SDP relaxations for some combinatorial optimization problems

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In this chapter we present recent developments on solving various combinatorial optimization problems by using semidefinite programming (SDP). We present several SDP relaxations of the quadratic assignment problem and the traveling salesman problem. Further, we show the equivalence of several known SDP relaxations of the graph equipartition problem, and present recent results on the bandwidth problem.

Notation

The space of $p \times q$ real matrices is denoted by $\mathbb{R}^{p\times q}$, the space of $k \times k$ symmetric matrices is denoted by $\mathcal{S}_k$, and the space of $k\times k$ symmetric positive semidefinite matrices by $\mathcal{S}_k^+$. We will sometimes also use the notation $X \succeq 0$ instead of $X \in \mathcal{S}_k^+$, if the order of the matrix is clear from the context.

For index sets $\alpha, \beta \subset \{1, \ldots, n\}$, we denote the submatrix that contains the rows of A indexed by α and the columns indexed by β as $A(\alpha, \beta)$. If $\alpha = \beta$, the principal submatrix $A(\alpha, \alpha)$ of A is abbreviated as $A(\alpha)$. The ith column of a matrix C is denoted by $C_{:,i}$.

We use I_n to denote the identity matrix of order n, and e_i to denote the i-th standard basis vector. Similarly, J_n and u_n denote the $n\times n$ all-ones matrix and all-ones n-vector respectively, and $0_{n\times n}$ is the zero matrix of order n. We will omit subscripts if the order is clear from the context. The set of $n \times n$ permutation matrices is denoted by Π_n. We set $E_{ij} = e_i e_j^{\mathrm{T}}$.

The 'vec' operator stacks the columns of a matrix, while the 'diag' operator maps an $n \times n$ matrix to the n-vector given by its diagonal. The adjoint operator of 'diag' we denote by 'Diag'. The trace operator is denoted by 'tr'.

The Kronecker product $A \otimes B$ of matrices $A \in \mathbb{R}^{p\times q}$ and $B \in \mathbb{R}^{r\times s}$ is defined as the $pr \times qs$ matrix composed of pq blocks of size $r \times s$, with block ij given by $a_{ij}B$, $i = 1, \ldots, p$, $j = 1, \ldots, q$.

1 The Quadratic Assignment Problem

The quadratic assignment problem (QAP) was introduced in 1957 by Koopmans and Beckmann as a mathematical model for assigning a set of economic activities to a set of locations. Nowadays, the QAP is widely considered as a classical combinatorial optimization problem. The QAP is also known as a generic model for various real-life problems, such as hospital layout [48, 27], balancing of turbine runners [49], decoding for multi-input multi-output systems [55, 56], etc. For a more detailed list on applications of the QAP see e.g., [11, 12, 15].

We study the Koopmans–Beckmann form of the QAP, which can be written as

$$\text{(QAP)} \qquad \begin{aligned} &\min \operatorname{tr}(AXB + C)X^{\mathrm{T}} \\ &\text{s.t.} \quad X \in \Pi_n, \end{aligned} \tag{1}$$

where A and B are given symmetric $n \times n$ matrices, and C is a square matrix of order n. It is well-known that the QAP contains the traveling salesman problem as a special case and is therefore NP-hard in the strong sense. Moreover, experience has shown that instances with $n = 30$ are already very hard to solve in practice. Thus it is typically necessary to use massive parallel computing to solve even moderately sized QAP instances.

The recent developments in algorithms as well as in computational platforms have resulted in a large improvement in the capability to solve QAPs exactly. Anstreicher et al. [4] made a break–through by solving a number of previously unsolved large QAPs from QAPLIB [10]. They solved to optimality several famous instances, including the problem of size $n = 30$ posed by Nugent et al. [57], and problems of size $n = 30, 32$ posed by Krarup and Pruzan [47]. Optimal solutions of the problems of size $n = 36$ posed by Steinberg [66] are reported in [8, 58]. For a detailed survey on recent developments regarding the QAP problem, see Anstreicher [2].

In [4], the authors incorporate a convex quadratic programming bound that was introduced by Anstreicher and Brixius in [3], into a branch and bound framework that was running on a computational grid. Their computations are considered to be among the most extensive computations ever performed to solve combinatorial optimization problems. The computational work to solve a problem of size $n = 30$ (in particular Nug30) took the equivalent of nearly 7 years of computation time on a single HP9000 C3000 workstation.

In the sequel we describe the quadratic programming bound (QPB) that is introduced in [3]. Let V be an $n \times (n-1)$ matrix whose columns form an orthonormal basis for the nullspace of u_n^{T}, and define $\hat{A} := V^{\mathrm{T}}AV$, $\hat{B} := V^{\mathrm{T}}BV$. The QPB bound is:

$$\text{(QPB)} \qquad \begin{aligned} &\min \operatorname{vec}(X)^{\mathrm{T}}Q\operatorname{vec}(X) + \operatorname{tr}(CX^T) + \sum_{i=1}^{n} \lambda(\hat{A})_i \lambda(\hat{B})_{n+1-i} \\ &\text{s.t. } Xu_n = X^{\mathrm{T}}u_n = u_n \\ &\qquad X \geq 0, \end{aligned}$$

where $Q := (B \otimes A) - (I \otimes V\hat{S}V^{\mathrm{T}}) - (V\hat{T}V^{\mathrm{T}} \otimes I)$, and $\lambda(\cdot)_1 \leq \ldots \leq \lambda(\cdot)_n$ are the eigenvalues of the matrix under consideration. The matrices $\hat{S}$ and $\hat{T}$ are optimal solutions of the following SDP problem

$$\begin{aligned} \mathrm{OPT}_{\mathrm{SDD}_{(\hat{A},\hat{B})}} := & \max \ \mathrm{tr}(\hat{S}) + \mathrm{tr}(\hat{T}) \\ & \text{s.t. } (\hat{B} \otimes \hat{A}) - (I \otimes \hat{S}) - (\hat{T} \otimes I) \succeq 0. \end{aligned}$$

It is shown by Anstreicher and Wolkowicz [5] that

$$\mathrm{OPT}_{\mathrm{SDD}_{(\hat{A},\hat{B})}} = \sum_{i=1}^{n} \lambda(\hat{A})_i \lambda(\hat{B})_{n+1-i},$$

and in [3] that optimal $\hat{S}$, $\hat{T}$ can be obtained from the spectral decomposition of $\hat{A}$ and $\hat{B}$. The objective in QPB is convex on the nullspace of the constraints $Xu = X^{\mathrm{T}}u = u$, or equivalently $(V^{\mathrm{T}} \otimes V^{\mathrm{T}})Q(V \otimes V) \succeq 0$. Therefore, QPB is a convex quadratic programming program.

In [3], the quadratic programming bounds are computed using a long-step path following interior point algorithm. However, it turned out to be too costly to use interior point methods (IPMs) in a branch and bound setting, particularly for the large scale problems. Therefore, in [4, 7] the Frank-Wolfe (FW) algorithm [30] is implemented to approximately solve QPB in each node of the branching tree. Although the FW method is known to have poor asymptotic performance, it seems to be a good choice in the mentioned branch and bound setting. Namely, each iteration of the FW algorithm requires the solution of a linear assignment problem that can be performed extremely rapidly, and the FW algorithm generates dual information that can be exploited while branching.

Another class of convex relaxations for the QAP are the semidefinite programming bounds. The following SDP relaxation of the QAP was studied by Povh and Rendl [61]:

$$(\mathrm{QAP}_{\mathrm{ZW}}) \quad \begin{aligned} \min \ & \mathrm{tr}(B \otimes A + \mathrm{Diag}(\mathrm{vec}(C)))Y \\ \text{s.t. } & \mathrm{tr}(I_n \otimes E_{jj})Y = 1, \quad \mathrm{tr}(E_{jj} \otimes I_n)Y = 1, \quad j = 1, \ldots, n \\ & \mathrm{tr}(I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y = 0 \\ & \mathrm{tr}(J_{n^2} Y) = n^2 \\ & Y \geq 0, \quad Y \succeq 0. \end{aligned}$$

We use the abbreviation ZW to emphasize that this model is motivated by Zhao et al. [68]. Namely, in [61] it is proven that the relaxation $\mathrm{QAP}_{\mathrm{ZW}}$ is equivalent to the earlier relaxation of Zhao et al. [68]. The SDP relaxation $\mathrm{QAP}_{\mathrm{ZW}}$ is also equivalent to the so-called $N^+(K)$-relaxation by Lovász and Schrijver [53] applied to the QAP, as was observed by Burer and Vandenbussche [9]. The equivalence between the two relaxations was also shown in [61].

