Chapter 1

Graph Matching

In this chapter we review basic definitions and notations from the graph theory used in this thesis and introduce different forms and formulations of the graph matching problem together with some algorithms for solving them. The classification we use is based on [14], although we concentrated our attention mainly on one specific group of algorithms: those, which consider the graph matching problem as a quadratic optimization problem. Not all algorithms, we present thereby, were initially mentioned in [14], but we also do not cover all of the resent ones due to their quantity. We focus our selfs specially on those, that are important for further reading of the thesis.

1.1 Basic definitions and notation

A *undirected graph* $G = (V, E)$ is defined as a pair of disjoint sets V, E, where $E \subseteq \{\{u, v\}|u, v \in V\}$ [15]. The elements of the set V are called *vertices* or *nodes*[1] 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 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 $e = \{v_i, v_{i'}\} \in E$. Each graph can be represented by its *adjacency matrix* $A=(a_{ij})_{n\times n}$, where

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

and n is the number of nodes in the graph.

A *path* in a graph $G = (V, E)$ is a sequence of nodes $\{v_0, v_1, \ldots, v_k\}$ connected by

[1] We use terms vertex and node further in the text as synonyms

the edges $\{v_0v_1, v_1v_2, \ldots, v_{k-1}v_k\}$, where $v_i \in V$ and $v_{i-1}v_i \in E$ for all $i = 0, \ldots, k$. 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. The subgraph G' of G is *induced by the set* $V' \subseteq V$, if $E' = \{(v_i, v_{i'})|v_i, v_{i'} \in V'\}$. Analog, the set $E' \subseteq E$ induces the subgraph G' of G, if $V' = \{v \in V|v \in e \text{ and } e \in E'\}$. For the induced subgraph we use the notation $G' = G[V']$ and $G' = G[E']$ [15], depending if it is node- or vertex-induced. We also define 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, whose each pair of nodes is connected by an edge is called *complete*. In case, when each node $v_i \in V$ of a graph G has an associated attribute $d_i \in D$, one speaks about *attributed graph* $G = (V, E, D)$. If in contract to this each edge of a graph has an associated weight, the graph is called *weighted graph*. A connected, undirected graph without cycles is called a *tree*. A *hypergraph* is graph, whose edges connect several vertices at the same time (*hyperedges*).

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 $m : V^I \to V^J$ 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 metric $S(G^I, G^J, m)$ to measure the quality of matching m. In this case, *Graph matching problem* between G^I and G^J can be defined as a problem of finding such a map $m : V^I \to V^J$, that maximizes the similarity score $S(G^I, G^J, m)$ between the graphs and fulfills some additional constraints:

$$m = \underset{\hat{m}}{\operatorname{argmax}}\, S(G^I, G^J, \hat{m}) \tag{1.1}$$

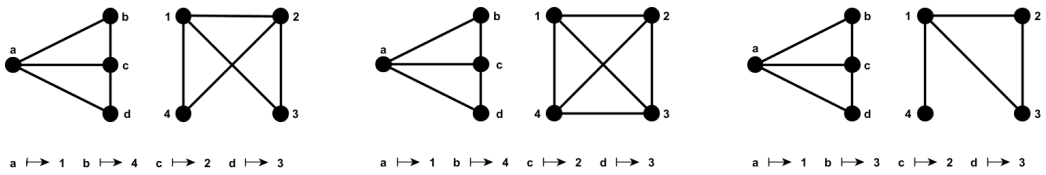
Based on the required properties of the mapping m the algorithms, that solve this problem, can be divided into two large groups [14]: *exact* and *inexact* graph matching methods. There are also variations inside of each group based on the definition of the similarity score between two graphs. In the following sections we will give an overview of the common exact and inexact graph matching algorithms.

1.2 Exact graph matching

The group of exact graph matching algorithms represents a class of more strict methods, that require the mapping between nodes of two graphs to be *edge preserving*. With other words: if $\{v_i, v_{i'}\} \in E^I$, then $\{m(v), m(v_{i'})\} \in E^J$ for all $v_i, v_{i'} \in V^I$. The graphs, considered in this case often do not have attributes.

