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On semidefinite programming relaxations of association schemes with application to combinatorial optimization problems

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Abstract

We construct convex, semidefinite programming (SDP) relaxations of the convex hull of association schemes with given parameters. As an application, we obtain new and known SDP relaxations of several combinatorial optimizations problems, including the traveling salesman and cycle covering problems (by considering the Lee association scheme) and the maximum p-section problem (by considering the scheme of the complete p-partite graph).

Thus, the approach in this paper may be seen as a unified framework to generate SDP relaxations of various combinatorial optimization problems.

Keywords: traveling salesman problem, maximum bisection, semidefinite programming, association schemes

AMS classification: 90C22, 20Cxx, 70-08

JEL code: C61

1 Introduction

Semidefinite programming (SDP) relaxations of combinatorial problems date back to the work of Lovász in 1979 [14], and received renewed interest following the seminal paper of Goemans and Williamson [9] on approved approximation algorithms using SDP.

Surveys on the application of SDP in combinatorial optimization are given in [13, 8].

The standard approach to obtaining SDP relaxations has been via binary variable formulations of the relevant combinatorial problems.

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Thus, for example, the convex hull of the set $\{vv^T \mid v \in \{-1,1\}^n\}$ is usually approximated by the convex *elliptope*:

$$\mathcal{E} := \{X = X^T \in \mathbb{R}^{n\times n} \ : \ X_{ii} = 1 \ (i = 1,\ldots,n), \ X \succeq 0\}$$

where $X \succeq 0$ means X is symmetric positive semidefinite. One can derive useful error bounds via this approximation, since

$$\frac{2}{\pi}\arcsin \mathcal{E} \subset \mathrm{conv}\{vv^T \mid v \in \{-1,1\}^n\} \subset \mathcal{E},$$

where the arcsin function is applied entry-wise (see e.g. [9, 18]).

Stronger SDP relaxations may then be obtained via so-called lift-and-project techniques, see e.g. [12].

In a recent paper [5] on SDP relaxations of the traveling salesman problem (TSP), a totally different approach to constructing SDP relaxations was introduced. This approach was based on the theory of association schemes in algebraic combinatorics.

In this paper we generalize the approach in [5] to obtain SDP relaxations of various combinatorial problems in a unified way. Thus we obtain known relaxations for the TSP and maximum bisection problems, and new ones for the cycle covering and maximum p-section problems.

Finally, we show that the approach may be generalized further to include all coherent configurations (and not only association schemes). Thus we may derive relaxations of problems like the maximum cut problem with specified cut sizes.

Notation

We use I_n to denote the identity matrix of order n. Similarly, J_n and e_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 the subscript if the order is clear from the context.

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 *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 $A_{ij}B$ $(i = 1,\ldots,p)$, $(j = 1,\ldots,q)$.

2 Preliminaries on Association Schemes

We will give a brief overview of this topic; for an introduction to association schemes, see Chapter 12 in [7], or §3.3 in the book by Cameron [2].

Definition 2.1 (Association scheme)**.** *Assume that a given set of zero-one $n \times n$ matrices $\mathcal{A} = \{A_0,\ldots,A_d\}$ has the following properties:*

(1) $A_0 = I$ and $\sum_{i=0}^{d} A_i = J$ (all-ones matrix).

(2) $A_i^T \in \mathcal{A}$ *for each* i*;*

(3) $A_i A_j = A_j A_i$ *for all* i, j*;*

(4) $A_i A_j \in span\{A_0, \ldots, A_d\}$ *for all* i, j*.*

Then $\mathcal{A}$ *is called an* association scheme *with* d *classes. If the* A_i*'s are also symmetric, then we speak of a* symmetric association scheme*.*

The complex span of the matrices $\{A_0, \ldots, A_d\}$ is a matrix $*$-algebra (i.e. a subspace of $\mathbb{C}^{n \times n}$ that is also closed under matrix multiplication and taking complex conjugate transposes), called the *Bose-Mesner* algebra of the association scheme.

Informally, one sometimes refers to a 'matrix from the association scheme' in stead of 'a matrix from the Bose-Mesner algebra of the association scheme. (The same abuse of terminology is common when speaking about a basis or generators of the Bose-Mesner algebra, etc.)

Note that, if $\{A_0, \ldots, A_d\}$ is an association scheme, and P a permutation matrix, then $\{PA_0P^T, \ldots, PA_dP^T\}$ is also an association scheme, and the two Bose-Mesner algebras are isomorphic as algebras.

Example 2.1. *The set of circulant matrices:*

$$\begin{bmatrix} c_0 & c_1 & c_2 & \cdots & & c_{n-1} \\ c_{n-1} & c_0 & c_1 & & \cdots & \\ & c_{n-1} & c_0 & c_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \\ & & & & & c_1 \\ c_1 & & \cdots & & c_{n-1} & c_0 \end{bmatrix}$$

are from an association scheme with n *classes. The natural 0-1 basis of the circulant matrices forms this association scheme.*

Likewise, the $n \times n$ *symmetric circulant matrices are from a symmetric association scheme with* $d = \lfloor n/2 \rfloor$ *classes.*

A graph with diameter d with adjacency matrix from $\mathcal{A}$ is called distance regular. Conversely, any distance regular graph with diameter d generates an association scheme with d classes as follows.