One may easily verify that $\mathrm{QAP}_{\mathrm{ZW}}$ is indeed a relaxation of the QAP (1) by noting that

$$Y := \mathrm{vec}(X)\mathrm{vec}(X)^{\mathrm{T}}$$

is a feasible point of $\mathrm{QAP}_{\mathrm{ZW}}$ for $X \in \Pi_n$, and that the objective value of $\mathrm{QAP}_{\mathrm{ZW}}$ at this point Y is precisely $\mathrm{tr}(AXB + C)X^{\mathrm{T}}$. The constraints involving E_{jj} are generalizations of the assignment constraints $Xu = X^{\mathrm{T}}u = u$, and the sparsity constraints i.e., $\mathrm{tr}(I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y = 0$ generalize the orthogonality conditions $XX^{\mathrm{T}} = X^{\mathrm{T}}X = I$. This sparsity pattern is sometimes called the *Gangster constraint* and is denoted by $\mathcal{G}(Y) = 0$, see e.g., [68].

The following lemma from [61] gives an explicit description of the feasible set of $\mathrm{QAP}_{\mathrm{ZW}}$.

Theorem 1 ([61], Lemma 6) *A matrix*

$$Y = \begin{pmatrix} Y^{(11)} & \cdots & Y^{(1n)} \\ \vdots & \ddots & \vdots \\ Y^{(n1)} & \cdots & Y^{(nn)} \end{pmatrix} \in \mathcal{S}^{+}_{n^2}, \quad Y^{(ij)} \in \mathbb{R}^{n \times n}, \quad i, j = 1, \ldots, n,$$

is feasible for $\mathrm{QAP}_{\mathrm{ZW}}$ *if and only if* Y *satisfies*

(i) $\mathcal{G}(Y) = 0$, $\mathrm{tr}(Y^{(ii)}) = 1$ *for* $1 \leq i \leq n$, $\sum_{i=1}^{n} \mathrm{diag}(Y^{(ii)}) = u$,

(ii) $u^{\mathrm{T}}Y^{(ij)} = \mathrm{diag}(Y^{(jj)})^{\mathrm{T}}$ *for* $1 \leq i, j \leq n$,

(iii) $\sum_{i=1}^{n} Y^{(ij)} = u\,\mathrm{diag}(Y^{(jj)})^{\mathrm{T}}$ *for* $1 \leq j \leq n$.

Bounds obtained by solving $\mathrm{QAP}_{\mathrm{ZW}}$ are quite good in practice, but computationally demanding for interior point solvers, even for relatively small instances (say $n \geq 15$). (Note that the matrix variable Y is a square matrix of order n^2, and that the relaxation has $O(n^4)$ sign constraints and $O(n^3)$ equality constraints.) Therefore, some alternative methods were used to solve $\mathrm{QAP}_{\mathrm{ZW}}$. A dynamic version of the bundle method is used in [63] to approximately solve QAPLIB [10] problems of sizes $n \leq 32$, and in [9] the augmented Lagrangian approach is implemented for solving problems with $n \leq 36$.

For QAP instances where the data matrices have large *automorphism groups*, the SDP bounds can be computed more efficiently by exploiting symmetry. This was shown in [20], see also the chapter by de Klerk, de Oliveira Filho, and Pasechnik in this handbook. In [20], $\mathrm{QAP}_{\mathrm{ZW}}$ bounds for Eschermann and Wunderlich [28] instances for n up to 128 are computed with interior point solvers. In these instances the automorphism group of B is the automorphism group of the Hamming graph (see e.g. [65], or Example 5.1 in [20]).

In Table 1, $\mathrm{QAP}_{\mathrm{ZW}}$ bounds are listed for Eschermann–Wunderlich instances of sizes $n = 32, 64, 128$ that are computed using symmetry reduction (for details see [20]). Note that bounds from [9] do not always give the same bounds as those from [20]. The reason for the difference is that the augmented

Lagrangian method does not always solve the SDP relaxation $\mathrm{QAP}_{\mathrm{ZW}}$ to optimality. The previous lower bounds for esc64a and esc128 given in Table 1 are the Gilmore-Lawler [34, 50] bounds.

Thus, in [20] it is shown that QAP instances where the data matrices have large automorphism groups, $\mathrm{QAP}_{\mathrm{ZW}}$ bounds can be computed efficiently by IPMs. Moreover, this approach gives an opportunity for solving strengthened $\mathrm{QAP}_{\mathrm{ZW}}$ relaxations.

As noted in [63], the SDP relaxation $\mathrm{QAP}_{\mathrm{ZW}}$ can be strengthened by adding the so called *triangle inequalities*

$$0 \le Y_{rs} \le Y_{rr} \tag{2}$$

$$Y_{rr} + Y_{ss} - Y_{rs} \le 1 \tag{3}$$

$$-Y_{tt} - Y_{rs} + Y_{rt} + Y_{st} \le 0 \tag{4}$$

$$Y_{tt} + Y_{rr} + Y_{ss} - Y_{rs} - Y_{rt} - Y_{st} \le 1, \tag{5}$$

which hold for all distinct triples (r, s, t). Note that there are $O(n^6)$ triangle inequalities. In [20] the following result is proven.

Lemma 2 [20] *If an optimal solution Y of $\mathrm{QAP}_{\mathrm{ZW}}$ has constant diagonal, then all the triangle inequalities (2)–(5) are satisfied.*

Since optimal solutions of $\mathrm{QAP}_{\mathrm{ZW}}$ for the instances solved in [20] have constant diagonal, the lower bounds can not be improved by adding the triangle inequalities (2)–(5).

In [21] it is shown how one may obtain stronger bounds than $\mathrm{QAP}_{\mathrm{ZW}}$ for QAP instances where one of the data matrices has a *transitive automorphism group*. The results in the sequel are restricted to the QAP where $C = 0$. The idea in [21] is to assign facility s to location r for a given arbitrary index pair (r, s). In other words, to fix entry (r, s) in the permutation matrix X to one. This leads to a QAP problem that is one dimension smaller than the original one, i.e., to the problem

$$\min_{X \in \Pi_{n-1}} \operatorname{tr}(A(\alpha)XB(\beta) + \bar{C}(\alpha, \beta))X^{\mathrm{T}}. \tag{6}$$

Here $\alpha = \{1, \ldots, n\} \backslash r$ and $\beta = \{1, \ldots, n\} \backslash s$, and

$$\bar{C}(\alpha, \beta) = 2A(\alpha, \{r\})B(\{s\}, \beta).$$

Further, in [21] it is suggested to solve relaxation $\mathrm{QAP}_{\mathrm{ZW}}$ for the corresponding smaller dimensional problem, i.e.,

$$(\mathrm{QAP}_{\mathrm{dKS}}) \quad \begin{aligned} \min\ & \operatorname{tr}(B(\beta) \otimes A(\alpha) + \operatorname{Diag}(\operatorname{vec}(\bar{C})))Y \\ \text{s.t.}\ & \operatorname{tr}(I_{n-1} \otimes E_{jj})Y = 1,\ \operatorname{tr}(E_{jj} \otimes I_{n-1})Y = 1,\ j = 1, \ldots, n-1 \\ & \operatorname{tr}(I_{n-1} \otimes (J_{n-1} - I_{n-1}) + (J_{n-1} - I_{n-1}) \otimes I_{n-1})Y = 0 \\ & \operatorname{tr}(J_{(n-1)^2}Y) = (n-1)^2 \\ & Y \ge 0, \quad Y \succeq 0. \end{aligned}$$

Note that here Y has size $(n-1)^2 \times (n-1)^2$. In [21] the symmetry reduction of the SDP problem $\mathrm{QAP}_{\mathrm{dKS}}$ is performed in order to solve the relaxation efficiently.