There are several forms of the exact graph matching. The most known one is *graph isomorphism*: two graphs are called *isomorph* ($G^I \simeq G^J$), if the edge preserving mapping between their nodes is bijective. This implies, that two graphs have the 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 graphs, the problem is called *subgraph isomorphism*. Its further extension is a isomorphism between subgraphs of the graphs. The last problem can obviously have several solutions, but one is normally interested in finding a common subgraph with 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 bijective. This problem is called *graph monomorphism*. The correspondences here are still one-to-one, but the second graph may contain additional nodes and edges, comparing to the first graph. Even weaker form of graph matching problem is *graph homomorphism*. It allows many-to-one mapping between nodes of two graphs, which means that the only one restriction on the mapping m is to be total. On the Fig. 1.1 one can see examples of different exact graph matching problems.



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

Figure 1.1: Exact graph matching problems

All problems except graph isomorphism are proofed to be $NP-$complete [17]. This can be shown through the reduction of the matching problem to the clique problem. The graph isomorphism is currently shown to be $NP-$hard [17, 33]. For special types of graphs there exist polynomial time algorithms (e.g. for trees [1, 17]).

The most widespread approach to solve exact graph matching problems is based on tree search with backtracking. The idea is to starts with an empty solution and try in each step to expend it based on some rules until the solution is found. If it happens, that on some step a current solution cannot be expend further due to problem's constraints, the current branch is cut and algorithm backtracks to the last feasible solution and tries to expand it in other way. Those algorithms are very slow, if they need to search through the whole tree, but can be speeded up by applying some heuristic 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 [29] algorithm.

The one of the first algorithms, that uses described techniques, is the one by Ullman [38]. Later it was extended and improved mostly by the suggestion a new pruning heuristics (see for example [21] for comparison of algorithms based on the same technique). We also want to mention here another well known algorithm, which uses the tree search method and is closely related to maximal common subgraph problem, - algorithm by Bron and Kerbosch [2] for finding cliques in an undirected graphs.

The other techniques, that were successfully applied for the (sub)graph isomorphism are decision trees [25, 36, 35] and group theory[24] for maximal subgraph matching.

1.3 Inexact graph matching

Sometimes it is difficult to apply the exact matching algorithms described in previous section to real world problems. There are two possible reasons for that. On the one hand, that are variations in the structure of graphs, that describe a same object. Those variations could be a consequence of natural deformations or noise influence, that can occur in some real word applications. On the other hand, solving the graph matching problem exactly can be time or memory consuming. As a consequence one can be interested in solving graph matching problem inexactly. In this case, no edge preserving mapping between the nodes of two graphs is required.

Let us recall the problem statement (1.1):

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

where $S(G^I, G^J, \hat{m})$ defines the similarity measure between the attributed graphs

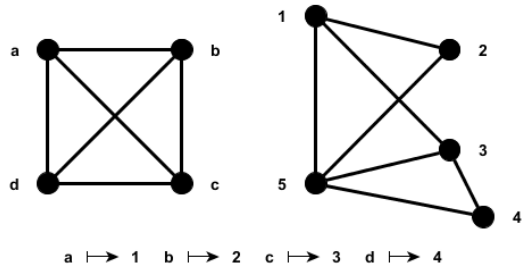


Figure 1.2: Inexact graph matching

$G^I = (V^I, E^I, D^I)$ and $G^J = (V^J, E^J, D^J)$. The mapping m is required to be total and sometimes also injective, to guarantee one-to-one matching.

Depending if an algorithm for solving (1.1) finds a global solution or not, it is called *optimal* or *suboptimal*. The choice, which algorithm to select depends on a specific problem. It should be noted, that an optimal inexact algorithms is not necessary faster than the exact one. 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 high number of different approaches inside the group of inexact graph matching algorithms. In the following section we summarized the most common form of objective function of the problem (1.1).