Theorem 2.1. *Given a distance regular graph* $G = (V, E)$ *with diameter* d*, define* $|V| \times |V|$ *matrices* $A^{(k)}$ $(k = 1, \ldots, d)$ *as follows:*

$$A_{ij}^{(k)} = \begin{cases} 1 & \text{if } dist(i,j) = k \\ 0 & \text{else,} \end{cases} \qquad (i, j \in V),$$

where $dist(i, j)$ *is the length of the shortest path from* i *to* j*.*

Then $\{I, A^{(1)}, \ldots, A^{(d)}\}$ *forms a symmetric association scheme on* d *classes.*

A proof of this result is given in [2] (Theorem 3/6(b) there.)

The matrices $A^{(k)}$ in the theorem are called the distance matrices of the graph G, with $A^{(1)}$ being its adjacency matrix.

Example 2.2. *The standard Hamiltonian cycle with adjacency matrix*

$$\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \\ 0 & & & & 0 & 1 \\ 1 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}$$

generates the association scheme of the symmetric circulant matrices.

The example is a particular case of what is known as a Lee association scheme. In particular, any association scheme obtained from the one in the example via permutations of rows and columns is called a Lee scheme.

2.1 Eigenvalues of association schemes

By definition, the Bose-Mesner algebra of an association scheme has a basis of zero-one matrices. By a fundamental result in commutative algebra, it also has a basis of idempotent matrices, as the following result shows.

Theorem 2.2. *An association scheme with d classes has an orthogonal basis $E_0, \ldots, E_d$ of self-adjoint idempotents that sum to I, i.e.*

$$E_i = E_i^2, \; E_i = E_i^* \quad (i = 0, \ldots, d),$$

with $E_0 = \frac{1}{n}J$ and $\sum_{i=0}^{d} E_i = I$.

Note that the matrices E_i are Hermitian positive semidefinite, since they are self-adjoint and have zero-one eigenvalues.

We may write the basis $\{A_0, \ldots, A_d\}$ in terms of the basis $\{E_0, \ldots, E_d\}$, and vice versa.

In particular, there exist constants $p_k(i)$, called eigenvalues of the scheme, such that

$$\sum_{i=0}^{d} p_j(i) E_i = A_j \quad (j = 0, \ldots, d).$$

Note that the value $p_j(i)$ is the ith eigenvalue of A_j. Also note that $p_j(0)$ is the valency of the graph with adjacency matrix A_j, since

$$A_j e = \sum_{i=0}^{d} p_j(i) E_i e = p_j(0), \quad (j = 1, \ldots, d),$$

since $E_i e = 0$ $(i = 1, \ldots, d)$.

Similarly, there exist constants $q_k(i)$, called dual eigenvalues, such that

$$\frac{1}{n}\sum_{i=0}^{d} q_j(i)A_i = E_j \succeq 0 \quad (j = 0, \ldots, d). \tag{1}$$

One has $q_0(i) = 1$ for all i.

It is customary to define primal and dual matrices of eigenvalues via

$$P_{ij} := p_j(i),\ Q_{ij} := q_j(i) \quad (i, j = 0, \ldots, d).$$

It is easy to show that $PQ = nI$.

Example 2.3. *The dual eigenvalues of the association scheme of the symmetric circulant matrices are (for odd n):*

$$q_i(j) = 2\cos(2\pi ij/n) \quad (i, j = 1, \ldots, d \equiv \lfloor n/2 \rfloor).$$

Moreover, $q_i(0) = 2$ for all i. (Recall that $q_0(j) = 1$ for all j.)

2.2 Strongly regular graphs

A graph from an association scheme with $d = 2$ classes is called a *strongly regular graph.*

An equivalent, and more insightful definition is as follows.

Definition 2.2. *A simple graph that is neither a clique nor a co-clique is called strongly regular if there exist parameters k, λ, μ such that*

- *each vertex is adjacent to k vertices;*
- *for each pair of adjacent vertices there are λ vertices adjacent to both;*
- *for each pair of non-adjacent vertices there are μ vertices adjacent to both.*

Example 2.4. *A simple example of a strongly regular graph that will be used later on is the complete bipartite graph $K_{m,m}$ on $2m$ vertices. Here $k = \mu = m$ and $\lambda = 0$.*

The eigenvalue matrices P and Q have closed form expressions for strongly regular graphs. The adjacency matrix of a strongly regular graph has an eigenvalue k corresponding to the eigenvector e (since it is k-regular). Eigenvalues that have eigenvectors orthogonal to e are called restricted eigenvalues. Note that k may also be a restricted eigenvalue. It follows that there are exactly two distinct restricted eigenvalues, that we will denote by r and s $(r > s)$.

Theorem 2.3. *Let $G = (V, E)$ be a strongly regular graph with parameters k, λ, μ and restricted eigenvalues r and s. Assume the multiplicity of the eigenvalue r (resp. s) is f (resp. g). One has*

$$P = \begin{bmatrix} 1 & k & |V| - k - 1 \\ 1 & r & -r - 1 \\ 1 & s & -s - 1 \end{bmatrix},\ Q = \begin{bmatrix} 1 & f & g \\ 1 & fr/k & gs/k \\ 1 & -\frac{f(r+1)}{|V|-k-1} & -\frac{g(s+1)}{|V|-k-1} \end{bmatrix}.$$

Example 2.5. *The association scheme of the complete bipartite graph* $K_{m,m}$ *is given (using a suitable labeling of the vertices) by*

$$\mathcal{A} = \left\{ A_0 = I_{2m},\ A_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes J_m,\ A_2 = I_2 \otimes (J_m - I_m) \right\}.$$

Thus the restricted eigenvalues of $K_{m,m}$ *are the eigenvalues* $r = 0$ *and* $s = -m$ *of* A_1*, so that*

$$P = \begin{bmatrix} 1 & m & m-1 \\ 1 & 0 & -1 \\ 1 & -m & m-1 \end{bmatrix},\ Q = \begin{bmatrix} 1 & 2(m-1) & 1 \\ 1 & 0 & -1 \\ 1 & -2 & 1 \end{bmatrix}.$$

One can verify that $PQ = |V|I = 2mI$*, as it should be.*

3 SDP relaxations of association schemes

For the purposes of deriving convex relaxations of association schemes, we summarize the results of the last section in the following way.

