Synthetic data

For the first set of tests we adopted a commonly used approach for evaluation of graph matching algorithms on two synthetic generated sets of points (see [14, 16, 44]). For this purpose one generates first a set  $V^I \subset \mathbb{R}^2$  of  $n_1$  standard normally distributed points on a plane:  $V^I = \{v_i = (x_i, y_i) | x_i \sim \mathcal{N}(0, 1), y_i \sim \mathcal{N}(0, 1), i =$

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<sup>1</sup>For more details see <http://mathworks.com/help/distcomp/parallel-pools.html>

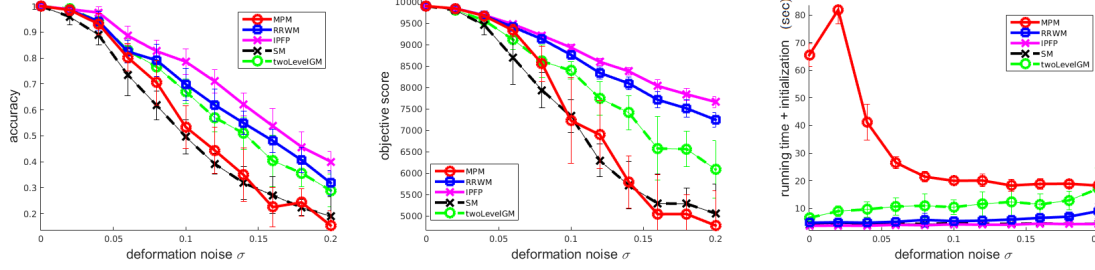
$1, \dots, n_1\}$ . In a second step  $V^J$  is generated, which represents a distorted copy of the first set with  $\bar{n}$  additional normally distributed points. The distortion is achieved by adding a normally distributed noise with zero mean and a variance  $\sigma^2$  to the coordinates of the points in  $V^I$ . This means, that the set  $V^J$  consists of  $n_2 = n_1 + \bar{n}$  nodes, where  $n_1$  points have a unique pair in  $V^I$  and are called inliers, whereby the other  $\bar{n}$  points are outliers. The task is to find correspondences between points in the two sets, which obviously can be formulated as a graph matching problem. For that we consider two fully connected graphs  $G^I$  and  $G^J$  with the nodes defined by the sets  $V^I$  and  $V^J$  respectively. We assume, that the graphs do not have attributes and each node in the first graph can be theoretically matched to each node in the second graph.

For the evaluation of our graph matching framework we follow the setup of the synthetic point set tests from the publications [16] and [48] and formulate four different kinds of tests. In the first test we set the number of outliers  $\bar{n}$  to zero and vary only the deformation noise  $\sigma^2$ . In the second test, we do not have a deformation noise ( $\sigma^2 = 0$ ) and compare the behavior of the different graph matching algorithms in case of an increasing number of outliers  $\bar{n}$ . In the third test, we perform the second test in presence of deformation in the second graph. For this we fix  $\sigma^2 = 0.03$  and increase iteratively the number of outliers  $\bar{n}$ . Finally, in the fourth test we consider again two graphs with the same size, but omit randomly  $(1 - \theta)$  percentage of edges in both graphs with increasing  $\theta$ . For performing the tests we adopted the supplemental MATLAB code provided by Minsu Cho et al. in their paper [16]. For simplicity we combine the described tests together in a first group of tests.

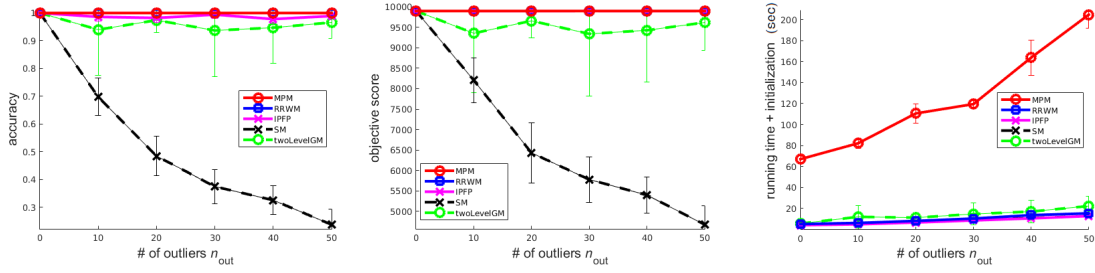
The first graphs we consider are relatively small: 100 – 150 nodes. The main reason for using small graphs is to compare the 2LevelGM with the following well known methods: MPM [16], RRWM [14], SM [43] and IPFP [44]<sup>2</sup>. The selection of the graph size was determined by application examples of the corresponding algorithms provided in the mentioned publications. To our best knowledge, those algorithms has not been applied directly to graphs with more than 150 nodes each without additional problem simplifications (for example reduction of the set of possible correspondences, which is difficult to achieve for non-attributed graphs). This restriction on the size of the graphs is determined mainly by the size of the dense affinity matrix  $S$ , which is used by all algorithms. The matrix  $S$  is calculated in

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<sup>2</sup>We used the implementation of those algorithms provided in [17].



**Figure 4.1:** Performance of the 2LevelGM with non-attributed anchor graphs on synthetic data: test 1 ( $n_1 = 100$ ,  $\bar{n} = 0$ ,  $\theta = 100\%$ )

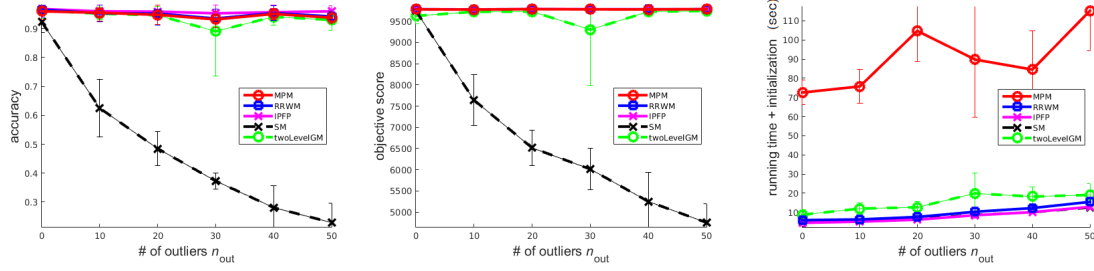


**Figure 4.2:** Performance of the 2LevelGM with non-attributed anchor graphs on synthetic data: test 2 ( $n_1 = 100$ ,  $\bar{n} \in [0, 50]$ ,  $\sigma^2 = 0$ ,  $\theta = 100\%$ )

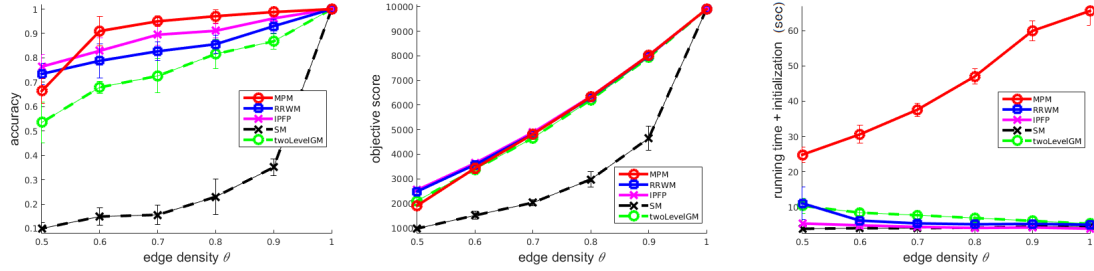
all cases using Eq. (3.10) with  $\sigma_s^2 = 0.15$ , where the value of the parameter  $\sigma_s^2$  is chosen according to the proposition made in [14]. To calculate affinity matrix on the anchor level we use  $\sigma_s^2 = 10$ .

