GNCGCP - Graduated NonConvexity and Graduated Concavity Procedure

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Abstract

In this paper we propose the Graduated NonConvexity and Graduated Concavity Procedure (GNCGCP) as a general optimization framework to approximately solve the combinatorial optimization problems on the set of partial permutation matrices. GNCGCP comprises two sub-procedures, graduated nonconvexity (GNC) which realizes a convex relaxation and graduated concavity (GC) which realizes a concave relaxation. It is proved that GNCGCP realizes exactly a type of convex-concave relaxation procedure (CCRP), but with a much simpler formulation without needing convex or concave relaxation in an explicit way. Actually, GNCGCP involves only the gradient of the objective function and is therefore very easy to use in practical applications. Two typical NP-hard problems, (sub)graph matching and quadratic assignment problem (QAP), are employed to demonstrate its simplicity and state-of-the-art performance.

Index Terms

Combinatorial optimization, Graduated optimization, Deterministic annealing, Subgraph matching, Quadratic assignment problem

I. INTRODUCTION

The recently proposed Path following and extended Path following algorithms exhibited state-of-the-art performances [1], [2] on equal-sized graph matching problems. As a typical NP-hard problem, equal-sized (with size \( N \)) graph matching under the one-to-one constraint can be formulated as follows,

\[
\min_X F(X), \quad \text{s.t. } X \in \mathcal{P}, \mathcal{P} := \{X | X_{ij} = \{0, 1\}, \sum_{j=1}^{N} X_{ij} = 1, \sum_{i=1}^{N} X_{ij} = 1, \forall i, j\},
\]

(1)

where \( \mathcal{P} \) denotes the set of \((N \times N)\) permutation matrices, \( F(X) \) is given later by (14) or (16). By relaxing \( \mathcal{P} \) to its convex hull, i.e., the set of \((N \times N)\) doubly stochastic matrices denoted by \( \mathcal{D} \), the (extended)
Path following algorithm proposed the convex and concave relaxation procedure (CCRP) formulated by a weighted linear combination of a convex relaxation $F_v(X)$ and a concave relaxation $F_c(X)$ of $F(X)$ as follows \[ F_\eta(X) = (1 - \eta)F_v(X) + \eta F_c(X), X \in \mathcal{D}. \tag{2} \]

In implementation, $\eta$ increases gradually from 0 to 1, making $F_\eta(X)$ become gradually from $F_v(X)$ to $F_c(X)$, whose minima locate exactly in $\mathcal{P}$. Similar to the graduated nonconvexity [4] algorithm, the (extended) Path following is a deterministic annealing method which usually finds a good suboptimal solution, but at a much less computational cost than stochastic simulated annealing techniques. As a state-of-the-art optimization algorithm, the (extended) Path following showed superior performance but has difficulties in finding convex or concave relaxation, which thus greatly hinders its practical applications. For instance, neither the convex nor concave relaxation proposed by (extended) Path following [1], [2] on equal-sized graph matching is applicable on the subgraph matching defined on the set of partial permutation matrices.

In this paper we will propose the Graduated NonConvexity and Graduated Concavity Procedure (GNCGCP) to equivalently realize the CCRP in (2) on partial permutation matrix (with permutation matrix as a special case), but in a much simpler way without involving the convex or concave relaxation explicitly. Actually, GNCGCP needs only the gradient of the objective function, making it very easy to use in practical applications. Two case studies on (sub)graph matching and quadratic assignment problem (QAP) witness the simplicity and state-of-the-art performance of GNCGCP. The GNCGCP is proposed in the next Section, followed by the (sub)graph matching and QAP problems discussed in Sections III and IV respectively, and finally Section V concludes this paper.

II. GRADUATED NONCONVEXITY AND GRADUATED CONCAVITY PROCEDURE

A. Formulation and Algorithm

In this paper we consider the optimizations on the set of $(M \times N)$ partial permutation matrices $\Pi$ as, $ \min_X F(X), \quad \text{s.t.} \, X \in \Pi := \{X | X_{ij} = \{0, 1\}, \sum_{j=1}^N X_{ij} = 1, \sum_{i=1}^M X_{ij} \leq 1, \forall i, j\}, \, M \leq N. \tag{3} $\] Such a formulation covers a wide range of important problems, such as correspondence, assignment, matching, and traveling salesman problem (TSP). Specific to graph matching, it defines a subgraph matching problem where each node in the smaller graph has to match exactly one node in the bigger one,
1: \( \zeta \leftarrow 1, X \leftarrow X^0 \)

2: \textbf{while} \( \zeta > -1 \land X \notin \Pi \) \textbf{do}

3: \hspace{1em} \textbf{while} \( X \) not converged \hspace{1em} \triangleright \text{Frank-Wolfe algorithm}

4: \hspace{2em} Y = \arg \min_Y \tr \nabla F_\zeta(X)^\top Y, \text{s.t.}\ Y \in \Omega

5: \hspace{2em} \alpha = \arg \min_\alpha F_\zeta(X + \alpha(Y - X)), \text{s.t.}\ 0 \leq \alpha \leq 1 \hspace{1em} \triangleright \text{line search}

6: \hspace{2em} X \leftarrow X + \alpha(Y - X)

7: \hspace{1em} \textbf{end while}

8: \hspace{1em} \zeta \leftarrow \zeta - d\zeta

9: \hspace{1em} \textbf{end while}

10: \textbf{return} \( X \)

Fig. 1. Algorithmic framework of GNCGCP.

and each node in the bigger graph can match at most one node in the smaller one. It obviously includes (11) as a special case when \( M = N \).

