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Semidefinite Programming Relaxations of the Traveling Salesman Problem and Their Integrality Gaps

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Abstract. The traveling salesman problem (TSP) is a fundamental problem in combinatorial optimization. Several semidefinite programming relaxations have been proposed recently that exploit a variety of mathematical structures including, for example, algebraic connectivity, permutation matrices, and association schemes. The main results of this paper are twofold. First, de Klerk and Sotirov [de Klerk E, Sotirov R (2012) Improved semidefinite programming bounds for quadratic assignment problems with suitable symmetry. *Math. Programming* 133(1):75–91.] present a semidefinite program (SDP) based on permutation matrices and symmetry reduction; they show that it is incomparable to the subtour elimination linear program but generally dominates it on small instances. We provide a family of simplicial TSP instances that shows that the integrality gap of this SDP is unbounded. Second, we show that these simplicial TSP instances imply the unbounded integrality gap of every SDP relaxation of the TSP mentioned in the survey on SDP relaxations of the TSP in section 2 of Sotirov [Sotirov R (2012) SDP relaxations for some combinatorial optimization problems. Anjos MF, Lasserre JB, eds., *Handbook on Semidefinite, Conic and Polynomial Optimization* (Springer, New York), 795–819.]. In contrast, the subtour linear program performs perfectly on simplicial instances. The simplicial instances thus form a natural litmus test for future SDP relaxations of the TSP.

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Keywords: traveling salesman problem • integrality gap • semidefinite programming

1. Introduction

In this paper, we consider relaxations of the traveling salesman problem (TSP) based on semidefinite programs. The TSP is a fundamental problem in combinatorial optimization, combinatorics, and theoretical computer science. An input consists of a set $[n] := \{1, 2, 3, \dots, n\}$ of n cities and, for each pair of cities $i, j \in [n]$, an associated cost or distance $d_{ij} \geq 0$ reflecting the cost or distance of traveling from city i to city j . Throughout this paper, we assume that the edge costs d_{ij} are *symmetric* (so that $d_{ij} = d_{ji}$ for all $i, j \in [n]$) and *metric* (so that $d_{ij} \leq d_{ik} + d_{kj}$ for all $i, j, k \in [n]$). The TSP is then to find a minimum-cost tour visiting each city exactly once. Treating the cities as vertices of the complete, undirected graph K_n and treating an edge $\{i, j\}$ of K_n as having cost d_{ij} , the TSP is equivalent to finding a minimum-cost Hamiltonian cycle on K_n .

The TSP (with the implicit assumptions that the edge costs are metric and symmetric) is a canonical nondeterministic polynomial-time-hard (NP-hard) problem; finding a polynomial-time approximation algorithm with as strong a performance guarantee as possible remains a major open question. Currently it is known to be NP-hard to approximate TSP solutions in polynomial time to within any constant factor $\alpha < 123/122$ (Karpinski et al. [19]). In contrast, the strongest positive performance guarantee dates back more than 40 years: the Christofides–Serdyukov algorithm (Christofides [3], Serdyukov [24]) finds a Hamiltonian cycle in polynomial time that is at most a factor of $\frac{3}{2}$ away from the optimal TSP solution.

One powerful technique for analyzing TSP approximation algorithms is to *relax* the discrete set of Hamiltonian cycles. The prototypical example is the subtour elimination linear program (LP), also referred to as the Dantzig–Fulkerson–Johnson relaxation (Dantzig et al. [6]) and the Held–Karp bound (Held and Karp [16]), which we will refer to as the *subtour LP*. The subtour LP is a *relaxation* of the TSP because (1) every Hamiltonian cycle has a corresponding feasible solution to the subtour LP, and (2) the value of the subtour LP for such a feasible solution equals the cost of the corresponding Hamiltonian cycle. As a result, the optimal value of the subtour LP is a lower bound on the optimal solution to the TSP. Wolsey [29], Cunningham [4], and Shmoys and Williamson [26] show that the Christofides–Serdyukov algorithm produces a (not necessarily optimal)

Hamiltonian cycle that is within a factor of $3/2$ of the optimal value of the subtour LP. Combining these two observations shows that the Christofides–Serdyukov algorithm satisfies the following chain of inequalities:

$$\begin{aligned} \text{Optimal TSP solution} &\leq \text{Cost of cycle produced by Christofides–Serdyukov algorithm} \\ &\leq \frac{3}{2} \text{Optimal value of subtour LP} \\ &\leq \frac{3}{2} \text{Optimal TSP solution.} \end{aligned}$$

Hence, the Christofides–Serdyukov algorithm is a $\frac{3}{2}$ -approximation algorithm for the TSP. Moreover, the *integrality gap* of the subtour LP, which measures the worst-case performance of a relaxation relative to the TSP, is at most $3/2$: for any instance, the ratio of the optimal TSP solution to the optimal value of the subtour LP cannot be more than $3/2$. If the subtour LP did not have a constant-factor integrality gap, it would not be possible to use the LP as before to show that a TSP algorithm was a constant-factor approximation algorithm. Goemans [12] conjectured that the integrality gap of the subtour LP is $4/3$, although the $3/2$ bound of Wolsey [29], Cunningham [4], and Shmoys and Williamson [26] remains state of the art.

More recently, several TSP relaxations based on semidefinite programs (SDPs) have been proposed; see section 2 of Sotirov [27] for a short survey. Cvetković et al. [5] gives a relaxation based on adjacency matrices and algebraic connectivity. De Klerk et al. [8] introduce a relaxation based on the theory of association schemes (see also de Klerk et al. [9]). Zhao et al. [30] introduce a relaxation to the more general quadratic assignment problem (QAP), a special case of which is the TSP. Their relaxation is based on properties of permutation matrices; de Klerk et al. [10] show that the optimal value of their SDP coincides with the optimal value of the SDP introduced by Zhao et al. [30] when specialized to the TSP. Sotirov [27] summarizes two interpretations of this latter SDP relaxation of the QAP. First, it is equivalent to a similar SDP relaxation of the QAP also based on permutation matrices from Povh and Rendl [23] (with equivalence shown in Povh and Rendl [23]). Second, it is equivalent to applying the N^+ lift-and-project operator of Lovász and Schrijver [22] to a QAP polytope; this equivalence is shown in Burer and Vandembussche [2] and Povh and Rendl [23]. Anstreicher [1] gives another SDP relaxation of the QAP. When specialized to the TSP, it is equivalent to the projected eigenvalue bound of Hadley et al. [15].

Most recently, de Klerk and Sotirov [8] apply symmetry reduction to strengthen the QAP relaxation of Povh and Rendl [23] in certain cases. This strengthened QAP relaxation can be applied to the TSP, and de Klerk and Sotirov [8] evaluate the strengthened QAP relaxation on the 24 classes of facet-defining inequalities for the TSP on eight vertices. Although solving the SDP is computationally demanding, their results are promising: the strengthened QAP performs at least as well as the subtour LP on all but one of the 24 instances, and it generally outperforms the subtour LP.

Although computationally involved, these SDPs are based on a broad variety of rich combinatorial structures that has led to several theoretical results. Goemans and Rendl [11] show that the SDP relaxation of Cvetković et al. [5] is weaker than the subtour LP in the following sense: any solution to the subtour LP implies an equivalent feasible solution for the SDP of Cvetković et al. [5] of the same cost. Both optimization problems are minimization problems, and the SDP is optimizing over a broader search set, so the optimal value for the SDP of Cvetković et al. [5] cannot be closer than the optimal value of the subtour LP to the optimal TSP cost. However, de Klerk et al. [10] show the exciting result that their SDP is incomparable with the subtour LP: there are instances where the optimal value of their SDP is closer to the optimal TSP cost than the optimal value of the subtour LP and vice versa. Moreover, de Klerk et al. [10] show that their SDP is stronger than the earlier SDP of Cvetković et al. [5]: any feasible solution for the SDP of de Klerk et al. [10] implies a feasible solution for the SDP of Cvetković et al. [5] of the same cost.

Gutekunst and Williamson [14] show that the SDP relaxations of both Cvetković et al. [5] and de Klerk et al. [10], however, have unbounded integrality gaps. Moreover, they have a counterintuitive nonmonotonicity property: in certain instances, it is possible to artificially add vertices (in a way that preserves metric and symmetric edge costs) and arbitrarily lower the cost of the optimal solution to the SDP. Such a property contrasts with both the TSP and subtour LP, which are known to be monotonic (see Section 4).

