Bounds for the Quadratic Assignment Problem Using Continuous Optimization Techniques

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Abstract

The *quadratic assignment problem* (denoted QAP), in the trace formulation over the permutation matrices, is

$$\min_{X \in \Pi} \ tr(AXB + C)X^t.$$

Several recent lower bounds for QAP are discussed. These bounds are obtained by applying continuous optimization techniques to approximations of this combinatorial optimization problem, as well as by exploiting the special matrix structure of the problem. In particular, we apply constrained eigenvalue techniques, reduced gradient methods, subdifferential calculus, generalizations of trust region methods, and sequential quadratic programming.

Keywords : Quadratic Assignment Problem, Bounds, Constrained Eigenvalues, Reduced Gradient, Trust Regions, Sequential Quadratic Programming.

1 Introduction

The *quadratic assignment problem*, denoted QAP, is a generalization of the linear sum assignment problem, i.e. given the set $N = \{1, 2, \ldots, n\}$ and three n by n matrices $A = (a_{ik})$, $B = (B_{jl})$, and $C = (c_{ij})$, find a permutation π of the set N which minimizes

$$\sum_{i=1}^{n} c_{i\pi(i)} \ + \ \sum_{i=1}^{n}\sum_{k=1}^{n} a_{ik} b_{\pi(k)\pi(i)}. \qquad (1)$$

Equivalently, see [5], the trace formulation of QAP is to find a permutation matrix X to solve

$$\textbf{QAP} \qquad \min_{X \in \Pi} \ tr(AXB + C)X^t,$$

where Π denotes the set of $n \times n$ permutation matrices. The linear sum assignment problem, $LSAP$, can be solved very efficiently since the constraint can be relaxed from $X \in \Pi$ to $X \in \Omega$, the set of doubly stochastic matrices. This illustrates that $LSAP$ is in fact a linear programming problem. However, QAP is an NP-hard problem. (It contains, as a special case, the Travelling Salesman Problem, *TSP*.) If we relax the constraint as we did for $LSAP$, then there does not necessarily exist an optimum at an extreme point (i.e. permutation matrix) unless the objective function is concave. In the concave case, we may have many extreme points as local optima resulting in a hard combinatorial problem. Moreover, even the problem of finding an ϵ-approximation of the optimal solution is NP-hard. Thus from a worst case point of view, QAP is extremely difficult to solve. In the general case QAP is also difficult to solve, e.g. general QAP's of size $n \geq 15$ can prove to be intractable. Current solution techniques employ branch and bound methods and it appears that the poor quality of the lower bounds is a major cause of the difficulties. Thus it is worthwhile to collect a 'toolbox' of various bounds.

In this paper we present several bounds for QAP based on techniques from continuous optimization. These bounds exploit the special structure of QAP and include several interesting theoretical results. In Section 2 we present some of the background needed, as well as give a short survey of known bounds and solution techniques. In Section 3 we look at several bounding techniques based on constrained eigenvalue problems. In particular, we provide a projection technique onto the space of matrices with row and column sums 1. This is a special application of the reduced gradient technique in nonlinear programming. Our projection preserves orthogonality as well as the special matrix structure of our problem. This section also includes heuristic and iterative techniques for improving bounds. The iterative technique employs subgradient maximization.

In Section 4 we show how to treat the nonsymmetric QAP, i.e. we provide a transformation from a nonsymmetric QAP to an Hermitian one, which allows the application of our eigenvalue bounds. This includes the introduction of an interesting class of matrices.

In Section 5 we apply generalizations of trust region techniques to QAP. This allows us to apply bounding techniques without splitting the objective function into two parts. Included is an interesting characterization of global optimality for the QAP when the orthogonality constraint is relaxed using the Löewner partial order.

The results in this paper are taken from the following papers which have been recently submitted and/or are in progress: [7, 8, 9, 17, 18].

2 Background

In this section we present some background material including a short summary of results on QAP. We first present some of the notation and well known basic results used in this paper.