Since our initial graphs  $G^I$  and  $G^J$  are not attributed, we first consider the formulation of 2LevelGM with non-attributed anchors graphs. The similarities between anchors are calculated in this case based on the matching score of the underlying subgraphs (see chapter 3.2.2). For the initialization of the initial subgraphs we use the grid method (see chapter 3.2.1) with  $2 \times 2$  cells. The average matching results of 10 runs in the four defined tests are illustrated in Figs. 4.1-4.4. The vertical bars at each point show the standard deviation of the measured mean value (accuracy, objective score and running time) for the corresponding problem setting.

From this results one can see that the SM algorithm has the worst matching quality in all cases. 2LevelGM performs little bit unstable, which is indicated by a relatively high standard deviation compared with other algorithms. For this reason the average performance (objective score and accuracy) of 2LevelGM is a little bit lower than the one of IPFP and RRWM, although in individual runs 2LevelGM is not worse. The running time of 2LevelGM is slower as of IPFP and RRWM. However this is



**Figure 4.3:** Performance of the 2LevelGM with non-attributed anchor graphs on synthetic data: test 3 ( $n_1 = 100$ ,  $\bar{n} \in [0, 50]$ ,  $\sigma^2 = 0.03$ ,  $\theta = 100\%$ )



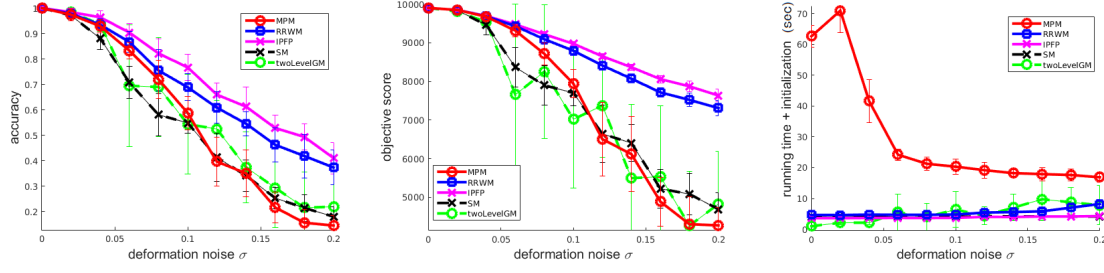
**Figure 4.4:** Performance of the 2LevelGM with non-attributed anchor graphs on synthetic data: test 4 ( $n_1 = n_2 = 100$ ,  $\sigma^2 = 0$ )

expected, because without anchor attributes 2LevelGM performs graph matching using RRWM on each pair of subgraphs. Although those subgraphs are smaller than the initial graphs, the overall complexity of 2LevelGM is in this case high as it of RRWM. This results in the longer runtime of 2LevelGM. The slowest algorithm is MPM. For that MPM have achieved best accuracy and objective score in three of four tests. However, it is outperformed by 2LevelGM in the first test (Fig. 4.1) with significantly smaller time demand<sup>3</sup>.

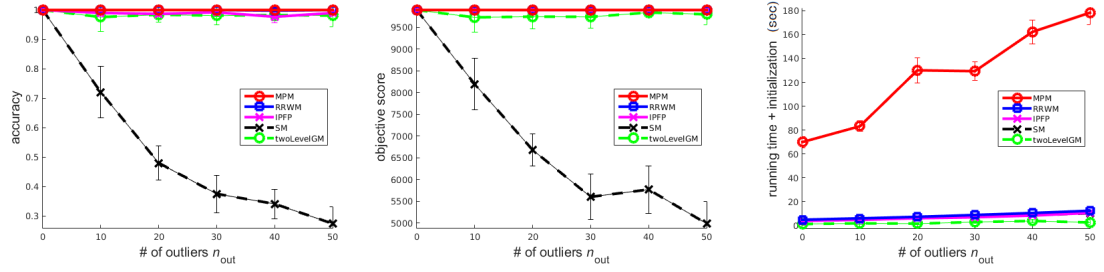
Below we present the results of testing on the first group of tests using 2LevelGM with attributed anchor graphs. For this purpose we use the attributes, that capture geometrical structure of the subgraphs (see chapter 3.2.2). We set the size of used histograms to 35 bins and the radius  $R$  of the circle region around each node to 2. The results of the comparison are presented in Figs. 4.5-4.8. One can directly see the improved performance time of the 2LevelGM algorithm in all tests. The proposed algorithm also shows a more stable performance in the second test. On the other side, 2LevelGM seems to be more susceptible to graph deformations (see

<sup>3</sup>The used implementations of 2LevelGM, SM and IPFP are purely MATLAB implementations, whereby some steps of MPM and RRWM were written using C++. This makes the comparison of the running time between algorithms difficult.

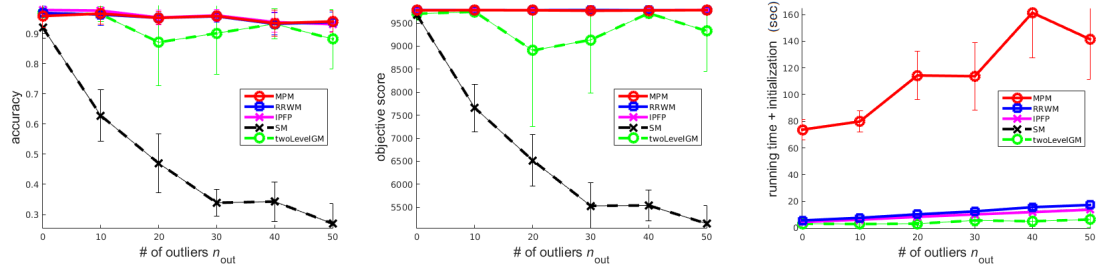
Figs. 4.5, 4.8). The reason for this lies in the selected anchor attributes, that are not sufficiently robust against deformations in the length of edges.



**Figure 4.5:** Performance of the 2LevelGM with attributed anchor graphs on synthetic data: test 1 ( $n_1 = 100$ ,  $\bar{n} = 0$ ,  $\sigma^2 = 0$ )



**Figure 4.6:** Performance of the 2LevelGM with attributed anchor graphs on synthetic data: test 2 ( $n_1 = 100$ ,  $\bar{n} \in [0, 50]$ ,  $\sigma^2 = 0$ ,  $\theta = 100\%$ )

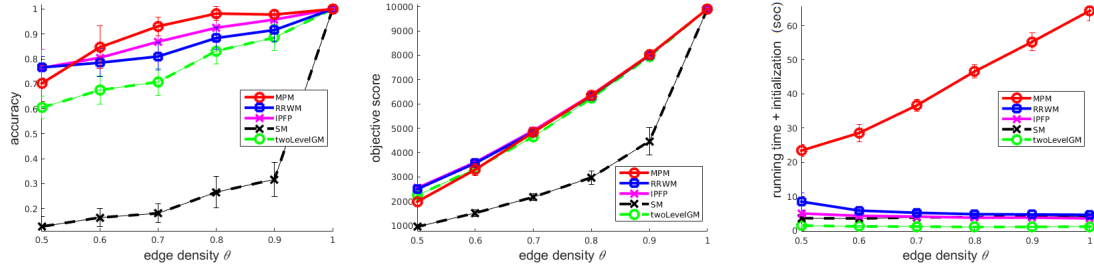


**Figure 4.7:** Performance of the 2LevelGM with attributed anchor graphs on synthetic data: test 3 ( $n_1 = 100$ ,  $\bar{n} \in [0, 50]$ ,  $\sigma^2 = 0.03$ ,  $\theta = 100\%$ )

To test the performance of our framework on bigger graphs we created another group of three tests and compare the results of 2LevelGM with those of the PATH [82]<sup>4</sup> and GLAG [27]<sup>5</sup> algorithms. In contrast to the graph matching problem formulation

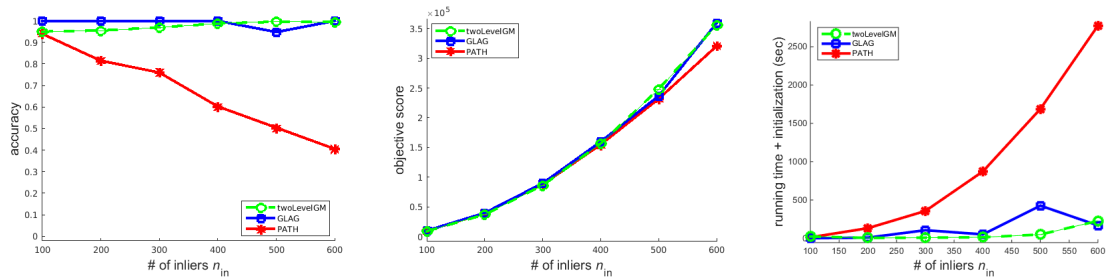
<sup>4</sup><http://cbio.enscm.fr/graphm/>

<sup>5</sup><http://www.fing.edu.uy/~mfiori/>. We replaced the default maximal number of iterations (30000) with 1000 to reduce the computational time.