The main results of this paper are to complete the characterization of integrality gaps of every SDP relaxation of the TSP mentioned in Sotirov [27] and to introduce a family of instances that implies that every such SDP has an unbounded integrality gap and is nonmonotonic. To do so, we show that the SDP of de Klerk and Sotirov [10] has an unbounded integrality gap (and, in turn, has the same nonmonotonicity property as those of Cvetković et al. [5] and de Klerk et al. [10]). Doing so further implies that no SDP relaxation of the TSP

surveyed in Sotirov [27] can be used in proving approximation guarantees on TSP algorithms in the same way as the subtour LP. The family of instances we use generalizes those from Gutekunst and Williamson [14] to a new family of TSP instances, which we call *simplicial TSP instances* because they can be viewed as placing groups of vertices at the extreme points of a simplex. This family forms an intriguing set of test instances for SDP relaxations of the TSP: the vertices of the TSP instance can be embedded into \mathbb{R}^d (for a d that grows as the integrality gap increases), the integrality gap of the subtour LP on these instances is one (i.e., the optimal value of the subtour LP on any instance in this family matches the cost of the TSP solution), but these instances imply an unbounded integrality gap for at least the following SDPs:

- The SDP TSP relaxation of Cvetković et al. [5] (based on algebraic connectivity);
- The SDP TSP relaxation of de Klerk et al. [10] based on the theory of association schemes (see also de Klerk et al. [9]);
- The SDP QAP relaxation of Zhao et al. [30], when specialized to the TSP (based on permutation matrices and shown by de Klerk et al. [10] to have an optimal value coinciding with the SDP of de Klerk et al. [10]);
- The SDP QAP relaxation of Povh and Rendl [23], when specialized to the TSP (based on permutation matrices and shown by Povh and Rendl [23] to be equivalent to the SDP of Zhao et al. [30]);
- The SDP QAP relaxation of de Klerk and Sotirov [8], when specialized to the TSP (obtained by performing symmetry reduction on the SDP of de Klerk et al. [10]); and
- The SDP QAP relaxation of Anstreicher [1], when specialized to the TSP (equivalent to the projected eigenvalue bound of Hadley et al. [15]).

In Section 2, we introduce the notation we will use and provide background on the SDP of de Klerk and Sotirov [8]. In Section 3, we show how the instances of Gutekunst and Williamson [14] directly imply that the integrality gap of the SDP of Povh and Rendl [23] is unbounded but only that the integrality gap of the SDP of de Klerk and Sotirov [8] is at least two. This result motivates the generalized simplicial instances we formalize in Section 4. In Section 4, we also prove our main result. We specifically show that for $z \in \mathbb{N}$, the simplicial instances in \mathbb{R}^{2z-1} imply an integrality gap for the SDP of de Klerk and Sotirov [8] of at least z . We do so by finding a family of instances where the SDP cost can be bounded by $2 + \varepsilon$ for any $\varepsilon > 0$ (with sufficiently large n), whereas the TSP cost grows arbitrarily. As a corollary, we show that the SDP of de Klerk and Sotirov [8] is again nonmonotonic. We conclude in Section 5 by discussing two open questions about SDP-based relaxations of the TSP.

2. SDP Relaxations of the TSP

2.1. Notation and Preliminaries

Throughout this paper, we use J_m and I_m to respectively denote the all-ones and identity matrix in $\mathbb{R}^{m \times m}$. We let $e_i^{(m)}$ denote the i th standard basis vector in \mathbb{R}^m and let $e^{(m)} := e_1^{(m)} + \dots + e_m^{(m)}$ denote the all-ones vector in \mathbb{R}^m . We let $E_{ij}^{(m)} := e_i^{(m)}(e_j^{(m)})^T$ denote the $m \times m$ matrix with a one in the i, j th position and zero elsewhere.

We let $\mathbb{S}^{m \times m}$ denote the set of real, symmetric matrices in $\mathbb{R}^{m \times m}$ and let Π_m be the set of $m \times m$ permutation matrices. The term $Y \geq 0$ denotes that Y is a positive semidefinite matrix; for $Y \in \mathbb{S}^{m \times m}$, $Y \geq 0$ means that all eigenvalues of Y are nonnegative. The term $Y \geq 0$ denotes that Y is a nonnegative matrix entrywise.

We will use several matrix operations from linear algebra. For a matrix $M \in \mathbb{R}^{m \times m}$ and $S_1, S_2 \subset [m]$, let $M[S_1, S_2]$ denote the submatrix of M with rows in S_1 and columns in S_2 . When $S_1 = S_2$, we simplify notation and write $M[S_1] := M[S_1, S_1]$. For a vector $x \in \mathbb{R}^m$, let $Diag(x)$ be the $m \times m$ diagonal matrix whose i, i th entry is x_i . For a matrix Y , let $\text{trace}(Y)$ denote the trace of Y , that is, the sum of its diagonal entries. For $A, B \in \mathbb{S}^{m \times m}$, note that

$$\text{trace}(AB) = \sum_{i=1}^m \sum_{j=1}^m A_{ij}B_{ij} = \langle A, B \rangle,$$

the matrix inner product. For an $m \times m$ matrix Y , let $\text{vec}(Y)$ be the vector in \mathbb{R}^{m^2} that stacks the columns of Y . Finally, for matrices A, B of arbitrary dimension, $A \otimes B$ denotes the Kronecker product of A and B . The Kronecker product has particularly nice spectral properties. If $A \in \mathbb{R}^{a \times a}$ and $B \in \mathbb{R}^{b \times b}$ have respective eigenvalues $\lambda_i(A)$ and $\lambda_j(B)$ for $i = 1, \dots, a$ and $j = 1, \dots, b$, the ab eigenvalues of $A \otimes B$ are the ab products $\lambda_i(A)\lambda_j(B)$ (theorem 4.2.12 of Horn and Johnson [17]).

We will regularly work with *circulant* matrices. A circulant matrix in $\mathbb{R}^{m \times m}$ has the form

$$\begin{pmatrix} c_0 & c_1 & c_2 & c_3 & \cdots & c_{m-1} \\ c_{m-1} & c_0 & c_1 & c_2 & \cdots & c_{m-2} \\ c_{m-2} & c_{m-1} & c_0 & c_1 & \ddots & c_{m-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_1 & c_2 & c_3 & c_4 & \cdots & c_0 \end{pmatrix} = (c_{(t-s) \bmod m})_{s,t=1}^m.$$

Such a matrix is symmetric if $c_i = c_{m-i}$ for $i = 1, \dots, m-1$. We use a standard basis of symmetric circulant matrices in $\mathbb{R}^{m \times m}$ consisting of matrices $C_0^{(m)}, C_1^{(m)}, \dots, C_d^{(m)}$, where, for $i = 1, \dots, d-1$, $C_i^{(m)}$ is the symmetric circulant $m \times m$ matrix with $c_i = c_{m-i} = 1$ and $c_j = 0$ otherwise. We set $C_0^m = 2I$ and, when m is even, set $C_{m/2}^{(m)}$ to be the matrix where $c_{m/2} = 2$ and $c_j = 0$ otherwise. Following these definitions, each $C_i^{(m)}$ has the property that all rows sum to two. When clear from context, we will suppress the dependence on the dimension and use, for example, C_i rather than $C_i^{(m)}$. We use $\mathcal{A}(G)$ to denote the adjacency matrix of a graph G and \mathcal{C}_m to denote the cycle graph on m vertices in lexicographic order. Note that $\mathcal{A}(\mathcal{C}_m) = C_1^{(m)}$.

Throughout the remainder of this paper, we take n to be the number of cities/vertices of a TSP instance. We will assume that n is even and let $d = n/2$. We reserve D as the matrix of edge costs or distances (so that for $1 \leq i \leq n$ and $1 \leq j \leq n$, $D_{ii} = 0$ and $D_{ij} = d_{ij}$ is the cost of traveling between cities i and j). We implicitly assume that the edge costs d_{ij} defining D are symmetric and metric.

Let $\text{OPT}_{\text{SDP}}(D)$ and $\text{OPT}_{\text{TSP}}(D)$, respectively, denote the optimal value to an SDP relaxation and the cost of an optimal TSP solution for a given matrix of costs D . If \mathcal{D} is the set of all cost matrices corresponding to metric and symmetric TSP instances, the *integrality gap* of the SDP is

$$\sup_{D \in \mathcal{D}} \frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)}.$$

This ratio is bounded below by one for any SDP that is a relaxation of the TSP (because the optimal TSP solution has a corresponding feasible SDP solution of cost $\text{OPT}_{\text{TSP}}(D)$). The ratio $\frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)}$ for any TSP cost matrix $D \in \mathcal{D}$ provides a lower bound on the integrality gap.