2.1 Notation and Basic Results

All matrices are assumed to be real and $n \times n$ unless stated otherwise. We let $u = \frac{1}{\sqrt{n}}(1,\ldots,1)^t \in \Re^n$ be the normalized n-vector of ones, and $u_i,\ i = 1,\ldots,n$ be the unit vectors in $\Re^n$. We let $\mathcal{E}$ be the set of $n \times n$ matrices having row and column sums of one, $\mathcal{N}$ be the set of $n \times n$ matrices with non-negative elements, and $\mathcal{O}$ be the set of $n \times n$ orthogonal matrices. I.e.

$$\begin{aligned} \mathcal{E} &= \left\{X \in \Re^{n\times n} : Xu = X^t u = u\right\}; \\ \mathcal{N} &= \left\{X \in \Re^{n\times n} : X \geq 0 \ \textit{elementwise}\right\}; \\ \mathcal{O} &= \left\{X \in \Re^{n\times n} : XX^t = I\right\}. \end{aligned} \tag{2}$$

By definition, the set of *doubly stochastic* matrices, denoted Ω, satisfies

$$\Omega = \mathcal{E} \cap \mathcal{N}.$$

It is well known that the set of *permutation* matrices, denoted Π, satisfies

$$\Pi = \mathcal{O} \cap \Omega = \mathcal{O} \cap \mathcal{E} \cap \mathcal{N}. \tag{3}$$

Furthermore, $\Pi = \mathcal{O} \cap \mathcal{N}$. The *linear sum assignment problem* with cost coefficients $C = (c_{ij})$, denoted $LSAP(C)$, is

$$\mathbf{LSAP(C)} \quad \min_{X\in\Pi} trCX^t.$$

$LSAP$ can be solved as a linear program by relaxing the constraints $X \in \Pi$ to $X \in \Omega$.

Given matrix A, the sum of the rows, columns, and elements of A are denoted by

$$r_A = \sqrt{n}Au,\ c_A = \sqrt{n}A^t u,\ \textit{and}\ s_A = nu^t Au,$$

respectively.

We assume the matrices A and B are symmetric with orthogonal diagonalizations $\Lambda_1 = Q_1^t A Q_1$ and $\Lambda_2 = Q_2^t B Q_2$, respectively, and eigenvalues $\lambda = (\lambda_i)$ and $\mu = (\mu_i)$, respectively. (The results in this paper can be extended to the case where neither A nor B are symmetric, see e.g. [8, 9]. We discuss this in Section 4.) If the vectors λ and μ are arranged in non-decreasing order then we get the *maximal scalar product*

$$< \lambda, \mu >_+ = \sum_i \lambda_i \mu_i,$$

and the *minimal scalar product*

$$< \lambda, \mu >_- = \sum_i \lambda_i \mu_{n-i+1}.$$

We also use the Löewner partial order, i.e. for symmetric matrices $A \preceq B$ ($A \prec B$) denotes $B - A$ is positive semidefinite (resp. positive definite).

2.2 Solution Techniques for QAP

As mentioned in the introduction QAP is *NP-hard*. Unlike the *Travelling Salesman Problem (TSP)*, a special case of QAP, it is generally accepted that QAP's of size $n > 15$ are intractable. This motivates the research of finding good, inexpensive, lower bounds for QAP to be implemented in a branch and bound procedure.

2.2.1 Lower Bounds for QAP

The classical lower bound for QAP is the Gilmore-Lawler bound [6, 12] which is based on a particular linear underestimation, $\tilde{C}$, of the objective function. The bound is given by the optimal function value of $LSAP(\tilde{C})$ and provides good bounds (relative to other known bounds). Unlike many other known bounds, the Gilmore-Lawler bound is not obtained by separating QAP into subproblems. We denote this bound by GLB.

In 1987, Finke, Burkard, and Rendl [5] introduced a new bound for QAP that is based on eigenvalue decompositions. Their bound is obtained by separating QAP into quadratic and linear subproblems. The linear subproblem can be solved exactly as an $LSAP$. The quadratic subproblem is relaxed to $X \in \mathcal{O}$ (from $X \in \Pi$). An optimal solution to the relaxed subproblem is characterized by the minimal scalar product of the eigenvalues of A and B. The bound is obtained by summing the optimal values of the relaxed subproblems, i.e.,

$$< \lambda, \mu >_- + LSAP(C). \tag{4}$$

We denote this eigenvalue based bound by *EVB1*.