In general, the bounds obtained from $\mathrm{QAP}_{\mathrm{dKS}}$ are not lower bounds for the original QAP problem, but if $\mathrm{aut}(A)$ or $\mathrm{aut}(B)$ is transitive then they are also global lower bounds.

Theorem 3 [21] *If aut(A) or aut(B) is transitive and $C = 0$, then any lower bound for the QAP subproblem (6) at the first level of the branching tree is also a lower bound for the original QAP.*

Note that if both $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ are transitive, then there is only one subproblem. However, if only one of the automorphisms groups of the data matrices is transitive, then the number of different subproblems depends on the automorphism group of the other data matrix. In any case, if only one of the automorphisms groups of the data matrices is transitive, the number of different subproblems is at most n, the order of the data matrices. The following lemma provides details.

Lemma 4 [21] *Let aut(B) be transitive. Then there are as many different child subproblems at the first level of the branching tree as there are orbits of aut(A).*

In the sequel we discuss the quality of the bounds $\mathrm{QAP}_{\mathrm{dKS}}$ obtained by fixing arbitrary (r, s). In order to do that, we need to show that the following SDP problem

$$
\begin{array}{rl}
\min & \mathrm{tr}(B \otimes A)Y \\
\text{s.t.} & \mathrm{tr}(I_n \otimes E_{jj})Y = 1, \mathrm{tr}(E_{jj} \otimes I_n)Y = 1, \quad j = 1, \ldots, n \\
& \mathrm{tr}(I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y = 0 \\
& \mathrm{tr}(J_{n^2} Y) = n^2 \\
& \mathrm{tr}(E_{ss} \otimes E_{rr})Y = 1 \\
& Y \geq 0, \quad Y \succeq 0,
\end{array}
\tag{7}
$$

is equivalent to $\mathrm{QAP}_{\mathrm{dKS}}$. Note that SDP relaxation (7) differs from $\mathrm{QAP}_{\mathrm{ZW}}$ by one additional constraint. For the proof of equivalence we will use the following lemmas.

Lemma 5 *Let Y be feasible for (7), then*

(a) $\mathrm{tr}(E_{jj} \otimes E_{rr})Y = 0$, $j = 1, \ldots, n$, $j \neq s$

(b) $\mathrm{tr}(E_{ss} \otimes E_{jj})Y = 0$, $j = 1, \ldots, n$, $j \neq r$

(c) $\mathrm{tr}(E_{ij} \otimes (E_{rk} + E_{kr}))Y = 0$, $i \neq j$, $k = 1, \ldots, n$

(d) $\mathrm{tr}((E_{sk} + E_{ks}) \otimes E_{ij})Y = 0$, $k \neq s$, $i \neq r$, $j \neq r$.

Proof. The results follow trivially from the generalized assignment constraints in (7), and from the fact that if $Y \in \mathcal{S}_n^+$ and $y_{ii} = 0$, then $y_{ij} = 0$, for all $j = 1, \ldots, n$. □

Lemma 6 *Let Y be feasible for (7), then*

$$\operatorname{diag}(Y) = Y_{:,(s-1)n+r}.$$

Proof. This follows from the fact that $u_n^{\mathrm{T}} Y^{(sj)} = \operatorname{diag}(Y^{(jj)})^{\mathrm{T}}$ for $1 \leq j \leq n$ (see Theorem 1) and (c)–(d) in Lemma 5. □

Now we can show that (7) and $\mathrm{QAP}_{\mathrm{dKS}}$ are equivalent. A similar proof was obtained by De Klerk (private communication, 2010).

Theorem 7 *Let $r, s \in \{1, \ldots, n\}$ be fixed. The semidefinite program (7) is equivalent to* $\mathrm{QAP}_{\mathrm{dKS}}$ *in the sense that there is a bijection between the feasible sets that preserves the objective function.*

Proof. Assume w.l.o.g. that $r = s = 1$. We show first that for any $Y \in \mathcal{S}_{n^2 \times n^2}$ that is feasible for (7), we can find exactly one matrix $Z = Z(Y) \in \mathcal{S}_{(n-1)^2 \times (n-1)^2}$ that is feasible for $\mathrm{QAP}_{\mathrm{dKS}}$. Consider the block form of Y as in Theorem 1. From Lemma 5 and Lemma 6 it follows that

$$Y_{rk}^{(ij)} = Y_{kr}^{(ij)} = 0 \quad i, j = 2 \ldots, n, \quad k = 1, \ldots, n,$$

and for $\alpha = \{2, \ldots, n\}$ the following principal submatrices are zero matrices, i.e.,

$$Y^{(1j)}(\alpha) = Y^{(j1)}(\alpha) = 0_{n-1}, \quad j = 1, \ldots, n,$$

and

$$Y_{:,1}^{(j1)} = \operatorname{diag}(Y^{(jj)}), \quad j = 1, \ldots, n.$$

Now, we define

$$Z^{(i-1,j-1)} := Y^{(ij)}(\alpha) \in \mathbb{R}^{(n-1)\times(n-1)}, \quad i, j = 2, \ldots, n,$$

and

$$Z(Y) := \begin{pmatrix} Z^{(11)} & \ldots & Z^{(1,n-1)} \\ \vdots & \ddots & \vdots \\ Z^{(n-1,1)} & \ldots & Z^{(n-1,n-1)} \end{pmatrix} \in \mathcal{S}_{(n-1)^2 \times (n-1)^2}.$$

Since $Z(Y)$ is a principal submatrix of the positive semidefinite matrix Y, it follows that $Z(Y) \succeq 0$. The other constraints from $\mathrm{QAP}_{\mathrm{dKS}}$ are trivially satisfied.

Conversely, let $Z \in \mathcal{S}^+_{(n-1)^2 \times (n-1)^2}$ be feasible for $\mathrm{QAP}_{\mathrm{dKS}}$. We construct $Y \in \mathcal{S}^+_{n^2 \times n^2}$ such that $Z = Z(Y)$ in the following way. In each block $Z^{(ij)}$, $i, j = 1, \ldots, n-1$, add the first row and column with all zeros and call these $n \times n$ blocks $\bar{Z}^{(ij)}$. Define n blocks $\widetilde{Z}^{(1j)} \in \mathbb{R}^{n \times n}$, $j = 1, \ldots, n$ in the following way

$$\widetilde{Z}_{ij}^{(11)} = \begin{cases} 1 & \text{for } \; i = j = 1 \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\widetilde{Z}^{(1j)}_{1,:} = \text{diag}(\bar{Z}^{(jj)})^{\mathrm{T}}, \quad \widetilde{Z}^{(1j)}_{kl} = 0, \quad l = 1,\ldots,n,\ k,j = 2,\ldots,n.$$

Finally, let

$$Y := \begin{pmatrix} \widetilde{Z}^{(11)} & \widetilde{Z}^{(12)} & \ldots & \widetilde{Z}^{(1n)} \\ (\widetilde{Z}^{(12)})^{\mathrm{T}} & \bar{Z}^{(11)} & \ldots & \bar{Z}^{(1,n-1)} \\ \vdots & \ddots & \vdots & \vdots \\ (\widetilde{Z}^{(1n)})^{\mathrm{T}} & \bar{Z}^{(n1)} & \ldots & \bar{Z}^{(n-1,n-1)} \end{pmatrix} \in \mathcal{S}_{n^2\times n^2}.$$

From Proposition 14 it follows that Y is a positive semidefinite matrix. Also the remaining constraints in (7) are satisfied, due to the construction of Y.

Finally, note that for any pair of feasible solutions $Y \in \mathcal{S}^+_{n^2\times n^2}$ of (7) and $Z = Z(Y) \in \mathcal{S}^+_{(n-1)^2\times(n-1)^2}$ of QAP_{dKS} it holds that

$$\text{tr}(B \otimes A)Y = \text{tr}(B(\beta) \otimes A(\alpha) + 2\text{Diag}(B(\beta,\{s\}) \otimes A(\alpha,\{r\})))Z.$$

□

Finally, we may conclude.

Corollary 8 *Fix $r, s \in \{1,\ldots,n\}$. Assume that aut(A) or aut(B) is transitive and $C = 0$. Then the SDP relaxation QAP_{dKS} dominates* QAP_{ZW}.