**Figure 4.8:** Performance of the 2LevelGM with attributed anchor graphs on synthetic data: test 4 ( $n_1 = n_2 = 100$ ,  $\sigma^2 = 0.00$ )

considered by 2LevelGM and previous algorithms the PATH and GLAG algorithms solve the minimization problem (2.2). However, they do not take into account node attributes, so the second term in (2.2) disappears. PATH and GLAG do not work with the affinity matrix  $S$  and therefore can be directly applied to bigger graphs without the necessity to reduce the set of possible candidate matches. This was the reason, why we have selected this algorithms to estimate matching results of our approach on bigger graphs. The results of the comparison in one run can be seen in Figs. 4.9-4.11<sup>6</sup>. We do not provide averaged results for this group of tests due to their high computational demand. The presented results were obtained by using  $5 \times 4$  grid to initialize 2LevelGM. The PATH and GLAG algorithms are initialized with the weighted adjacency matrices of the initial graph, whereby weights are defined by the length of the edges.

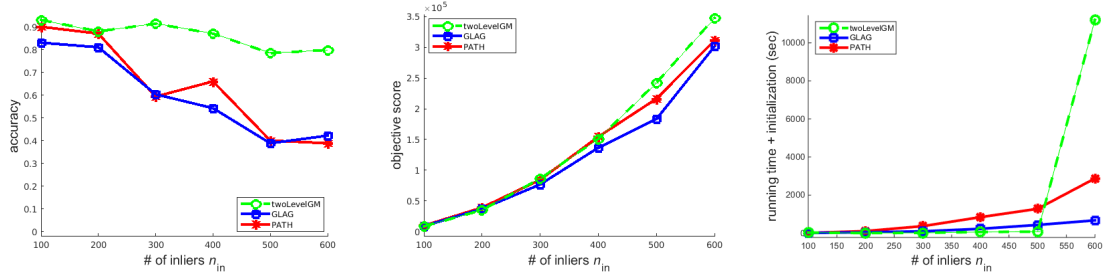


**Figure 4.9:** Performance comparison of 2LevelGM, GLAG and PATH on bigger graphs ( $\bar{n} = 0$ ,  $\sigma^2 = 0$ ,  $\theta = 100\%$ )

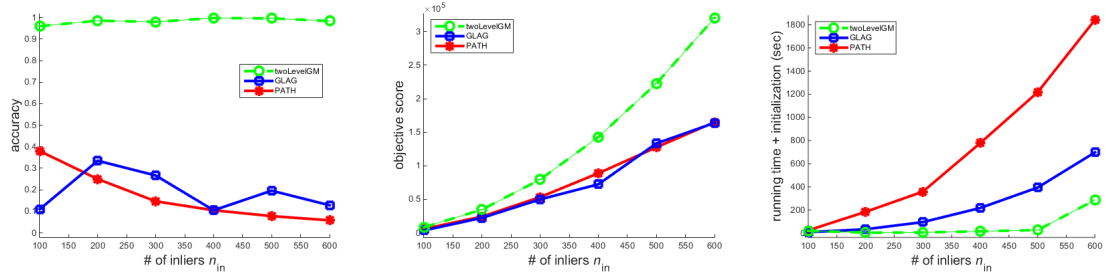
All performed tests for bigger graphs can be considered as instances of the graph isomorphism problem in exact (Fig. 4.9) and inexact (Figs. 4.10, 4.11) forms. We investigate the matching score, accuracy and running time of the graph matching

<sup>6</sup>This group of tests was executed on a desktop PC with an 2.67GHz Intel(R) Xeon(R) CPU with 4 cores. 4 MATLAB workers were used





**Figure 4.10:** Performance comparison of 2LevelGM, GLAG and PATH on bigger graphs ( $\bar{n} = 0$ ,  $\sigma^2 = 0.03$ ,  $\theta = 100\%$ )



**Figure 4.11:** Performance comparison of 2LevelGM, GLAG and PATH on bigger graphs ( $\bar{n} = 0$ ,  $\sigma^2 = 0$ ,  $\theta = 90\%$ )

algorithms as functions of number of nodes in the initial graphs. In all cases the proposed two level graph matching framework outperforms both GLAG and PATH in objective score and especially in running time with one exception. This one is the running time of the last iteration in Fig. 4.10. We consider it as an individual case and suppose, that an imbalanced graph partitioning of initial graphs causes the jump in the running time. Overall 2LevelGM shows a high matching accuracy in all three tests. Additionally we believe it is possible to improve the framework by solving instability issues, which we saw in previous cases.

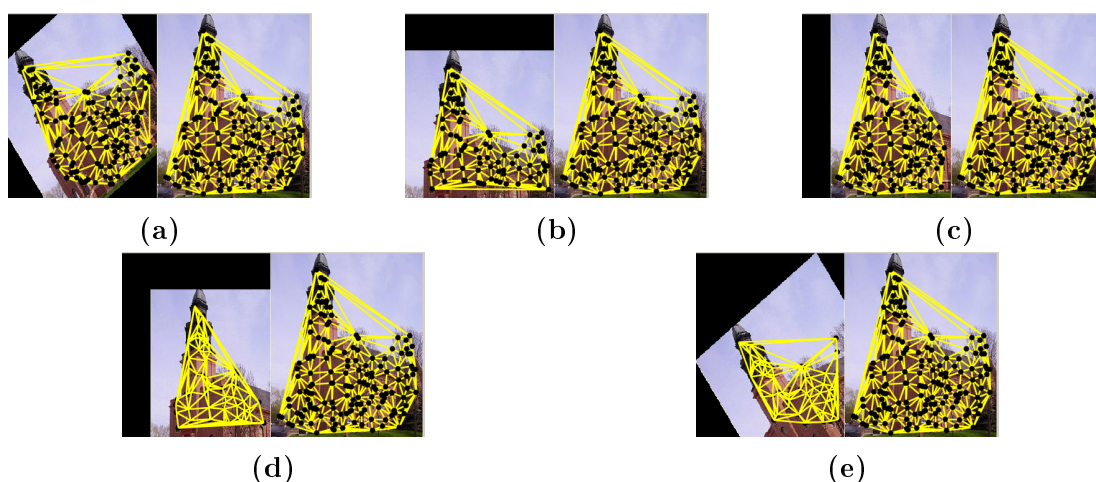
## 4.2 Real data tests

In the following sections we use the developed two level graph matching algorithm for finding correspondences between features on a pair of images. To formulate this problem as a graph matching problem we use the standard approach settled in computer vision literature [14, 15, 48, 49, 59]. For that we extract SIFT features [47] of two images around keypoints, that were located using some feature detector (we used MSER [51]). Given the extracted features of two images we construct two attributed graphs  $G^I = (V^I, E^I, D^I)$  and  $G^J = (V^J, E^J, D^J)$  for each image re-

spectively. The nodes of those graphs are placed at the locations of the detected keypoints with their features as node attributes. To connect nodes via edges one can use Delaunay triangulation [49, 59], nearest neighbors relations between nodes [67] or consider complete graphs [15, 16].