Lemma 3.1. *Let* $\{A_0, \ldots, A_d\}$ *be an association scheme. One has*

$$\sum_{i=0}^{d} q_j(i) A_i = nE_j \quad \succeq \quad 0 \quad (j = 0, \ldots, d),$$

where the $q_j(i)$ $(i, j = 0, \ldots, d)$ *are the dual eigenvalues of the scheme, and* $\{E_0, \ldots, E_d\}$ *is the idempotent basis of the scheme.*

As a consequence we may define a convex set that contains a given association scheme $\{A_0, \ldots, A_d\}$ as the solution set of the following the linear matrix inequalities:

$$\sum_{i=0}^{d} q_j(i) X_i \quad = \quad nY_j \quad (j = 0, \ldots, d), \tag{2}$$

$$X_i \quad \geq \quad 0 \quad (i = 1, \ldots, d),\ X_0 = I, \tag{3}$$

$$Y_i \quad \succeq \quad 0 \quad (i = 1, \ldots, d),\ Y_0 = \frac{1}{n} J. \tag{4}$$

Note that the system (2—4) has a solution given by $X_i = A_i$ and $Y_i = E_i$ $(i = 0, \ldots, d)$. Also, every other association scheme with the same eigenvalues corresponds to a solution.

The following theorem shows that several important equalities are already implied by (2—4).

Theorem 3.1. *Assume* X_i *and* Y_i $(i = 0, \ldots, d)$ *satisfy the system (2—4). Then the following holds:*

1. $\sum_{j=0}^{d} Y_j = I$,
2. $Y_j e = 0 \quad (j = 1, \ldots, d)$,
3. $\sum_{i=0}^{d} p_j(i) Y_i = X_j \quad (j = 1, \ldots, d)$,
4. $X_j e = p_j(0) e \quad (j = 1, \ldots, d)$.

Proof. Using $\sum_{i=0}^{d} q_j(i) A_i = nE_j$ $(j = 0, \ldots, d)$ and $\sum_{j=0}^{d} E_j = I$, one has

$$\sum_{i=0}^{d} \left(\sum_{j=0}^{d} q_j(i) \right) A_i = nI.$$

Since $A_0 = I$ and the A_i's are linearly independent this implies:

$$\sum_{j=0}^{d} q_j(0) = n \text{ and } \sum_{j=0}^{d} q_j(i) = 0 \;\; (i = 1, \ldots, d). \tag{5}$$

Now note that (2) implies

$$\sum_{i=0}^{d} \left(\sum_{j=0}^{d} q_j(i) \right) X_i = \sum_{j=0}^{d} Y_j,$$

and we thus obtain $\sum_{j=0}^{d} Y_j = I$ by using (5) and $X_0 = I$.

Now using

$$J + \sum_{j=1}^{d} Y_j = nI,$$

we obtain $\sum_{j=1}^{d} Y_j e = 0$, which in turn implies $Y_j e = 0$ $(j = 1, \ldots, d)$, since $Y_j \succeq 0$ $(j = 1, \ldots, d)$.

To prove item 3 of the theorem, we note that the coefficient matrix in the linear system (2) is Q^T. Since $PQ = nI$ we have $Q^{-T} = \frac{1}{n} P^T$, which implies the required result.

Finally, we have

$$\sum_{i=0}^{d} p_j(i) Y_i e = X_j e \quad (j = 1, \ldots, d),$$

and using $Y_j e = 0$ $(j = 1, \ldots, d)$ yields item 4 of the theorem. □

In addition to the linear equalities that are implied by the relaxation (2—4), all linear matrix inequalities of a certain type are implied, as the next result shows.

Theorem 3.2. *Assume that the linear matrix inequality*

$$\sum_{i=0}^{d} \alpha_i X_i \succeq 0, \tag{6}$$

where $\alpha_1, \ldots, \alpha_d$ are given scalars, is satisfied by $X_i = A_i$ $(i = 1, \ldots, d)$, where $\{A_0, \ldots, A_d\}$ is an association scheme with dual eigenvalues $q_j(i)$ $(i, j = 0, \ldots, d)$.

Then (6) may be written as a conic linear combination of the linear matrix inequalities

$$\sum_{i=0}^{d} q_j(i) X_i \succeq 0 \quad (j = 1, \ldots, d) \text{ and } \sum_{i=0}^{d} X_i = J.$$

Proof. We have that

$$\sum_{i=0}^{d} \alpha_i A_i =: Y \succeq 0,$$

say. Since $Y \succeq 0$ is in the Bose-Mesner algebra of the scheme, there exist nonnegative scalars $\beta_0, \ldots, \beta_d$ such that

$$Y = \sum_{i=0}^{d} \beta_i E_i$$

where the E_i's form the idempotent basis of the algebra, as before. (The values β_i are precisely the nonnegative eigenvalues of Y). Substituting

$$\sum_{i=0}^{d} q_j(i) A_i = n E_j \quad (j = 0, \ldots, d)$$

yields

$$\sum_{i=0}^{d} \alpha_i A_i = \sum_{j=0}^{d} \frac{\beta_j}{n} \left[\sum_{i=0}^{d} q_j(i) A_i \right]$$

as required. □

4 SDP relaxations of combinatorial optimization problems

In this section we apply the SDP relaxation (2—4) to different combinatorial optimization problems, by considering different association schemes.