2.2. SDP Relaxations

The QAP was introduced in Koopmans and Beckmann [20]. Let matrices $A, B \in \mathbb{S}^{n \times n}$, respectively, encode the pairwise distances between a set of n locations and the pairwise flows between n different facilities. Let $C = (c_{ij})$ be a matrix of placement costs where c_{ij} denotes the cost of placing facility i at location j . The QAP is to assign each facility to a distinct location to minimize total cost, where the cost depends quadratically on flows and distances and linearly on placement costs:

$$\min\{\text{trace}((AXB + C)X^T) : X \in \Pi_n\},$$

where $A, B \in \mathbb{S}^{n \times n}$ and $C \in \mathbb{R}^{n \times n}$. The TSP for n cities is obtained in the special case where $B = D, A = \frac{1}{2}\mathcal{A}(C_n) = \frac{1}{2}C_1^{(n)}$, and $C = 0$ (the all-zeros matrix). In this case, using the cyclic and linear properties of trace, the objective function becomes

$$\text{trace}\left(\frac{1}{2}C_1^{(n)}XDXT\right) = \frac{1}{2}\langle X^T C_1^{(n)}X, D \rangle,$$

so the permutation matrix X can be interpreted as finding the optimal tour and relabeling the vertices according to the order of that tour; $X^T C_1^{(n)}X$ is then the adjacency matrix of the relabeled tour.

The SDP QAP relaxation of Povh and Rendl [23], when specialized to the TSP, is

$$\begin{aligned}
 & \min \quad \frac{1}{2} \text{trace} \left((D \otimes C_1^{(n)}) Y \right) \\
 & \text{subject to} \quad \text{trace} \left((I_n \otimes E_{jj}^{(n)}) Y \right) = 1 && j = 1, \dots, n, \\
 & \quad \text{trace} \left((E_{jj}^{(n)} \otimes I_n) Y \right) = 1 && j = 1, \dots, n, \\
 & \quad \text{trace}((I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n) Y) = 0 \\
 & \quad \text{trace}(J_{n^2} Y) = n^2 \\
 & \quad Y \geq 0, Y \geq 0, Y \in \mathbb{S}^{n^2 \times n^2}.
 \end{aligned} \tag{1}$$

That this is a valid relaxation can be seen by setting $Y = \text{vec}(X)\text{vec}(X)^T$ for any permutation matrix $X \in \Pi_n$. Letting $X_{:i} = X[[n], \{i}]$ denote the i th column of X , that is,

$$\text{vec}(X) = \begin{pmatrix} X_{:1} \\ X_{:2} \\ \vdots \\ X_{:n} \end{pmatrix},$$

we see that Y has the block structure

$$Y = \begin{pmatrix} Y^{(11)} & Y^{(12)} & \dots & Y^{(1n)} \\ Y^{(21)} & Y^{(22)} & \dots & Y^{(2n)} \\ \vdots & \vdots & \ddots & \vdots \\ Y^{(n1)} & Y^{(n2)} & \dots & Y^{(nn)} \end{pmatrix},$$

where $Y^{(ij)} = X_{:i} X_{:j}^T \in \mathbb{R}^{n \times n}$. If X is a permutation matrix, each $Y^{(ij)} = E_{st}^{(n)}$ for some s, t . Specifically, $Y^{(ij)} = E_{st}^{(n)}$ for the s, t such that $Xe_i = e_s$ and $Xe_j = e_t$. That the constraints hold then readily follows: each $Y^{(ii)} = E_{ss}^{(n)}$ for some s (so that $\text{trace}((E_{ii}^{(n)} \otimes I_n) Y) = 1$), and because X is a permutation matrix, $Y^{(ii)} \neq Y^{(kk)}$ for $i \neq k$ (so that $\text{trace}((I_n \otimes E_{jj}^{(n)}) Y) = 1$). Similarly, each $Y^{(ii)}$ is diagonal, whereas each $Y^{(ij)}$ with $i \neq j$ has zero diagonal (so that $\text{trace}((I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n) Y) = 0$), and because each of the n^2 blocks $Y^{(ij)}$ consists of a single one and zeros elsewhere, the sum of all entries in Y is n^2 ; that is, $\text{trace}(J_{n^2} Y) = n^2$. The factored form $Y = \text{vec}(X)\text{vec}(X)^T$ implies that Y is a rank-one positive semidefinite matrix, and because Y is 0–1, $Y \geq 0$. Finally, $(Y^{(ij)})^T = (X_{:i} X_{:j}^T)^T = X_{:j} X_{:i}^T = Y^{(ji)}$, so Y is symmetric. As we show explicitly in Section 3, results from Gutekunst and Williamson [14] and de Klerk et al. [10] imply that SDP (1) has an unbounded integrality gap.

In de Klerk and Sotirov [8], symmetry reduction is applied to SDP (1) to obtain the following SDP relaxation of the TSP:

$$\begin{aligned}
 & \min \quad \text{trace} \left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n)}[\alpha] + \text{Diag}(\bar{c}) \right) Y \right) \\
 & \text{subject to} \quad \text{trace} \left((I_{n-1} \otimes E_{jj}^{(n-1)}) Y \right) = 1 && j = 1, \dots, n-1 \\
 & \quad \text{trace} \left((E_{jj}^{(n-1)} \otimes I_{n-1}) Y \right) = 1 && j = 1, \dots, n-1 \\
 & \quad \text{trace}((I_{n-1} \otimes (J_{n-1} - I_{n-1}) + (J_{n-1} - I_{n-1}) \otimes I_{n-1}) Y) = 0 \\
 & \quad \text{trace}(J_{(n-1)^2} Y) = (n-1)^2 \\
 & \quad Y \geq 0, Y \geq 0, Y \in \mathbb{S}^{(n-1)^2 \times (n-1)^2},
 \end{aligned} \tag{2}$$

where $s, r \in [n]$, $\alpha = [n] \setminus r$ and $\beta = [n] \setminus s$, and $\bar{c} = \text{vec}(C_1[\alpha, \{r\}]D[\{s\}, \beta])$. All that matters for the TSP is the order in which the vertices are visited in the optimal tour; there are $(n-1)!/2$ distinct tours but $n!$ permutation matrices. One way to interpret the symmetry reduction intuitively is that, without loss of generality, one may assume that an optimal solution $X \in \Pi_n$ is such that $X_{r,s} = 1$ (i.e., that the s th vertex visited is vertex r): an

optimal tour includes vertex r and can be reindexed (without changing the cost of the tour) so that vertex r is the s th vertex visited. Making this assumption leaves the $n - 1$ vertices α to be visited at the $n - 1$ positions β , so one can effectively write a QAP for $X[\alpha, \beta] \in \Pi_{n-1}$ (the submatrix of X for which entries are not fixed by $X_{r,s} = 1$). Following through this process results in a QAP on $(n - 1)$ vertices; appropriately adjusting the objective function and writing the SDP relaxation of the QAP on $(n - 1)$ vertices yield the SDP relaxation (2). See de Klerk and Sotirov [8] for full details.

We analyze the integrality gap of SDP (2) in Sections 3 (showing that it is at least two) and 4 (showing that it is unbounded). In both cases, we will find a set of instances on n vertices and an associated feasible $Y \in \mathbb{S}^{n^2 \times n^2}$ that together imply an unbounded integrality gap for SDP (1). We note that up to dimension, the constraints of SDPs (1) and (2) are exactly the same. Any feasible Y for an instance on n vertices of SDP (1) thus gives a feasible solution to SDP (2), but in this latter SDP, Y is a feasible solution for instances with one more vertex. After finding an instance of n vertices and feasible Y for SDP (1), our approach will be to add a single vertex and then use the same Y to bound the integrality gap of SDP (2) (accounting for the adjusted objective function). It will thus be convenient to view SDP (2) as an SDP for $n + 1$ vertex instances (with n still even). The SDP then becomes

$$\begin{aligned} \min \quad & \text{trace} \left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c}) \right) Y \right) \\ \text{subject to} \quad & \text{trace} \left(\left(I_n \otimes E_{jj}^{(n)} \right) Y \right) = 1 & j = 1, \dots, n, \\ & \text{trace} \left(\left(E_{jj}^{(n)} \otimes I_n \right) Y \right) = 1 & j = 1, \dots, n, \\ & \text{trace} \left((I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n) Y \right) = 0 \\ & \text{trace} \left((J_n \otimes J_n) Y \right) = n^2 \\ & Y \geq 0, Y \geq 0, Y \in \mathbb{S}^{n^2 \times n^2}, \end{aligned}$$

where $s, r \in [n + 1]$ and $\alpha = [n + 1] \setminus r$ and $\beta = [n + 1] \setminus s$ and where $\bar{c} = \text{vec}(C_1[\alpha, \{r\}]D[\{s\}, \beta])$. We also refer to this form of the SDP on $n + 1$ vertices as SDP (2).