### 4.2.1 Image affine transformation

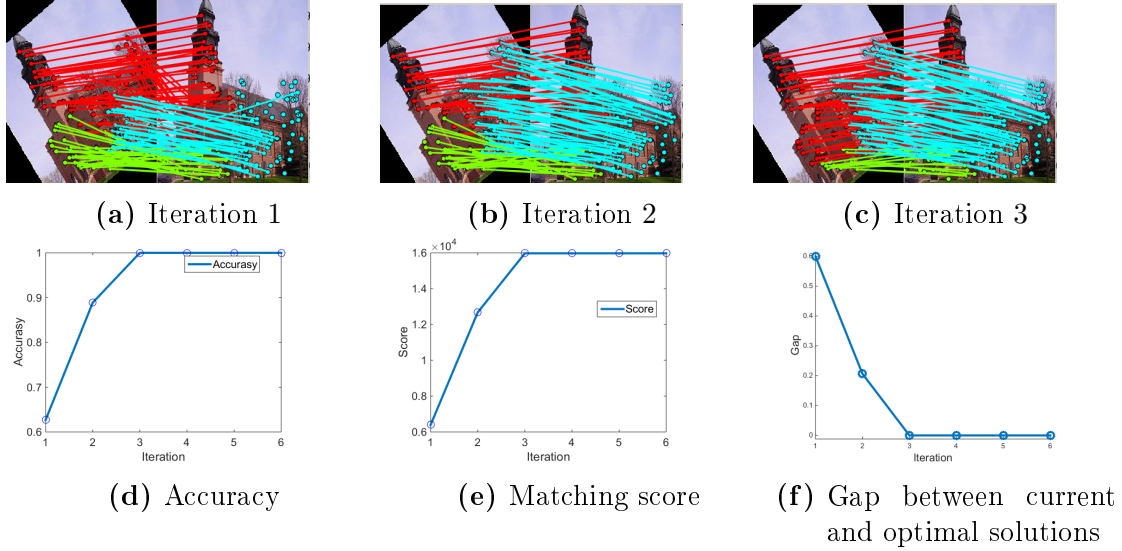
The first image set we consider can be seen as a synthetic data set of real images. It consists of image pairs, where one image in each pair is the same in all cases and the second image represent a rotated/shifted copy of the first one with additional Gaussian noise added to its pixels (see Fig. 4.12<sup>7</sup>). On this simple examples we want to demonstrate the work of the update rule inside 2LevelGM algorithm (see chapter 3.2.5).



**Figure 4.12:** Synthetic image data set: first image [81] in each pair is a transformed copy of the second image with Gaussian noise added to its pixels. Keypoints are extracted on the second image in each pair using MSER feature detector [51] and inherited by the first image. The edges between nodes are built using Delaunay triangulation procedure [49, 59]

To create the anchor graphs we used the HEM coarsening algorithm (see Alg. 2) with a fixed number of anchors. Since the initial graphs are not big (the right image in each pair contains 152 keypoints), we set the number of anchors to 3 for all anchor graphs. In this case the subgraphs are big enough to guaranty a robust estimation of an affine transformation between them. The work of 2LevelGM is illustrated in Fig. 4.13 on the example of the first image pair (Fig. 4.12a). The nodes in the

<sup>7</sup>The presented image of a church is taken from the SUN[81] dataset (category "church outdoor").



**Figure 4.13:** Result of applying 2LevelGM to the image pair 4.12a. Nodes of the matched subgraphs have the same color.

matched subgraphs have the same color. One can see how the initial graph partition changes through the iterations, which leads to the improvement in both accuracy and objective score (see Figs. 4.13d-4.13e). Fig. 4.13f shows additionally the decrease of the gap  $\frac{x_i - x_{\text{opt}}}{x_{\text{opt}}}$  between the optimal solution  $x_{\text{opt}}$  and solution in the  $i$ -th iteration  $x_i$ . It is easy to see that three iterations are sufficient. Further iterations do not improve matching.

In Fig. 4.14 we present the results of matching of all 5 image pairs with 2LevelGM in comparison with the results obtained with ProgGM [15], GLAG [27] and PATH [82]. In 2LevelGM and ProgGM we use Eq. (3.10) with  $\sigma_s^2 = 0.15$  to calculate the affinity matrix for the initial graphs and their subgraphs. For the anchor graphs we use the same formula, but with  $\sigma_s^2 = 10$ . The size of the set of initial candidate matches used by ProgGM is limited by 3000 pairs. For the rest we use the default parameters of ProgGM suggested by the authors with RRWM as its graph matching module. The PATH and GLAG algorithms are used with the same settings as in the previous test on the synthetic data sets.

It is pleasant to see that 2LevelGM is able to find the absolutely correct matching for the whole set except one image pair and therefore shows better results in objective score and accuracy than ProgGM, PATH and GLAG do. The result of matching of the last image pair is roughly the same for 2LevelGM and ProgGM. We notice that

2LevelGM is not able to improve graph partitioning further in this case, although some nodes from the true matches belonged to different subgraphs. Regarding the running time ProgGM is the fastest algorithm. 2LevelGM is a little bit slower than ProgGM, but still much faster than PATH and GLAG. However we should point out, that ProgGM directly stops as soon as the matching score does not increase any more. In contrast to that, our 2LevelGM has to make some additional iterations at the end to ensure that a local minimum is found. This is done intentionally, as we cannot make certain statements about the convergence of our framework.

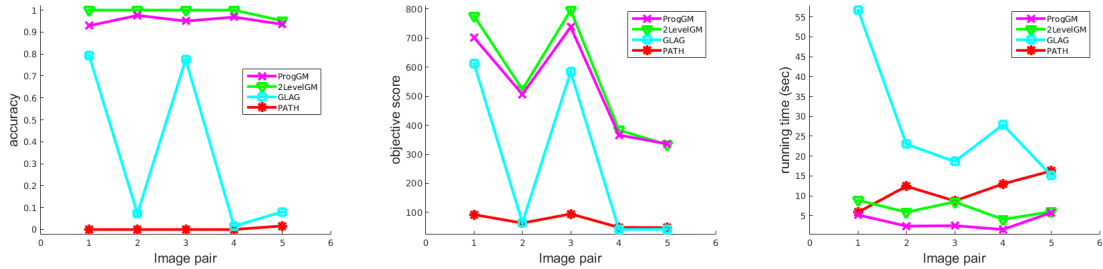


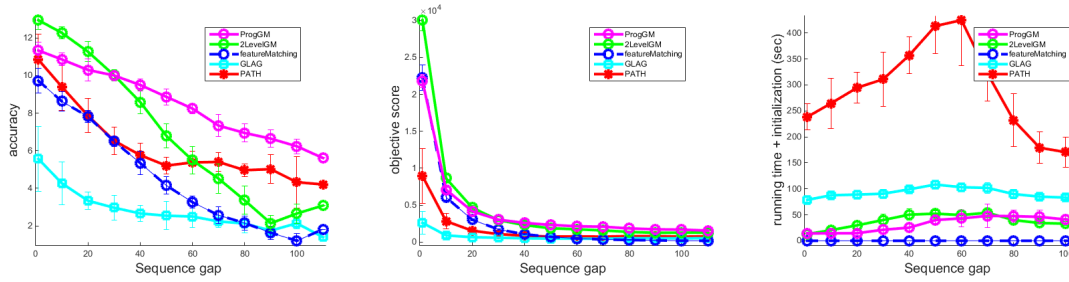
Figure 4.14: Evaluation of 2LevelGM on the synthetic image dataset (see Fig. 4.12)