The eigenvalue bound *EVB1* is, in general, very poor unless some reductions are applied to the matrices A and B. In order to maintain the symmetry of A and B, and the trace structure of the objective function of QAP, reductions are restricted to the following scheme (see e.g. [5]): Let $e, g, r, s \in \Re^n$ and define

$$E = \sqrt{n}(eu^t + ue^t);$$

$$G = \sqrt{n}(gu^t + ug^t);$$

$$R = diag(r); \ \ and \ S = diag(s).$$

The two reduction rules we use are (see e.g. [5]):

[Rd1] Set $A = \tilde{A} + E$ and $B = \tilde{B} + G$. Then for every $X \in \Pi$,
$tr(AXB + C)X^t = tr(\tilde{A}X\tilde{B} + \tilde{C})X^t$ with
$\tilde{C} = C + 2(\tilde{A}G + EB)$.

[Rd2] Set $A = \tilde{A} + R$ and $B = \tilde{B} + S$. Then for every $X \in \Pi$,
$tr(AXB + C)X^t = tr(\tilde{A}X\tilde{B} + \tilde{C})X^t$ holds with
$\tilde{C} = C + (diag\tilde{A}) \cdot s^t + r \cdot (diag\tilde{B})^t + r \cdot s^t$.

Note that these reductions do not affect the objective function value of QAP, but in general affect the bounds. A reduction scheme that minimizes the variance of the eigenvalues of A and B can be easily characterized, see e.g. [5, 17]. This scheme attempts to reduce the influence of the quadratic part of QAP, the part that is not solved exactly in *EVB1*. We denote the eigenvalue bound, applied after the variance minimizing reduction, by *EVB2*.

2.2.2 Exact Algorithms

To date, the most successful algorithms for QAP are branch and bound algorithms which, at any stage, consider a single assignment and either fix it or disallow it (i.e., set x_{ij} to either 1 or 0.). On a sequential machine, the most successful implementation is given in [1]; while the good implementations on parallel processors can be found in [16, 20].

There also exist algorithms based on cutting planes. Unlike TSP where cutting plane methods are very successful, these methods can only solve QAP's of size less than or equal to 8. However, cutting plane methods have proved to be the basis for some of the best heuristics for QAP.

For a further discussion and survey of solution techniques see [9].

3 New Eigenvalue Based Bounds

In this section we discuss new lower bounds for QAP based on constrained eigenvalue techniques, see e.g. [7, 17]. These bounds improve on the eigenvalue bounds $EVB1$ and $EVB2$.

3.1 Gradient Projection

A standard way of treating equality constraints in optimization is known as *gradient projection* (or *reduced gradient*) methods. Consider the linearly constrained optimization problem

$$\begin{array}{rl} min & f(x) \\ subject\ to & Dx = b, \end{array} \tag{5}$$

and let Z be a matrix whose columns are a basis for the null space of D. Then (5) is equivalent to the unconstrained optimization problem

$$\min_d \ f(x_0 + Zd)$$

for any x_0 such that $Dx_0 = b$.

We can similarly eliminate the linear equality constraints $X \in \mathcal{E}$ of QAP. This is done by exploiting the fact that u, the normalized n-vector of ones, is both a right and left eigenvector (with eigenvalue 1) of every permutation matrix X. Rather than relaxing to $X \in \mathcal{O}$ from $X \in \Pi$ as was done for $EVB1$ and $EVB2$, we maintain the constraint $X \in \mathcal{E}$ by restricting ourselves to the orthogonal matrices acting on the orthogonal complement of u, $\{u\}^\perp$. Projecting QAP orthogonally onto $\{u\}^\perp$ we are able to obtain an equivalent problem, denoted EP, see below. The objective function of EP has the same trace structure as QAP and also constrains the (matrix) variables to be orthogonal.