3. An Integrality Gap of at Least Two

We first show how results from Gutekunst and Williamson [14] and de Klerk et al. [10] imply that the integrality gap of SDP (1) is unbounded, whereas the integrality gap of SDP (2) is at least two. De Klerk et al. [10, theorem 3] show that the optimal value of SDP (1) coincides with the optimal value of an SDP relaxation of the TSP based on association schemes; Gutekunst and Williamson [14] give a family of instances that show that this latter SDP has an unbounded integrality gap. By combining the same family of instances as Gutekunst and Williamson [14] and the relationship between the SDPs from de Klerk et al. [10, theorem 3], we obtain that the integrality gap of SDP (1) is unbounded, whereas the integrality gap of SDP (2) is at least two.

Theorem 1. *Let $d = \frac{n}{2}$, where n is even, and define*

$$a_i = \frac{2}{n-2} \left(\cos\left(\frac{\pi i}{d}\right) + 1 \right), \quad i = 1, \dots, d,$$

and

$$b_i = \begin{cases} \frac{2}{n} (1 - \cos(\frac{\pi i}{d})), & \text{if } i = 1, \dots, d-1, \\ \frac{2}{n}, & \text{if } i = d. \end{cases}$$

Let $A = \sum_{i=1}^d a_i C_i$ and $B = \sum_{i=1}^d b_i C_i$. Then

$$Y = \frac{1}{2n} ((I_2 \otimes J_d - I_n) \otimes A + (J_2 - I_2) \otimes J_d \otimes B + 2I_n \otimes I_n)$$

is feasible for SDP (1).

Note that Y is an $n^2 \times n^2$ symmetric matrix that can be partitioned into blocks of size $n \times n$. The n blocks on the diagonal are scaled copies of the identity matrix. The other blocks are all scaled copies of A or B . For example, when $n = 6$, we have

$$Y = \frac{1}{2n} \begin{pmatrix} 2I & A & A & B & B & B \\ A & 2I & A & B & B & B \\ A & A & 2I & B & B & B \\ B & B & B & 2I & A & A \\ B & B & B & A & 2I & A \\ B & B & B & A & A & 2I \end{pmatrix}.$$

To prove Theorem 1, we will make use of the following facts from Gutekunst and Williamson [14]. For completion, we sketch their proofs in the appendix. For $k = 0, \dots, n - 1$, define

$$a^{(k)} = \sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) a_i, \quad b^{(k)} = \sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) b_i.$$

Note that

$$\cos\left(\frac{2\pi i(n-k)}{n}\right) = \cos\left(2\pi i - \frac{2\pi ik}{n}\right) = \cos\left(\frac{2\pi ik}{n}\right),$$

so $a^{(k)} = a^{(n-k)}$ and $b^{(k)} = b^{(n-k)}$.

Proposition 1. (a) The a_i and b_i parameters sum as follows: $\sum_{i=1}^d a_i = \sum_{i=1}^d b_i = 1$. Equivalently, $a^{(0)} = b^{(0)} = 1$, (b) $b^{(k)} = -(1 - \frac{2}{n})a^{(k)} - \frac{2}{n}$, (c) For $k = 1, \dots, d$,

$$a^{(k)} = \begin{cases} \frac{d-2}{n-2}, & \text{if } k = 1, \\ -\frac{2}{n-2}, & \text{otherwise.} \end{cases}$$

(d) $b_1 \leq \frac{4\pi^2}{n^3}$.

To show that Y is positive semidefinite, we also use properties of circulant matrices.

Lemma 1 (Gray [13]). The circulant matrix $M = (m_{(t-s) \bmod n})_{s,t=1}^n$ has eigenvalues

$$\lambda_t(M) = \begin{cases} \sum_{s=0}^{n-1} m_s e^{-\frac{2\pi i s t \sqrt{-1}}{n}}, & \text{if } t = 1, \dots, n-1, \\ \sum_{s=0}^{n-1} m_s, & \text{if } t = n. \end{cases}$$

The eigenvector corresponding to eigenvalue λ_t is $v_t = (1, w_t, w_t^2, \dots, w_t^{n-1})$ for $t = 0, 1, \dots, n-1$ with $w_t = e^{-\frac{2\pi i \sqrt{-1}}{n}}$.

To avoid ambiguity with index variables and imaginary numbers, we explicitly write $\sqrt{-1}$ whenever working with imaginary numbers and reserve i and j as index variables.

We first show that Y satisfies each of the constraints of SDP (1).

Claim 1. Y satisfies the following SDP constraint: $\text{trace}((I_n \otimes E_{jj})Y) = 1$ and $\text{trace}((E_{jj} \otimes I_n)Y) = 1$ for $j = 1, \dots, n$.

Proof. Each of the n^2 diagonal entries of Y is $\frac{1}{n}$. Both $I_n \otimes E_{jj}$ and $E_{jj} \otimes I_n$ are diagonal matrices with exactly n nonzero entries, all of which are equal to one. \square

Claim 2. Y satisfies the following SDP constraint: $\text{trace}((I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y) = 0$.

Proof. The $n \times n$ blocks of Y have sparsity patterns that imply this constraint: I is a diagonal matrix, whereas A and B have zero diagonal (there is no coefficient of C_0 in the sums defining A and B). \square

Claim 3. Y satisfies the following SDP constraint: $\text{trace}(J_{n^2}Y) = n^2$.

Proof. To show that this constraint holds, we note that Y is expressed in terms of n^2 blocks, each of size $n \times n$ and each of which is either $\frac{1}{2n}A$, $\frac{1}{2n}B$, or $\frac{1}{n}I$. In the first row of A , we have that $A_{1,i} = a_i = a_{n-i}$ for $i = 1, \dots, d-1$, whereas $A_{1,d} = 2a_d$. Because A is circulant, each of the n rows of A then sums to $2 \sum_{i=1}^d a_i$. Using the first result of Proposition 1,

the entries in A sum to $2n$ so that $\text{trace}(J_n \frac{1}{2n} A) = 1$. Analogously, $\text{trace}(J_n \frac{1}{2n} B) = \text{trace}(J_n \frac{1}{n} I_n) = 1$. That is, each of the n^2 blocks defining Y sums to one so that when we sum all the entries in Y ,

$$\text{trace}(J_{n^2} Y) = n^2. \quad \square$$

Claim 4. Y satisfies the following SDP constraint: $Y \geq 0$.

Proof. The penultimate constraint follows because $a_i, b_i \geq 0$. \square

To show feasibility, we thus must finally show the following.

Claim 5. Y satisfies the following SDP constraint: $Y \geq 0$.

Proof. From Lemma 1, we have that the eigenvectors of a circulant matrix with first row $(m_0, m_1, \dots, m_{n-1})$ are of the form $v_j = (1, w_j, w_j^2, \dots, w_j^{n-1})$ for $j = 0, 1, \dots, n-1$ with $w_j = e^{-\frac{2\pi i j \sqrt{-1}}{n}}$. The eigenvalue corresponding to v_j is

$$\lambda_j = m_0 + m_1 w_j + m_2 w_j^2 + \dots + m_{n-1} w_j^{n-1}.$$

Hence, v_j is a simultaneous eigenvector of A, B , and I_n . Let λ_j^A and λ_j^B , respectively, indicate the eigenvalues of A and B corresponding to v_j . Note that

$$\begin{aligned} w_j^i + w_j^{n-i} &= e^{-\frac{2\pi i j \sqrt{-1}}{n}} + e^{-\frac{2\pi i (n-i) \sqrt{-1}}{n}} \\ &= \cos\left(-\frac{2\pi i j}{n}\right) + \sqrt{-1} \sin\left(-\frac{2\pi i j}{n}\right) + \cos\left(-\frac{2\pi (n-i) j}{n}\right) + \sqrt{-1} \sin\left(-\frac{2\pi (n-i) j}{n}\right) \\ &= 2 \cos\left(\frac{2\pi i j}{n}\right). \end{aligned}$$

Then, because $A_{1,i} = A_{1,n-i} = a_i$ for $i = 1, \dots, d-1$ and $A_{1,d} = 2a_d$,

$$\lambda_j^A = \left(\sum_{i=1}^{d-1} a_i (w_j^i + w_j^{n-i}) \right) + 2a_d w_j^d = 2 \sum_{i=1}^d a_i \cos\left(\frac{2\pi i j}{n}\right) = 2a^{(j)}.$$

Similarly, $\lambda_j^B = 2b^{(j)}$.