1.3.1 Graph Matching Objective Function

In some literature instead of defining the similarity function as in (1.1) one speaks about dissimilarity between two graphs cite or matching score cite. The goal in this case is to minimize those values. Two versions of the problem formulation are however equivalent and one can easy transform one into other.

Quadratic Optimization Problem

The objective of graph matching is to find a mapping between two attributed graphs $G^I = (V^I, E^I, D^I)$ and $G^J = (V^J, E^J, D^J)$. 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 $n_1 \leq n_2$. Here and further, we require the mapping m in (1.1) 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 with a even stricter assumption, that $n_1 = n_2 = n$ and the matching is bijective. In this case a mapping between nodes of the two graphs defines a permutation σ of the set $\{1, \ldots, n\}$. Each permutation σ 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 Π_n the set of all feasible permutations:

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

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 weighed graphs, the adjacency matrices contain edge weights, instead of binary values. We can now formulate the graph matching problem as (compare with [23, 31]cite):

$$P = \underset{\hat{P} \in \Pi_n}{\operatorname{argmin}} \|A^I - \hat{P} A^J \hat{P}^T\|^2 + \operatorname{tr}(D\hat{P}^T) \tag{1.2}$$

where $\|\cdot\|$ is the matrix Frobenius norm and the matrix $D \in \mathbb{R}^{n \times n}$ represent the pairwise dissimilarity[2] between node attribute sets D^I and D^J. Some authors [39] use slightly different reformulation of it, namely:

$$P = \underset{\hat{P} \in \Pi_n}{\operatorname{argmin}} \|A^I \hat{P} - \hat{P} A^J\|^2, \tag{1.3}$$

After some transformations, the problem (1.2) can be reformulated as (see [7], Appendix A):

$$P = \underset{\hat{P} \in \Pi_n}{\operatorname{argmin}} \, vec(\hat{P})^T (-(A^J)^T \otimes (A^I)^T) vec(\hat{P}) + \operatorname{tr}(D\hat{P}^T) \tag{1.4}$$

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

[2]We will discuss later, how to calculate the dissimilarity between node attributes.

The objective function of (1.4) is a negation of the objective of the *quadratic assignment problem*, which is know to be $NP-$hard [7, 32].

The both formulations have their advantages and disadvantages. The main benefit of (1.2) is the low space complexity $\mathcal{O}(n^2)$, where the space requirement of (1.4) estimates with $\mathcal{O}(n^4)$. This makes the second formulation 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 (1.2). In this sense the last formulation can be easily generalized in the way, we represent below.

We return back to the case where $n_1 \neq n_2$. Let 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 necessary 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 complicated form $x_{(j-1)n_1+i}$.

To measure a similarity between graphs one consider 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 $s_E : E^I \times E^J \to \mathbb{R}$ and should penalize disagreements in the structure of two graphs. The second one $s_V : V^I \times V^J \to \mathbb{R}$ represent additional constrains on the possible node correspondences.

Using the introduced notation and definitions of the node and edge similarity functions the function $S(G^I, G^J, m)$ in (1.1) can be now rewrite as follows:

$$S(G^I, G^J, m) = \sum_{\substack{x_{ij}=1 \\ x_{i'j'}=1}} s_E(e_{ij}, e_{i'j'}) + \sum_{x_{ij}=1} s_V(v_i, v_j) \tag{1.5}$$

This formula can be also expressed in matrix form. We define an *affinity* or *similarity matrix* $A \in \mathbb{R}^{n_1 n_2 \times n_1 n_2}$, whose diagonal elements are $s_V(v_i, u_j)$ and non-diagonal elements are $s_E(e_{ii\prime}, e_{jj\prime})$. Using this matrix we become the following formulation of the graph matching problem as an quadratic optimization problem [8, 10, 11, 14]:

$$\operatorname*{argmax}_x x^T S x \tag{1.6}$$

$$\text{s.t. } x \in \{0,1\}^{n_1 n_2} \tag{1.7}$$

$$\sum_{i=1\ldots n_1} x_{ij} \leq 1 \tag{1.8}$$

$$\sum_{j=1...n_2} x_{ij} \leq 1 \tag{1.9}$$

We notice, that in the case, where $n_1 = n_2$, both conditions (1.8) and (1.9) will be fulfilled with equality.