The basic idea is as follows: if the combinatorial optimization problem in question may be restated as finding a certain distance regular subgraph of minimum (or maximum) weight in a given weighted graph, then the the SDP relaxation (2—4) applies.

For example, the traveling salesman problem (TSP) may be stated as looking for a minimum weight Hamiltonian cycle in a given weighted graph. Similarly, the maximum bisection problem may be viewed in finding a maximum weight complete bipartite graph $K_{m,m}$ in a given weighted graph on $2m$ vertices.

4.1 The traveling salesman and related problems

Given is a matrix D with positive off-diagonal entries, which we view as edge weights in a complete graph. The TSP is to find a Hamiltonian cycle of minimum weight in this graph.

The association scheme of a Hamiltonian cycle is the Lee Scheme (see Example 2.3).

Applying the SDP relaxation (2—4) with the suitable objective function yields the SDP problem (after eliminating the Y_i variables):

$$\min \frac{1}{2}\mathrm{trace}(DX_1) \tag{7}$$

subject to

$$\begin{aligned} I + \sum_{k=1}^{d} X_k &= J \\ I + \sum_{k=1}^{d} \cos\left(\frac{2\pi i k}{n}\right) X_k &\succeq 0 \quad (i = 1, \ldots, d), \\ X_i &\geq 0 \quad (i = 1, \ldots, d), \end{aligned}$$

where the values $q_j(i) = 2\cos\left(\frac{2\pi i j}{n}\right)$ are the dual eigenvalues for the Lee scheme (see Example 2.3).

This is precisely the SDP relaxation of TSP introduced in the paper [5].

Remark

One may use Theorem 3.2 to show that this relaxation of the TSP is tighter than the SDP relaxation of Cvetkovích et al. [3]. This was already shown in [5] (Theorem 4.1 there), but the proof may be simplified greatly using the more general Theorem 3.2.

4.1.1 The k-cycle covering problem

Consider the problem of partitioning the vertices of a complete weighted graph into k vertex disjoint cycles of equal length, such that the sum of the edge lengths appearing in the cycles is minimal.

This problem was studied by Goemans and Williamson [10] (see also [15]), who showed that a 4-approximation algorithm exists when the weights satisfy the triangle inequality.

Now let $n_k := n/k$ be integer. The matrix variable X_{n_k} now corresponds to the adjacency matrix of k disjoint cycles of length n_k.

In other words, we obtain a new SDP relaxation for the k-cycle covering problem by replacing the objective function (7) by $\min \frac{1}{2}\mathrm{trace}(DX_{n_k})$.

4.2 The maximum bisection problem

Here we are given a matrix W with nonnegative entries that we view as edge weights of a graph $G = (V, E)$ with $|V| = 2m$.

The goal is to find a complete bipartite subgraph $K_{m,m}$ of G of maximum weight.

The association scheme generated by $K_{m,m}$ is described in Example 2.4 and its eigenvalues in Example 2.5.

Applying the SDP relaxation (2—4) yields the SDP problem:

$$\max \frac{1}{2}\mathrm{trace}(WX_1) \tag{8}$$

subject to

$$\begin{array}{rcl} I_{2m} + X_1 + X_2 & = & J_{2m} \\ (m-1)I_{2m} - X_2 & \succeq & 0 \\ I_{2m} - X_1 + X_2 & \succeq & 0 \\ X_1, X_2 & \geq & 0. \end{array}$$

An earlier SDP relaxation of the maximum bisection problem due to Frieze and Jerrum [6] (see also Ye [18]) is the following.

$$\max \left\{ \frac{1}{4}\mathrm{trace}((W - J_{2m})X) \mid \mathrm{diag}(X) = e_{2m},\ Xe_{2m} = 0,\ X \succeq 0 \right\}. \tag{9}$$

To see that this is a relaxation of the maximum bisection problem, set $X = vv^T$, where $v \in \{-1, 1\}^{2m}$ gives the optimal equipartition of the vertex set.

We will show next that these two SDP relaxations actually provide the same upper bound.

Theorem 4.1. *The optimal values of the SDP problems (8) and (9) coincide.*

Proof. Given an optimal solution X_1, X_2 of (8), set

$$X := I_{2m} - X_1 + X_2 \succeq 0.$$

Using part 4 of Theorem 3.1 we have

$$\begin{array}{rcl} Xe_{2m} & = & e_{2m} - X_1 e_{2m} + X_2 e_{2m} \\ & = & e_{2m} - me_{2m} + (m-1)e_{2m} = 0, \end{array}$$

where we have used that $A_1e_{2m} = me_{2m}$ and $A_2e_{2m} = (m-1)e_{2m}$ for the association scheme of $K_{m,m}$ (see Example 2.5). Moreover, it is easy to verify that $\mathrm{diag}(X) = e_{2m}$ and $\frac{1}{4}\mathrm{trace}((W-J)X) = \frac{1}{2}\mathrm{trace}(WX_1)$.