To approximate the integer program (3) by a relaxation technique, \( \Pi \) is firstly relaxed to its convex hull, i.e., the set of \((M \times N)\) doubly sub-stochastic matrices \( \Omega \) [5],

\[
\Omega := \{X | X_{ij} \geq 0, \sum_{j=1}^{N} X_{ij} = 1, \sum_{i=1}^{M} X_{ij} \leq 1, \forall i, j\}. \tag{4}
\]

Then, we propose the Graduated NonConvexity and Graduated Concavity Procedure (GNCGCP) to approximately solve it as follows,

\[
F_\zeta(X) = \begin{cases} 
(1 - \zeta)F(X) + \zeta \tr X^\top X & \text{if } 1 \geq \zeta \geq 0, \\
(1 + \zeta)F(X) + \zeta \tr X^\top X & \text{if } 0 > \zeta \geq -1,
\end{cases}, X \in \Omega. \tag{5}
\]

In GNCGCP, \( \zeta \) decreases gradually from 1 to -1, implying that the objective function \( F_\zeta(X) \) becomes gradually from \( \tr X^\top X \) to \( F(X) \) (graduated nonconvexity) and finally to \( -\tr X^\top X \) (graduated concavity). For each currently fixed \( \zeta \), \( F_\zeta(X) \) is minimized by the Frank-Wolfe algorithm [6], using the minimum of the previous \( F_\zeta(X) \) as the starting point. Here and hereafter, \( F(X) \) is assumed to be neither convex nor concave, or otherwise, (5) is further simplified accordingly. That is, the equation on \( 1 \geq \zeta \geq 0 \) \((0 > \zeta \geq -1)\) is removed in case \( F(X) \) itself is convex (concave).

The algorithmic framework of GNCGCP is given by the algorithm in Figure 1. In the algorithm, the
gradient $\nabla F_\zeta(X)$ takes the form
\[
\nabla F_\zeta(X) = \begin{cases} 
(1 - \zeta)\nabla F(X) + 2\zeta X & \text{if } 1 \geq \zeta \geq 0, \\
(1 + \zeta)\nabla F(X) + 2\zeta X & \text{if } 0 > \zeta \geq -1.
\end{cases}
\] (6)

The linear program $Y = \arg \min_Y \text{tr} \nabla F_\zeta(X)^\top Y$, s.t. $Y \in \Omega$ can be solved by the non-square Hungarian algorithm [7], and line search $\alpha = \arg \min_\alpha F_\zeta(X+\alpha(Y-X))$ can be efficiently solved by the backtracking algorithm [8]. The convergence of $X$ is confirmed by checking whether
\[
\text{tr} \nabla F_\zeta(X)^\top (Y - X) < \varepsilon |F_\zeta(X) + \text{tr} \nabla F_\zeta(X)^\top (Y - X)|.
\] (7)

Once $X$ becomes discrete, the algorithm is terminated, even if $\zeta$ has not reached -1.

Without considering sparsity (of the adjacency matrix), storage complexity of the algorithm is $O(N^2)$, and the computational complexity is roughly $O(N^3)$ resulting from matrix multiplication. Both complexities are comparable with those of the (extended) Path following algorithm [1], [2].

B. Discussions and Interpretations

1) GNCGCP realizes a type of CCRP:

Theorem 1: GNCGCP (5) realizes a convex and concave relaxations procedure (2), with the convex and concave relaxations respectively given by
\[
F_v(X) = F(X) - \lambda_{\min} \text{tr} (X^\top X - JX),
\]
\[
F_c(X) = F(X) - \lambda_{\max} \text{tr} (X^\top X - JX),
\] (8)

where $J := 1_{N \times M}$ denotes the unit matrix consisting of all 1s, $\lambda_{\min}$ and $\lambda_{\max}$ denote the minimal and maximal eigenvalues of the Hessian matrix of $F(X)$, respectively.