One can easily see, that the formulation (1.4) can be obtained from (1.2)-(1.9) by setting $S = -(A^J)^T \otimes (A^I)^T$.

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

- Node similarity

  The most frequently used approach to define a node similarity is to compare attributes of the corresponding nodes. In most of seen literature, the node attributes are represented by $d-$dimensional real vectors : $D^i, D^J \subset \mathbb{R}^d$. One of the simplest ways to define a node similarity in this case is to use a distance metric:

  $$s_V(v_i, v_j) = dist(d_i, d_j), \text{ for } \forall v_i \in V^I, \forall v_j \in V^J \tag{1.10}$$

  It can be, for example, an euclidean distance ([10]cite). The other widely used alternative to define node similarity, is to use cosine similarity[3] of node attributes [27]cite: $dist_c(d_i, d_j) = \frac{d_i \cdot d_j}{\|d_i\|_2 \|d_j\|_2}$, where dot denotes scalar product of two vectors.

- Edge similarity

  One possible approach to calculate edge similarity is to calculate *edge dissimilarity* $d_E : E^I \times E^J \to \mathbb{R}$ first and then transform it into similarity by using, for example, one of the following functions [8, 9, 10, 11]:

  - $s_E(e_{ii\prime}, e_{jj\prime}) = exp(-\frac{d_(e_{ii\prime}, e_{jj\prime})^2}{\sigma_s^2})$
  - $s_E(e_{ii\prime}, e_{jj\prime}) = \max(\beta - d_(e_{ii\prime}, e_{jj\prime})/\sigma_s^2, 0)$

  where $e_{ii\prime} \in E^I$ and $e_{jj\prime} \in E^J$. The parameters σ_s and β 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 a weights of the edges, if such are provided. An other alternative could be to use length of the edges [8, 9, 10, 11], if coordinates of the nodes in some system (usually, Cartesian coordinates) are known. It

[3] Cosine similarity is not distance metric, because it does not fulfill the triangular inequality.

a significant assumptions, which holds however for almost all graphs arose in practical application.

If the nodes of the graphs is described not only by their location, but also by some affine region around the nodes, one can use so-called geometric dissimilarity [9, 11]:

$$d(e_{ij}, e_{i'j'}) = \frac{1}{2}(d_{geo}(m_j|m_i) + d_{geo}(m_i|m_j)) \tag{1.11}$$

$$d_{geo}(m_j|m_i) = \frac{1}{2}(\|x_{j'} - H_i x_j\| + \|x_j - H_i^{-1} x_{j'}\|) \tag{1.12}$$

$$d_{geo}(m_i|m_j) = \frac{1}{2}(\|x_{i'} - H_j x_i\| + \|x_i - H_j^{-1} x_{i'}\|) \tag{1.13}$$

where m_i is a correspondence between nodes v_i and $v_{i'}$ and H_i is a homography from v_i to $v_{i'}$ defined by the provided affine regions around each node.

Error correcting graph matching

Another way to measure the similarity between two graphs is based on *graph edit distance* [5]. The graph edit distance is defined through costs of *graph edit operations*, that transform on graph into another. Those operations are insertion, deletion and substitution of the both nodes and edges. The algorithms, that uses graph edit distance for graph matching, are often called *error correcting* [14].

Consider two attributed graphs $G^I = (V^I, E^I, D^I)$ and $G^J = (V^J, E^J, D^J)$ and 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 [3]:

- 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 $V^I \backslash \bar{V}^I$ are *deleted*
- nodes in $V^J \backslash \bar{V}^J$ are *inserted*.

An edit operation of an edge is defined based on the transformations applied to it's end nodes. For example, if a node $v_j \in V^J$ was inserted, then all edges incident to this node are also inserted. Alternatively, if a node $v_i \in V^I$ was 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 $v_j, v_{j'}$.