The numerical results in [21] (see also Table 1) show that the SDP lower bounds QAP_{dKS} can be significantly better than the SDP bounds QAP_{ZW}. The authors in [21] were not able to form QAP_{dKS} relaxation for esc128 problem due to the memory issues.

instance	previous l.b.	QAP_{ZW}	QAP_{dKS}	best known u.b.
esc32a	103 ([9])	104	107	130
esc32h	424 ([9])	425	427	438
esc64a	47	98	105	116
esc128	2	54	n.a.	64

Table 1. Optimal values for the larger esc instances.

The SDP bound QAP_{dKS} has several potential areas of application. In particular, it is applicable for all QAP instances where the automorphism group of one of the data matrices is transitive. Famous examples of such instances are the traveling salesman problem and the graph equipartition problem, which will be discussed in the next sections.

2 The Traveling Salesman Problem

Let $K_n(D)$ be a complete graph on n vertices with edge lengths $D_{ij} = D_{ji} > 0$ $(i \neq j)$. The traveling salesman problem (TSP) is to find a Hamiltonian circuit of minimum length in $K_n(D)$. The n vertices are often called cities, and the Hamiltonian circuit of minimum length the optimal tour. Here we present two SDP relaxations for the traveling salesman problem.

Cvetković et al. [14] derived a semidefinite programming relaxation for the TSP that is motivated by the algebraic connectivity of graphs. (The algebraic connectivity of a graph is defined as the second smallest eigenvalue of the Laplacian of the graph, see (8).) In particular, Cvetković at al. [14] exploit the fact that the Laplacian eigenvalues of the Hamiltonian circuit are $2(1 - \cos(\frac{2k\pi}{n}))$ for $k = 0, \dots, n-1$, and the second smallest eigenvalue is

$$h_n := 2\left(1 - \cos\left(\frac{2\pi}{n}\right)\right).$$

In [14] it is concluded that if X is in the convex hull of all Hamiltonian cycles (represented by their adjacency matrices) through n vertices, then its algebraic connectivity is at least h_n. This eigenvalue constraint is reformulated as a semidefinite constraint, and the resulting SDP relaxation for the TSP from [14] is:

$$(\mathrm{TSP_{CK}}) \qquad \begin{aligned} \min\ & \tfrac{1}{2}\operatorname{tr}(DX) \\ \text{s.t. } & Xu_n = 2u_n \\ & \operatorname{diag}(X) = 0 \\ & 0 \le X \le J \\ & 2I - X + 2\left(1 - \cos\left(\tfrac{2\pi}{n}\right)\right)(J - I) \succeq 0. \end{aligned}$$

It was shown by Goemans and Rendl [35] that the well known Held-Karp linear programming bound [17, 39] dominates the SDP relaxation $\mathrm{TSP_{CK}}$. In the sequel we present the most recent SDP bound for the TSP. This bound dominates $\mathrm{TSP_{CK}}$ and is independent of the Held-Karp bound.

In [19], a new SDP relaxation of the TSP is derived. This relaxation coincides with the SDP relaxation for the QAP introduced in [68] when applied to the QAP reformulation of the TSP. Indeed, it is well known that the TSP is a special case of the QAP, and can be stated as

$$(\mathrm{TSP}) \qquad \min_{X \in \Pi_n} \operatorname{tr}\left(\frac{1}{2} D X C_n X^{\mathrm{T}}\right),$$

where C_n is the adjacency matrix of the canonical circuit on n vertices:

$$C_n := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \\ 0 & & & & 0 & 1 \\ 1 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix},$$

and D is the matrix of edge lengths. Thus, the following SDP relaxation of the TSP is derived in [19] from $\mathrm{QAP_{ZW}}$ (see p. 3) by symmetry reduction, see also the chapter entitled "Relaxations of combinatorial problems via association schemes" in this handbook.

$$(\mathrm{TSP_{dKPS}})\qquad \begin{array}{lll} \min \frac{1}{2}\operatorname{tr}\left(DX^{(1)}\right) & & \\ \text{s.t. } \sum_{k=1}^{d} X^{(k)} = J - I & & \\ \quad I + \sum_{k=1}^{d} \cos\left(\frac{2\pi i k}{n}\right) X^{(k)} \succeq 0 & & i = 1,\dots,d \\ \quad X^{(k)} \geq 0, \quad X^{(k)} \in \mathcal{S}_n, & & k = 1,\dots,d, \end{array}$$

where $d = \lfloor \frac{1}{2} n \rfloor$ is the diameter of the canonical circuit on n vertices. In [19] it is proven that $\mathrm{TSP_{dKPS}}$ dominates the relaxation due to Cvetković et al. [14], and is not dominated by the Held-Karp linear programming bound (or vice versa). In [22] it is shown that when the matrix of distances between cities D is symmetric and circulant, the SDP relaxation $\mathrm{TSP_{dKPS}}$ reduces to a linear programming problem.

Following the idea on improving $\mathrm{QAP_{ZW}}$ by fixing one position in the permutation matrices, one can strengthen $\mathrm{TSP_{dKPS}}$ as well. This approach is applicable to the TSP since the automorphism group of C_n is the dihedral group, which is transitive. Preliminary results in [21] show that the lower bounds so obtained are very promising. Finally, we note here that the SDP bound $\mathrm{TSP_{dKPS}}$ is hard to compute for large size problems; however it provides a new polynomial-time convex approximation of the TSP with a rich mathematical structure.

3 The Graph Equipartition Problem

The *k-equipartition problem* (k-GP) is defined as follows. Consider an undirected graph $G = (V, E)$ with vertex set V, $|V| = n = km$, and edge set E. The goal is to find a partition of the vertex set into k sets $S_1, \dots, S_k$ of equal cardinality, i.e., $|S_i| = m$, $i = 1, \dots, k$ such that the total weight of edges joining different sets S_i is minimized. If there is no restriction on the size of the sets, then we refer to this as the *graph partition* problem.

We denote by A the *adjacency matrix* of G. For a given partition of the graph into k subsets, let $X = (x_{ij})$ be the $n \times k$ matrix defined by

$$x_{ij} = \begin{cases} 1 \text{ if node } i \text{ is in } S_j \\ 0 \text{ if node } i \text{ is not in } S_j. \end{cases}$$

It is clear that the jth column $X_{:,j}$ is the characteristic vector of S_j, and k-partitions are in one-to-one correspondence with the set

$$\mathcal{P}_k := \left\{ X \in \mathbb{R}^{n \times k} : \; Xu_k = u_n, \; X^{\mathrm{T}} u_n = m u_k, \; x_{ij} \in \{0, 1\} \right\}.$$

For each $X \in \mathcal{P}_k$, it holds that

- $\operatorname{tr} X^{\mathrm{T}} D X = \operatorname{tr} D$, if D is diagonal.
- $\frac{1}{2} \operatorname{tr} X^{\mathrm{T}} A X$ gives the total weight of the edges within the subsets S_j.

Therefore, the total weight of edges cut by X, i.e., those joining different sets S_j is

$$w(E_{\text{cut}}) := \frac{1}{2} \operatorname{tr}(X^{\mathrm{T}} L X),$$

where

$$L := \operatorname{Diag}(A u_n) - A \tag{8}$$

is the Laplacian matrix of the graph. The *k-equipartition problem* in a trace formulation can then be written:

$$\text{(k–GP)} \quad \begin{array}{l} \min \frac{1}{2} \operatorname{tr}(X^{\mathrm{T}} L X) \\ \text{s.t.} \;\; X \in \mathcal{P}_k \end{array}$$

It is easy to verify that for $X \in \mathcal{P}_k$ it follows:

$$\operatorname{tr}(X^{\mathrm{T}} L X) = \operatorname{tr}(X^{\mathrm{T}} A X (J_k - I_k)), \tag{9}$$

where J_k is the $k \times k$ all-ones matrix and I_k the identity matrix of order k.

The graph partition problem has many applications such as VLSI design [51], parallel computing [6] and floor planing [16]. The equipartition problem also plays a role in telecommunications, see e.g., [52]. For more applications of the k–equipartition problem see Lengauer [43] and the references therein.