To prove Theorem 1, we derive $F_\zeta(X)$ by adding a constant $-\zeta M$ as follows,
\[
\arg \min_X F_\zeta(X) = \arg \min_X [F_\zeta(X) - \zeta M] = \arg \min_X [F_\zeta(X) - \zeta \text{tr} JX], X \in \Omega.
\] (9)

Therefore, $F_\zeta(X)$ can be equivalently rewritten by $\hat{F}_\zeta(X)$ as
\[
\hat{F}_\zeta(X) = F_\zeta(X) - \zeta \text{tr} JX = \begin{cases} 
(1 - \zeta)F(X) + \zeta \text{tr} (X^\top X - JX) & \text{if } 1 \geq \zeta \geq 0, \\
(1 + \zeta)F(X) + \zeta \text{tr} (X^\top X - JX) & \text{if } 0 > \zeta \geq -1.
\end{cases}
\] (10)

To prove that (10) realizes exactly a CCRP, two Propositions were firstly given as follows.

Proposition 2.1: There always exists a $\zeta_u = \frac{\lambda_{\min}}{\lambda_{\min} - 1} \in (0, 1)$ making $\hat{F}_\zeta(X)$ convex as $1 \geq \zeta \geq \zeta_u$, where $\lambda_{\min}$ denotes the smallest eigenvalue of the Hessian matrix $H_X$ of $F(X)$. 

Proof: The Hessian matrix $\hat{H}_X$ of $\hat{F}_\zeta(X)$ takes the form $(1 - \zeta)H_X + \zeta I$. To make $\hat{H}_X$ positive definite, $\zeta$ should satisfy $\zeta \geq \frac{\lambda_{\min}}{\lambda_{\min} - 1}$. As $F(X)$ is neither convex nor concave, $\lambda_{\min}$ is a negative number, which makes $0 < \frac{\lambda_{\min}}{\lambda_{\min} - 1} < 1$. Thus, choosing $\zeta_u = \frac{\lambda_{\min}}{\lambda_{\min} - 1}$, any $\zeta$ satisfying $1 \geq \zeta \geq \zeta_u$ will make $\hat{H}_X$ positive definite and consequently $\hat{F}_\zeta(X)$ convex. □

**Proposition 2.2:** There always exists a $\zeta_l = \frac{-\lambda_{\max}}{\lambda_{\max} + 1} \in (-1, 0)$ making $\hat{F}_\zeta(X)$ concave as $\zeta \geq \zeta_l \geq -1$, where $\lambda_{\max}$ denotes the biggest eigenvalue of the Hessian matrix of $F(X)$.

**Proof:** The proof can be accomplished in a similar way as that of Proposition 2.1. □

Then, based on the above two Propositions, we get the following two Lemmas.

**Lemma 2.1:** The value range $1 \geq \zeta \geq 0$ in (10) can be equivalently shrunk to $\zeta_u \geq \zeta \geq 0$ with $\zeta_u$ given by Proposition 2.1.

**Proof:** $\hat{F}_{\zeta_l}(X)$ is a convex function, whose global minimum is obtainable without depending on the previous results gotten on $1 \geq \zeta > \zeta_u$. Thus, the value range of $1 \geq \zeta \geq 0$ can be equivalently shrunk to $\zeta_u \geq \zeta \geq 0$ for (10). □

**Lemma 2.2:** The value range $0 \geq \zeta \geq -1$ in (10) can be equivalently shrunk to $0 \geq \zeta \geq \zeta_l$ with $\zeta_l$ given by Proposition 2.2.

**Proof:** $\hat{F}_{\zeta_l}(X)$ is a concave function, implying that minimization of $\hat{F}_{\zeta_l}(X)$ will result in a discrete solution $\hat{X} \in \Pi$. As $\zeta$ decreases further from $\zeta_l$ to $-1$, $\hat{X}$ will keep unchanged because it remains to be a local minimum of $\hat{F}_\zeta(X)$. Thus, the value range of $0 \geq \zeta \geq -1$ can be equivalently shrunk to $0 \geq \zeta \geq \zeta_l$ for (10). □

**Comments:** Actually, once $\zeta$ reaches $\zeta_l$, the GNCGCP will terminate according to the algorithm in Figure 1. Therefore, Lemma 2.2 holds naturally in the context of GNCGCP.

Finally, we prove Theorem 1.

**Proof of Theorem 1** Based on Lemmas 2.1 and 2.2, $\hat{F}_\zeta(X)$ in (10) (or $F_\zeta(X)$ in (5)) is equivalently rewritten as

$$
\hat{F}_\zeta(X) = \begin{cases} 
(1 - \zeta)F(X) + \zeta \text{tr} (X^T X - JX) & \text{if } \zeta_u \geq \zeta \geq 0, \\
(1 + \zeta)F(X) + \zeta \text{tr} (X^T X - JX) & \text{if } 0 \geq \zeta \geq \zeta_l.
\end{cases}
$$

Then, for each fixed $\zeta$, $\hat{F}_\zeta(X)$ is normalized by a constant $1 - \zeta$ or $1 + \zeta$, making

$$
\hat{F}_\zeta(X) = \begin{cases} 
F(X) + \frac{\zeta}{1 - \zeta} \text{tr} (X^T X - JX) & \text{if } \zeta_u \geq \zeta \geq 0, \\
F(X) + \frac{\zeta}{1 + \zeta} \text{tr} (X^T X - JX) & \text{if } 0 \geq \zeta \geq \zeta_l.
\end{cases}
$$
or equivalently,
\[ \hat{F}_\gamma(X) = F(X) + \gamma \text{tr} \left( X^T X - JX \right), \quad -\lambda_{\text{min}} \geq \gamma \geq -\lambda_{\text{max}}, \quad (11) \]
where \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) are defined in propositions 2.1 and 2.2 respectively.