We assume, that all operations can be performed simultaneously. Let $S = \{s_1, s_2, \ldots, s_k\}$ 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 then as $\sum_{i=1}^{k} c(s_i)$. Using this one define a *edit distance* between the graphs G^I and G^J as follows [5, 40]:

$$dist(G^I, G^J, m) = \min_{S=\{s_1,\ldots,s_k\}} c(S) \tag{1.14}$$

The cost functions are often defined as a functions of edge weights and node attributes. Their exact definitions depend however on an application. Sometimes, it can helpful, when the distance measure (1.14) defines a metric, which is not automatically the case. A list of restrictions on the cost functions, that ensure the distance (1.14) to be a metric, is provide i.e. in [5]. The same author in [6] provides a direct formulation of an edit distance measure, with metric properties without direct specification of cost functions.

An interesting question is, how does the error corrected graph matching problem correspond to the other matching problems. Some authors have shown, that some particular constrains on the graph edit costs allow to transform the first problem to the other or the other way round. In [4] it was shown, that graph isomorphism, subgraph isomorphism and maximum common subgraph problems can be considered as a special cases of the error correcting graph matching.

It is also easy to show, how to reformulate (1.14) into (1.2). The objective function of the last formulation can be rewritten as $\sum_{i=1}^{n}\sum_{j=1}^{n}(A^I_{ii'} - A^J_{\sigma(i)\sigma(i')})^2$. Comparison of the last expression with the definition (1.14) leads us direct to the idea, how to select the edge insertion/deletion/substitution cost functions, to make the problem formulations equivalent:

$$c(e_{\text{subst}}) = (A^I_{ii'} - A^J_{\sigma(i)\sigma(i')})^2 \quad c(e_{\text{insert}}) = (A^J_{\sigma(i)\sigma(i')})^2 \quad c(e_{\text{del}}) = (A^I_{ii'})^2$$

1.4 Approaches for solving graph matching problem

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

1.4.1 Discrete optimization

Tree search methods

Similar to the exact graph matching problems the tree based methods with backtracking were successfully applied also to inexact matching problems. They were especially wild used for the error-correcting graph matching. The searching procedure often can be guided, so that the required time is shorter, than exponential time, which is needed by a blind searching. To traverse a tree effectively one uses score of the current achieved partial matching together with a heuristic estimate for the score of the remaining nodes. The most algorithms in this groups differ in a suggested heuristics to estimate future costs and in a rules, for tree traversing. The most used methods for the last are depth-first-search and A^*-Algorithm [18]. The first algorithm for inexact graph matching based on the three search was presented in [37]. It is an optimal inexact graph matching algorithm. For further examples of the three search methods for inexact graph matching we refer to [5, 34, 40].

Simulated Annealing

Simulated annealing is a heuristic for searching the global optimum of a given energy function [7]. It is an extension of the Metropolis Algorithm [26], that was suggesting for finding an equilibrium of a physic system with many particles. Speaking in terms of a combinatorial optimization problem, feasible solutions of a problem define states of a system and corresponding objective scores it's energy. The idea is find the state with the lowest energy by performing some random changes in a system. A change, that pushes system into a state with lower energy, is always accepted. On the other side, a change, that increases energy function, is accepted with some probability. This probability and number of changes per iteration is controlled by the temperature parameter T. The bigger T the viewer changes are allowed and the smaller the accepted probability is.

The application of the simulated annealing to the graph matching problems can be found in [19]. It is also a common used heuristic used for quadratic assignment problem [7].

1.4.2 Continuous optimization

This group is one of the biggest and deep investigated. The main idea is to relax the integer constraints in the discrete optimization problems (1.2), (1.6) and apply

continuous optimization algorithms to solve them. The found solution must be converted afterwards back in the discrete domain. We list further some of the techniques applied for solving relaxed problems.

The first subgroup of the algorithms, that use techniques of the continuous optimization, are those, who work directly with the objective function of (1.2) or (1.6).