Recall that

$$Y = \frac{1}{2n} (((I_2 \otimes J_d) - I_n) \otimes A + (J_2 - I_2) \otimes J_d \otimes B + 2I_n \otimes I_n).$$

By finding a shared set of eigenvectors of $(I_2 \otimes J_d) - I_n$, $(J_2 - I_2) \otimes J_d$, and $2I_n$, we can use properties of the Kronecker product to explicitly compute the eigenvalues of Y as a function of the $a^{(j)}$ and $b^{(j)}$; the remaining results from Proposition 1 will suffice to show that they are all nonnegative. We use the following as our shared set of eigenvectors.¹ We first have $u_1 = e^{(n)}$ and $u_2 = (e_1^{(2)} - e_2^{(2)}) \otimes e^{(d)}$. The remaining u_3, \dots, u_n are the $n-2$ vectors of the form $e^{(2)} \otimes (e_1^{(d)} - e_i^{(d)})$ and $(e_1^{(2)} - e_2^{(2)}) \otimes (e_1^{(d)} - e_i^{(d)})$ for $i = 2, \dots, d$ (in any order). Denote by μ_j^A and μ_j^B the respective eigenvalues of $(I_2 \otimes J_d) - I_n$ and $(J_2 - I_2) \otimes J_d$ associated with u_j . Then

$$\mu_1^A = d-1, \quad \mu_2^A = d-1, \quad \mu_j^A = -1 \text{ otherwise}$$

and

$$\mu_1^B = d, \quad \mu_2^B = -d, \quad \mu_j^B = 0 \text{ otherwise.}$$

Now note that

$$(((I_2 \otimes J_d) - I_n) \otimes A + (J_2 - I_2) \otimes J_d \otimes B + 2I_n \otimes I_n)(u_i \otimes v_j) = (\mu_i^A \lambda_j^A + \mu_i^B \lambda_j^B + 2)(u_i \otimes v_j),$$

so the eigenvalues of $2nY$ must be the values of $(\mu_i^A \lambda_j^A + \mu_i^B \lambda_j^B + 2)$ over $i = 1, \dots, n$ and $j = 0, \dots, n-1$. That is,

$$2(\mu_i^A a^{(j)} + \mu_i^B b^{(j)} + 1), i = 1, \dots, n; j = 0, \dots, n-1.$$

To show $Y \geq 0$, it suffices to show that these are all nonnegative. For $j = 0$, we have that $a^{(0)} = b^{(0)} = 1$ and thus that

$$\mu_i^A a^{(0)} + \mu_i^B b^{(0)} + 1 = \begin{cases} d - 1 + d + 1 = 2d \geq 0, & i = 1, \\ d - 1 - d + 1 = 0 \geq 0, & i = 2, \\ -1 + 0 + 1 = 0 \geq 0, & i \geq 3. \end{cases}$$

Otherwise, for $j \neq 0$, we have

$$\mu_i^A a^{(j)} + \mu_i^B b^{(j)} + 1 = \begin{cases} (d - 1)a^{(j)} + db^{(j)} + 1, & i = 1, \\ (d - 1)a^{(j)} - db^{(j)} + 1, & i = 2, \\ -a^{(j)} + 1, & i \geq 3. \end{cases}$$

Using $b^{(k)} = -\left(1 - \frac{2}{n}\right)a^{(k)} - \frac{2}{n}$ from Proposition 1:

$$= \begin{cases} 0, & i = 1, \\ (n - 2)a^{(j)} + 2, & i = 2, \\ -a^{(j)} + 1, & i \geq 3. \end{cases}$$

By the final case of Proposition 1, for $j = 1, \dots, d$,

$$a^{(j)} = \begin{cases} \frac{d-2}{n-2}, & \text{if } j = 1, \\ -\frac{2}{n-2}, & \text{otherwise} \end{cases}$$

Hence, the eigenvalues are all nonnegative. and $Y \geq 0$. \square

Proof of Theorem 1. Claims 1–5 imply that Y is feasible for SDP (1). \square

Corollary 1. *The integrality gap of SDP (1) is unbounded.*

To show that the integrality gap is unbounded, we consider the cost matrix

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

used in Gutekunst and Williamson [14]. This cost matrix is that of a *cut semimetric*: there are two equally sized groups of vertices $\{1, \dots, d\}$ and $\{d + 1, \dots, n\}$; the cost of traveling between two vertices in the same group is zero, whereas the cost of traveling between two vertices in different groups (i.e., crossing the cut defined by $\{1, \dots, d\}$) is one.

Proof. The integrality gap of SDP (1) is at least

$$\frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)}.$$

Note that $\text{OPT}_{\text{TSP}}(D) \geq 2$, because a minimum-cost Hamiltonian cycle must cross the cut defined by $\{1, \dots, d\}$ twice; the tour $1, 2, \dots, d, d + 1, \dots, n, 1$ realizes this cost so that $\text{OPT}_{\text{TSP}}(D) = 2$. We then bound $\text{OPT}_{\text{SDP}}(D)$ using Y as a feasible solution to SDP (1). When computing the cost, we evaluate $\text{trace}((D \otimes C_1)Y)$. The $n^2 \times n^2$ matrix $D \otimes C_1$ consists of $n \times n$ blocks, either of which is an $n \times n$ block of zeros (exactly where Y has a $\frac{1}{2n}A$ block or a $\frac{1}{n}I$ block) or a C_1 (exactly in the $2d^2$ places where Y has a $\frac{1}{2n}B$ block). Hence,

$$\begin{aligned} \text{OPT}_{\text{SDP}}(D) &\leq \frac{1}{2} \text{trace}((D \otimes C_1)Y) \\ &= \frac{1}{2} 2d^2 \frac{1}{2n} \text{trace}(C_1 B) \\ &= \frac{d^2}{2n} 2nb_1 \\ &= d^2 b_1 \\ &\leq 4\pi^2 \frac{d^2}{n^3}, \end{aligned}$$

using the final result of Proposition 1. Thus, $\text{OPT}_{\text{SDP}}(D) \leq c \frac{1}{n}$ for some constant c . Hence, the integrality gap is at least

$$\frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)} \geq \frac{2}{c \frac{1}{n}} = \frac{2}{c} n,$$

which grows without bound. \square

This instance and feasible solution Y do not, however, show that the integrality gap of SDP (2) is unbounded. Instead, they imply the following.

Corollary 2. *The integrality gap of SDP (2) is at least two.*

We consider an instance of SDP (2) on $n + 1$ vertices. This change of bookkeeping implies that the feasible solution Y from Theorem 1 is feasible for SDP (2).

Proof. We consider an instance on $n + 1$ vertices with two groups of vertices, $\{1, \dots, d, d + 1\}$ and $\{d + 2, \dots, n + 1\}$. As before, we define the cost of traveling between vertices in the same group to be zero and the cost of traveling between vertices in distinct groups to be one. By taking $r = s = 1$, we have that

$$D[\beta] = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes J_d$$

and $C_1^{(n+1)}[\alpha] \leq C_1^{(n)}$ entrywise. As in Corollary 1, the integrality gap is at least

$$\frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)},$$

and again $\text{OPT}_{\text{TSP}}(D) = 2$. To upper bound the denominator, we note that the feasibility of Y implies that

$$\begin{aligned} \text{OPT}_{\text{SDP}}(D) &\leq \text{trace} \left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c}) \right) Y \right) \\ &= \text{trace} \left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] \right) Y \right) + \text{trace}(\text{Diag}(\bar{c})Y). \end{aligned}$$

We can bound the first term by Corollary 1 because

$$\text{trace} \left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] \right) Y \right) \leq \text{trace} \left(\left(\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes J_d \right) \otimes \frac{1}{2} C_1^{(n)} \right) Y \right) \leq c \frac{1}{n}.$$

We can compute the second term. Note that $C_1[\alpha, \{r\}] = e_1^{(n)} + e_n^{(n)}$ and $D[\{s\}, \beta] = (e_{d+1}^{(n)} + e_{d+2}^{(n)} + \dots + e_n^{(n)})^T$. Thus, $C_1[\alpha, \{r\}]D[\{s\}, \beta]$ is an $n \times n$ matrix with exactly n ones and all other entries zero. Hence,

$$\text{Diag}(\bar{c}) = \text{Diag}(\text{vec}(C_1[\alpha, \{r\}]D[\{s\}, \beta]))$$

is a diagonal matrix with exactly n ones on the diagonal. Because each diagonal entry of Y is $\frac{1}{n}$, we have

$$\text{trace}(\text{Diag}(\bar{c})Y) = 1.$$

Putting everything together, we get that

$$\text{OPT}_{\text{SDP}}(D) \leq 1 + \frac{c}{n},$$

so the integrality gap is at least

$$\frac{\text{OPT}_{\text{TSP}}(D)}{\text{OPT}_{\text{SDP}}(D)} \geq \frac{2}{1 + \frac{c}{n}} = \frac{2n}{n + c}$$

for some constant c , which gets arbitrarily close to two as n grows. \square

The solution Y is not necessarily optimal for SDP (2), and hence, this family of instances may in fact imply an integrality gap larger than two. Numerical experiments on this family suggest that the optimal solutions to

SDP (2) have value strictly less than one as n grows sufficiently large but are far less structured than Y . To show that the integrality gap of SDP (2) is unbounded, we instead modify the family of instances considered.