On the other hand, based on the convex and concave relaxations given by (8), a CCRP is constructed as follows,
\[ F_\eta(X) = (1 - \eta)F_v(X) + \eta F_c(X) = F(X) - [(1 - \eta)\lambda_{\text{min}} + \eta \lambda_{\text{max}}] \text{tr} \left( X^T X - JX \right). \quad (12) \]
By defining \( \gamma = (1 - \eta)\lambda_{\text{min}} + \eta \lambda_{\text{max}} \), \( 0 \leq \eta \leq 1 \), \( F_\eta(X) \) above can be equivalently written as
\[ F_\gamma(X) = F(X) + \gamma \text{tr} \left( X^T X - JX \right), \quad -\lambda_{\text{min}} \geq \gamma \geq -\lambda_{\text{max}}. \quad (13) \]
Exact (11)! Therefore, the GNCGCP realizes a CCRP with the convex and concave relaxations given by (8). □

It is worth discussing the case of \( F(X) \) being non-quadratic (such as a quartic function like (14)) where \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) are in general dependent on \( X \). If \( X \) is unconstrained/unbounded, \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) might become \( -\infty \) and \( +\infty \) respectively, implying that any \(-1 < \zeta < 1\) will result in \( F_\zeta(X) \) neither convex nor concave (see Propositions 2.1 and 2.2). Fortunately, because \( X \) here is constrained as a doubly substochastic matrix, i.e., each element is bounded by \( 0 \leq x \leq 1 \), both \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) must be some finite numbers, meaning that we can always get a convex relaxation by some \( \zeta < 1 \) and a concave relaxation by some \( \zeta > -1 \). The point here is that GNCGCP does not need to figure out the number (\( \lambda \) or corresponding \( \zeta \)) explicitly, which is realized in an implicit way.

A simple illustration of the convex and concave relaxations in (8) is shown in Figure 2 (the sub-figure on the left-hand side).

Fig. 2. Illustration of the construction of convex and concave relaxations (the one on the left-hand side), and the convergence processes of CCRP and GNCGCP.
2) **GNCGCP versus CCRP**: Basically, without involving convex or concave relaxation explicitly, GNCGCP provides a very simple way to construct a CCRP algorithm; by contrast, the problem specific relaxation is typically difficult to construct. A typical example is the complicated concave relaxations used by (E)PATH [1], [2], which are applicable only on equal-sized graph matching. Similarly, it is also usually difficult to calculate $\lambda_{\text{max}}$ or $\lambda_{\text{min}}$ in (8), especially on non-quadratic functions.

Another interesting difference between GNCGCP and CCRP lies in the construction of relaxation functions. A convex or concave relaxation will certainly reshape the original relaxed function when $X \in \Omega$ or $\in \mathcal{D}$. By introducing the simple quadratic function $\zeta \text{tr} X^T X$, GNCGCP reshapes the relaxed function in a symmetric way, and meanwhile, as $\zeta \to 0$, GNCGCP approaches the original relaxed function. By contrast, other types of relaxations in general have no chance to directly optimize it. This is probably the main reason GNCGCP exhibited a better or at least a no worse performance than some other types of CCRP, especially on the QAP discussed in Section [V].

A simple comparison between the convergence of CCRP and GNCGCP is given by Figure 2, where it is observed that CCRP starts with a convex relaxation and ends with a concave relaxation but GNCGCP starts with $\text{tr} X^T X$ and ends with $-\text{tr} X^T X$, with the convex and concave relaxations realized implicitly during the process (see Lemmas 2.1 and 2.2).

Based on the GNCGCP algorithm in Figure [I] to utilize GNCGCP the only thing we need to do is to find the gradient of the objective function. Thus, any optimization problems on $\Pi$ with a differentiable objective function can be directly approximated by GNCGCP. Below we use (sub)graph matching and quadratic assignment problem to demonstrate this simple process.