The k–equipartition problem is NP-hard, even for $k = 2$, see [31]. The graph equipartition problem is extensively studied and many heuristics are suggested, see e.g., Kernighan and Lin [46], Fiduccia and Mattheyses [29]. In [32], a branch-and-cut algorithm based on SDP is implemented for the minimum k–partition problem. The authors here compute globally optimal solutions for dense graphs up to 60 vertices, for grid graphs with up to 100 vertices, and for different values of k. Also, there are several known relaxations of the problem, and we list some of them below. In 1973, Donath and Hoffman [25] derive an eigenvalue based bound for k–GP that was further improved by Rendl and Wolkowicz [64] in 1995. In [1], Alizadeh shows that the Donath–Hoffman bound can be obtained as the dual of a semidefinite program. A detailed description of these bounds and their relationships are given by Karisch and Rendl [45]. In the same paper bounds are derived that are stronger than the mentioned eigenvalue based bounds, whereas Wolkowicz and Zhao [69] derive bounds for the general graph partition problem.

In the sequel we derive an SDP relaxation from [45], which is based on matrix lifting, and an SDP relaxation from [69], which is based on vector lifting, and show that they are *equivalent*. Moreover, we relate these relaxations with an SDP relaxation of k–equipartition problem that is derived from the SDP relaxation of the quadratic assignment problem. In particular, we first derive the SDP relaxation k–GP_{KR} [45] whose matrix variable is in $\mathcal{S}_n^+$. Then, we derive the SDP relaxation k–GP_{ZW} [69] that also includes nonnegativity constraints and whose matrix variable is in $\mathcal{S}^+_{nk+1}$. Furthermore, we introduce a new relaxation k–GP$_{\rm RS}$ with matrix variable in $\mathcal{S}^+_{nk}$ that we prove is dominated by k–GP$_{\rm ZW}$ and which dominates k–GP$_{\rm KR}$. Finally, we introduce an SDP relaxation for the graph equipartition problem that is derived as a special case of the QAP in [23] and that is known to be equivalent to k–GP$_{\rm KR}$, and show that this relaxation dominates k–GP$_{\rm ZW}$. From this follows the equivalence of all these formulations.

Very recently, a preprint [26] has appeared in which it is also shown that SDP relaxations based on vector-lifting and on matrix lifting for quadratically constrained quadratic programs with matrix variables provide equivalent bounds, under mild assumptions.

At the end of this section, we present a relaxation for the k–equipartition problem that was recently derived by De Klerk et al. [23] and that dominates all the above-mentioned relaxations.

One way to obtain a relaxation of the k-equipartition is to linearize the objective function $\operatorname{tr}(X^{\rm T}LX) = \operatorname{tr}(LXX^{\rm T})$ by replacing $XX^{\rm T}$ by a new variable Y. This yields the following feasible set of k–GP:

$$P_k := \operatorname{conv}\{Y : \exists X \in \mathcal{P}_k \;\text{ such that }\; Y = XX^{\rm T}\}.$$

In order to obtain tractable relaxations for k–GP one needs to approximate the set P_k by larger sets containing P_k. Karisch and Rendl [45] impose on elements $Y \in P_k$ the following set of constraints

$$\{Y \in \mathcal{S}_n : \operatorname{diag}(Y) = u_n,\; Yu_n = mu_n,\; Y \geq 0,\; Y \succeq 0\}\,,$$

and consequently obtain the SDP relaxation:

$$(\text{k–GP}_{\rm KR})\qquad \begin{array}{c} \min \tfrac{1}{2}\operatorname{tr}(LY) \\ \text{s.t. } \operatorname{diag}(Y) = u_n, Yu_n = mu_n \\ Y \geq 0,\; Y \succeq 0. \end{array}$$

The nonnegativity constraints in k–GP$_{\rm KR}$ are redundant when $k = 2$, see [45]. In [45] it is further suggested to add to k–GP$_{\rm KR}$ the *independent set constaints*

$$\sum_{i<j, ij\in I} y_{ij} \geq 1,\; \text{ for all } I \text{ with } |I| = k+1, \tag{10}$$

and the *triangle constraints*

$$y_{ij} + y_{ik} \leq 1 + y_{jk} \text{ for all triples } (i,j,k). \tag{11}$$

Adding these two sets of constraints to k–GP$_{\rm KR}$ results in a model that contains $\begin{pmatrix} n \\ k+1 \end{pmatrix}$ additional inequalities from (10) and $3\begin{pmatrix} n \\ 3 \end{pmatrix}$ from (11). The resulting relaxation is currently the strongest known relaxation for the k–equipartition problem. However, it is computationally demanding to obtain the resulting bounds due to the large number of constraints.

Another approach to obtain tractable relaxations of k–GP is to linearize the objective function by lifting into the space of $(nk+1)\times(nk+1)$ matrices as described in [69]. In [69], Wolkowicz and Zhao derive an SDP relaxation for the general graph partition problem. Here, we restrict their approach to the equipartition problem.

For $X \in \mathcal{P}_k$ we define $y := \operatorname{vec}(X)$ and $Y := yy^{\mathrm{T}}$. We write Y in block form

$$Y = \begin{pmatrix} Y^{(11)} & \dots & Y^{(1k)} \\ \vdots & \ddots & \vdots \\ Y^{(k1)} & \dots & Y^{(kk)} \end{pmatrix}, \tag{12}$$

where

$$Y^{(ij)} := X_{:,i}X_{:,j}^{\mathrm{T}} \in \mathbb{R}^{n\times n}, \quad i,j = 1,\dots,k.$$

Finally, we associate $X \in \mathcal{P}_k$ with a rank-one matrix $Y_X \in \mathcal{S}^+_{nk+1}$ in the following way:

$$Y_X := \begin{pmatrix} 1 \\ \operatorname{vec}(X) \end{pmatrix} \begin{pmatrix} 1 \\ \operatorname{vec}(X) \end{pmatrix}^{\mathrm{T}} = \begin{pmatrix} 1 & y^{\mathrm{T}} \\ y & Y \end{pmatrix}, \tag{13}$$

which has block form

$$Y_X = \begin{pmatrix} 1 & \left(y^{(1)}\right)^{\mathrm{T}} & \cdots & \left(y^{(k)}\right)^{\mathrm{T}} \\ y^{(1)} & Y^{(11)} & \dots & Y^{(1k)} \\ \vdots & \vdots & \ddots & \vdots \\ y^{(k)} & Y^{(k1)} & \dots & Y^{(kk)} \end{pmatrix}, \tag{14}$$

where $y^{(i)} = X_{:,i}$, $i = 1,\dots,k$. The matrix Y_X has the *sparsity pattern*

$$\operatorname{tr}(E_{ll}Y^{(ij)}) = 0, \quad \forall i,j = 1,\dots,k,\ i \neq j, \quad l = 1,\dots,n,$$

and any $Y \in \mathcal{S}_{nk}$, $Y \geq 0$ has the same sparsity pattern if and only if

$$\operatorname{tr}((J_k - I_k)\otimes I_n)Y = 0. \tag{15}$$

This sparsity pattern, which is similar to that described for $\mathrm{QAP}_{\mathrm{ZW}}$ in Section 1, is sometimes called the Gangster constraint, see [69].