Conversely, assume that X is feasible for (9). It is straightforward to verify that setting

$$X_1 := \frac{1}{2}(J_{2m} - X),\ X_2 := \frac{1}{2}(J_{2m} + X) - I_{2m}$$

yields a feasible solution of (8) with the same objective value. □

4.3 Max-p-section

The max-p-section problem is the generalization of max bisection, where the aim is to find a complete p-partite subgraph of maximum total edge weight in a given weighted graph.

The association scheme generated by the complete p-partite graph on pm vertices has the eigenvalue matrices:

$$P = \begin{pmatrix} 1 & m(p-1) & m-1 \\ 1 & 0 & -1 \\ 1 & -m & m-1 \end{pmatrix},\ Q = \begin{pmatrix} 1 & p(m-1) & p-1 \\ 1 & 0 & -1 \\ 1 & -p & p-1 \end{pmatrix}.$$

Applying the SDP relaxation (2—4) yields the SDP problem:

$$\max \frac{1}{2}\mathrm{trace}(WX_1) \tag{10}$$

subject to

$$\begin{aligned} I_{pm} + X_1 + X_2 &= J_{pm} \\ (m-1)I_{pm} - X_2 &\succeq 0 \\ (p-1)I_{pm} - X_1 + (p-1)X_2 &\succeq 0 \\ X_1, X_2 &\geq 0. \end{aligned}$$

Note that this coincides with the relaxation (8) in the bisection ($p = 2$) case.

A different SDP relaxation for the max-p-section problem was introduced in [1].

5 Exact conic programming reformulations

In this section we give an exact description of the conic hull of all association schemes with the same parameters.

To be precise, we fix an association scheme $\{A_0, \ldots, A_d\}$ and consider

$$\mathrm{conv}\left\{\{P^TA_0P, \ldots, P^TA_dP\}\ :\ P \in \Pi_n\right\} \subset \mathbb{R}^{n\times n},$$

where Π_n denotes the set of $n \times n$ permutation matrices.

In order to describe this convex hull we use a result by Povh and Rendl [16]. To this end, recall that a matrix Y is called completely positive if $Y = \sum_i y_i y_i^T$ for some nonnegative vectors y_i.

It will be convenient to use the following notation for block matrices: If an $n^2 \times n^2$ matrix Y is partitioned into $n \times n$ blocks $Y^{(ij)}$ $(i, j = 1, \ldots, n)$ we will write $Y = [Y^{(ij)}]_{i,j=1,\ldots,n}$.

Lemma 5.1 ([16]). *Consider the set*

$$\mathcal{Y} := \Big\{ Y = [Y^{(ij)}]_{i,j=1,\ldots,n} \in \mathcal{C}_{n^2} \;\Big|$$

$$\sum_{i=1}^{n} Y^{(ii)} = I,\ trace(Y^{(ij)}) = \delta_{ij}\ (i, j = 1, \ldots, n), trace(JY) = n^2 \Big\},$$

where $\mathcal{C}_n$ is the cone of $n \times n$ completely positive matrices, and δ_{ij} the Kronecker delta. One has

$$\mathcal{Y} = conv\left\{ vec(P)vec(P)^T \ :\ P \in \Pi_n \right\}.$$

Using the lemma, it is straightforward to show the following.

Lemma 5.2. *Let $A \in \mathbb{S}^{n\times n}$ be given. The following two sets coincide:*

- $conv\left\{P^T AP \ :\ P \in \Pi_n\right\}$
- $\left\{M \in \mathbb{S}^{n\times n} \ :\ M_{ij} = trace(AY^{(ij)})\ (i, j = 1, \ldots, n),\ Y \in \mathcal{Y}\right\}$

where $Y \in \mathbb{S}^{n^2\times n^2}$ is the block matrix with blocks $Y^{(ij)}$ $(i, j = 1, \ldots, n)$, as before.

Proof. Let $P \in \Pi_n$ and $A \in \mathbb{S}^{n\times n}$ be given and fix $i, j \in \{1, \ldots, n\}$. Define $E^{(ij)} \in \mathbb{S}^{n\times n}$ as the matrix with ones in positions (i, j) and (j, i) and zeros elsewhere. One has:

$$\begin{aligned}(P^T AP)_{ij} &= \frac{1}{2}\text{trace}(E^{(ij)}P^T AP) \\ &= \frac{1}{2}\text{trace}\left[(E^{(ij)} \otimes A)(\text{vec}(P)\text{vec}(P)^T)\right] \\ &= \text{trace}(AY^{(ij)})\end{aligned}$$

for some $Y \in \mathcal{Y}$. □

Using the lemma, we may describe the convex hull of association schemes with given eigenvalues.

Theorem 5.1. *Given is an association scheme $\mathcal{A} = \{A_0, \ldots, A_d\}$ with idempotent basis $\{E_0, \ldots, E_d\}$ and dual eigenvalues $q_j(i)$ $(i, j = 0, \ldots, d)$. Consider the following system:*

$$\sum_{i=0}^{d} q_j(i)X_i = Y_j \quad (j = 0, \ldots, d), \tag{11}$$

$$X_i \geq 0 \quad (i = 0, \ldots, d), \tag{12}$$

where

$$(Y_j)_{rs} = trace\left(E_j Y^{(rs)}\right) \quad (j = 0, \ldots, d), \ (r, s = 1, \ldots, n), \tag{13}$$

where $Y \in \mathcal{Y}$ *is the block matrix* $Y = [Y^{(rs)}]_{r,s=1,\ldots,n}$ $(r, s = 1, \ldots, n)$.