### III. Case Study 1: (Sub)Graph Matching

#### A. Problem Formulation

(Sub)Graph matching as a fundamental problem in theoretical computer science finds wide applications in computer vision and machine learning [9], [10], [11], [12], [1], [2], [13]. Given two graphs $G_D$ and $G_M$ to be matched, the (sub)graph matching problem is formulated as follows,

$$\min_X F(X) = \text{tr}(A_M - XA_D X^T)^T (A_M - XA_D X^T), \text{s.t. } X \in \Pi, \quad (14)$$

where $A_M \in \mathbb{R}^{N_M \times N_M}$ and $A_D \in \mathbb{R}^{N_D \times N_D}$ denote the adjacency matrices of $G_M$ and $G_D$, respectively, and $N_M \leq N_D$. To use GNCGCP to approximate it, we need just to relax $\Pi$ to $\Omega$ and find $\nabla F(X)$ as,

$$\nabla F(X) = 2X(A_D^T X A_D + A_D X^T X A_D^T) - 2(A_M X A_D^T + A_M^T X A_D). \quad (15)$$
Below we denote by GNCGCP\_SGM the above (sub)graph matching algorithm, which is applicable on both equal-sized and subgraph matching problems, and is applicable on any types of graph provided that it can be represented by an adjacency matrix.

In case the two graphs take exactly the same size $N$ which implies that $\Pi$ degenerates to $\mathcal{P}$, the objective function in (14) can be derived as \cite{1},

\[
F(X) = \text{tr}(A_M - XA_DX^\top)(A_M - XA_DX^\top) = \text{tr}(A_MX - XA_D)(A_MX - XA_D), \quad X \in \mathcal{P}. \quad (16)
\]

Then, by relaxing $\mathcal{P}$ to $\mathcal{D}$, GNGGCP is implementable by finding

\[
\nabla F(X) = A_M^\top A_MX - A_M^\top XA_D - A_M XA_D^\top + XA_D A_D^\top. \quad (17)
\]

Because $F(X)$ with $X \in \mathcal{D}$ in (16) itself becomes a convex function, GNCGCP is further simplified by removing the equation on $1 \geq \zeta \geq 0$, that is, $\zeta$ needs just to decrease from 0 to $-1$ but not 1 to $-1$. The algorithm is denoted by GNCGCP\_GM, which is closely related to the Path following \cite{1} (on undirected graph) and extended Path following \cite{2} algorithms, with the same convex relaxation but a different concave relaxation.

B. Experimental Results

1) overview: Both synthetic and real data were employed to evaluate the GNCGCP algorithms.

On equal-sized graph matching, six algorithms including 1:) Umeyama’s spectral decomposition (U for short) \cite{9}, 2:) graduated assignment (GA) \cite{10}, 3:) path following algorithm (PATH, for undirected graph only) \cite{1}, 4:) extended path following (EPATH, for directed graph only) \cite{2}, 5:) GNCGCP\_SGM, and 6:) GNCGCP\_GM were experimentally compared. Considering space limit we are not to compare their complexities in detail. Actually, in all the following experiments, the time-cost of GNCGCP is comparable with that of (E)PATH.

On subgraph matching, four algorithms including GNCGCP\_SGM, GA, spectral relaxation matching (SM for short) \cite{14}, and probabilistic spectral matching (PSM) \cite{15} were experimentally compared.

All of the algorithms were implemented by Matlab\footnote{The source codes of all the (sub)graph matching and QAP algorithms used in the experiments are available at \url{http://www.escience.cn/people/zylu/GNCGCP.html}} and for GNCGCP\_SGM, GNCGCP\_GM and (E)PATH, the same parameter settings were used as follows: the learning step $d\zeta = d\eta = 0.001$ and the stopping parameter $\varepsilon = 0.001$ in (7).
2) on synthetic data: Synthetic graphs were generated according to three options:

- directed (abbreviated by D) or undirected (U);
- degree distribution: a binomial (B) \( P(k) = C_N^k p^k (1-p)^{1-k} \) (with \( p = 0.5 \)) or a power (P) \( P(k) \propto k^{-\alpha} \) law (scale-free graph with a fixed \( \alpha = 1.5 \) in all of the experiments);
- weight distribution: a standard log-normal (L) \( p(w) = \frac{1}{w\sqrt{2\pi}} e^{-\frac{\ln^2 w}{2}}, w > 0 \) or absolute normal \( p(w) = \frac{2}{\sqrt{2\pi}} e^{-\frac{w^2}{2}}, w \geq 0 \).

Therefore, there are totally eight types of graphs, each of which is abbreviated by a sequential three-character notation. For instance, DBL denotes the directed graphs with a binomial degree distribution and a log-normal weight distribution.

Two experiments were conducted on equal-sized graphs, with the first one to evaluate the noise resistance ability of the algorithms, and the second one to evaluate their scalabilities with respect to graph size. In the first experiment, the graph size \( N \) was fixed at 8, and for each graph pair, \( G_M \) was generated by adding \( \beta |E_D| \) edges into \( G_D \), where \( |E_D| \) denotes the number of edges of \( G_D \), and \( \beta \) is the parameter that controls the noise level. In the experiment \( \beta \) was increased from 0 to 1 by a step size 0.1, and on each noise level, 50 graph pairs were randomly generated. The experimental results on the eight types of graphs are shown in Figure 3, where OPT denotes the optimal result obtained by an exhaustive search.

