Inexact Graph Matching Using Centrality Measures

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Abstract

Graph matching is the process of computing the similarity between two graphs. Depending on the requirement, it can be exact or inexact. Exact graph matching requires a strict correspondence between nodes of two graphs, whereas inexact matching allows some flexibility or tolerance during the graph matching. In this chapter, we describe an approximate inexact graph matching by reducing the size of the graphs using different centrality measures. Experimental evaluation shows that it can reduce running time for inexact graph matching.

1 Introduction

Graph Matching (GM) is one of the important research areas in graph-based representation in structural pattern recognition. GM is the process of computing the similarity between the two graphs. Depending on the nature of the matching, it has been broadly classified into two varieties, exact GM and inexact or error-tolerant GM. For exact GM, strict correspondence is necessary between each node and edge of the first graph to the corresponding nodes and edges of the second graph. Exact GM is like a graph isomorphism problem in which a bijective mapping is required from the nodes of the first graph to the nodes of the second graph.

Exact GM although theoretically appealing, may not be useful in many real-world applications, as due to the existence of noise or distortion during the processing, the input graph data may be altered. In such situations, we use inexact GM or error-tolerant GM due to its flexibility to accommodate errors during the process of matching. Polynomial time solution for GM is not available. Graph isomorphism problem is neither shown to be in NP-complete nor in P. On the other hand, the subgraph isomorphism problem is known to be NP-complete. Due to non-availability of exact polynomial time algorithms for GM problem, several approximation algorithms and heuristic have been proposed.

An extensive survey of different GM methods is explained in [7] and [15]. In [4] author describes a precise framework for inexact GM. A-star search technique for finding minimum cost paths is described in [17]. Inexact GM of the attributed relational graphs (ARG) is described in [32]. In [29] authors introduced a distance measure for non-hierarchical ARG by considering the cost of recognition of nodes.

A category of GM algorithms utilizing the spectral technique of algebraic graph theory has been introduced [5], which depend on the fact that adjacency matrices of similar graphs will have a similar decomposition [28], [30].

A novel class of GM techniques based on the so-called graph kernel, which uses the concept of kernel machines to graph domain, is described in [16], [21]. Graph kernel enables us to utilize

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statistical pattern recognition methods to the structural pattern. The essential types of graph kernels are convolution kernel, diffusion kernel and random walk kernel [18], [19].

Another technique of GM is based on geometric graphs in which each vertex has its associated coordinate in two-dimensional space [11], [12]. Geometric GM using the edit distance approach is demonstrated to be \(NP\)-hard in [6]. Geometric GM using a probabilistic approach is described in [2] and in the paper, [23] authors have presented geometric GM based on Monte Carlo tree search.

Graph Edit Distance (GED) is one of the important techniques used for inexact GM [3], [29]. GED between two graphs is defined as the minimum edit operations needed to convert the first graph into another one. GED is the generalization of string edit distance. Exact algorithms for GED are computationally expensive and are exponential on input graphs’ size. To make GED computation feasible, many approximate methods using local search, greedy method, neighborhood search, bipartite GED, homeomorphic, GED etc. have been proposed [9], [14], [20], [25], [26], [31], [13], [8].

In [10], the authors proposed an approach to inexact GM by contracting the nodes from the graphs based on their degree centrality. In this chapter, we describe this approach to perform inexact GM by reducing the size of the graphs using different centrality measures such as eigenvector, betweenness and PageRank centrality. It leads to a reduction in search space needed to compute GED between two graphs. We perform the experimental evaluation to demonstrate that these centrality measures can be used as a trade-off for running time and accuracy for GM algorithms.

This chapter is organized as follows. Section 2, contains preliminaries and motivation. Section 3, presents inexact GM using centrality measures. Section 4, describes the experimental evaluation and finally section 5, contains the conclusion.

### 2 Preliminaries and motivation

In this section we explain the basic definitions related to GM. For a detailed description the reader is referred to [1], [21]. We also describe the motivation for our work.

