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LETTER

A New Model for Graph Matching and Its Algorithm*

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SUMMARY Graph matching is a NP-Hard problem. In this paper, we relax the admissible set of permutation matrices and meantime incorporate a barrier function into the objective function. The resulted model is equivalent to the original model. Alternate iteration algorithm is designed to solve it. It is proven that the algorithm proposed is locally convergent. Our experimental results reveal that the proposed algorithm outperforms the algorithm in [1].

key words: *graph matching; alternate iteration algorithm; permutation matrix*

1. Introduction

Graphs are commonly used as abstract representations for complex structures, including DNA sequences, documents, text, and images. A graph G is an ordered pair $G = (V, W)$, where V is a set of n vertices in the graph, and W is a weighting function, which gives a real nonnegative value $W(v_i, v_j)$ to each pair of vertices (v_i, v_j). The adjacency matrix of a graph $G = (V, W)$ is given by $A = (a_{ij})_{nn}$, where $a_{ij} = W(v_i, v_j)$. The problem of matching two graphs $\bar{G} = (\bar{V}, \bar{W})$ and $\tilde{G} = (\tilde{V}, \tilde{W})$ consists of finding a permutation π from the set $\bar{V} = \{\bar{v}_1, \bar{v}_2, \cdots, \bar{v}_{\bar{n}}\}$ to $\tilde{V} = \{\tilde{v}_1, \tilde{v}_2, \cdots, \tilde{v}_{\tilde{n}}\}$ (generally, $\bar{n} \le \tilde{n}$), that makes $\bar{G}$ and $\tilde{G}$ as close as possible with respect to a certain matching cost. In this paper, we consider the following graph matching model:

$$\pi^* \in arg \min_{\pi \in S_{\bar{n},\tilde{n}}} \left\{ \sum_{i=1}^{\bar{n}} \sum_{j=1}^{\bar{n}} (\bar{a}_{ij} - \tilde{a}_{\pi(i)\pi(j)})^2 \right\}, \tag{1}$$

where $S_{\bar{n},\tilde{n}}$ is the set of permutations from $\{\bar{v}_1, \bar{v}_2, \cdots, \bar{v}_{\bar{n}}\}$ to $\{\tilde{v}_1, \tilde{v}_2, \cdots, \tilde{v}_{\tilde{n}}\}$.

This model has been widely studied during the past thirty years [2], [3]. However, it has been proved that (1) is NP-hard [3]. Indeed, when $\bar{n} = \tilde{n}$, (1) is a quadratic assignment problem. Researchers have showed that the quadratic assignment problem with more 30 nodes are practically intractable [4]. There has been no polynomial time algorithm that can directly solve it with 0-1 integer solutions. A wise method is to find a good approximate solution or a sub-optimality solution in reasonable time. Continuous optimization method is one of the most important methods for graph matching, such as graduated assignment [5], RKHS methods [6], alternate iteration method [1], *etc.* The common principle of continuous optimization algorithm for graph matching algorithm is to cast graph matching, which is a inherently discrete optimization problem, into a continuous optimization problem. There are many optimization algorithms that can be used to find a solution of this continuous optimization problem. But these algorithms do not ensure the optimality of the solution. Furthermore, the solution of continuous optimization must be converted back from the continuous domain into the initial discrete domain by a heuristic process.

The aim of this paper is to present a new equivalent model of (1) and avoid heuristic process which is a common process in most of continuous optimization methods for graph matching with same size. The resulted model is as follows:

$$(X^*, Y^*) \in arg \min\{G_\alpha(X, Y) | X \in \mathcal{P}(n), Y \in \Omega\} \tag{2}$$