Matrices $\{X_0, \ldots, X_d\}$ *form a solution of this system if and only if they are a convex combination of association schemes of the form* $\{PA_0P^T, \ldots, PA_dP^T\}$, *where* $P \in \Pi_n$.

Proof. The matrices $\{X_0, \ldots, X_d\}$ in a solution of the system is uniquely determined by the matrices $\{Y_0, \ldots, Y_d\}$ via (11). Indeed, the linear operator defined by (11) is invertible, since its matrix representation is the (nonsingular) matrix Q^T of dual eigenvalues.

Thus we only need to show that, if $\{Y_0, \ldots, Y_d\}$ is a solution of the system, then it may be written as a convex combination of sets of the form $\{PE_0P^T, \ldots, PE_dP^T\}$, where $P \in \Pi_n$. This follows immediately from Lemma 5.2. □

It is not immediately obvious that the SDP relaxation (2 — 4) is implied by the exact formulation in the theorem, i.e. that the conditions $Y_j \succeq 0$ $(j = 0, \ldots, d)$ are implied. To show this, we may assume without loss of generality that the matrices $Y^{(rs)}$ $(r, s = 1, \ldots, n)$ in Theorem 5.1 belong to the Bose-Mesner algebra of the association scheme $\mathcal{A}$.

Thus, the expression (13) in the theorem reduces to:

$$\text{trace}\left(E_j Y^{(rs)}\right) = p_j(0)\lambda_j(Y^{(rs)}) \quad (r, s = 1, \ldots, n), (j = 0, \ldots, d),$$

where $\lambda_j(Y^{(rs)})$ is the eigenvalue of $Y^{(rs)}$ that corresponds to the eigenspace spanned by the columns of E_j, and $p_j(0)$ is its multiplicity, as before.

We now perform a unitary transformation on $Y = [Y^{(ij)}]_{i,j=1,\ldots,n}$ in order to obtain a block matrix with diagonal blocks. If U denotes the unitary matrix that block diagonalizes the Bose-Mesner algebra of $\mathcal{A}$, then $I_n \otimes UY(I_n \otimes U)^* := [\bar{Y}^{(ij)}]_{i,j=1,\ldots,n}$ where

$$\bar{Y}^{(ij)} = \text{Diag}(\lambda_1(Y^{(ij)}), \ldots, \lambda_d(Y^{(ij)})),$$

i.e. each block $Y^{(ij)}$ is replaced by a diagonal block containing its eigenvalues (with multiplicities).

Now notice that, for any fixed $j \in \{1, \ldots, d\}$, the matrix

$$[\lambda_j(Y^{(rs)})]_{r,s=1,\ldots,n} \tag{14}$$

is a principal submatrix of $\bar{Y} := [\bar{Y}^{(ij)}]_{i,j=1,\ldots,n}$. Since $\bar{Y} = (I_n \otimes U)Y(I_n \otimes U)^* \succeq 0$, it follows that the matrix in (14) is positive semidefinite too, as required. As already mentioned, this means that $Y_j \succeq 0$.

6 Generalization to coherent configurations

An association scheme is a special case of a so-called *coherent configuration*. In particular, a set of matrices that meets all the conditions in Definition 2.1 except possibly condition 3 (commutativity) and $A_0 = I$ forms a coherent configuration.

Definition 6.1 (Coherent configuration)**.** *Assume that a given set of zero-one $n \times n$ matrices $\{A_1, \ldots, A_d\}$ has the following properties:*

(1) $\sum_{i \in \mathcal{I}} A_i = I$ *for some index set* $\mathcal{I} \subset \{1, \ldots, d\}$ *and* $\sum_{i=1}^{d} A_i = J$*.*

(2) $A_i^T \in \mathcal{A}$ *for each* i*;*

(3) $A_i A_j = A_j A_i$ *for all* i, j*;*

(4) $A_i A_j \in span\{A_1, \ldots, A_d\}$ *for all* i, j*.*

Then $\{A_1, \ldots, A_d\}$ *is called a* coherent configuration*.*

Thus, a coherent configuration is a basis of zero-one matrices of a (possibly non-commutative) matrix $*$-algebra.

A coherent configuration does not necessarily have a self-adjoint idempotent basis, but it does have a basis of positive semidefinite Hermitian matrices. This is a consequence of the structural theorem for matrix $*$-algebras. In stating the theorem, we require the following notation for the direct sum of two matrix algebras $\mathcal{A}_1$ and $\mathcal{A}_2$:

$$\mathcal{A}_1 \oplus \mathcal{A}_2 := \left\{ \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix},\ A_1 \in \mathcal{A}_1,\ A_2 \in \mathcal{A}_2 \right\}.$$

Theorem 6.1 (Wedderburn [17]; see also §2.2 in [4])**.** *If $\mathcal{A} \in \mathbb{C}^{n \times n}$ is a matrix $*$-algebra, then there exist a unitary matrix U and positive integers p and n_i, t_i $(i = 1, \ldots, p)$ such that*

$$U^* \mathcal{A} U = \oplus_{i=1}^{p} t_i \odot \mathbb{C}^{n_i \times n_i}$$

where

$$t_i \odot \mathbb{C}^{n_i \times n_i} := \left\{ I_{t_i} \otimes M \mid M \in \mathbb{C}^{n_i \times n_i} \right\} \quad (i = 1, \ldots, p).$$

Corollary 6.1. *Any matrix $*$-algebra has a basis of Hermitian positive semidefinite matrices.*

Proof. Follows from Theorem 6.1 and that fact that $\mathbb{C}^{n \times n}$ has a basis of Hermitian positive semidefinite matrices. □

Now let $Z_1, \ldots, Z_d$ denote a Hermitian positive semidefinite basis of the algebra spanned by $\{A_1, \ldots, A_d\}$. As in the association scheme case (where the

Z_i's are also idempotent), we again have parameters $q_j(i)$ $(i, j = 1, \ldots, d)$ so that

$$\sum_{i=1}^{d} q_j(i) A_i = Z_j \succeq 0 \quad (j = 1, \ldots, d).$$

Note that we have used the same notation $q_j(i)$ as for the dual eigenvalues of association schemes, to emphasize the generalization.