The constraints $Xu_k = u_n$ and $X^{\mathrm{T}}u_n = mu_k$ are equivalent to

$$T\begin{pmatrix} 1 \\ \operatorname{vec}(X) \end{pmatrix} = 0, \tag{16}$$

where

$$T := \begin{pmatrix} -mu_k & I_k \otimes u_n^{\mathrm{T}} \\ -u_n & u_k^{\mathrm{T}} \otimes I_n \end{pmatrix}.$$

Constraint (16) may be rewritten as

$$\operatorname{tr}(T^{\mathrm{T}}TY_X) = 0,$$

where

$$T^{\mathrm{T}}T = \begin{pmatrix} km^2 + n & -(m+1)u_{nk}^{\mathrm{T}} \\ -(m+1)u_{nk} & I_k \otimes J_n + J_k \otimes I_n \end{pmatrix}.$$

For any $Y \geq 0$ that satisfies (15), one has

$$\operatorname{tr}\left(T^{\mathrm{T}}T \begin{pmatrix} 1 & y^{\mathrm{T}} \\ y & Y \end{pmatrix}\right) = (km^2 + n) - 2(m+1)u_{nk}^{\mathrm{T}}y + \operatorname{tr}(I_k \otimes J_n)Y + \operatorname{tr}(Y).$$

Thus the condition

$$\operatorname{tr}\left(T^{\mathrm{T}}T \begin{pmatrix} 1 & y^{\mathrm{T}} \\ y & Y \end{pmatrix}\right) = 0 \tag{17}$$

becomes

$$\operatorname{tr}(I_k \otimes J_n)Y + \operatorname{tr}(Y) = (m+1)(2u_{nk}^{\mathrm{T}}y - n).$$

Finally, by relaxing the rank-one condition on Y_X (see (13)) to $Y_X \in \mathcal{S}_{nk+1}^{+}$ we obtain an SDP relaxation of the k–equipartition problem (see also [69]):

$$(\text{k–GP}_{\text{ZW}}) \qquad \begin{array}{ll} \min & \frac{1}{2}\operatorname{tr}(I_k \otimes L)Y \\ \text{s.t.} & \operatorname{tr}((J_k - I_k) \otimes I_n)Y = 0 \\ & \operatorname{tr}(I_k \otimes J_n)Y + \operatorname{tr}(Y) = (m+1)(2u_{nk}^{\mathrm{T}}y - n) \\ & \begin{pmatrix} 1 & y^{\mathrm{T}} \\ y & Y \end{pmatrix} \in \mathcal{S}_{nk+1}^{+}, \quad Y \geq 0. \end{array}$$

In [69], the nonnegativity constraints are not imposed in the relaxation. Although Wolkowicz and Zhao [69] do not include these $O(n^4)$ inequalities, they conclude that it would be worth adding them. The following theorem lists the valid constraints that are implied by the constraints of the SDP problem k–GP$_{\text{ZW}}$.

Theorem 9 ([69], Lemma 4.1) *Assume that $Y \in \mathcal{S}_{nk}$ and $y \in \mathbb{R}^{nk}$ are such that*

$$\bar{Y} := \begin{pmatrix} 1 & y^{\mathrm{T}} \\ y & Y \end{pmatrix} \succeq 0,$$

and $\bar{Y}$ has the block form (14) and satisfies (17). Then

(i) $\sum_{i=1}^{k} y^{(i)} = u_n, \;\; u_n^{\mathrm{T}}y^{(i)} = m, \; i = 1, \ldots k.$

(ii) $m(y^{(j)})^{\mathrm{T}} = u_n^{\mathrm{T}}Y^{(ij)}, \; i, j = 1, \ldots, k.$

(iii) $\sum_{i=1}^{k} Y^{(ij)} = u_n(y^{(j)})^{\mathrm{T}}, \; j = 1, \ldots, k.$

(iv) $\sum_{i=1}^{k} \operatorname{diag}(Y^{ij}) = y^{(j)}, \; j = 1, \ldots, k.$

Proof. The proof follows from the fact that $T\bar{Y} = 0$. □

The following corollary is an immediate consequence of part (iv) of the previous theorem.

Corollary 10 *Assume that $Y \in \mathcal{S}_{nk}$ and $y \in \mathbb{R}^{nk}$ are as in Theorem 9. If $Y \geq 0$ also satisfies (15), then* $\operatorname{diag}(Y) = y$.

We now introduce the SDP relaxation k–GP$_{\rm RS}$ as an intermediate step to show the equivalence of k–GP$_{\rm ZW}$ and k–GP$_{\rm KR}$. In particular, we first show that the following SDP problem is dominated by k–GP$_{\rm ZW}$:

$$
(\text{k–GP}_{\rm RS}) \qquad
\begin{aligned}
\min\ & \tfrac{1}{2}\operatorname{tr}(I_k \otimes L)Y \\
\text{s.t. } & \operatorname{tr}((J_k - I_k) \otimes I_n)Y = 0 \\
& \operatorname{tr}(I_k \otimes E_{jj})Y = 1, \quad j = 1, \dots, n \\
& m \operatorname{diag}(Y^{(ii)}) = Y^{(ii)} u_n, \quad i = 1, \dots, k \\
& \operatorname{tr}(I_k \otimes J_n)Y = km^2 \\
& \operatorname{tr}((J_k - I_k) \otimes J_n)Y = n(n-m) \\
& Y \in \mathcal{S}_{nk}^+, \quad Y \geq 0,
\end{aligned}
$$

where Y has block form (12). In the following two theorems we compare the relaxations k–GP$_{\rm ZW}$, k–GP$_{\rm RS}$ and k–GP$_{\rm KR}$.

Theorem 11 *The SDP relaxation* k$-$GP$_{\rm ZW}$ *dominates the SDP relaxation* k$-$GP$_{\rm RS}$.

Proof. Because the objective functions are the same, it suffices to show that if (Y, y) is feasible for k–GP$_{\rm ZW}$, then Y is feasible for k–GP$_{\rm RS}$. Assume that Y has block form (12).

It is clear that $Y \succeq 0$, $Y \geq 0$ and $\operatorname{tr}((J_k - I_k) \otimes I_n)Y = 0$. From Theorem 9 it follows that $\operatorname{tr}(I_k \otimes E_{jj})Y = 1$, $j = 1, \dots, n$, and $m \operatorname{diag}(Y^{(ii)}) = Y^{(ii)} u_n$, $i = 1, \dots, k$. Furthermore, from $u_n^{\rm T} Y^{(jj)} = m(\operatorname{diag}(Y^{(jj)}))^{\rm T}$, $j = 1, \dots, k$, we have $u_n^{\rm T} Y^{(jj)} u_n = m^2$, and hence constraint $\operatorname{tr}(I_k \otimes J_n)Y = km^2$ is satisfied. Similarly $\operatorname{tr}((J_k - I_k) \otimes J_n)Y = n(n-m)$ follows. □

Theorem 12 *The SDP relaxation* k$-$GP$_{\rm RS}$ *dominates the SDP relaxation* k$-$GP$_{\rm KR}$.

Proof. Let $Y \in \mathcal{S}_{nk}$ be feasible for k–GP$_{\rm RS}$ with block form (12). We construct from Y a feasible point $\widetilde{Y} \in \mathcal{S}_n$ for k–GP$_{\rm KR}$ in the following way:

$$
\widetilde{Y} := \sum_{j=1}^{k} Y^{(jj)}.
$$

Clearly, $\widetilde{Y} \succeq 0$ and $\widetilde{Y} \geq 0$. From $\operatorname{tr}(I_k \otimes E_{jj})Y = 1$, $j = 1, \dots, n$, it follows that

$$\operatorname{diag}(\widetilde{Y}) = \operatorname{diag}(\sum_{j=1}^{k} Y^{(jj)}) = u_n,$$

and from $Y^{(ii)}u_n = m \operatorname{diag}(Y^{(ii)})$, $i = 1, \ldots, k$, that

$$\widetilde{Y}u_n = \sum_{j=1}^{k} Y^{(jj)}u_n = m \sum_{j=1}^{k} \operatorname{diag}(Y^{(jj)}) = mu_n.$$

It remains to show that the objectives agree. Indeed,

$$\operatorname{tr}(I_k \otimes L)Y = \sum_{j=1}^{k} \operatorname{tr}(LY^{(jj)}) = \operatorname{tr}(L\widetilde{Y}).$$