A graph \(G\) is defined as \(G = (V, E, \mu, \nu)\), where \(V\) is the set of vertices, \(E\) is the set of edges, \(\mu\) is a node labeling function \(\mu : V \rightarrow L_V\), and \(\nu\) is edge labeling function \(\nu : E \rightarrow L_E\). Here, \(L_V\) is the node label set and \(L_E\) is the edge label set. A graph \(G_1\) is called subgraph of another graph \(G_2\), when \(V_1 \subseteq V_2\); \(E_1 \subseteq E_2\); for each node \(u\) of graph \(G_1\), we have \(\mu_1(u) = \mu_2(u)\); similarly, for each edge \(e\) of \(G_1\), we have \(\nu_1(e) = \nu_2(e)\).

A sequence of edit operations that convert one graph \(G_1\) to another graph \(G_2\) is called edit path from \(G_1\) to \(G_2\). The simple edit operations include insertion, deletion and substitution nodes and edges. Insertion and deletion of node \(u\) is denoted respectively by \(\epsilon \rightarrow u\) and \(u \rightarrow \epsilon\), whereas substitution of node \(u\) by node \(v\) is denoted by \(u \rightarrow v\). Similarly insertion and deletion of edge \(e\) is represented respectively by \(\epsilon \rightarrow e\) and \(e \rightarrow \epsilon\), while substitution of edge \(e\) by edge \(f\) is denoted by \(e \rightarrow f\).

The GED between two graphs \(G_i = (V_i, E_i, \mu_i, \nu_i)\) for \(i = 1, 2\) is defined by

\[
GED(G_1, G_2) = \min_{(e_1, \ldots, e_k) \in \varphi(G_1, G_2)} \sum_{i=1}^{k} c(e_i)
\]

where \(c(e_i)\) is the cost of edit operation \(e_i\) and \(\varphi(G_1, G_2)\) represents the set of all edit path transforming \(G_1\) to \(G_2\).

Node contraction is the process of deleting nodes and its associated edges provided it is not a cut vertex [10]. \(k\)-degree node contraction on a graph \(G\) is the process of contracting all nodes of
degree \( k \) in graph \( G \). \( k^*-\)degree node contraction is the task of applying \( k \)-degree node contraction iteratively on a graph \( G \), from \( i = 1 \) to \( k \). \( k^*-GED \) is defined as GED between \( G_1 \) and \( G_2 \), with \( k^*-\)degree node contraction applied on both \( G_1 \) and \( G_2 \).

The applications of exact GM to real-world applications is rather limited due to the presence of noise or error during the processing of the graphs. Inexact GM offers an alternative to perform approximate GM. Due to exponential complexity associated with GED, other methods have been introduced to perform efficient GM at the cost of a slight decrease in accuracy. A technique proposed in [10] is based on removing the nodes based on their degree centrality to decrease the size of the matching graphs. However, degree centrality may not always be the best criteria to ignore the nodes. Depending on the structure and properties of the different dataset, we can select the appropriate centrality measure to delete the nodes for reducing the size of the graphs. In this chapter, we use eigenvector, betweenness and PageRank centrality in addition to degree centrality to reduce the size of the graphs for estimating an early approximate GM between two graphs.

Now we briefly explain the above centrality measures [22]. Centrality of the node in a graph signifies its relative importance in the graph. The centrality measures aim to find the most important or central nodes of a graph or network. Simplest centrality measure is degree centrality, which simply refers to the degree of the given node. A node with more adjacent nodes or neighbors will have higher degree centrality as compared to nodes with a fewer connection. Betweenness centrality of a node is based on the extent by which this node lies on the paths between other nodes. Eigenvector centrality is a generalization of degree centrality, which assigns each node a value proportionate to the sum of the values of its neighbors. For a node \( u_i \), its eigenvector centrality is given by \( x_i = \kappa_1^{-1} \sum_j A_{ij}x_j \), where \( \kappa_1 \) is the largest eigenvalue of adjacency matrix \( A \) and \( A_{ij} \) is an element of \( A \). In PageRank centrality, the centrality of a node is proportionate to the centrality of its neighbors divided by their outgoing degree. The PageRank centrality is defined by \( x_i = \alpha \sum_j A_{ij} \frac{x_j}{k_j} + \gamma \), where \( \alpha \) is a free parameter, \( k_j \) is the outgoing degree and \( \gamma \) is a constant.

### 3 Inexact graph matching

To reduce the computation time of inexact GM, we ignore the nodes from the graphs with less centrality value before computing a similarity score using GED between two graphs.

**Definition 1.** \( t \)-centrality node contraction is the process of contracting \( t \) nodes from a graph \( G \) with least centrality values of a given centrality measure.