We will specifically look for instances D where $\text{OPT}_{\text{TSP}}(D)$ grows arbitrarily large while $\text{OPT}_{\text{SDP}}(D) \leq a + \frac{b}{n}$ for constants a and b ; as in the preceding proof, we bound $\text{trace}(\text{Diag}(\bar{c})Y)$ by an absolute constant (a) and show that $\text{trace}(D[\beta] \otimes \frac{1}{2}C_1^{(n+1)}[\alpha])Y$ decays with $\frac{1}{n}$ (with a constant b that does not depend on n). We also want to find feasible (but not necessarily optimal) solutions that retain the structure of Y : a matrix with a simple block structure that respects that of the cost matrix; that can be decomposed into terms, each of which is the Kronecker product of a matrix constructed using J and I and a circulant matrix; and that we will thus be able to explicitly write down their eigenvalues.

4. Unbounded Integrality Gap

We now generalize the results of Section 3 to a more involved set of instances that allow us to prove our main theorem.

Theorem 2. *Let $z \in \mathbb{N}$. Then the integrality gap of SDP (2) is at least z .*

An immediate corollary is as follows.

Corollary 3. *The integrality gap of SDP (2) is unbounded.*

As before, we first start by finding feasible solutions to SDP (1). We then modify these solutions so that they are feasible to SDP (2).

4.1. Feasible Solutions to SDP (1)

To generalize the preceding example, we consider an instance with g equally sized groups of n/g vertices. If u, v are two vertices in the same group, then the cost of traveling between u and v is zero; otherwise, the cost is one. Labeling the vertices so that the i th group consists of vertices $\{(i-1)\frac{n}{g} + 1, \dots, i\frac{n}{g}\}$, the cost matrix is

$$D = (J_g - I_g) \otimes J_{n/g}.$$

The instances in Section 3 are the special case where $g = 2$. These instances are metric and can be viewed as Euclidean TSP in \mathbb{R}^{g-1} ; we refer to this family of instances as *simplicial TSP instances*. In a regular $g-1$ simplex, there are g extreme points, each pair of which is a distance one apart. One way to interpret an instance with g groups is as embedded into a regular $g-1$ simplex in \mathbb{R}^{g-1} , where each group of $\frac{n}{g}$ vertices is placed at an extreme point of the simplex.

To prove Theorem 2, we take $g = 2z$. To simplify our proofs, we thus assume that g is even throughout. These instances generalize and extend the results from Section 3, which studied the simpler case with $g = 2$ groups.

We use solutions of the form

$$Y = \frac{1}{2n} [(J_g - I_g) \otimes J_{n/g} \otimes B + I_g \otimes J_{n/g} \otimes A + I_g \otimes I_{n/g} \otimes (2I_n - A)], \quad (3)$$

where

$$A = \sum_{i=1}^d a_i C_i, \quad B = \sum_{i=1}^d b_i C_i$$

are symmetric circulant matrices defined in terms of parameters a_1, \dots, a_d and b_1, \dots, b_d . We set

$$a_i = \begin{cases} \frac{1}{n-g} \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \right], & i < d \\ \frac{1}{n-g} \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \right], & i = d. \end{cases}$$

We also set²

$$b_i = \begin{cases} \frac{2g - (n-g)a_i}{n(g-1)}, & i < d \\ \frac{g - (n-g)a_i}{n(g-1)}, & i = d. \end{cases}$$

We will often take sums of the a_i or b_i . It will be helpful to note that

$$a_d = \frac{1}{n-g} \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi dj}{d}\right) \right] - \frac{1}{n-g} \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j) \cos(\pi j) \right]$$

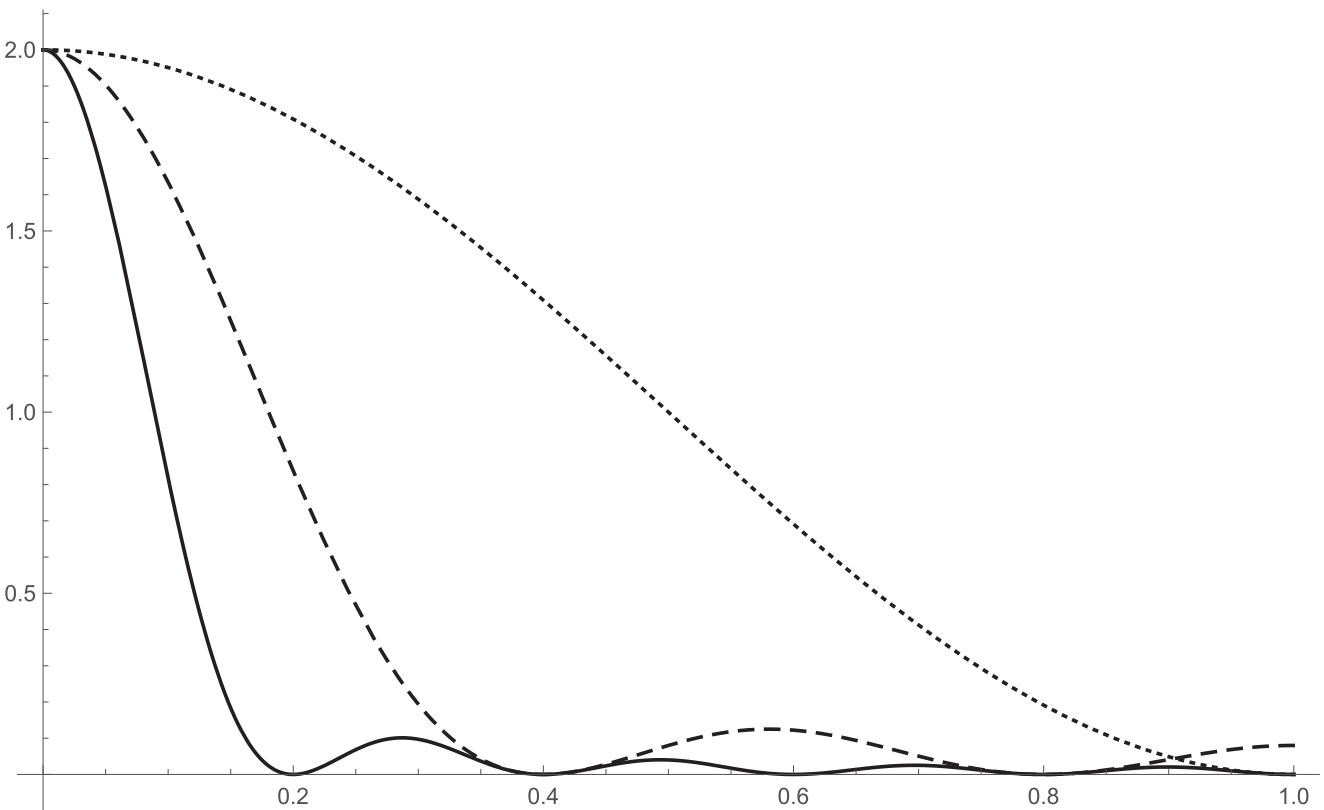
and

$$b_d = \frac{2g - (n-g)a_d}{n(g-1)} - \frac{g}{n(g-1)}.$$

Figure 1 provides intuition for how the a_i depend on g . The a_i can be viewed as uniform samples from a sum of cosines that places a larger weight on smaller values of i . As g increases, the proportion of the a_i that are close to zero grows. As in Section 3, the only parameter that OPT_{SDP} depends on will be b_1 , and large a_1 implies small b_1 .

Note that Y is a large block matrix that respects the symmetry of our cost matrix D in the exact same way as in Section 3: Each diagonal block is $\frac{1}{n}I_n$; everywhere else that D has a zero, Y places a block $\frac{1}{2n}A$; everywhere that D has a one, Y has a block $\frac{1}{2n}B$. In the later proofs, it will help to refer to multiple types of blocks of Y . Also, Y can be partitioned into larger blocks of size $\frac{n^2}{g} \times \frac{n^2}{g}$, each of which is either $J_{n/g} \otimes \frac{1}{2n}B$ or $\frac{1}{2n}((J_{n/g} \otimes A) + I_{n/g} \otimes (2I_n - A))$; we refer to these blocks as *major blocks*. The former are off-diagonal, so we refer to them as *major off-diagonal blocks*, whereas the latter are on the diagonal of Y , so we refer to them as *major diagonal blocks*. Each of these major blocks consists of $(n/g)^2$ smaller $n \times n$ blocks, each of which is a $\frac{1}{2n}A, \frac{1}{2n}B$, or $\frac{1}{n}I_n$. We refer to each as a *minor block*. We refer to each of the n blocks of $\frac{1}{n}I_n$ as a *minor diagonal block*, and we refer to the remaining $n \times n$ blocks (each of which is a single $n \times n$ block equal to $\frac{1}{2n}A$ or $\frac{1}{2n}B$) as a *minor off-diagonal blocks*.