where $G_\alpha(X, Y) = \|\bar{A}Y - Y\tilde{A}\| + \alpha\|X - Y\|$, $\|.\|$ is Frobenius norm, α is a barrier coefficient, $\mathcal{P}(n)$ denotes the set of permutation matrices and $\Omega \subset \mathcal{P}(n)$. Let (X^*, Y^*) be an optimal solution of (2), then it is proved that X^* is an optimal solution of (1) if $\alpha \ge \|\bar{A}\| + \|\tilde{A}\|$. This avoids the heuristic process in most of continuous optimization methods. Meantime, alternate iteration algorithm is designed to solve it in this paper. It is proved that the algorithm proposed is locally convergent. A related work of this paper appears in [1], but, the model in [1] is not a equivalent model of model (1) and it does not avoid heuristic process. The rest of this paper can be organized as follows. In Sect. 2, A new model for graph matching with same size is proposed. The experimental results given in Sect. 3 show the effectiveness of the proposed algorithm. This paper is concluded in Sect. 4.

2. A New Model for Graph Matching

It is easy to know that model (1) can also be formulated in matrix form as follows when $\bar{n} = \tilde{n} = n$:

$$X^* \in arg \min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\} \tag{3}$$

where $\|.\|$ denotes Frobenius norm $\|X\| = tr(XX^T)^{0.5}$ and $\mathcal{P}(n)$ denotes the set of permutation matrices. The relation between π^* in (1) and P^* in (3) is $P^*(1, 2, \cdots, \tilde{n})^T =$

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$(\pi_1^*, \pi_2^*, \cdots, \pi_n^*)^T$.

In solving the graph matching problem (1) or (3), the combinatorial nature of the set of permutations is the biggest challenge. So, most of researchers want to find a good approximate solution in reasonable time by a approximate model. Continuous optimization model is one of the important models. The common principle is to relax the set of corresponding matrices. Generally, it includes the following two steps [1], [6]:

step 1. Formulate a relax optimization model for graph matching and solve it.

step 2. Derive a sub-optimal matching from relaxation solution by a heuristic process. For example, a permutation matrix which is the closest to the relaxation solution with mean-square-error is chosen, etc.

In order to obtain an equivalent model of model (3) and avoid heuristic process, we relax the admissible set of permutation matrices and meantime incorporate a barrier function into the objective function. The resulted model appears in model (2),which is equivalent to the model (3).

Theorem 1: If $\alpha \geq \|\bar{A}\| + \|\tilde{A}\|$ and $\Omega \supset \mathcal{P}(n)$, then (2) is equivalent to (3),that is:

(1) $\min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\} = \min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$;

(2) If $X^* \in \min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(\bar{n}, \tilde{n})\}$, then, $(X^*, X^*) \in arg\min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$;

(3) If $(X^*, Y^*) \in arg\min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$, then, $X^* \in \min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\}$.

Proof. (1) $\forall X \in \mathcal{P}(n), Y \in \Omega$,

$$\begin{aligned}\|\bar{A}X - X\tilde{A}\| &= \|(\bar{A}Y - Y\tilde{A}) + (\bar{A}X - \bar{A}Y) + (Y\tilde{A} - X\tilde{A})\| \\ &\leq \|\bar{A}Y - Y\tilde{A}\| + \|\bar{A}\|\|X - Y\| + \|\tilde{A}\|\|X - Y\| \\ &\leq \|\bar{A}Y - Y\tilde{A}\| + \alpha\|X - Y\|\end{aligned}$$

So, $\min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\} \leq \min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$. It is obvious that $\min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\} \geq \min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$, and hence, $\min\{\|\bar{A}X - X\tilde{A}\| | X \in \mathcal{P}(n)\} = \min\{G_\alpha(X, Y) | Y \in \Omega, X \in \mathcal{P}(n)\}$. It is easy to know that (2) and (3) hold from (1). □

Note 1. A similar model appears in [1]. But, the model in [1] is not a equivalent of model (3) and its sub-optimal solution must be derived from relaxation solution by a heuristic process. The model in [1] is as follows:

$$(X^*, Y^*) = arg\min\{F_\alpha(X, Y) | X \in M^+(n), Y \in O(n)\}. \quad (4)$$

where $F_\alpha(X, Y) = \|\bar{A}X - X\tilde{A}\|^2 + \alpha\|X - Y\|^2$, $\alpha > 0$ is a barrier parameter, and $O(n)$ and $\mathcal{M}^+(n)$ are the set of orthogonal matrices and the set of non-negative matrices of order n, respectively.