Given the parameters $q_j(i)$ $(i, j = 1, \ldots, d)$, we may again construct (approximations of) the convex hull of coherent configurations with these parameters, by replacing the A_i's by nonnegative matrix variables X_i as before, with the additional constraint that $\sum_{i=1}^{d} X_i = J$.

Finally, the constraints $\mathrm{trace}(X_i) = \mathrm{trace}(A_i)$ and $\mathrm{trace}(JX_i) = \mathrm{trace}(JA_i)$ $(i = 1, \ldots, d)$ may be added. By Theorem 3.1, these constraints are already implied for association schemes, but we show below that this is not necessarily true for more general coherent configurations.

Thus far we have derived the following SDP relaxation:

$$\begin{aligned}
\sum_{i=1}^{d} q_j(i) X_i &\succeq 0 \quad (j = 1, \ldots, d), && (15)\\
\sum_{i=1}^{d} X_i &= J, && (16)\\
\sum_{i \in \mathcal{I}} X_i &= I, && (17)\\
\mathrm{trace}(X_i) &= \mathrm{trace}(A_i) \quad (i = 1, \ldots, d), && (18)\\
\mathrm{trace}(JX_i) &= \mathrm{trace}(JA_i) \quad (i = 1, \ldots, d), && (19)\\
X_i &\geq 0 \quad (i = 1, \ldots, d). && (20)
\end{aligned}$$

Unfortunately, Theorem 3.2 does not hold for general coherent configurations. Thus there may be (infinitely many) additional valid linear matrix inequalities of the type

$$\sum_{i=1}^{d} \alpha_i X_i \succeq 0$$

where $\alpha_1, \ldots, \alpha_d$ are scalars.

The difference with the association scheme case may be explained as follows. All Hermitian positive semidefinite matrices from an association scheme lie in the polyhedral cone generated by the idempotent basis $\{E_0, \ldots, E_d\}$. In the general case, the corresponding cone is not polyhedral.

We note, however, that it is still possible to optimize over this infinite set of valid linear matrix inequalities in polynomial time using the ellipsoid method. Indeed, for given $\{X_1, \ldots, X_d\}$ one may decide using SDP whether there exist values $\alpha_1, \ldots, \alpha_d$ such that

$$\sum_{i=1}^{d} \alpha_i A_i \succeq 0 \text{ and } \sum_{i=1}^{d} \alpha_i X_i \not\succeq 0.$$

This provides the necessary separation oracle for the ellipsoid method.

In the next section we illustrate these ideas by considering the coherent configurations associated with cuts of specified size in graphs. We will not consider all possible linear matrix inequalities, but will limit the discussion to the SDP relaxation (15)— (20).

6.1 The maximum cut problem with specified cut size

Consider the generalization of the maximum bisection problem where the vertex set must now be partitioned into two subsets of cardinality k and $\ell := n-k$ for a given k. (Note that $k = n/2$ reduces to the maximum bisection problem).

Thus we consider the coherent configuration associated with the complete bipartite graph $K_{k,\ell}$.

The coherent configuration has dimension 6 and consists of the following matrices:

$$A_1 = \begin{pmatrix} I_k & 0_{k\times\ell} \\ 0_{\ell\times k} & 0_{\ell\times\ell} \end{pmatrix},\ A_2 = \begin{pmatrix} J_k - I_k & 0_{k\times\ell} \\ 0_{\ell\times k} & 0_{\ell\times\ell} \end{pmatrix},\ A_3 = \begin{pmatrix} 0_{k\times k} & J_{k\times\ell} \\ 0_{\ell\times k} & 0_{\ell\times\ell} \end{pmatrix},$$

$$A_4 = \begin{pmatrix} 0_{k\times k} & 0_{k\times\ell} \\ J_{\ell\times k} & 0_{\ell\times\ell} \end{pmatrix},\ A_5 = \begin{pmatrix} 0_{k\times k} & 0_{k\times\ell} \\ 0_{\ell\times k} & I_{\ell\times\ell} \end{pmatrix},\ A_6 = \begin{pmatrix} 0_{k\times k} & 0_{k\times\ell} \\ 0_{\ell\times k} & J_\ell - I_\ell. \end{pmatrix},$$

and its complex span is isomorphic (as a $*$-algebra) to $\mathbb{C}\oplus\mathbb{C}\oplus\mathbb{C}^{2\times 2}$. The relevant $*$-isomorphism, say ϕ, satisfies:

$$\phi(A_1) = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 1 & 0 \\ & & 0 & 0 \end{pmatrix},\ \phi(A_2) = \begin{pmatrix} -1 & & & \\ & 0 & & \\ & & k-1 & 0 \\ & & 0 & 0 \end{pmatrix},\ \phi(A_3) = \sqrt{k\ell}\begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & 1 \\ & & 0 & 0 \end{pmatrix},$$

$$\phi(A_4) = \sqrt{k\ell}\begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & 0 \\ & & 1 & 0 \end{pmatrix},\ \phi(A_5) = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 0 & 0 \\ & & 0 & 1 \end{pmatrix},\ \phi(A_6) = \begin{pmatrix} 0 & & & \\ & -1 & & \\ & & 0 & 0 \\ & & 0 & \ell-1 \end{pmatrix}.$$