In 1996 Gold and Rangarajan [12] presented an iterative algorithm applied to the formulation (1.6) which uses *deterministic annealing*[4]. They use Taylor series approximation to relax the initial quadratic assignment problem to linear assignment problem, which they solve using *soft-assign*. The basic idea of the soft-assigned is to a binary correspondence matrix to a doubly stochastic one. The determenistic annealing was also used in [28] to solver Lagrangian Relaxation of the problem (1.2). Also in [13] the similar technique was applied to the point set matching. 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.

Two Algorithms suggested in [39] and [22] uses *Frank-Wolfe algorithm* [16], that solves originally a convex quadratic program. The both algorithms starts with some solution (continuous in [39] and continuous or discrete in [22]) and iteratively improve this solution. The improvement step is an application of the *Frank-Wolfe algorithm* to the graph matching problem. It processes in two steps: it finds first a search direction by solving an linear assignment problem, which arises by the minimizing the first-order Tailor series approximation to the objective function; then the second step maximizes the continuous relaxation of the original problem along found direction. A continuous solution can be mapped afterward back in the discrete domain. Although, both algorithms use the same technique, they are applied to different formulations of the graph matching problem. The authors in [39] consider the formulation (1.4), whereby the work [22] uses more general case of the problem formulation (1.6). Avoiding the usage of the similarity matrix S gives the first algorithm a big advantage of the less complexity and space requirement, which make it possibly to work with graphs of a big size.

[4]Deterministic annealing is similar to the simulated annealing, but uses determenistic techniques to find the closest local minimum by value of the temperature parameter [30].

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 to minimize the summary cost of the assignment. Let $D = (d_{kl}), F = (f_{kl}), B = (b_{ik}) \in \mathbb{R}^{n\times n}$ be a real matrices that define a distances and flow between the locations, as well as opening costs. The problem defined above can then be formulated as an integer quadratic program [7, 20]:

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

where Σ_n is a set of all possible permutations of the set $\{1,\ldots,n\}$, and is called *Koopmans-Beckmann version of the quadratic assignment problem* (further *QAP*).

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

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

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

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

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

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

From the definition of the matrix trace follows cite:

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

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

$$\operatorname{vec}(APB) = (B^T \otimes A)\operatorname{vec}(P). \tag{A.5}$$

We can now apply the equality 2 and 3 in (A.4) to the formulation (A.2) and get the *trace formulation of QAP* [7]:

$$P = \underset{\hat{P}\in\Pi_n}{\operatorname{argmin}} \operatorname{tr}(F\hat{P}D^T\hat{P}^T + B\hat{P}^T). \tag{A.6}$$

The objective function of (A.6) can be further rewritten based on the last equality in (A.4) and property (A.5) as follows:

$$\begin{aligned} \operatorname{tr}(F\hat{P}D^T\hat{P}^T + B\hat{P}^T) &= \operatorname{tr}(\hat{P}(F\hat{P}D^T)^T) + \operatorname{vec}(B)^T \operatorname{vec}(\hat{P}) \\ &= \operatorname{vec}(\hat{P})^T \operatorname{vec}(F\hat{P}D^T) + \operatorname{vec}(B)^T \operatorname{vec}(\hat{P}) \\ &= \operatorname{vec}(\hat{P})^T (D \otimes F) \operatorname{vec}\hat{P} + \operatorname{vec}(B)^T \operatorname{vec}(\hat{P}). \end{aligned} \tag{A.7}$$

Based on this formulation the matrix B is called sometimes *linear cost matrix* and the matrix $D \otimes F$ the *quadratic costs matrix*. If we assume the matrix B be a constant matrix with the same values, that it does not have any influence on the optimization process. In this case setting matrix F to $-(A^I)^T$ and matrix D to $(A^J)^T$ lead us to the formulation (1.3). Similarly, denoting the Kronecker product $(-D \otimes F)$ as S results in the formulation (1.5).

It remains to show, that (1.2) is equivalent to (A.6). Indeed, consider the objective

function in (1.2):

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

The first and the last term are obviously constant, and thus can be ignored in optimization. Finally, substitution of $F = -(A^I)^T$, $D = (A^J)^T$ leads us to the formulation (A.6). That is exactly, what we wanted to show.

Appendix B

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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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