Figure 1. A plot showing $\frac{n-g}{g}a_i$ for $g = 2, 5$, and 10 . For each curve (and any value of n), the values a_1, \dots, a_{d-1} are taken by sampling the curve at $x = \frac{1}{d}, \frac{2}{d}, \dots, \frac{d-1}{d}$; the value of a_d is half the value at $x = 1$. The dotted curve shows $g = 2$, the dashed curve shows $g = 5$, and the remaining curve shows $g = 10$.



Example 1. Suppose that $g = 3$ and $n = 12$. Pictorially, the minor blocks are those blocks proportional to I_n, A , and B ; the major blocks are those delineated next that each consist of 16 minor blocks:

$$Y = \frac{1}{2n} \begin{pmatrix} 2I_n & A & A & A & | & B & B & B & B & | & B & B & B & B \\ A & 2I_n & A & A & | & B & B & B & B & | & B & B & B & B \\ A & A & 2I_n & A & | & B & B & B & B & | & B & B & B & B \\ A & A & A & 2I_n & | & B & B & B & B & | & B & B & B & B \\ \hline B & B & B & B & | & 2I_n & A & A & A & | & B & B & B & B \\ B & B & B & B & | & A & 2I_n & A & A & | & B & B & B & B \\ B & B & B & B & | & A & A & 2I_n & A & | & B & B & B & B \\ B & B & B & B & | & A & A & A & 2I_n & | & B & B & B & B \\ \hline B & B & B & B & | & B & B & B & B & | & 2I_n & A & A & A \\ B & B & B & B & | & B & B & B & B & | & A & 2I_n & A & A \\ B & B & B & B & | & B & B & B & B & | & A & A & 2I_n & A \\ B & B & B & B & | & B & B & B & B & | & A & A & A & 2I_n \end{pmatrix}$$

We now show that this solution meets each SDP constraint.

Proposition 2. *The matrix Y , as given by Equation (3), is feasible for SDP (1).*

Claim 6. For each $j = 1, \dots, n$, we have

$$\text{trace}((I_n \otimes E_{jj})Y) = 1 \quad \text{and} \quad \text{trace}((E_{jj} \otimes I_n)Y) = 1.$$

Proof. These constraints only depend on the diagonal entries of Y , each of which is equal to $\frac{1}{n}$. The constraint $\text{trace}((I_n \otimes E_{jj})Y) = 1$ expands as

$$Y_{jj} + Y_{n+j,n+j} + Y_{2n+j,2n+j} + \dots + Y_{(n-1)n+j,(n-1)n+j} = 1.$$

The constraint $\text{trace}((E_{jj} \otimes I_n)Y) = 1$ expands as

$$Y_{(j-1)n+1,(j-1)n+1} + Y_{(j-1)n+2,(j-1)n+2} + \dots + Y_{(j-1)n+n,(j-1)n+n} = 1.$$

Both summands consist of n terms, each of which is equal to $\frac{1}{n}$, so both hold immediately. \square

Claim 7. Y satisfies the following SDP constraint: $\text{trace}((I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n)Y) = 0$.

Proof. This constraint holds because of Y 's sparsity pattern: first note that

$$\text{trace}((I_n \otimes (J_n - I_n))Y) = 0,$$

because each $n \times n$ minor diagonal block of Y is $\frac{1}{n}I_n$, which is diagonal. Second

$$\text{trace}(((J_n - I_n) \otimes I_n)Y) = 0,$$

because every minor diagonal block is either $\frac{1}{2n}A$ or $\frac{1}{2n}B$; the matrices A and B are a linear combination of C_1, \dots, C_d , all of which have every diagonal entry zero. \square

Claim 8. Y satisfies the following SDP constraint: $\text{trace}(J_{n^2}Y) = n^2$.

This proof involves some involved bookkeeping and uses a handful of lemmas. We use $\mathbb{1}_{\{\circ\}}$ to denote the indicator function that is one if event \circ happens and zero otherwise.

Lemma 2. *Let n be even and $0 < k < n$ be an integer. Then*

$$\sum_{j=1}^d \cos\left(\frac{\pi jk}{d}\right) = \frac{-1 + (-1)^k}{2}.$$

This identity is a consequence of Lagrange’s trigonometric identity; see the appendix for a more detailed proof.

Lemma 3. *Let g be even. Then*

$$\sum_{j=1}^{g-1} (g-j) \mathbb{1}_{\{j \text{ odd}\}} = \frac{g^2}{4} \text{ and } \sum_{j=1}^{g-1} (g-j)(-1)^j = -\frac{g}{2}.$$

Proof. The first claim of this lemma readily follows from the fact that the sum of the first m positive odd integers is m^2 . Thus,

$$\sum_{j=1}^{g-1} (g-j) \mathbb{1}_{\{j \text{ odd}\}} = (g-1) + (g-3) + \dots + 1 = \left(\frac{g}{2}\right)^2,$$

where we note that we added $\frac{g}{2}$ odd numbers. The second claim follows because

$$\begin{aligned} \sum_{j=1}^{g-1} (g-j)(-1)^j &= [-(g-1) + (g-2)] + [-(g-3) + (g-4)] + \dots + [-3 + 2] - 1, \\ &= -1 \frac{g-2}{2} - 1 \\ &= -\frac{g}{2}. \quad \square \end{aligned}$$

Lemma 4. *The a_i sum to 1: $\sum_{i=1}^d a_i = 1$.*

Proof. This lemma follows by direct computation using the preceding identities:

$$\begin{aligned} \sum_{i=1}^d a_i &= \left(\sum_{i=1}^d \frac{1}{n-g} \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \right] \right) - \frac{1}{n-g} \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j) \cos(\pi j) \right] \\ &= \frac{1}{n-g} \left(2d + \frac{4}{g} \left[\sum_{i=1}^d \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \right] - 1 - \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right) \\ &= \frac{1}{n-g} \left(2d + \frac{4}{g} \left[\sum_{j=1}^{g-1} (g-j) \sum_{i=1}^d \cos\left(\frac{\pi ij}{d}\right) \right] - 1 - \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right). \end{aligned}$$

By Lemma 2:

$$\begin{aligned} &= \frac{1}{n-g} \left(2d + \frac{4}{g} \left[\sum_{j=1}^{g-1} (g-j) \frac{(-1) + (-1)^j}{2} \right] - 1 - \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right) \\ &= \frac{1}{n-g} \left(2d - \frac{4}{g} \left[\sum_{j=1}^{g-1} (g-j) \mathbb{1}_{\{j \text{ odd}\}} \right] - 1 - \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right). \end{aligned}$$

By Lemma 3, and using that g is even:

$$\begin{aligned} &= \frac{1}{n-g} \left(2d - \frac{4}{g} \left[\frac{g^2}{4} \right] - 1 + \frac{2g}{g2} \right) \\ &= \frac{1}{n-g} (2d - g) \\ &= 1, \end{aligned}$$

because $n = 2d$. \square

Lemma 5. *The b_i sum to 1: $\sum_{i=1}^d b_i = 1$.*

Proof. This lemma readily follows from the definition of the b_i in terms of the a_i :

$$\begin{aligned} \sum_{i=1}^d b_i &= \left(\sum_{i=1}^d \frac{2g - (n-g)a_i}{n(g-1)} \right) - \frac{g}{n(g-1)} \\ &= \frac{2gd}{n(g-1)} - \frac{n-g}{n(g-1)} \sum_{i=1}^d a_i - \frac{g}{n(g-1)}. \end{aligned}$$

By Lemma 4:

$$\begin{aligned} &= \frac{2gd}{n(g-1)} - \frac{n-g}{n(g-1)} - \frac{g}{n(g-1)} \\ &= \frac{1}{n(g-1)} (ng - n + g - g) \\ &= \frac{1}{n(g-1)} (n(g-1)) \\ &= 1. \quad \square \end{aligned}$$

Proof of Claim 8. To show that $\text{trace}(J_{n^2}Y) = n^2$, we want to sum the entries of Y . We mirror the proof of Claim 3 and first compute the sum of the entries in each minor block, which is either a $\frac{1}{n}I_n$, $\frac{1}{2n}A$, or $\frac{1}{2n}B$. As in Claim 3, Lemma 4 implies that $\text{trace}(J_n \frac{1}{2n}A) = \frac{1}{2n} 2n \sum_{i=1}^d a_i = \frac{1}{2n} 2n = 1$, and analogously, Lemma 5 implies that $\text{trace}(J_n \frac{1}{2n}B) = 1$. Moreover, $\text{trace}(J_n \frac{1}{n}I_n) = 1$. Hence, each of the n^2 minor blocks of Y sums to one, so the total sum of entries in Y is

$$\text{trace}(J_{n^2}Y) = n^2. \quad \square$$

Claim 9. Y satisfies the following SDP constraint: $Y \geq 0$.