![Figure 3: Matching errors on the eight types of graphs with respect to noise levels, summarized from 50 random runs on each noise level.](image)
In the second experiment, 10 groups of graph pairs were generated for each of the eight types, with the graph size increasing from 5 to 50 by a step size 5. For each group 50 graph pairs were randomly generated in the same way as the first experiment with a fixed noise level 0.2. The experimental results are shown in Figure 4.

Two observations could be summarized from the above experimental results. First, (E)PATH, GNCGCP_GM and GNCGCP_SGM outperformed significantly U and GA. This witnessed the superiority of CCRP and also GNCGCP. Second, GNCGCP_SGM exhibited a slightly better or at least a no worse performance than GNCGCP_GM and (E)PATH (see for instance UPL and DPL in Figure 4), and meanwhile GNCGCP_GM exhibited a comparable performance with (E)PATH, echoed by the discussions in Section II-B2.

On subgraph matching, $G_D$ and $G_M$ were generated in the following way. The bigger graph $G_D$ with $N_D = 20$ was firstly randomly generated, then a smaller graph $G_M$ with $N_M = 10$ was randomly extracted out from $G_D$, and finally $G_M$ was generated by adding some noises to $G_M$ in the same manner as the first experiment by setting $\beta = 0.5$. The experimental results are shown in Figure 5 where GNCGCP_SGM achieved the best performance on all of the eight types of graphs.

3) on real data: The real data experiments were conducted on the 6 eiffel and 6 revolver samples shown in Figure 6 which were fetched from the Caltech-256 Database \[16\]. The first one and first five
leftmost samples of *eiffel* and *revolver* in Figure 6 were chosen as the model samples to match the rest five and one samples, respectively. Total 35 and 20 feature points (typically corner points) were marked manually for the *eiffel* and *revolver* models respectively, and all of the points are linked each other to construct their undirected graph representation. The edge attribute comprises two parts, i.e., the normalized distance and direction, and the unary term or appearance cue was not incorporated into the model.

The equal-sized graph matching results are shown in Figure 7 (the upper row), including both the matching error and summed number of correct matchings (whole numbers are 175 and 100 for *eiffel* and *revolver* respectively), and some typical matchings are shown in Figure 8 (the upper row). It is observed that on *eiffel* GNCGCP_SGM got slightly better results, and on *revolver* all the four algorithms got quite good results, with the number of correct matchings being 100, 100, 98, and 100 respectively.

We then conducted subgraph matching on the data, by taking the one *eiffel* and five *revolver* model samples as smaller models, and randomly adding some outlier points to the rest samples to get the larger one. The algorithms were evaluated on five levels of the number of added outliers, i.e., 4, 8, 12, 16, and 20 respectively. The experimental results are shown in Figure 7 (the lower row), and some typical results by adding 12 outliers are shown in Figure 8 (the lower row). We can observe that GNCGCP_GCP got the best results on both criterions, and meanwhile, though the performance became in general worse as the number of outliers became bigger, the decline of GNCGCP_SGM was the slowest one.
IV. Case Study 2: Quadratic Assignment Problem

The quadratic assignment problem (QAP) is a well-known combinatorial optimization problem in operations research and discrete optimization [17], [18], [19], and is closely related to the equal-sized graph matching problem. Given two equal-sized matrices $A, B$, and without considering the linear term, QAP formally takes the following form,

$$\min_{X} F(X) = \text{tr}(AXB^\top X^\top), \quad \text{s.t.} X \in \mathcal{P}. \quad (18)$$

By relaxing $\mathcal{P}$ to $\mathcal{D}$, the GNCGCP is applicable by finding

$$\nabla F(X) = AXB^\top + A^\top XB. \quad (19)$$

The algorithm is denoted by GNCGCP_QAP.
GNCGCP_QAP was compared with PATH and EPATH on both the symmetric and asymmetric QAPLib benchmark datasets [20] used respectively in [1] and [2]. GNCGCP_SGM and GNCGCP_GM were also included in the experiments. The parameter settings of different algorithms were the same as those in the previous (sub)graph matching experiments. The experimental results are listed in Tables I and II respectively, where the results except for the three types of GNCGCP algorithms are directly fetched from [1] and [2] respectively, OPT denotes the currently known best result, and for each algorithm, 'awar(%)' (average wrong assignment ratio) = \( \frac{1}{n} \sum_{i=1}^{n} (cost_i - opt_i)/opt_i \) indicates its average deviation from OPT.