The above definition implies that starting from the node with the lowest centrality value in a graph \( G \), up to \( t \) nodes are deleted provided they are not a cut vertex. Depending on the centrality measure used \( t \)-centrality node contraction (\( t \)-NC) can be \( t \)-degree centrality node contraction (\( t \)-DC-NC), \( t \)-betweenness centrality node contraction (\( t \)-BC-NC), \( t \)-eigenvector node contraction (\( t \)-EV-NC) and \( t \)-PageRank node contraction (\( t \)-PR-NC).

**Definition 2.** \( t \)-degree centrality node contraction is the operation of contracting \( t \) nodes of the smallest degree from a graph \( G \).

When \( t \) is equal to the number of nodes of degree \( k \) in a graph, then \( t \)-degree centrality node contraction corresponds to \( k \)-degree node contraction.
**Definition 3.** $t$-betweenness centrality node contraction is the operation of contracting $t$ nodes with the lowest betweenness score from a graph $G$.

**Definition 4.** $t$-eigenvector centrality node contraction is the process of contracting $t$ nodes with the lowest eigenvector centrality from a graph $G$.

**Definition 5.** $t$-PageRank centrality node contraction is the process of contracting $t$ nodes with the lowest PageRank score from a graph $G$.

**Definition 6.** $t$-centrality GED computation between two graphs $G_1$ and $G_2$ is defined as GED between these graphs, when $t$ nodes of least centrality of both graphs $G_1$ and $G_2$ have been contracted.

In the above definition depending on the actual centrality criteria used $t$-centrality GED computation ($t$-GED) corresponds to $t$-degree centrality GED computation ($t$-DC-GED), $t$-betweenness centrality GED computation ($t$-BC-GED), $t$-eigenvector GED computation ($t$-EV-GED) and $t$-PageRank GED computation ($t$-PR-GED).

### 3.1 Edit Cost

We can define the edit cost of $t$-GED by using an additional operation $c(u \to \epsilon) = 0$, for $t$ vertices of the graph $G$ having the lowest score of the given centrality measure.

$t$-GED utilizes the Euclidean distance and allocates the constant cost to insertion, deletion and substitution of vertices and links. For two graphs $G_1$ and $G_2$, having vertices $u \in V_1$, $v \in V_2$ and links $e \in E_1$, $f \in E_2$, we specify the extended edit cost function as given below.

\[
c(u \to v) = x_{node}
\]
\[
c(\epsilon \to v) = x_{node}
\]
\[
c(u \to v) = y_{node} \cdot ||\mu_1(u) - \mu_2(v)||
\]
\[
c(\epsilon \to \epsilon) = x_{edge}
\]
\[
c(\epsilon \to f) = x_{edge}
\]
\[
c(\epsilon \to f) = y_{edge} \cdot ||\nu_1(e) - \nu_2(f)||
\]
\[
c(u \to \epsilon) = 0, \text{ if } u \text{ is one of the } t \text{ nodes of the lowest centrality value and is not a cut vertex.}
\]

Here $x_{node}$, $y_{node}$, $x_{edge}$, $y_{edge}$ are positive constants.

### 3.2 Algorithm

The computation of inexact GM using $t$-centrality node contraction is outlined in Algorithm 1. The input to the $t$-Centrality-Graph-Edit-Distance algorithm is two graphs $G_1 = (V_1, E_1, \mu_1, \nu_1)$, $G_2 = (V_2, E_2, \mu_2, \nu_2)$ and a parameter $t$. The output to the algorithm is the minimum cost $t$-GED between $G_1$ and $G_2$. The algorithm calls the procedure $t$-Centrality-Node-Contraction in lines 1–2 for graphs $G_1$ and $G_2$ respectively to remove $t$ nodes having the lowest centrality value provided they are not cut vertex. $G_1'$ and $G_2'$ are the resultant graphs obtained after performing $t$-Centrality-Node-Contraction on $G_1$ and $G_2$ respectively, such that $V_1' = \{u_1', ..., u_{n'}\}$ and $V_2' = \{v_1', ..., v_{m'}\}$. Line 3 initializes an empty set $A$. The vertex $u_1'$ of $G_1'$ is substituted by each vertex $v_j'$ of $G_2'$ in the for loop of lines 3–6, and deletion of $u_1'$ is performed in line 7. The computation of the minimum cost edit path is performed in the while loop of lines 8–27. If loop in line 10 check, whether $C_{min}$ is a complete edit path, so that it completely transform $G_1'$ to $G_2'$. If all nodes $V_2'$ are processed (line 13), then remaining nodes of $V_2'$ are simply inserted in $C_{min}$ in for loop of lines 14–16. Similarly,
all unprocessed vertices of $V'_1$ is substituted by all vertices of $V'_2$ along with the deletion of vertices of $V'_1$ in the for loop of lines 19–23, and $A$ is updated in line 24.