We need to define the following:

$$P := [u \vdots V], \ with\ V^t u = 0 \ and\ V^t V = I_{n-1}; \tag{6}$$

$Q := VV^t$ is the orthogonal projection on $\{u\}^\perp$;

$$P^tAP = \begin{bmatrix} \alpha & a^t \\ a & \hat{A} \end{bmatrix}; \ P^tBP = \begin{bmatrix} \beta & b^t \\ b & \hat{B} \end{bmatrix}; \ P^tCP = \begin{bmatrix} \gamma & c_1^t \\ c_2 & \hat{C} \end{bmatrix}; \tag{7}$$

where

$$\begin{gathered} \hat{A} = V^tAV; \ \hat{B} = V^tBV; \ \hat{C} = V^tCV; \\ a = V^t r_A/\sqrt{n}; \ b = V^t r_B/\sqrt{n}; \\ c_1 = V^t r_{C^t}/\sqrt{n}; \ c_2 = V^t r_C/\sqrt{n}; \\ \alpha = s_A/n; \ \beta = s_B/n; \ \gamma = s_C/n. \end{gathered}$$

Now define the following programming problem in the matrix variable $Y \in \Re^{(n-1)\times(n-1)}$

$$\mathbf{EP} \qquad \begin{array}{rc} min & tr(\hat{A}Y\hat{B}Y^t + (2ab^t + \hat{C})Y^t) + \alpha\beta + \gamma \\ subject\ to & Y^tY = I, \ VYV^t \geq -uu^t. \end{array}$$

We will see that EP is equivalent to QAP. This is based on the following characterization of permutation matrices.

Lemma 3.1 *[7] $X \in \Pi$ if and only if*

$$X = PY_1P^t \text{ with } Y_1 = \begin{bmatrix} 1 & 0 \ldots 0 \\ 0 & \\ \vdots & Y \\ 0 & \end{bmatrix}, \tag{8}$$

for some orthogonal Y in $\Re^{(n-1)\times(n-1)}$ satisfying

$$VYV^t \geq -uu^t. \tag{9}$$

Using this lemma we are able to prove the following theorem.

Theorem 3.1 *[7] The matrix Y solves EP if and only if the matrix X defined by (8) solves QAP.*

Since EP and QAP are equivalent, a lower bound for QAP can be obtained by finding a lower bound for EP. As was done in [5] for *EVB1* and *EVB2*, we separate EP into quadratic and linear subproblems, solve the linear subproblem exactly and solve the quadratic subproblem with the linear inequality constraints ignored. Relaxing the inequality constraints in EP is equivalent to considering orthogonal matrices having row and column sums of one in QAP. It is important to notice that the variables Y in EP are $(n-1)\times(n-1)$ matrices as oppposed to $n \times n$ matrices, i.e., the projection has reduced the dimension of the problem.

Theorem 3.2 *[7] Let $\hat{\lambda}$ and $\hat{\mu}$ be the eigenvalues of $\hat{A}$ and $\hat{B}$, repectively. Set*

$$D = V(2ab^t + \hat{C})V^t,$$

and define the LSAP

$$z^{opt} = \min_{X\in\Pi} tr DX^t.$$

Then a lower bound for QAP is

$$< \hat{\lambda}, \hat{\mu} >_- + z^{opt} + (\alpha\beta + \gamma).$$

We denote the above lower bound by *IVB*. In the case that the linear term, C, of QAP is zero, the lower bound can be simplified, see e.g. [7],

$$< \hat{\lambda}, \hat{\mu} >_- + \frac{2}{n} < r_A, r_B >_- - \frac{s_A s_B}{n^2}. \tag{10}$$

The following theorem shows that reductions of type [Rd1], discussed in Section 2.2.1, do not affect the new bound.

Theorem 3.3 *[7] Suppose that the reduction [Rd1] is applied to A and B. Then the lower bound in Theorem 3.2 is unchanged.*

We can however try to find a 'good' reduction using [Rd2] as was done for the bound in [5] and discussed in Section 2.2.1 above.