| Data     | OPT   | U    | GA   | QPB  | PATH  | GNCGCP_QAP | GNCGCP_SGM | GNCGCP_GM |
|----------|-------|------|------|------|-------|------------|------------|-----------|
| chr12c   | 11156 | 40370| 19014| 20306| 18048 | 11566      | 17020      | 21818     |
| chr15a   | 9896  | 60986| 30370| 26132| 19088 | 12402      | 10840      | 19186     |
| chr15c   | 9504  | 76318| 23686| 29862| 16206 | 15080      | 14890      | 19942     |
| chr20b   | 2298  | 10022| 6290 | 6674 | 5560  | 3164       | 3452       | 5286      |
| chr22b   | 6194  | 13118| 9658 | 9942 | 8500  | 6918       | 7858       | 8358      |
| rou12    | 235528| 297572|273438|278834|256320 |238134     |238954      |264324     |
| rou15    | 354210| 480352|457908|381016|391270 |374932     |377898      |391768     |
| rou20    | 72522 | 905246|840120|804676|778284 |729542     |747322      |772100     |
| tai10a   | 135028| 189852|168096|165364|152534 |138306     |138306      |147092     |
| tai15a   | 388214| 483596|451164|455778|419224 |392268     |396596      |419328     |
| tai17a   | 491812| 620964|589814|550852|530978 |514224     |531732      |545802     |
| tai20a   | 703482| 915144|871480|799790|753712 |736710     |746766      |778154     |
| tai30a   | 1818146|2213846|2077958|1996442|1903872|1856666   |1874642     |1917674    |
| tai35a   | 2422002|2925390|2803456|2720986|2555110|2470186   |2482652     |2544354    |
| tai40a   | 3139370|3727478|3668044|3529402|3281830|3180740   |3224410     |3342272    |
| awar(%)  | 0     |146.5|56.6 |56.5 |32.1 |10.9       |15.6        |34.7       |

It is observed that GNCGCP_QAP exhibited the best performance. Specifically, it achieved the best results on 27 out of the 31 datasets, and in average, GNCGCP_QAP outperformed all of the competitors on both the symmetric and asymmetric datasets. It is also interesting to observe that GNCGCP_SGM outperformed (or achieved the same best results on some asymmetric datasets) both (E)PATH and GNCGCP_GM on all of the 31 datasets.

Actually, by setting \( A_M := -A^T \) and \( A_D := B^T \), to utilize GNCGCP_SGM to solve (18), one needs
TABLE II

Comparative results on some asymmetric QAPLib benchmark data sets.

| Data     | OPT | U | QCV | GA | EPATH | GNCGCP_QAP | GNCGCP_SGM | GNCGCP_GM |
|----------|-----|---|-----|----|-------|------------|------------|------------|
| lipa20a  | 3683| 3925 | 3902 | 3909 | 3885  | 3789       | 3823       | 3860       |
| lipa20b  | 27076 | 35213 | 34827 | 27076 | 32081  | 27076      | 27076      | 32207      |
| lipa30a  | 13178 | 13841 | 13787 | 13668 | 13577  | 13459      | 13485      | 13628      |
| lipa30b  | 151426 | 196088 | 189496 | 151426 | 151426  | 151426     | 151426     | 151426     |
| lipa40a  | 31538 | 32663 | 32647 | 32590 | 32247  | 32024      | 32204      | 32012      | 32356      |
| lipa40b  | 476581 | 626004 | 572039 | 476581 | 476581  | 476581     | 476581     | 476581     |
| lipa50a  | 62093 | 64138 | 63930 | 63730 | 63399  | 62901      | 63032      | 63414      |
| lipa50b  | 1210244 | 1569908 | 1468492 | 1210244 | 1210244 | 1210244    | 1210244    | 1210244    |
| lipa60a  | 107218 | 110196 | 110075 | 109809 | 109168  | 108445     | 108679     | 109079     |
| lipa60b  | 2520135 | 3305286 | 3131985 | 2520135 | 2520135 | 2520135    | 2520135    | 2520135    |
| lipa70a  | 169755 | 173906 | 173496 | 173172 | 172209  | 171421     | 171723     | 172519     |
| lipa70b  | 4603200 | 5974833 | 5576103 | 4603200 | 4603200 | 4603200    | 4603200    | 4603200    |
| lipa80a  | 253195 | 258262 | 258140 | 258218 | 256601  | 255639     | 255546     | 256430     |
| lipa80b  | 7763962 | 10079359 | 9703626 | 7763962 | 7763962 | 7763962    | 7763962    | 7763962    |
| lipa90a  | 360630 | 367756 | 367250 | 366743 | 365233  | 363480     | 364319     | 364900     |
| lipa90b  | 12490441 | 16271254 | 13870571 | 12490441 | 12490441 | 12490441   | 12490441   | 12490441   |