Obviously, model (3) is a linear assignment problem on variable X and is a convex optimization programming on variable Y. Thus, we design alternate iteration algorithm to solve it.

Alternate Iteration Algorithm for same size graphs (AIA):
Step 0. Given tolerance $\epsilon > 0$, a barrier parameter$\alpha > 0$, a initial point $Y^0 \in \Omega$, $k = 0$;
Step 1. Solve the following linear assignment problem:

$$X^k \in arg\min\{\|X - Y^k\|^2 | X \in \mathcal{P}(n)\} \quad (5)$$

If $k > 1$ and $G_\alpha(X^{k-1}, Y^{k-1}) - G_\alpha(X^k, Y^k) \geq \epsilon$, stop; otherwise, $k = k + 1$, and goto *Step 2*.
Step 2. Solve the following programming

$$Y^k \in arg\min\{G_\alpha(X^{k-1}, Y) | Y \in \Omega\} \quad (6)$$

goto *Step 1*.

Below is the convergence theorem for the alternate iteration algorithm.

Theorem 2: The algorithm always converges monotonically to a local minimum. That is, $G_\alpha(X^k, Y^k) \geq G_\alpha(X^{k+1}, Y^{k+1})$, where $\{X^k, Y^k\}_{k=1}^{+\infty}$ are the iterative sequences.

Proof. According to $X^k \in arg\min\{\|X - Y^k\|^2 | X \in \mathcal{P}(n)\}$ and $Y^{k+1} \in arg\min\{\|\bar{A}Y - Y\tilde{A}\| + \|Y - X^k\| | Y \in \Omega\}$, we have $0 \leq G_\alpha(X^{k+1}, Y^{k+1}) \leq G_\alpha(X^k, Y^{k+1}) \leq G_\alpha(X^k, Y^k)$. So, the sequence $\{F(X^k, Y^k)\}$ is non-increasing and bounded below. It means that alternate iteration algorithm converge monotonically to a local minimum. □

Obviously, the programming (5) is equivalent to the following linear assignment problem:

$$X^k \in arg\min\{tr(-Y^{kT}X) | X \in \mathcal{P}(n)\} \quad (7)$$

A typical linear assignment algorithm, such as the Kuhn-Munkres algorithm, has a complexity $O(n^3)$ [8]. And the programming (6) is a convex programming if Ω is the set of doubly stochastic matrices. The rest process of alternate iteration algorithm consists of the following two subproblems:

(1) *The choice of relaxation set* Ω. Theoretically, it only requires that Ω includes the set of permutation matrices. But, due to the local property of the proposed algorithm, the relaxation set must be as compact as possible. Meantime, (5) and (6) must be easy to solve. By Birkhoff theorem [7], any doubly stochastic matrix is a convex combination of finitely many permutation matrices. So, we let Ω be the set of doubly stochastic matrices in this paper.

(2) *The choice of initial point.* Since the algorithm is local, the choice of initial point is very important. We here suggest choosing the solution of the quadratic convex programming:

$$Y^0 = arg\min\{\|\bar{A}Y - Y\tilde{A}\|^2 | Ye = e, Y^T e = e, Y \geq 0\}$$

as initial point, where e is a vector of length n with entry 1.