## 4.2.2 House dataset

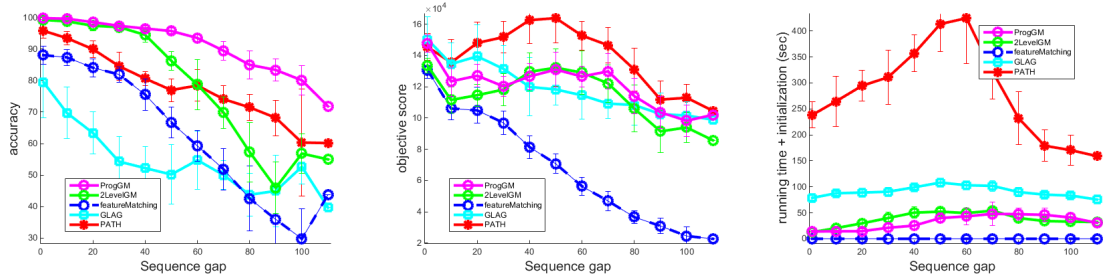
Our next data set is the well known CMU House sequence [1] which consists of 111 images of a toy house taken from different viewpoints. It was widely used for the evaluation of graph matching algorithms [3, 11, 14, 25, 48, 49]. The provided ground truth [57] consists of 30 feature points presented in all frames in the sequence. Due to that reason most authors considered for matching small graphs with 30 nodes. By analogy with the previous experiment we used MSER to extract around 250 key-points on each image in the sequence with SIFT descriptors and use all of them to build the initial graphs to be matched. The provided ground truth is extrapolated to neighboring features in the same way it was done in [15]<sup>8</sup>. We perform matching between pairs of images spaced by 1, 10, 20, ..., 110 frames. However we match at maximum 10 image pairs for each gap (i.e. detachment between frames). Further we analyze the averaged matching score, accuracy and running time of 2LevelGM, ProgGM, PATH, GLAG and simple feature matching [47] as functions of the sequence gap. Notice that the bigger the gap the stronger the deformation between the object on two images and the more difficult the matching problem is.

<sup>8</sup>We set the radius of extrapolation to 10.

The results of matching can be seen in Figs. 4.15-4.16, where each figure represents one group of results. The difference between two provided groups lies in the post-processing step, which has been applied to the final solutions of all algorithms in the second group. This post processing step is initially used only by ProgGM to extrapolate the obtained graph matching solution in the same way as it is done for the ground truth [15]. This leads to the possibly not unique correspondences between node sets of initial graphs and, in our opinion, significantly increases the accuracy of the solution (compare images in Fig. 4.17). To make the comparison fairer we applied the same post-processing step also to the solutions of 2LevelGM, PATH, GLAG and feature matching.



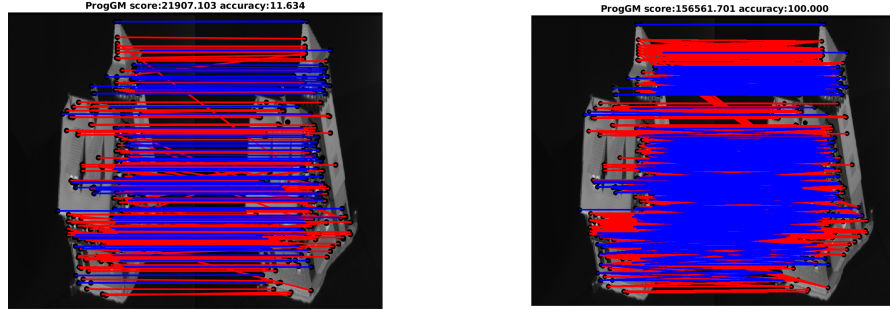
**Figure 4.15:** Evaluation of 2LevelGM on the CMU House sequence: not extrapolated solution



**Figure 4.16:** Evaluation of 2LevelGM on the CMU House sequence: extrapolated solution

For ProgGM we have used the same parameters as for the synthetic image set matching from the previous section. The same holds true for the PATH and GLAG algorithms. In 2LevelGM we have used the grid initialization with  $2 \times 2$  cells, which worked better in this case than HEM or LEM algorithms did. Those coarsening algorithms created very unbalanced subgraphs, which caused problems in time performance and space allocation during the matching process. To perform matching on the higher level we have assigned attributes to the anchors. In application for the house sequence this approach showed the same results regarding matching accuracy

and objective score as the idea to use subgraph matchings to calculate similarities between anchors. Additionally it is much faster. To define anchor attributes we used only the provided node attributes. We also tried to include structure information of the subgraphs into the anchor attributes or use only the structure based attributes, but the impact on the results was minimal.



(a) solution ProgGM, accuracy 11.63%      (b) extrapolated solution ProgGM, accuracy 100%

**Figure 4.17:** Result of extrapolation of matching solution: multiple correspondences, higher accuracy and objective score. The blue color denotes correct matches and the red color the wrong ones.

Summarizing we have to admit that ProgGM shows better matching accuracy over the majority of the House sequence compared with the other methods. In contrast to this, the simple feature matching and GLAG have the lowest accuracy. PATH shows the third best result. For small sequence gap, its accuracy is clearly lower, than those of ProgGM and 2LevelGM. However, PATH seems to be more robust against deformations in the graph structure, which follows from the very slow decrease in its accuracy for the higher sequence gap. Remarkable is, that the both GLAG and PATH algorithms achieve high objective score in case of extrapolated solutions. They outperform ProgGM and 2LevelGM, although the accuracy of PATH and GLAG is almost always lower than that of ProgGM and 2LevelGM. Regarding the running time PATH and GLAG are very slow compared to the other three used algorithms. The running time of 2LevelGM and ProgGM lie in the same range. The objective score and accuracy of 2LevelGM is also comparable with the results of ProgGM for small values of the sequence gap. 2LevelGM even outperforms ProgGM in case of not extrapolated solutions and a small sequence gap (see the first plot in Fig. 4.15). The accuracy falls however rapidly down after the gap exceeds the value 40. During the investigation of this behavior we found out, that there are two reasons responsible for the achieved matching results of 2LevelGM. The

first one lies in the disability of the used matching algorithm (RRWM) to find good correspondences between correctly matched subgraphs. The cause is a strong distortion in positions of the nodes in both subgraphs. The higher the deformation the worse the matching accuracy and therefore the objective score are [14]. The second reason is the ineffectiveness of our update rule to improve graph partitions in this case. According to the formulation in chapter 3.2.5 2LevelGM tries to estimate affine transformation between the nodes in the matched subgraphs, but in case of the house sequence this transformation is not affine. The attempt to improve the update rule by estimating a projective transformation between two sets of nodes was not successful as different groups of nodes inside one cluster have different transformations.

## 4.3 Discussion

In this chapter we have performed an evaluation of the suggested two level graph matching framework on synthetic graphs and real image examples. We have compared it with different state-of-the-art algorithms and presented the results of matching by measuring the reached objective score, accuracy of the obtained solution and the required running time in seconds.

In the first group of tests we have evaluated how well our two level approach treats graphs, which still can be matched directly with existing algorithms based on the same problem formulation (RRWM [14], MPM [16], SM [43] and IPFP [44]). The results show, that in the case of subgraph isomorphism and homomorphism, our approach gains results, which are close to those of RRWM, IPFP and MPM, and outperforms SM. However it shows a little bit weaker results than other algorithms in case of high deformation between matched graphs. Although even in this case it is able to outperform MPM and SM.

In the second group we have tested the ability of 2LevelGM to solve (sub)graph isomorphism and homomorphism problems on graphs with up to 600 nodes. In this case the proposed approach outperforms both GLAG [27] and PATH [82] in accuracy, objective score and running time.

At the end, in the third group of tests we have used 2LevelGM for finding correspondences between keypoints of two images. We have shown that in the case, when changes in the positions of keypoints on two images can be described by an affine transformation, 2LevelGM outperforms such algorithms as ProgMG [15], PATH [82]

and GLAG [27]. On the other side, in case of complex transformations between key-points, the used graph partition update rule is getting less effective. This can be seen on the evaluation results on the CMU House sequence [1].



# Chapter 5

## Conclusions and discussion

The present master thesis addresses the problem of graph matching and its application for finding correspondences between points on two images. The task of the graph matching problem is to find a mapping between node set of one graph and node set of the other graph that satisfies some predefined conditions. In the chapter 2 we have formally defined the graph matching problem and its possible specifications based on the different requirements on a desired matching. Additionally we have provided an extensive overview of classical and recent algorithms for solving graph matching problems.