□

Finally, to show equivalence of the SDP relaxations $\mathrm{k-GP_{KR}}$ and $\mathrm{k-GP_{ZW}}$ we introduce one more relaxation of the k–equipartition problem. That relaxation is related to the quadratic assignment problem. Namely, it is well known that the graph equipartition problem is a special case of the QAP. To show this, we recall that the sets Π_n and $\mathcal{P}_k$ are related in the following way (see e.g., [44]). If $Z \in \Pi_n$ then $X = Z(I_k \otimes u_m) \in \mathcal{P}_k$. Conversely, each $X \in \mathcal{P}_k$ can be written as $X = Z(I_k \otimes u_m)$ with $Z \in \Pi_n$. For such a related pair (Z, X) it follows that

$$\operatorname{tr}(X^{\mathrm{T}}AX(J_k - I_k)) = \operatorname{tr}(Z^{\mathrm{T}}AZ(I_k \otimes u_m)(J_k - I_k)(I_k \otimes u_m)^{\mathrm{T}}) = \operatorname{tr}(Z^{\mathrm{T}}AZB),$$

where

$$B := (J_k - I_k) \otimes J_m \in \mathcal{S}_n. \tag{18}$$

Therefore, the k–equipartition problem may be formulated as the QAP

$$\min_{Z \in \Pi_n} \frac{1}{2} \operatorname{tr} AZBZ^{\mathrm{T}},$$

where A is the adjacency matrix of G, and B is of the form (18). In [23] it is suggested to use the SDP relaxation $\mathrm{QAP_{ZW}}$ (see p. 3) of the quadratic assignment problem as an SDP relaxation of the k-equipartition problem. Here we call that relaxation $\mathrm{k–GP_{QAP}}$:

$$(\mathrm{k–GP_{QAP}}) \qquad \begin{array}{ll} \min & \frac{1}{2}\operatorname{tr}(B \otimes A)Y \\ \text{s.t.} & \operatorname{tr}(I \otimes E_{jj})Y = 1, \;\; \operatorname{tr}(E_{jj} \otimes I)Y = 1 \quad j = 1, \ldots, n \\ & \operatorname{tr}(I \otimes (J - I)) + (J - I) \otimes I)Y = 0 \\ & \operatorname{tr}(J_{n^2}Y) = n^2 \\ & Y \succeq 0, \;\; Y \geq 0. \end{array}$$

This relaxation can be reduced by using symmetry reduction, as is shown by Dobre [24]. By using the reduced formulation of $\mathrm{k–GP_{QAP}}$, he proves the following result.

Theorem 13 [24] *The SDP problems* $\mathrm{k-GP_{KR}}$ *and* $\mathrm{k-GP_{QAP}}$ *are equivalent.*

In the following theorem we relate k–$\mathrm{GP_{QAP}}$ and k–$\mathrm{GP_{ZW}}$. To prove that k–$\mathrm{GP_{ZW}}$ is dominated by k–$\mathrm{GP_{QAP}}$, we need the following proposition.

Proposition 14 ([33], Proposition 7) *Let* $A \in \mathcal{S}_n$ *such that* $\mathrm{diag}(A) = cAu_n$ *for some* $c \in \mathbb{R}$, *and*

$$\bar{A} = \begin{pmatrix} 1 & a^{\mathrm{T}} \\ a & A \end{pmatrix}$$

where $a := \mathrm{diag}(A)$. *Then the following are equivalent:*

(i) $\bar{A}$ *is positive semidefinite,*
(ii) A *is positive semidefinite and* $\mathrm{tr}(J_n A) \geq (\mathrm{tr}\, A)^2$.

Theorem 15 *The SDP relaxation* $\mathrm{k-GP_{QAP}}$ *dominates the SDP relaxation* $\mathrm{k-GP_{ZW}}$.

Proof. Let $Y \in \mathcal{S}^+_{n^2}$ be feasible for k–$\mathrm{GP_{QAP}}$ with block form (12) where $k = n$ and $Y^{(ij)} \in \mathbb{R}^{n\times n}$, $i, j = 1, \ldots, n$. We construct from $Y \in \mathcal{S}^+_{n^2}$ a feasible point (W, w) with $W \in \mathcal{S}_{nk}$ for k–$\mathrm{GP_{ZW}}$ in the following way. First, define blocks

$$W^{(pq)} := \sum_{i=(p-1)m+1}^{pm} \sum_{j=(q-1)m+1}^{qm} Y^{(ij)}, \quad p, q = 1, \ldots, k, \tag{19}$$

and then collect all k^2 blocks into the matrix:

$$W = \begin{pmatrix} W^{(11)} & \cdots & W^{(1k)} \\ \vdots & \ddots & \vdots \\ W^{(k1)} & \cdots & W^{(kk)} \end{pmatrix}, \tag{20}$$

and set $w = \mathrm{diag}(W)$. The sparsity pattern $\mathrm{tr}((J_k - I_k) \otimes I_n)W = 0$ follows from the sparsity pattern of Y, i.e., from $\mathrm{tr}((J_n - I_n) \otimes I_n)Y = 0$. By direct verification it follows that

$$\mathrm{tr}(I_k \otimes J_n)W + \mathrm{tr}(W) = (m + 1)(2u_{nk}^{\mathrm{T}} w - n).$$

To prove that

$$\begin{pmatrix} 1 & w^T \\ w & W \end{pmatrix} \succeq 0, \tag{21}$$

we use Proposition 14. From the valid equalities for k–$\mathrm{GP_{QAP}}$ (see Theorem 1) it follows that

$$W^{(pp)}u_n = m\,\mathrm{diag}(W^{(pp)}) \text{ and } W^{(pq)}u_n = m\,\mathrm{diag}(W^{(pp)}), \quad p, q = 1, \ldots, k.$$

Therefore, the assumptions of Proposition 14 are satisfied. Further, from

$$u_{nk}^{\mathrm{T}} W u_{nk} = n^2 \quad \text{and} \quad \mathrm{tr}(W) = n,$$

we have that $\mathrm{tr}(J_n W) \geq (\mathrm{tr}\, W)^2$. Finally, for any $x \in \mathbb{R}^{nk}$ let $\widetilde{x} \in \mathbb{R}^{n^2}$ be defined by

$$\widetilde{x}^{\mathrm{T}} := \left[u_m^{\mathrm{T}} \otimes x_{1:n}^{\mathrm{T}}, \ldots, u_m^{\mathrm{T}} \otimes x_{n(k-1)+1:nk}^{\mathrm{T}} \right]$$

then

$$x^{\mathrm{T}} W x = \widetilde{x}^{\mathrm{T}} Y \widetilde{x} \geq 0,$$

since $Y \succeq 0$. Now (21) follows from Proposition 14.

It remains to show that for any pair of feasible solutions $(Y, (W, w))$, which are related as described, the objective values coincide. From (19) and (9) we have

$$\mathrm{tr}\left((J_k - I_k) \otimes (J_m \otimes A)\right) Y = \mathrm{tr}\left((J_k - I_k) \otimes A\right) W,$$

which finishes the proof. □

We have now shown the following sequence:

$$\text{k–GP}_{\mathrm{ZW}} \geq \text{k–GP}_{\mathrm{RS}} \geq \text{k–GP}_{\mathrm{KR}} \equiv \text{k–GP}_{\mathrm{QAP}} \geq \text{k–GP}_{\mathrm{ZW}},$$

where $A \geq B$ means that A dominates B. Hence, we can finally conclude that all formulations are equivalent.

In [23], the authors derive an SDP relaxation for the k–equipartition problem that dominates the previously described relaxations. That relaxation coincides with the relaxation for the quadratic assignment problem $\mathrm{QAP}_{\mathrm{dKS}}$ (see p. 5) where B is as in (18) and A is the adjacency matrix of the graph. After applying symmetry reduction to $\mathrm{QAP}_{\mathrm{dKS}}$ the relaxation from [23] takes the form

$$(\text{k–GP}_{\mathrm{SYM}}) \quad \begin{array}{ll} \min & a^{\mathrm{T}} \mathrm{diag}(X_5) + \frac{1}{2} \mathrm{tr}\, \bar{A}(X_3 + X_4 + X_7) \\ \text{s.t.} & X_1 + X_5 = I_{n-1} \\ & \sum_{t=1}^{7} \mathrm{tr}(J X_t) = (n-1)^2 \\ & \mathrm{tr}(X_1) = m - 1 \\ & \mathrm{tr}(X_5) = (k-1)m \\ & \mathrm{tr}(X_2 + X_3 + X_4 + X_6 + X_7) = 0 \\ & X_3 = X_4^{\mathrm{T}} \\ & \begin{pmatrix} \frac{1}{m-1}(X_1 + X_2) & \frac{1}{\sqrt{(k-1)m(m-1)}} X_3 \\ \frac{1}{\sqrt{(k-1)m(m-1)}} X_4 & \frac{1}{(k-1)m}(X_5 + X_6 + X_7) \end{pmatrix} \succeq 0 \\ & X_1 - \frac{1}{m-2} X_2 \succeq 0 \\ & X_5 - \frac{1}{m-1} X_6 \succeq 0 \\ & X_5 + X_6 - \frac{1}{k-2} X_7 \succeq 0 \\ & X_i \geq 0, \; i = 1, \ldots, 7, \end{array}$$

where the X_i are all of order $n-1$, $a = A_{:,j}$, and $\bar{A} = A(\{1, \ldots j-1, j+1, \ldots, n\})$ is the principal submatrix of A, for some (fixed) $j = 1, \ldots, n$. The relaxation k–GP$_{\mathrm{SYM}}$ gives a lower bound for the original problem k–GP since the automorphism group of B is transitive, see Theorem 3.