Theorem 3.4 *[7] The optimal real diagonal shift $A - R$, with $R = diag(r)$, that minimizes the variance of the eigenvalues of $V^t(A-R)V$ is defined by*

$$Q = VV^t; \; \delta = \left(\frac{n-1}{n}\right) trQA; \tag{11}$$

$$r_i = \frac{\delta}{n-1} + \frac{n}{n-1}(QAQ)_{ii} - \frac{1}{n}(trAQ).$$

3.2 Iterative Improvement

The eigenvalue bounds discussed above, *EVB1*, *EVB2*, *IVB*, rely on splitting QAP into linear and quadratic subproblems. Reductions may then be applied to attempt to increase the lower bound of the quadratic subproblem. The approach in [17] finds reductions to improve the lower bound by taking into account the effect of the reductions on *both* subproblems. Recall a lower bound for QAP can be obtained by the sum

$$m = < \tilde{\lambda}, \tilde{\mu} >_- + LSAP(\tilde{C}),$$

where $\tilde{A}$, $\tilde{B}$, and $\tilde{C}$ are given by [Rd1] and [Rd2], and $\tilde{\lambda}$, $\tilde{\mu}$ are the eigenvalues of $\tilde{A}$ and $\tilde{B}$, respectively. To improve the lower bound for QAP, (i.e. increase m), we use the derivative of the minimal scalar product, $< \lambda, \mu >_-$, as well as the subdifferential of the lower bound for $LSAP(C)$. A bundle and trust region subgradient routine from [21] was used to perform the maximization.

Assuming simple eigenvalues, the gradient of the minimal scalar product, say $d_1 = (e_1^t, g_1^t, r_1^t, s_1^t)^t$, can be obtained using the derivatives of the eigenvalues and the chain rule. (In the problems tested multiplicities of eigenvalues did not occur. The case of multiple eigenvalues can be handled using subdifferentials as well, see e.g. [15] for related problems.) The gradient of the lower bound for $LSAP(C)$ exists if the optimal solution is unique. This is equivalent to saying the optimal basis does not change for sufficiently small perturbations of C. In the event the optimal basis changes, it is shown that the direction of steepest ascent (subgradient) for the linear subproblem, say d_2, is the element of minimal norm of the subdifferential, see e.g. [4, 19].

For problems of size $n \geq 12$, the bound obtained by this algorithm is the best to date. One drawback to this bound is that it is much more expensive to obtain than *GLB, EVB1, EVB2* and *IVB.* We denote this bound by *EVB3.*

3.3 Numerical Results

In this section we present a comparison of the eigenvalue based bounds, *EVB1, EVB2, EVB3, IVB*, with the Gilmore-Lawler bound *GLB*, on both random problems and standard test problems found in the literature.

The first 8 examples in table 1 are taken from [14] and the last 5 are taken from [2]. The examples from [14] were also used in [5, 17]. The examples from [2] are all of size $n = 10$ and were generated in the following way; the matrix A is symmetric with entries uniformly drawn from the integers 0,1,...,10, the matrix C also has entries drawn uniformly from the integers 0,1,...,10 but C is not necessarily symmetric. Finally the matrix B represents the squared Euclidean distances of 10 points drawn randomly from the integer lattice $(0, 1, ..., 10) \times (0, 1, ..., 10)$.

First note that the bound *IVB* outperforms the 'classical' bound *GLB* for problems of size $n \geq 15$. Comparing *EVB1* and *IVB* we see that the additional constraint $X \in \mathcal{E}$ drastically improves the lower bound. While the computation times of *GLB*, *EVB1*, *EVB2*, and *IVB* are comparable, each iteration of *EVB3* takes about the same amount of time. Thus we see that *IVB* is the best 'inexpensive' bound for QAP. Tests indicate that it takes approximately 20-30 iterations before *EVB3* outperforms *IVB*. However, each iteration of the iterative improvement bound *EVB3* is about as expensive as computing *IVB*. Moreover, it can be shown that there exists reductions of type [Rd1] and [Rd2] for QAP such that the new bound IVB is no worse than the bound EVB2, see [7].