In this work we have concentrated ourselves on the problems, that formulate graph matching problem in an inexact way. In the most general case such problems use a so-called affinity matrix to measure similarity between two graphs. As it has been shown, this problem formulation represents a special case of the quadratic assignment problem, which is known to be NP-hard. Due to the big size of the affinity matrix most of the existing graph matching algorithms, which solve inexact graph matching problem based on this formulation, become fast intractable for relatively small<sup>1</sup> graphs due to time and memory demands. Due to that reason we have suggested a framework (2LevelGM), which allows the application of existing algorithms to bigger graphs. The detailed explanation of the proposed technique is given in chapter 3. There we have presented a two level graph matching algorithm, which is based on a variation of the well known divide and conquer paradigm. Initially provided graphs represent the lower level in our matching schema. To reduce the

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<sup>1</sup>The exact size of the graphs, that still can be handled by those algorithms, depends on the used implementation and on the hardware they are executed on. The used implementation of RRWM was able to match graphs with roughly up to 150 nodes each.

problem size we have replaced initial graphs by new smaller graphs (anchor graphs), which we have placed on the higher level. Each node (anchor) of such a graph represents a subgraph of the corresponding initial graph. Given such a two level structure our method proceeds as follows:

1. it finds correspondences between nodes of the anchors graphs (higher level);
2. finds for each pair of matched anchors a mapping between the nodes of the underlying subgraphs (lower level);
3. updates subgraphs;
4. runs further through steps 1 – 3 until it does not achieve any improvement in the overall solution in several successive iterations.

Under an overall solution we understand a union of the local solutions of the subproblems. To perform matching between anchor graphs and subgraphs of the initial graphs we have used the Reweighted Random Walk algorithm [14].

For partitioning the initial graph we have suggested two methods. The first one lays a grid with a fixed number of cells over the graphs and captures nodes inside one cell into one cluster. The second method iteratively replaces edges in the independent edge sets of the initial graphs with a single node until the desirable size of graphs is reached. Generally any other partition method can be used instead. However, there is one requirement to a selected partition method: it should create similar anchor graphs for similar initial graphs. Both of the proposed techniques have approved themselves to be able to guaranty this requirement. However, we have noticed, that the second method tends to create more anchors in the areas of high node density in the original graph. As a result in the case of initial graphs with different regions of high node density the resulting anchor graphs could be substantially different.

On the higher level we have matched the anchor graphs again by using a similarity matrix between anchor graphs. To calculate it we have proposed a technique for defining anchor attributes. Alternatively one can use the matching score of the underlying subgraphs.

To improve the initial partition we have suggested an update procedure, which allows the existing subgraphs to exchange nodes with their neighbors based on the current matching solution. The formulated update rule is based on the consideration, that in case of correct matching locally connected groups of nodes should underlie the same local transformation, which we assumed to be affine.

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How well the proposed framework works is evaluated in chapter 4 on some synthetic graphs and real image examples. We have performed a comparison with the different state-of-the-art algorithms (RRWM [14], MPM [16], SM [43], IPFP [44], GLAG [27], PATH [82] and ProgGM [15]) and reported the results of matching by measuring the reached objective score, the accuracy of the obtained solution and the required running time. After summarizing the results of different tests we came to the following conclusions:

- The usage of anchor attributes for anchor graph matching is preferred, as it improves the runtime performance of our approach. When using attributed anchor graphs, 2levelGM was in most cases at least exactly as fast as the other algorithms or even faster, when running on graphs with up to 600 nodes. The only one exception is ProgGM, which is faster compared to 2LevelGM. However ProgGM considers one reduced version of an initial matching problem, where we create a whole set of smaller subproblems. Consequently, the reason for better running time lies in the fact, that we solve summary more graph matching problems.
- Both ways to match anchor graphs lead to similar results in accuracy and objective score. Although, we have to admit, that the defined structure based attributes, when they are used alone, are susceptible to graph deformations and causes some instability issues in the matching results. This instability probably comes from sometimes wrongly matched anchors.
- In case of (sub)graph isomorphism problems, our approach shows positive results. In single runs it performs on the same level as RRWM, MPM, IPFP, when applied to graphs, which still can be matched directly with those algorithms. However due to some stability issues in its performance the averaged values are a little bit lower than those of the mentioned algorithms. For graphs with up to 600 nodes, our approach outperforms both GLAG and PATH algorithms, that use a less memory demand formulation of the graph matching problem.
- 2LevelGM has a less good accuracy and objective score on graphs with high deformation rate, which however is also the case for most of the other algorithms. In case of smaller graphs and the usage of subgraph matching to compare anchor graphs, the results achieved with 2LevelGM are close to those of RRWM and therefore are better than those of MPM. The usage of anchor attributes

in this case decreases the matching quality of our approach. This happens likely because the defined anchor attributes do not provide enough resistance against structural deformation. In case of bigger graphs 2LevelGM showed better results than GLAG and PATH also in presence of small deformation in the structure of one of the graphs.

- Applied to the problem of matching synthetically generated image pairs, where one image represent a rotated and/or translated copy of the other one, 2LevelGM showed very good results. Those examples demonstrate the usefulness of the proposed subgraph update rule.
- Evaluation on the CMU House sequence [1] shows, that 2LevelGM has troubles with the matching of image pairs with non-affine transformation between them.
- In comparison with GLAG and PATH 2LevelGM shows big potential to be applied to really big graphs.

Based on the made conclusions we have several thought how 2LevelGM can be improved in a future work. Possible ways of further development are shortly given below.

The method probably can be further improved by adopting more sophisticated graph partitioning techniques. Ideally, two graphs should be clustered jointly to guaranty better matching after the first iteration. There are some techniques, that solve this problem in case of a provided information about correct matches between some nodes, however we did not see similar algorithms for an completely unsupervised case.

We also believe, that the defined anchor attributes can be further improved. One of possible ways is to include not only length information of the edges in the underlying subgraphs, but also angles. A further improvement could be to connect results of the anchor matching in the successive iterations of the algorithm to improve its quality.

Since our current update rule is less effective in case of non-affine transformation between matched clusters, we have tried to improve it already during our work on the thesis via the estimation of non-rigid transformation. However achieved improvement of 2LevelGM is not significant in case of the CMU House sequence. We suppose, that the reason for this lies in the fact, that our subgraphs are too big for estimating a one common transformation for all nodes inside them. Therefore a next step of the improvement could be a subdivision of matched subgraphs into

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smaller groups of nodes, which have similar transformations.

Currently, the performance of 2LevelGM depends strongly on the selected parameters, such as number of anchors, number of clusters to create a codebook of node attributes and so on. In future one can think about a way to parameter reduction or an automatic selection their best suitable values depending on a given problem.

Concerning future work it would be interesting to generalize the proposed framework using a probabilistic matching framework. Further tests on graphs bigger than those, which were considered in this thesis, can be performed as well. However for the better performance the current two level approach should be extended to an hierarchical one. The reason for this is the following consideration. To preserve subgraph problems sufficiently small one needs to increase the number of anchors. Consequently on some point the anchor graphs will become too big to be matched directly and need to be subdivided into smaller subproblems to perform further. According to the seen results of comparison we are right to expect, that a hierarchical modification of our two level framework will show good matching results and time performance. Our results should be considered as completed important stage that gives a base for further development and research.



# Appendix A

## Quadratic Assignment Problem

Consider a problem of assignment of  $n$  facilities to  $n$  locations given the transportation costs between the locations depending on the flow between them and opening costs of facilities in certain locations. The aim is the cost minimization of the assignment. Let  $D = (d_{kl}), F = (f_{kl}), B = (b_{ik}) \in \mathbb{R}^{n \times n}$  be real matrices that define a distances and flow between the locations, as well as the opening costs. The problem defined above can then be formulated as an integer quadratic program [10, 39]:

$$P = \operatorname{argmin}_{\hat{\sigma} \in \Sigma_n} \sum_{i=1}^n \sum_{j=1}^n f_{ij} d_{\hat{\sigma}(i)\hat{\sigma}(j)} + \sum_{i=1}^n b_{i\hat{\sigma}(i)}, \quad (\text{A.1})$$

where  $\Sigma_n$  is a set of all possible permutations of the set  $\{1, \dots, n\}$ . Eq. (A.1) is called *Koopmans-Beckmann version of the quadratic assignment problem* [10] (further *QAP*).