In [23] it is shown that the SDP relaxation k–GP$_{\mathrm{SYM}}$ dominates k–GP$_{\mathrm{KR}}$, and consequently all of the equivalent bounds presented here. However, k–GP$_{\mathrm{SYM}}$ does not dominate bounds obtained by adding constraints (10) and (11) to k–GP$_{\mathrm{KR}}$.

4 The Bandwidth Problem in Graphs

Let $G = (V, E)$ be an undirected graph with $|V| = n$ vertices and edge set E. A bijection $\phi : V = \{v_1, \ldots, v_n\} \to \{1, \ldots, n\}$ is called a *labeling* of the vertices of G. The bandwidth of the labeling ϕ is defined as

$$\max_{(i,j)\in E} |\phi(i) - \phi(j)|.$$

The bandwidth $\sigma_\infty(G)$ of a graph G is the minimum of this number over all labelings, i.e.,

$$\sigma_\infty(G) := \min \left\{ \max_{(i,j)\in E} |\phi(i) - \phi(j)|;\ \phi : V \to \{1, \ldots, n\} \right\}.$$

In terms of matrices, the bandwidth problem asks for a simultaneous permutation of the rows and columns of the adjacency matrix of G such that all nonzero entries are as close as possible to the main diagonal. The bandwidth problem is NP-hard [60].

The bandwidth problem originated in the 1950s from sparse matrix computations, and received much attention since Harary's description of the problem [37], and Harper's paper on the bandwidth of the n-cube [38]. The bandwidth problem arises in many different engineering applications which try to achieve efficient storage and processing. For more information on the bandwidth problem see, e.g. [13, 42, 18], and the references therein.

The bandwidth problem is related to the QAP. Indeed, let A be the adjacency matrix of G and $B = (b_{ij})$ defined by

$$b_{ij} := \begin{cases} 1 & \text{for } |i-j| > k \\ 0 & \text{otherwise.} \end{cases}$$

Then, if an optimal value of the corresponding QAP (see (1)) is zero, then the bandwidth of G is at most k. Since it is difficult to solve QAPs in practice for sizes greater than 30, other approaches to derive bounds for the bandwidth of a graph are necessary.

Several lower bounds for the bandwidth of a graph are established in [41, 40, 62]. In those papers, the basic idea to obtain lower bounds on $\sigma_\infty(G)$

is connecting the bandwidth minimization problem with the following graph partition problem. Let (S_1, S_2, S_3) be a partition of V with $|S_i| = m_i$ for $i = 1, 2, 3$. The *min-cut* problem is:

$$\text{(MC)} \qquad \begin{aligned} \text{OPT}_{\text{MC}} := \min & \sum_{i \in S_1, j \in S_2} a_{ij} \\ \text{s.t.} \quad & (S_1, S_2, S_3) \ \text{ partitions } \ V \\ & |S_i| = m_i, \quad i = 1, 2, 3, \end{aligned}$$

where $A = (a_{ij})$ is the adjacency matrix of G. Now, if $\text{OPT}_{\text{MC}} > 0$ then

$$\sigma_\infty(G) \geq m_3 + 1, \tag{22}$$

as noted in [41, 40, 62].

Helmberg et al. [40] use the following relaxation of MC to compute a bound for OPT_{MC}:

$$(\text{MC}_{\text{HW}}) \qquad \begin{aligned} \text{OPT}_{\text{HW}} := \min & \ \tfrac{1}{2} \operatorname{tr}(\hat{A} X D X^{\text{T}}) \\ \text{s.t.} \quad & X^{\text{T}} X = \operatorname{Diag}(m) \\ & X u_3 = u_n \\ & X^{\text{T}} u_n = m, \end{aligned}$$

where $m = [m_1, m_2, m_3]^{\text{T}}$, $\hat{A} = A + \frac{1}{n}(u_n^{\text{T}} A u_n) I_n - \operatorname{Diag}(A u_n)$, and

$$D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

They also prove that

$$\text{OPT}_{\text{HW}} = -\frac{1}{2}\mu_2 \lambda_2 - \frac{1}{2}\mu_1 \lambda_n, \tag{23}$$

where λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G, respectively, and values of μ_1, μ_2 ($\mu_1 \geq \mu_2$) are given by

$$\mu_{1,2} = \frac{1}{n} \left(-m_1 m_2 \pm \sqrt{m_1 m_2 (n - m_1)(n - m_2)} \right).$$

To show (23), the authors combine a projection technique for partitioning nodes of a graph [64] and a generalization of the Hoffman–Wielandt inequality (see e.g., [59]). By using (22) and (23), Helmberg et al. [40] derive the following result.

Theorem 16 [40] *Let G be an undirected graph on n vertices with at least one edge. Let λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G, respectively. Let $\alpha = \lfloor n\lambda_2/\lambda_n \rfloor$.*

1. *If* $\alpha \geq n-2$, *then* $G = K_n$ *and* $\sigma_\infty(G) = n-1$.
2. *If* $\alpha \leq n-2$ *and* $n-\alpha$ *is even, then* $\sigma_\infty(G) \geq \alpha + 1$.
3. *Otherwise* $\sigma_\infty(G) \geq \alpha$.

A proof of Theorem 16 that is based on interlacing of Laplacian eigenvalues, is given by Haemers [36].

Povh and Rendl [62] show that $\mathrm{MC}_{\mathrm{HW}}$ is equivalent to the following SDP problem:

$$(\mathrm{MC}_{\mathrm{PR}}) \quad \begin{array}{lll} \min & \frac{1}{2}\operatorname{tr}(D \otimes \hat{A})Y & \\ \text{s.t.} & \frac{1}{2}\operatorname{tr}((E_{ij}+E_{ji}) \otimes I_n)Y = m_i\delta_{ij}, & 1 \leq i \leq j \leq 3 \\ & \operatorname{tr}(J_3 \otimes E_{ii})Y = 1, & 1 \leq i \leq n \\ & \operatorname{tr}(V_i^{\mathrm{T}} \otimes W_j)Y = m_i, & 1 \leq i \leq 3, \quad 1 \leq j \leq n \\ & \frac{1}{2}\operatorname{tr}((E_{ij}+E_{ji}) \otimes J_n)Y = m_i m_j, & 1 \leq i \leq j \leq 3 \\ & Y \in \mathcal{S}_{3n}^{+}, & \end{array}$$

where $V_i = e_i u_3^{\mathrm{T}} \in \mathbb{R}^{3\times 3}$ and $W_j = e_j u_n^{\mathrm{T}} \in \mathbb{R}^{n\times n}$, $1 \leq i \leq 3$, $1 \leq j \leq n$. Note that adding the constraint $X \geq 0$ to the relaxation $\mathrm{MC}_{\mathrm{HW}}$ leads to an intractable model, while $\mathrm{MC}_{\mathrm{PR}}$ does permit tractable refinements. Therefore, in [62] it is suggested to tighten $\mathrm{MC}_{\mathrm{PR}}$ by adding nonnegativity constraints. This leads to a strengthened SDP relaxation of the min–cut problem and the following result.

Proposition 17 *Let* G *be an undirected and unweighted graph. If for some* $m = (m_1, m_2, m_3)$ *it holds that* $\mathrm{OPT}_{\mathrm{MC}} \geq \alpha > 0$, *then*

$$\sigma_\infty(G) \geq \max\{m_3 + 1, m_3 + \lceil \sqrt{2\alpha}\, \rceil - 1\}.$$

The numerical results in [62] show that this new bound is significantly better than the bounds obtained from the spectral bound.

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