4 Symmetrization and the Hermitian QAP

As mentioned above, the results in Section 3 can be extended to the case where both A and B are non-symmetric. In order to apply eigenvalue based bounds (see e.g. [5, 7, 17], Section 3), one must have real eigenvalues. Restricting ourselves to real matrices implies that A and B must be symmetric. However if we consider complex matrices we can relax the symmetric assumption to a Hermitian assumption. In [5] it is shown that if one of A or B is symmetric, then there exists an equivalent QAP with both matrices being symmetric. If we consider QAP as a quadratic form using the Kronecker product of A and B, then we can apply the standard symmetrization using the transpose; however, we lose the important trace structure of our problem. In this section we show that given any (real) QAP there does exist an equivalent (complex) QAP such that the matrices A and B are Hermitian and C is real. The reductions discussed in Section 2.2.1 can be extended to the Hermitian case (and even to the quaternions), see [9]. This allows for extensions of

Size n	Best known Value	GLB	$X \in \mathcal{O}$ EVB1	EVB2	EVB3	$X \in \mathcal{O} \cap \mathcal{E}$ IVB
5	50	50	-86	47	50	47
6	86	82	-160	70	70	69
7	148	137	-251	123	130	125
8	214	186	-409	160	174	167
12	578	493	-909	446	495	472
15	1150	963	-1745	927	989	973
20	2570	2057	-3198	2075	2229	2196
30	6124	4539	-7836	4982	5349	5265
10	4954	3586		2774	4541	4079
10	8082	6139		6365	7617	7211
10	8649	7030		6869	8233	7837
10	8843	6840		7314	8364	8006
10	9571	7627		8095	8987	8672

Table 1: Lower Bounds for QAP

eigenvalue based bounds to the *Hermitian-*QAP and hence permits the use of eigenvalue bounds for **all** real QAPs.

4.1 New Classes of Matrices

In order to describe how we transform a non-symmetric QAP to an equivalent *Hermitian-*QAP we need to describe several classes of matrices.

As is standard in the literature we let

$$A_+ = (A + A^*)/2,$$

denote the *Hermitian* part of A, and

$$A_- = (A - A^*)/2,$$

denote the *skew-Hermitian* part of A, where $\cdot^*$ denotes conjugate transpose. It immediately follows that $A = A_+ + A_-$. Letting $i = \sqrt{-1}$, we introduce two new classes of matrices. We define the *positive Hermitian* part of A as

$$\tilde{A}_+ = (A_+ + iA_-),$$

and the *negative Hermitian* part of A as

$$\tilde{A}_- = (A_+ - iA_-).$$

These new classes of matrices give rise to new results in matrix theory, e.g. an extension of the Hoffman-Wielandt inequality [10] to nonnormal matrices, see e.g. [8, 9].

Using these matrices and basic properties of the trace of a matrix we get the following theorem.

Theorem 4.1 *Given real matrices A, B, and C, the following problems are equivalent;*

$$QAP(A, B, C,),\ QAP(\tilde{A}_+, \tilde{B}_-, C),\ \textit{and}\ QAP(\tilde{A}_-, \tilde{B}_+, C).$$

This gives us the following lower bound for $QAP(A, B, C)$.

Theorem 4.2 *Given real matrices A, B, and C, a lower bound for $QAP(A, B, C)$ is*

$$< \tilde{\lambda}_+, \tilde{\mu}_- >_- + LSAP(C),$$

where $\tilde{\lambda}_+$ and $\tilde{\mu}_-$ are the eigenvalues of $\tilde{A}_+$ and $\tilde{B}_-$, respectively.

5 Further Nonlinear Programming Techniques

The bounds discussed in Section 3 dealt with the quadratic and linear parts of QAP separately. The iterative improvement technique of Section 3.2 attempted to bring these two parts back together. This outperformed all the other techniques as seen by our numerical tests. In this section we outline the approach taken in [18] which treats the two parts of QAP together. This involves the notions of trust regions, active sets, and sequential quadratic programming from nonlinear programming theory. Included is a characterization of optimality for a generalized trust region problem, see Theorem 5.1 below.