**Proposition 1.** $t$-Centrality-Graph-Edit-Distance algorithm performs inexact GM of $G'_1$ and $G'_2$.

Using the properties of the edit costs of $t$-GED, the Algorithm 1 return minimum cost of complete edit path which transform input graph $G'_1$ to output graph $G'_2$, so that every vertex of $G'_1$ is uniquely corresponds to a vertex of $G'_2$. Also the procedure $t$-Centrality-Node-Contraction ensures that $V'_1 \subset V_1$ and $V'_2 \subset V_2$.

**Proposition 2.** The procedure $t$-Centrality-Node-Contraction executes in $O(n)$ time.

We can check whether a node $u$ is a cut vertex in $O(n)$ time. Therefore the for loop of the procedure takes $O(t.n)$ time, that is $O(n)$.

The worst case computational complexity of the $t$-Centrality-Graph-Edit-Distance algorithm is exponential in the number of vertices in input graphs. We can use an appropriate variable $t$ to minimize the overall computation time.

4 Experimental evaluation

In this section, we apply $t$-Centrality-Graph-Edit-Distance algorithm for inexact GM using the degree, betweenness, eigenvector and PageRank centrality. We use IAM graph database [24] for the comparison of execution time and accuracy obtained by these centrality techniques. We use letter and AIDS dataset for the evaluation of the proposed inexact GM scheme.

Letter dataset contains fifteen capital letters of English alphabets, written through straight lines. For each instance of a graph, deformation of three distinct and increasing levels are applied to construct low, medium and high samples of graph dataset. Every vertex of letter graphs have an associated $(x, y)$ coordinates in the two-dimensional plane. Letter graphs with high distortion level contain the average number of vertices as 4.7 and the average number of links is 4.5. AIDS dataset consists of graph specifying chemical compounds. It contains two class of molecules, confirmed active and confirmed inactive. Graph molecules in active class exhibit activity against HIV, whereas molecules of inactive class show inactivity against HIV. Labels on node represent chemical symbol whereas labels on edge denote valence. The average number of vertices per graph in AIDS dataset is 15.7, whereas the average number of links are 16.2 edges.

4.1 Execution time comparison

For the comparison purpose, we have used the value of $t^*$ in $t^*$-GED to be equal to the number of nodes which would be considered for contraction in $k^*$-degree node contraction. Therefore the value of 1* in 1*-GED is the number of nodes of degree 1, value of 2* in 2*-GED is the number of nodes of degree 1 followed by degree 2, similarly the value of 3* in 3*-GED is the number of nodes of degree 1 followed by degree 2 and degree 3. Comparison of the average execution time of GM in milliseconds using $t$-Centrality-Graph-Edit-Distance algorithm as applied to letter A and E of high distortion letter dataset using different centrality measures in shown in Fig.1 and Fig.2 respectively.

We can observe that GM time using eigenvector criteria is least, whereas time using degree centrality is higher. Computation time for letter E is higher as it contains more nodes than letter
Algorithm 1: $t$-Centrality-Graph-Edit-Distance ($G_1, G_2$)

Require: Two Graphs $G_1, G_2$, where $V_1 = \{u_1, ..., u_n\}$ and $V_2 = \{v_1, ..., v_m\}$ and a parameter $t$