Note that $\phi(A_i)$ $(i = 1,\ldots,6)$ forms a basis of $\mathbb{C}\oplus\mathbb{C}\oplus\mathbb{C}^{2\times 2}$, as it should. A rank-one, Hermitian positive semidefinite basis is given by:

$$\phi(A_1+A_2),\ \phi(A_5+A_6),\ \phi(A_1+A_2-\imath\,(A_3-A_4)+A_5+A_6),$$

$$\phi(A_1+A_2-(A_3+A_4)+A_5+A_6),\ \phi((\ell-1)A_5-A_6),\ \phi((k-1)A_1-A_2)),$$

where $\imath := \sqrt{-1}$.

Thus the matrix with entries $Q_{ij} = q_j(i)$ is given by

$$Q = \begin{pmatrix} 1 & 0 & 1 & 1 & 0 & k-1 \\ 1 & 0 & 1 & 1 & 0 & -1 \\ 0 & 0 & -1 & -\imath & 0 & 0 \\ 0 & 0 & -1 & \imath & 0 & 0 \\ 0 & 1 & 1 & 1 & \ell-1 & 0 \\ 0 & 1 & 1 & 1 & -1 & 0 \end{pmatrix},$$

and the SDP relaxation of the maximum $k-\ell$ cut problem becomes

$$\max \frac{1}{2}\mathrm{trace}(W(X_3+X_4))$$

subject to

$$\begin{aligned}
\sum_{i=1}^{6} X_i &= J \\
\sum_{i=1}^{6} q_j(i) X_i &\succeq 0 \quad (j = 1, \ldots, 6) \\
X_i &\geq 0 \quad (i = 1, \ldots, 6), \\
X_3 &= X_4^T, \\
X_1 + X_5 &= I, \\
\mathrm{trace}(X_1) &= k, \\
\mathrm{trace}(JX_3) &= k\ell \\
\mathrm{trace}(JX_2) &= k(k-1) \\
\mathrm{trace}(JX_6) &= \ell(\ell-1).
\end{aligned}$$

Note that the X_i matrix variables are real, but the p.s.d. condition should be read as 'Hermitian positive semidefinite', since some of the parameters $q_j(i)$ are complex.

Substituting $X_1 + X_5 = I$, the linear matrix inequalities in the relaxation become:

$$\begin{aligned}
X_1 + X_2 &\succeq 0 \\
X_5 + X_6 &\succeq 0 \\
I + X_2 - (X_3 + X_3^T) + X_6 &\succeq 0 \\
I + X_2 - \imath(X_3 - X_3^T) + X_6 &\succeq 0 \\
(\ell - 1)X_5 - X_6 &\succeq 0 \\
(k-1)X_1 - X_2 &\succeq 0.
\end{aligned}$$

In any solution of these linear matrix inequalities, we may replace X_3 by its symmetric part to obtain another solution. Indeed, if

$$I + X_2 - (X_3 + X_3^T) + X_6 \succeq 0$$

then, for $\bar{X}_3 := \frac{1}{2}(X_3 + X_3^T)$

$$I + X_2 - (\bar{X}_3 + \bar{X}_3^T) + X_6 \succeq 0$$

and

$$I + X_2 - \imath(\bar{X}_3 - \bar{X}_3^T) + X_6 = I + X_2 + X_6 \succeq 0.$$

Moreover, replacing X_3 by $\frac{1}{2}(X_3 + X_3^T)$ does not change the objective value, since

$$\mathrm{trace}(W(\bar{X}_3 + \bar{X}_3^T)) \equiv \mathrm{trace}(W(X_3 + X_3^T)).$$

Thus the complex linear matrix inequality is redundant, and we may rewrite the SDP relaxation as

$$\max \frac{1}{2}\text{trace}(WX)$$

subject to

$$\begin{aligned}
X_1 + X_5 &= I \\
I + X_2 + X + X_6 &= J \\
X_1 + X_2 &\succeq 0 \\
X_5 + X_6 &\succeq 0 \\
I + X_2 - X + X_6 &\succeq 0 \\
(\ell - 1)X_5 - X_6 &\succeq 0 \\
(k - 1)X_1 - X_2 &\succeq 0 \\
\text{trace}(X_1) &= k \\
\text{trace}(JX) &= 2k\ell \\
\text{trace}(JX_2) &= k(k-1) \\
\text{trace}(JX_6) &= \ell(\ell-1) \\
X, X_1, X_2, X_5, X_6 &\geq 0.
\end{aligned}$$

The new variable X is the relaxation of the adjacency matrix of $K_{k,\ell}$.

Remarks

1. Note that the 'trace' constraints are not redundant. Indeed, if these constraints are omitted, a feasible point is given by $X_1 = I$, $X_2 = J - I$, $X = X_5 = X_6 = 0$. This confirms that Theorem 3.1 cannot be extended to more general coherent configurations than association schemes.

2. It is straightforward to show that we regain the SDP relaxation (8) of the maximum bisection problem if $k = \ell$.

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