5.1 Trust Regions

The orthogonal constraint $XX^t = I$ resembles in form the quadratic vector norm constraint, $||x||^2 = x^t x = \delta_c^2$, $x \in \Re^n$, with $\delta_c = 1$. This latter constraint, when applied to the minimization of a quadratic form on $\Re^n$, results in an eigenvalue problem. Therefore, the eigenvalue bounds discussed above are intuitively not surprising. When δ_c is arbitrary, the norm constraint is often referred to as a trust region constraint, see e.g. [13]. Trust region algorithms are used for unconstrained minimization. Given the real, twice continuously differentiable, function $f(x)$ on $\Re^n$, a current estimate x_c, the gradient g_c at x_c, and an estimate of the Hessian H_c at x_c, then trust region approaches choose an approximate step length δ_c and find the next iterate x_+ as an approximate solution of the constrained quadratic model

$$\begin{array}{rc} \min & f(x_c) + g_c^t d + \frac{1}{2} d^t H_c d \\ \text{subject to} & ||d|| \leq \delta_c. \end{array} \tag{12}$$

The radius of the trust region δ_c is increased or decreased depending on whether we get a satisfactory decrease in the objective function. The trust region subproblem (12) has several interesting properties. Surprisingly, it allows a characterization of optimality independent of the convexity of the quadratic objective function, i.e. there is no gap between necessary and sufficient optimality conditions for a global minimum for (12). This holds for the equality constrained trust region problem $||d|| = \delta_c$ as well. Moreover, the characterization of optimality allows an approximation to the optimum to be obtained very efficiently. However, these nice properties do not follow through if we add additional trust region constraints. Even two trust regions prove to be a very hard problem, see e.g. [3].

Since the orthogonality constraint $XX^t = I$ resembles a trust region constraint, let us relax the orthogonality constraint to

$$XX^t \preceq I, \tag{13}$$

where $\preceq$ denotes the Löewner partial order. This constraint now resembles the vector norm constraint. However, the partial order constraint (13) requires many inequalities to be verified, i.e. it is equivalent to checking that all the principal minors of $XX^t - I$ are nonpositive. In [18] it is shown that, surprisingly, we get the following complete characterization of optimality for the relaxation *TR* defined below. (We add a factor of $\frac{1}{2}$ to the quadratic part of QAP for notational convenience.)

Theorem 5.1 *Consider the relaxation of QAP*

$$\begin{array}{lrc} \textbf{TR} & \min & q(X) = tr \frac{1}{2} AXBX^t + CX^t \\ & \text{subject to} & \frac{1}{2}(XX^t - I) \preceq 0. \end{array}$$

Suppose that $XX^t \preceq I$. Define the optimality conditions

$$\begin{array}{rc} (i) & S \succeq 0, \\ (ii) & AXB + C + SX = 0, \\ (iii) & tr\ S(XX^t - I) = 0, \\ (iv) & tr\ (AhBh^t + hSh^t) \geq 0, \ \text{if the matrix } h \text{ satisfies } Xh^t + hX^t \text{ is psd on } \mathcal{N}(XX^t - I). \end{array} \tag{14}$$

Then:

a) X is a global minimum for TR *if and only if (14)(i)-(iv) holds;*

b) if (14)(i)-(iv) holds with $S \succ 0$, then X is a global minimum of TR *and $XX^t = I$.*

We can, in addition, guarantee that the optimum of *TR* is orthogonal, i.e. we can replace the constraint $XX^t \preceq I$ with $XX^t = I$. This involves applying [Rd2] reductions to guarantee the singular value condition in the following.