Ensure: A minimum cost $t$-GED between $G_1$ and $G_2$

1: $G'_1 \leftarrow t$-Centrality-Node-Contraction ($G_1, t$)
2: $G'_2 \leftarrow t$-Centrality-Node-Contraction ($G_2, t$)
3: $A \leftarrow \emptyset$
4: for each ($v'_j \in V'_2$) do
5:   $A \leftarrow A \cup \{u'_1 \rightarrow v'_j\}$
6: end for
7: $A \leftarrow A \cup \{u'_1 \rightarrow \epsilon\}$
8: while (True) do
9:   Compute minimum cost edit path $C_{min}$ from $A$
10:   if ($C_{min}$ is a complete edit path) then
11:      return $C_{min}$
12:   else
13:      if (all vertices ($u'_i \in V'_1$) are visited) then
14:         for all unvisited ($v'_j \in V'_2$) do
15:            $C_{min} \leftarrow C_{min} \cup \{\epsilon \rightarrow v'_j\}$
16:         end for
17:         $A \leftarrow A \cup \{C_{min}\}$
18:      else
19:         for (all unvisited vertices ($u'_i \in V'_1$)) do
20:            for (each ($v'_j \in V'_2$)) do
21:               $C_{min} \leftarrow C_{min} \cup \{u'_i \rightarrow v'_j\} \cup \{u'_i \rightarrow \epsilon\}$
22:            end for
23:         end for
24:         $A \leftarrow A \cup \{C_{min}\}$
25:      end if
26:   end if
27: end while
28: procedure $t$-Centrality-Node-Contraction($G, t$)
29: for ($i \leftarrow 1$ to $t$) do
30:   Select node $u$ with minimum centrality
31:   if ($u$ is not cut vertex) then
32:      $V \leftarrow V \setminus \{u\}$
33:      $E \leftarrow E \setminus \{(u, v) | (u, v) \in E, \forall v \in G\}$
34:   end if
35: end for
36: return $G$
37: end procedure
A. Comparison of the average running time of GM in milliseconds using beam search heuristic (beam width $w = 10$) for the four different centrality measures for the active class of AIDS dataset are shown in Fig.3. From this figure, we observe that Algorithm 1 usually takes less time using eigenvector and betweenness centrality as compared to the degree and PageRank centrality.

Fig.4 shows the corresponding average execution time of graphs for inactive AIDS dataset using the four centrality measures. Here again, the computation time using eigenvector and betweenness criteria take less time than the degree and PageRank, and between these two the average time using PageRank is less than degree centrality.

4.2 Accuracy comparison

For accuracy assessment, we consider the problem of classification of graphs by the nearest neighbor classifier. Letter dataset of high distortion level consists of 750 graphs for both training as well as test sets. Each of these training, as well as test dataset, contains 50 graphs for every 15 letters. Classification accuracy of proposed GM for letter A of high distortion using the four centrality indicators is given in Fig.5, while the accuracy of GM for letter E for the same measures are shown in Fig.6.
Figure 3. Comparison of execution time for active class of AIDS dataset

Figure 4. Comparison of execution time for inactive class of AIDS dataset

Figure 5. Comparison of accuracy ratio of letter A dataset
Here we note that accuracy of letter A for degree centrality is lower than the other three measures by contracting $t$ nodes, where $t$ is equal to nodes with degree 1 in the input graphs ($1^*\text{-GED}$). We can also observe that for letter E, the accuracy ratio using betweenness and PageRank is usually higher than that of degree centrality even though they take less computation time.

To find the accuracy on AIDS dataset, we utilize test dataset consisting of 300 graphs from active class and 1200 graphs from inactive class, whereas training dataset consists of 50 graphs from active class and 200 graphs from the inactive class of AIDS dataset. We can observe the accuracy ratio of the proposed inexact scheme using the four different centrality measure in Fig. 7. In this figure, we observe that the accuracy obtained using degree and PageRank centrality are generally higher than that of eigenvector and betweenness centrality. Here we notice the time versus accuracy trade-off, the centrality criteria which takes less time leads to less accuracy, whereas the centrality techniques which are more accurate take more computation time.

Fig. 8 shows the comparison of accuracy for the inactive class of AIDS dataset using the four centrality measures. In this figure also degree and PageRank criteria lead to higher accuracy for the classification of graphs of AIDS dataset.
5 Conclusion

In this chapter, we presented a technique to approximate GM utilizing the concept of centrality measure to reduce the size of the graphs by ignoring the nodes with a lower value of given centrality criteria. In particular, we have used eigenvector, betweenness and PageRank centrality apart from degree centrality to perform the node contraction for the computation for inexact GM. Experimental results show that these centrality criteria can be used as computation time versus accuracy trade-off for different graph dataset.

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