We can assign a permutation matrix  $P = (P_{ij}) \in \{0, 1\}^{n \times n}$  to each permutation  $\sigma$ , where  $P_{i\sigma(i)} = 1$  and 0 elsewhere. The set of all feasible permutation matrices is defined as

$$\Pi_n = \{P \in \{0, 1\}^{n \times n} \mid \sum_{i=1}^n P_{ij} = \sum_{j=1}^n P_{ij} = 1 \quad \forall i, j = 1, \dots, n\}.$$

It is easy to see that, the formulation in Eq. (A.1) is equivalent to

$$P = \operatorname{argmin}_{\hat{P} \in \Pi_n} (F \cdot \hat{P} D \hat{P}^T) + B \cdot \hat{P}, \quad (\text{A.2})$$

where  $\cdot$  denotes the Frobenius inner product of two square matrices defined as  $A \cdot B = \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij}$ .

We recall shortly the definition of the Kronecker product of two matrices and it's

connection with the Frobenius inner product of two matrices and matrix trace.

The Kronecker product of two matrices  $A = \{A_{ij}\}, B = \{B_{ij}\} \in \mathbb{R}^{n,n}$  is a new  $n^2 \times n^2$  matrix  $C$

$$C = A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{n1}B \\ \vdots & \ddots & \vdots \\ a_{1n}B & \dots & a_{nn}B \end{pmatrix}. \quad (\text{A.3})$$

From the definition of the matrix trace follows:

$$A \cdot B = \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij} = \sum_{i=1}^n (AB^T)_{ii} = \text{tr}(AB^T). \quad (\text{A.4})$$

We also can write

$$A \cdot B = \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij} = \text{vec}(A)^T \text{vec}(B), \quad (\text{A.5})$$

where  $\text{vec}(A)$  denotes the column-wise vectorization of a matrix  $A$ . Additionally, it holds [36]:

$$\text{vec}(APB) = (B^T \otimes A) \text{vec}(P). \quad (\text{A.6})$$

We can now use Eq. (A.4) in Eq. (A.2) to obtain the *trace formulation of QAP* [10]:

$$P = \underset{\hat{P} \in \Pi_n}{\text{argmin}} \text{tr}(F \hat{P} D^T \hat{P}^T + B \hat{P}^T). \quad (\text{A.7})$$

The objective function of the trace formulation of QAP can be further rewritten based on the properties in Eqs. (A.5) and (A.6) as follows:

$$\begin{aligned} \text{tr}(F \hat{P} D^T \hat{P}^T + B \hat{P}^T) &= \text{tr}(\hat{P} (F \hat{P} D^T)^T) + \text{vec}(B)^T \text{vec}(\hat{P}) \\ &= \text{vec}(\hat{P})^T \text{vec}(F \hat{P} D^T) + \text{vec}(B)^T \text{vec}(\hat{P}) \\ &= \text{vec}(\hat{P})^T (D \otimes F) \text{vec}(\hat{P}) + \text{vec}(B)^T \text{vec}(\hat{P}). \end{aligned} \quad (\text{A.8})$$

Based on this formulation the matrix  $B$  is called sometimes *linear cost matrix* and the matrix  $D \otimes F$  *quadratic costs matrix* [10, 64]. If we replace the matrix  $F$  with  $-(A^I)^T$ , the matrix  $D$  with  $(A^J)^T$  and the matrix  $B$  with  $D^I (D^J)^T$ , we obtain the formulation in Eq. (2.4) from chapter 2. Analog, if we define a matrix  $S = (-D \otimes F)$  with the vector  $\text{vec}(B)$  on the diagonal, we come to the formulation in Eq. (2.6).

It remains to show, that the problem in Eq. (2.2) is equivalent to the trace formulation of QAP (A.7). Indeed, consider the first term of the objective function in



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Eq. (2.2):

$$\begin{aligned}
\|A^I - \hat{P}A^J\hat{P}^T\|^2 &= \text{tr}((A^I - \hat{P}A^J\hat{P}^T)^T(A^I - \hat{P}A^J\hat{P}^T)) \\
&= \text{tr}(((A^I)^T - \hat{P}(A^J)^T\hat{P}^T)(A^I - \hat{P}A^J\hat{P}^T)) \\
&= \text{tr}((A^I)^T A^I - (A^I)^T \hat{P}A^J\hat{P}^T - \hat{P}(A^J)^T\hat{P}^T A^I + \hat{P}(A^J)^T\hat{P}^T \hat{P}A^J\hat{P}^T) \\
&= \text{tr}((A^I)^T A^I - 2(A^I)^T \hat{P}A^J\hat{P}^T + A^J(A^J)^T).
\end{aligned}$$

The first and the last terms are obviously constant and thus can be ignored during optimization. Consequently, it holds:

$$\underset{\hat{P} \in \Pi_n}{\text{argmin}} \|A^I - \hat{P}A^J\hat{P}^T\|^2 = \underset{\hat{P} \in \Pi_n}{\text{argmin}} -\text{tr}((A^I)^T \hat{P}A^J\hat{P}^T). \quad (\text{A.9})$$

We perform the same transformations with the second term:

$$\begin{aligned}
\|D^I - \hat{P}D^J\|^2 &= \text{tr}((D^I - \hat{P}D^J)^T(D^I - \hat{P}D^J)) \\
&= \text{tr}((D^I)^T D^I) - 2(D^I)^T \hat{P}D^J + (D^J)^T D^J \\
&= \text{tr}((D^I)^T D^I) - 2D^I(D^J)^T \hat{P} + (D^J)^T D^J
\end{aligned}$$

Also here the first and the last terms can be ignored during optimization, so that we can write:

$$\underset{\hat{P} \in \Pi_n}{\text{argmin}} \|D^I - \hat{P}D^J\|^2 = \underset{\hat{P} \in \Pi_n}{\text{argmin}} -\text{tr}(D^I(D^J)^T \hat{P}). \quad (\text{A.10})$$

The combination of the results in Eqs. (A.9) and (A.10) with the substitution  $F = -(A^I)^T$ ,  $D = (A^J)^T$  and  $B = -D^I(D^J)^T$  proof the equivalence of the problems (2.2) and (A.7). That is exactly, what we wanted to show.



# Appendix B

## Reweighted random walks for graph matching (RRWM)

The presented algorithm is developed by Minsu Cho et al. [14] and interprets the graph matching problem (2.6):

$$\operatorname{argmax}_x x^T S x \quad (2.6)$$

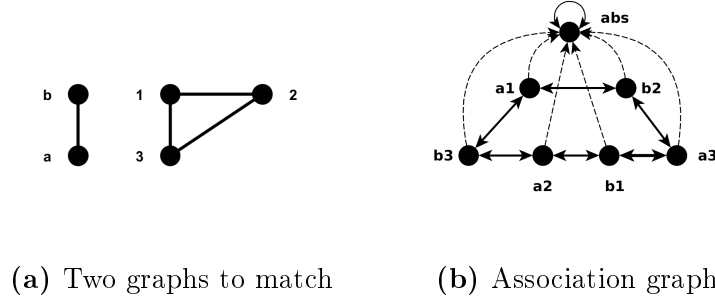
$$\text{s.t. } x \in \{0, 1\}^{n_1 n_2} \quad (2.7)$$

$$\sum_{i=1 \dots n_1} x_{ij} \leq 1 \quad (2.8)$$

$$\sum_{j=1 \dots n_2} x_{ij} \leq 1 \quad (2.9)$$

between two graphs  $G^I = (V^I, E^I, D^I)$ ,  $G^J = (V^J, E^J, D^J)$  in a random walk view. For that purpose the authors defined an association graph  $G^{rw} = (V^{rw}, E^{rw}, D^{rw})$  based on the affinity matrix  $S$ . The set of nodes  $V^{rw}$  of the new graph is represented by all possible correspondences between nodes in  $V^I$  and  $V^J$ . This means, that  $|V^{rw}| = n_1 n_2$ , where  $|V^I| = n_1$  and  $|V^J| = n_2$ . We refer to a node of the graph  $G^{rw}$  as  $v_{ij}$  if it represents a correspondence pair  $(v_i, v_j)$ ,  $v_i \in V^I, v_j \in V^J$ . The entry  $S_{ij, i'j'}$  of the matrix  $S$  defines the weight of the edge  $\{v_{ij}, v_{i'j'}\} \in E^{rw}$ . We denote the weighted adjacency matrix of the graph  $G^{rw}$  as  $W$ . An example of the construction is illustrated in Fig. B.1b. Note, that we omitted contradicting edges, whose weights are equal to zero, for example  $\{a1, b1\}$ .