Corollary 5.1 *Suppose that the smallest singular value*

$$\sigma_n(A^{-1}CB^{-1}) > 1.$$

Then the second order conditions (14) characterize optimality of X for TR, with X orthogonal, i.e. X orthogonal solves TR if and only if the first order conditions (14)(i)-(iii) hold and

$$tr(AhBh^t + hSh^t) \geq 0 \text{ if } Xh^t + hX^t \succeq 0.$$

The above characterizations of a global optimum of *TR* are of theoretical interest in that they extend the vector trust region results which hold only for a single trust region. It remains to develope fast approximate solution techniques based on these characterizations, just as was done for vector trust region algorithms for unconstrained minimization, see e.g. [13].

5.2 Sequential Quadratic Programming and Active Sets

In Section 3.2 we introduced a projection onto $\mathcal{E}$, the smallest linear manifold containing the matrices with row and column sums 1. This yielded the following equivalent problem to QAP

$$\textbf{EP} \qquad \begin{array}{rc} min & tr(\hat{A}Y\hat{B}Y^t + (2ab^t + \hat{C})Y^t) + \alpha\beta + \gamma \\ subject\ to & Y^tY = I,\ VYV^t \geq -uu^t, \end{array}$$

where the optimal permutation for QAP and the optimal orthogonal Y for EP are related by

$$X = P\begin{bmatrix} 1 & \\ & Y \end{bmatrix}P^t;\ P = [u \,\vdots\, V];\ PP^t = I.$$

The projection eliminated the constraints of $\mathcal{E}$ while maintaining the special trace structure as well as the orthogonality constraint of our problem. Being able to maintain this structure is what enabled us to obtain the eigenvalue bound *IVB*. The constraint $VYV^t \geq -uu^t$ corresponds to the nonnegativity constraint of QAP, i.e. $X \geq 0$. Thus

$$X_{ij} = 0 \text{ if and only if } V_iYV_j^t = \frac{-1}{n}, \tag{15}$$

where V_k is the *k-th* row of V.

To solve *EP* we need to apply the trust region results presented above with a branch and bound procedure applied to an active set approach. The active set is obtained by fixing $X_{ij} = 1$ or $X_{ij} = 0$. If $X_{ij} = 1$ is fixed, then we can simultaneously fix the rest of the *i-th* row and *j-th* column of X to 0. This results in a *QAP* of smaller dimension.

Handling $X_{ij} = 0$ fixed is somewhat harder. We first apply the projection and work with the equivalent problem *EP* and the constraint $V_iYV_j^t = \frac{-1}{n}$ fixed. Let $V_k^t = U_k\Sigma_k$ be the singular value decomposition of V_k^t; thus we have $U_k^tU_k = I$ and $\Sigma_k = diag(\sigma_k\, 0 \ldots 0)^t \in \Re^{(n-1)\times(n-1)}$. Substitute $Y = U_iZU_j^t$ in *EP* to get a new equivalent program in $Z \in \mathcal{O}$ with the added constraint that $Z_{11} = \frac{-1}{\sigma_i\sigma_j}$ corresponding to $X_{ij} = 0$. This problem can be handled with a sequential quadratic programming technique, where the orthogonality constraint $ZZ^t = I$ can be handled as an eigenvalue constraint on $ZZ^t - I$, with the Z_{11} element of Z fixed. Thus when we treat the inequality constraints in *EP* with an active set approach in this way, we can maintain both the orthogonality and trace structures. This allows us to apply eigenvalue based bounds. However, we can do even more by substituting the matrix exponential $Z = e^{iT}$, where $i = \sqrt{-1}$ and $T = T^t$ is symmetric. This parametrization of the orthogonal matrices actually yields all the complex orthogonal matrices, see [11] Problem 27.6.4. This eliminates all the constraints except for the nonnegativity ones. If we relax our problem by ignoring the nonnegativity constraints only, then we are left with an unconstrained minimization problem in only $n(n+1)/2$ constraints and we have not split up the objective function into linear and quadratic parts. We can also apply reductions to improve this bound, i.e. we are left with the max-min (or parametric minimization) problem

$$\max_{e,g,r,s} \quad \min_{T=T^t} \; tr(\hat{A}w(T)\hat{B}w(T) + (2ab^t + \hat{C})w(T)) + \alpha\beta + \gamma, \tag{16}$$

where $w(T)$ denotes the real part of e^{iT}.

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