3. Experiments

The performance of alternate iteration algorithm (AIA) is compared with the performance of the algorithm in [1] (Z-AIA) and relaxation method (RGM). The (RGM) consists the following two steps:

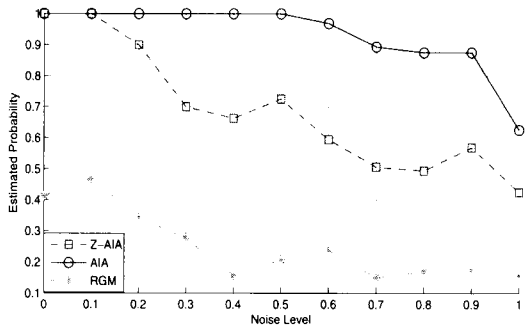

Fig. 1 Estimated Probability of correct vertex-vertex matching versus noise level ϵ[n = 8, α = 1].

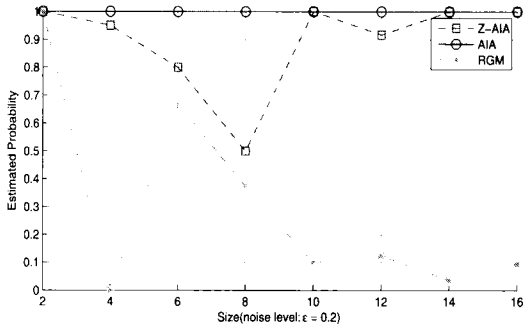

Fig. 2 Estimated Probability of correct vertex-vertex matching versus size of graph [α = 1,noise level: ϵ = 0.2].

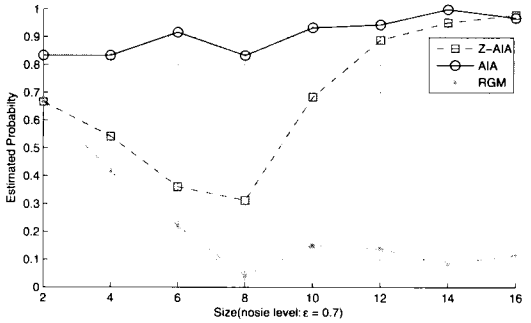

Fig. 3 Estimated Probability of correct vertex-vertex matching versus size of graph [α = 1, noise level: ϵ = 0.7].

step 1. Solve the following convex quadratic programming:

$$Y^* \in arg\min\{\|\tilde{A}Y - Y\tilde{A}\|^2 | Ye = e, Y^T e = e, Y \geq 0\}$$

step 2. Solve the following linear assignment problem:

$$X^* \in arg\min\{\|X - Y^*\|^2 | X \in \mathcal{P}(n)\}$$

X^* is chosen as the approximate solution of (RGM) and Y^* is chosen as the initial point of (AIA) in this paper.

In order to evaluate the performance of AIA, the following procedure is used. Weighted graphs set is randomly generated, where each graph has weights ranging from 0 to 1. Matching graph H is generated from each graph G in the set by adding uniformly distributed noise in the range of 0 to 1 to each weight in G, and then shuffling the order of nodes. Then, the above three graph matching algorithms are applied to graph matching for every pair H and G. The estimated probability of a correct vertex-vertex assignment is calculated for a given noise level ϵ, after 20 trials for each algorithm. From a point of view of probability, this reflects how well an algorithm performs for a given noise level. All programs are written in Matlab7.0 and run by PC with Pentium (R) Dual-Core CPU E5200 and 2 G RAM.

The results of estimated probability of correct vertex-vertex matching versus noise level are displayed in Fig. 1 and Fig. 2. The result of estimated probability of correct vertex-vertex matching versus size is displayed in Fig. 3. All results show that the matching of (AIA) is best than (Z-AIA) and (RGM) for the pairs of graph of uniformly distribute.

4. Conclusions

In this paper, a new equivalent model of (1) for graph matching with same size is proposed. It avoid heuristic process which is a common process in most of continuous optimization methods for graph matching. And alternate iteration algorithm is designed to solve it. It is proved that this algorithm is locally convergent. The experiments done in this paper show that the proposed algorithm outperforms the algorithm in [1] and its matching performance is very good when the graph is similar. But the matching performance is strongly dependent on the choices of initial point and the relaxation set because it is a local algorithm. It is the emphasis of our future work.

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