It is obvious, that the graph matching problem between two graphs  $G^I$  and  $G^J$  is equivalent to finding a subset of nodes in the associated graph  $G^{rw}$ , so that the respective node correspondences between  $V^I$  and  $V^J$  satisfy the matching criteria



**Figure B.1:** Association Graph of two given graphs for Reweighted Random Walk Method (compare with [14])

of the initial problem. For finding such a subset the authors adopt the page ranking algorithm based on a random walk, which is assumed to be a Markov chain [58]. To describe a Markov chain one defines a transition matrix  $P$ . An usual approach to define a transition matrix of a wighted graph  $G^{rw}$  is to convert the weighted adjacency matrix  $W$  of the graph into a stochastic matrix by the following normalization  $P = D^{-1}W$ , where  $D$  is a diagonal matrix with entries  $D_{kk} = \sum_l W_{kl}$ . This method was, for example, used in the PageRank algorithm [58]. It is however not suitable for the graph matching purposes, as it treats false correspondences equal to all other correspondences. To avoid this problem Cho et al. introduced an additional absorbing node  $v_{abs}$  (see Fig. B.1b) in the Graph  $G^{rw}$ . This node represents a state, that can be reached from each node  $v_k = v_{ij} \in V^{rw}$  with the probability  $1 - D_{kk}/D_{\max}$ ,  $D_{\max} = \max_k D_{kk}$ . Once reached the node  $v_{abs}$  can not be left any more. Using  $D_{\max}$  the matrix  $W$  is converted into a stochastic matrix by its multiplication with the factor  $1/D_{\max}$ . Summarizing the transition matrix  $P \in \mathbb{R}^{(n_1n_2+1) \times (n_1n_2+1)}$  is defined as

$$P = \begin{pmatrix} W/D_{\max} & \mathbf{1} - d/D_{\max} \\ 0 \dots 0 & 1 \end{pmatrix} \quad (\text{B.1})$$

and update formula of the probability distribution of the Markov chain is defined as

$$\left( x^{(n+1)T}, x_{\text{abs}}^{(n+1)} \right) = \alpha \left( x^{(n)T}, x_{\text{abs}}^{(n)} \right) P + (1 - \alpha)r^T, \quad (\text{B.2})$$

where  $\mathbf{1}$  in (B.1) denotes a vector of size  $\mathbb{R}^{n_1n_2 \times 1}$  with all entries equal to 1,  $d = (D_{11}, \dots, D_{n_1n_2})$  is the diagonal of the matrix  $D$ ,  $\alpha$  is a weighted factor and  $r \in \mathbb{R}^{n_1n_2+1}$  is a *reweighted jump vector*.

A Markov chain, defined by Eq. (B.2) without the second term, is denoted by the

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authors as an *affinity-preserving random walk*. The distribution  $\bar{\mathbf{x}}$  of unabsorbed random walks at time  $n$  is defined as follows:

$$\bar{\mathbf{x}}_{ij}^{(n)} = P(X^{(n)} = v_{ij} | X^{(n)} \neq v_{\text{abs}}) = \frac{x_{ij}^{(n)}}{1 - x_{\text{abs}}^{(n)}}, \quad (\text{B.3})$$

where  $X^{(n)}$  is the current location of a random walker at time  $n$ . The authors call  $\bar{\mathbf{x}}$  a *quasi-stationary distribution* of the absorbed Markov chain. They proof, that the distribution  $\bar{\mathbf{x}}$  is proportional to the left principal eigenvector of  $W$  and can be efficiently computed with the power iteration method [32].

The second summand in Eq. (B.2) represents the possibility of a random walker to make a jump with probability  $(1 - \alpha)$  into some constrained node, instead of following the edge. This term was proposed by the authors based on an personalization approach for web page ranking [41] as a way to include the matching constraints (2.8), (2.9) into random walk. The authors are pointing out, that without this term the matching constraints are incorporated only in the last discretization step of the algorithm, which leads to a weak local maximum.

A procedure of generation the jump vector  $r$  from a current quasi-stationary distribution  $\bar{\mathbf{x}}$  consists of two steps. In the first step (*inflation*) unreliable correspondences (i.e. small values in the vector  $\bar{\mathbf{x}}$ ) are damped and the good correspondences are boosted at the same time. The second step (*bistochastic normalization*) forces the matching constraints by transforming the matrix form of  $\bar{\mathbf{x}}$  into a double stochastic matrix using the normalization scheme of Sinkhorn [73].

The described steps are summarized in Algorithm 4 below. The discretization step in line 16 can be done by using any method, which solves the linear assignment problem, i.e. the Hungarian algorithm [40] or greedy heuristic as in [43].

There are some similarities between RRWM and some algorithms, described in chapter 2. For example, the authors notice, that line 6 of Algorithm 4 can be considered as the power iteration version of SM [43]. Also the Sinkhorn normalization (line 8-11) was used in soft-assign step in [31].

The complexity of the algorithm is  $\mathcal{O}(|E^I||E^J|)$  per iteration, whereby the quasi-stationary distribution  $\bar{\mathbf{x}}$  in line 6 was computed with the power iteration method [32].

---

**Algorithm 4:** Reweighted Random Walks Method, compare to [14]

---

**Input:** weight matrix  $W$ , the reweight factor  $\alpha$ , the inflation factor  $\beta$

**Output:** distribution  $\mathbf{x}$

```

1 set  $W_{ij,i'j'}=0$  for all conflicting match pairs, i.e.  $(v_{ij}, v_{i'j'})$  and  $(v_{ij}, v_{i'j})$ 
2  $D_{\max} = \max_{ij} \sum_{i'j'} W_{ij,i'j'}$ 
3  $P = W/D_{\max}$ , initialize starting probability  $\mathbf{x}$  as uniform
4 repeat
    /* Affinity preserving random walking by edges */
6    $\bar{\mathbf{x}} = \mathbf{x}^T P$ 
    /* Reweighting with two-way constraints */
    /* step 1 inflation: */
7    $\mathbf{y}^T = \exp(\beta \bar{\mathbf{x}} / \max \bar{\mathbf{x}})$ 
    /* step 2 bistochastic normalization : */
8   repeat
9     normalize across rows by  $\mathbf{y}_{ij} = \mathbf{y}_{ij} / \sum_j \mathbf{y}_{ij}$ 
10    normalize across columns by  $\mathbf{y}_{ij} = \mathbf{y}_{ij} / \sum_i \mathbf{y}_{ij}$ 
11  until  $\mathbf{y}$  converges;
12   $\mathbf{y} = \mathbf{y} / \sum \mathbf{y}_{ij}$ 
    /* Affinity-preserving random walking with reweighted jumps */
13   $\mathbf{x}^T = \alpha \bar{\mathbf{x}}^T + (1 - \alpha) \mathbf{y}^T$ 
14   $\mathbf{x} = \mathbf{x} / \sum \mathbf{x}_{ij}$ 
15 until  $\mathbf{x}$  converges;
16 discretize  $\mathbf{x}$  by the matching constraints

```

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# Appendix C

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# Appendix D

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