Avar(%) | 0 | 16.81 | 12.62 | 1.48 | 2.30 | 0.72 | 0.86 | 2.36 |

To add the term

$$F_1(X) = \text{tr}(XAX^T A_D X^T A_D X^T)$$

into (14) to get (18). Similarly, the term

$$F_2(X) = \text{tr}(X^TA^T A_M A_D X) + \text{tr}(A_D^T X^T A_D X)$$

has to be added into (16) to get (18). Both $F_1(X)$ and $F_2(X)$ become constant when $X \in \mathcal{P}$, implying that all of the GNCGCP_SGM, GNCGCP_GM and (E)PATH implement a CCRP algorithm to solve QAP. But when $X \in \mathcal{D}$, $F_1(X)$ and $F_2(X)$ will certainly reshape or provide some biases on the original relaxed function; as discussed in Section II-B2, this is probably the main reason GNCGCP_QAP achieved the best results. Meanwhile, it seems that $F_1(X)$ which involves only $A_D$ has less impact than $F_2(X)$ which involves both $A_M$ and $A_D$, and therefore GNCGCP_SGM achieved better results than both (E)PATH and GNCGCP_GM.
V. CONCLUSIONS

The GNCGCP is proposed as a general optimization framework for the discrete optimization problems on the set of partial permutation matrices, including a wide range of classic discrete optimization problems as its special cases, matching, assignment, and traveling salesman problem (TSP), to name a few. GNCGCP has its root in the CCRP, but it does not need to figure out the convex or concave relaxation explicitly, and is thus very easy to use in practical applications. Two case studies on (sub)graph matching and QAP witness the simplicity as well as state-of-the-art performance of GNCGCP.

REFERENCES

[1] M. Zaslavskiy, F. Bach, and J. P. Vert, “A path following algorithm for the graph matching problem,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 31, no. 12, pp. 2227–2242, 2009.
[2] Z. Y. Liu, H. Qiao, and L. Xu, “An extended path following algorithm for graph matching problem,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 34, no. 7, pp. 1451–1456, 2012.
[3] Z. Y Liu and H. Qiao, “A convex-concave relaxation procedure based subgraph matching algorithm,” Journal of Machine Learning Research: W&CP, vol. 25, pp. 237 – 252, 2012.
[4] A. Blake and A Zisserman, Visual Reconstruction, MIT Press, Cambridge, MA, USA, 1987.
[5] J. Maciel and J. P. Costeira, “A global solution to sparse correspondence problems,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 25, no. 2, pp. 187–199, 2003.
[6] M. Frank and P. Wolfe, “An algorithm for quadratic programming,” Naval Research Logistics Quarterly, vol. 3, no. 1-2, pp. 95–110, 1956.
[7] Francois Bourgeois and Jean-Claude Lassalle, “An extension of the munkres algorithm for the assignment problem to rectangular matrices,” Communications of the ACM, vol. 14, no. 802-804, pp. 12, 1971.
[8] S. Boyd and L. Vandenberghe, Convex Optimization, Cambridge University Press, 2004.
[9] S. Umeyama, “An eigendecomposition approach to weighted graph matching problems,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 10, no. 5, pp. 695–703, 1988.
[10] S. Gold and A. Rangarajan, “A graduated assignment algorithm for graph matching,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 18, no. 4, pp. 377–388, 1996.
[11] D. Conte, P. Foggia, C. Sansone, and M. Vento, “Thirty years of graph matching in pattern recognition,” International Journal of Pattern Recognition and Artificial Intelligence, vol. 18, no. 3, pp. 265–298, 2004.
[12] M. Leondeau, M. Hebert, and R. Sukthankar, “An integer projected fixed point method for graph matching and map inference,” in Proceedings Neural Information Processing Systems, 2009.
[13] F. Zhou and F. D. Torre, “Factorized graph matching,” in Proceedings of CVPR 2012, 2012.
[14] M. Leondeau and M. Hebert, “A spectral technique for correspondence problems using pairwise constraints,” in IEEE International Conference on Computer Vision (ICCV), 2005, vol. 2, pp. 1482–1489.
[15] A. Egozi, Y. Keller, and H. Guterman, “A probabilistic approach to spectral graph matching,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 35, no. 1, pp. 18 – 27, 2013.
[16] G. Griffin, A. Holub, and P. Perona, “Caltech-256 object category dataset,” Tech. Rep., California Institute of Technology, 2007.
[17] A. Rangarajan, A.L. Yuille, S. Gold, and E. Mjolsness, “A convergence proof for the softassign quadratic assignment problem,” in Proceedings Neural Information Processing Systems, 1996.
[18] A. Misevicius, “A modified simulated annealing algorithm for the quadratic assignment problem,” *Informatica*, vol. 14, no. 4, pp. 497–514, 2003.

[19] E. M. Loiola, N. M. M. Abreu, P. O. Boaventura-Netto, P. Hahn, and T. Querido, “A survey for the quadratic assignment problem,” *European Journal of Operational Research*, vol. 176, no. 2, pp. 657–690, 2007.

[20] R. E. Burkard, S. E. Karisch, and F. Rendl, “Qaplib - a quadratic assignment problem library,” *Journal of Global Optimization*, vol. 10, no. 4, pp. 391–403, 1997.