To show that $Y \geq 0$, we show that the a_i and b_i are nonnegative. We will use the following trigonometric identity.

Lemma 6. We have the following trigonometric identity:

$$(2 \cos(\theta) - 2) \sum_{j=1}^{g-1} (g-j) \cos(j\theta) = \cos(g\theta) - g \cos(\theta) + (g-1).$$

Proof.

$$\begin{aligned} &(2 \cos(\theta) - 2) \sum_{j=1}^{g-1} (g-j) \cos(j\theta) \\ &= 2 \sum_{j=1}^{g-1} (g-j) \cos(j\theta) \cos(\theta) - 2 \sum_{j=1}^{g-1} (g-j) \cos(j\theta). \end{aligned}$$

Applying the product-to-sum identity for cosine :

$$= \sum_{j=1}^{g-1} (g-j) \cos((j+1)\theta) + \sum_{j=1}^{g-1} (g-j) \cos((j-1)\theta) - 2 \sum_{j=1}^{g-1} (g-j) \cos(j\theta).$$

Reindexing to combine terms :

$$\begin{aligned} &= \sum_{j=2}^g (g-j+1) \cos(j\theta) + \sum_{j=0}^{g-2} (g-j-1) \cos(j\theta) - 2 \sum_{j=1}^{g-1} (g-j) \cos(j\theta) \\ &= \sum_{j=1}^{g-1} [(g-j+1) + (g-j-1) - 2(g-j)] \cos(j\theta) + \cos(g\theta) - g \cos(\theta) + (g-1) \cos(0) - 0 \\ &= \cos(g\theta) - g \cos(\theta) + (g-1). \quad \square \end{aligned}$$

Proof of Claim 9. We first show that the a_i are nonnegative. Recall that

$$a_i \propto 2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right)$$

(where the constant of proportionality is different for a_1, \dots, a_{d-1} and for a_d but in both cases is positive). To show that the a_i are nonnegative, we thus want to show that for $i = 1, \dots, d$,

$$\frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \geq -2,$$

or, equivalently,

$$\sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \geq -\frac{g}{2}.$$

We appeal to Lemma 6 with $\theta = \frac{\pi i}{d}$. For $i = 1, \dots, d$, $\cos(\theta) \neq 1$, so we have that

$$\begin{aligned} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) &= \frac{\cos(g\theta) - g \cos(\theta) + g - 1}{2 \cos(\theta) - 2} \\ &= \frac{g(1 - \cos(\theta))}{2(\cos(\theta) - 1)} + \frac{\cos(g\theta) - 1}{2 \cos(\theta) - 2} \\ &= -\frac{g}{2} + \frac{1 - \cos(g\theta)}{2 - 2 \cos(\theta)} \\ &\geq -\frac{g}{2}, \end{aligned}$$

because $1 - \cos(g\theta) \geq 0$ and $2 - 2 \cos(\theta) \geq 0$.

We now need only show that the $b_i \geq 0$. Recall that

$$b_i = \begin{cases} \frac{2g - (n-g)a_i}{n(g-1)}, & i < d, \\ \frac{g - (n-g)a_i}{n(g-1)}, & i = d. \end{cases}$$

For $i = 1, \dots, d-1$, it suffices to show that $2g \geq (n-g)a_i$. In these cases, we have

$$(n-g)a_i = 2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right).$$

Using $\cos(\theta) \leq 1$,

$$\begin{aligned} &\leq 2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \\ &= 2 + \frac{4}{g} (1 + 2 + \dots + (g-1)) \\ &= 2 + \frac{4(g-1)g}{g \cdot 2} \\ &= 2 + 2(g-1) \\ &= 2g, \end{aligned}$$

as desired.

For $i = d$, the situation is analogous. We want $(n - g)a_d \leq g$, which follows by the previous exact computations:

$$\begin{aligned} (n - g)a_d &= \frac{1}{2} \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g - j) \cos\left(\frac{\pi dj}{d}\right) \right] \\ &\leq \frac{1}{2} 2g \\ &= g. \quad \square \end{aligned}$$

Proposition 3. Y satisfies the following SDP constraint: $Y \geq 0$.

As before, define $a^{(k)} = \sum_{i=1}^d a_i \cos(2\pi ik/n)$ and $b^{(k)} = \sum_{i=1}^d b_i \cos(2\pi ik/n)$. Recall, as in Claim 5, that the eigenvectors of a general circulant matrix are of the form $v_j = (1, w_j, w_j^2, \dots, w_j^{n-1})$ for $j = 0, 1, \dots, n - 1$.

Claim 10. Matrices A and B are simultaneously diagonalizable. The eigenvalues of A are

$$\lambda_k(A) = 2a^{(k)}$$

for $k = 0, \dots, n - 1$. The eigenvalues of B are

$$\lambda_k(B) = 2b^{(k)}$$

for $k = 0, \dots, n - 1$, where $\lambda_k(A)$ and $\lambda_k(B)$ correspond to the same eigenvector v_k .

Proof. This is exactly as in Claim 5, because A and B are constructed using the same basis of symmetric circulant matrices. \square

Claim 11. The distinct eigenvalues of $2nY$ are

$$\begin{cases} 2(g - 1)\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}), \\ -2\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}), \\ 2 - 2a^{(k)}, \end{cases}$$

over $k = 0, \dots, n - 1$.

Proof. Note that

$$2nY = (J_g - I_g) \otimes J_{n/g} \otimes B + I_g \otimes J_{n/g} \otimes A + I_g \otimes I_{n/g} \otimes (2I_n - A).$$

Claim 10 gives a set of simultaneous eigenvectors/eigenvalues for B and A (and thus also $2I_n - A$), which we denote by v_k , for $k = 1, \dots, n$. We can similarly obtain a simultaneous set of eigenvectors/eigenvalues of $(J_g - I_g) \otimes J_{n/g}$, $I_g \otimes J_{n/g}$ and $I_g \otimes I_{n/g}$, so we will again use properties of the Kronecker product to explicitly compute the eigenvalues of Y as a function of the $a^{(k)}$ and $b^{(k)}$. Note that $(J_g - I_g) \otimes J_{n/g}$ has three distinct eigenvalues: $J_g - I_g$ has two distinct eigenvalues ($g - 1$ with associated eigenvector $e^{(g)}$ and -1 with associated eigenvectors $e_1^{(g)} - e_i^{(g)}$, for $i = 2, \dots, g$), and $J_{n/g}$ has two distinct eigenvalues (n/g with associated eigenvector $e^{(n/g)}$ and zero with associated eigenvectors $e_1^{(n/g)} - e_i^{(n/g)}$, for $i = 2, \dots, \frac{n}{g}$). Hence, spectral products of Kronecker products imply that the distinct eigenvalues of $(J_g - I_g) \otimes J_{n/g}$ are

$$\mu_i^B := \begin{cases} (g - 1) \times \frac{n}{g}, & i = 1 \left(\text{using } e^{(g)} \otimes e^{(n/g)} \right), \\ -1 \times \frac{n}{g}, & i = 2 \left(\text{using } \left(e_1^{(g)} - e_i^{(g)} \right) \otimes e^{(n/g)} \right), \\ (g - 1) \times 0 = -1 \times 0, & i = 3 \left(\text{using } e^{(g)} \otimes \left(e_1^{(n/g)} - e_i^{(n/g)} \right) \text{ or } \left(e_1^{(g)} - e_i^{(g)} \right) \otimes \left(e_1^{(n/g)} - e_i^{(n/g)} \right) \right). \end{cases}$$

In exactly the same way, the distinct eigenvalues of $I_g \otimes J_{n/g}$ are

$$\mu_i^A := \begin{cases} 1 \times \frac{n}{g}, & i = 1 \left(\text{using } e^{(g)} \otimes e^{(n/g)} \right) \\ 1 \times \frac{n}{g}, & i = 2 \left(\text{using } \left(e_1^{(g)} - e_i^{(g)} \right) \otimes e^{(n/g)} \right) \\ 1 \times 0, & i = 3 \left(\text{using } e^{(g)} \otimes \left(e_1^{(n/g)} - e_i^{(n/g)} \right) \text{ or } \left(e_1^{(g)} - e_i^{(g)} \right) \otimes \left(e_1^{(n/g)} - e_i^{(n/g)} \right) \right). \end{cases}$$

For $1 \leq i \leq 3$, let u_i be a shared eigenvector of $(J_g - I_g) \otimes J_{n/g}$ and $I_g \otimes J_{n/g} \otimes A$ with respective associated eigenvalues μ_i^B and μ_i^A . Then

$$\left((J_g - I_g) \otimes J_{n/g} \otimes B + I_g \otimes J_{n/g} \otimes A + I_g \otimes I_{n/g} \otimes (2I_n - A) \right) (u_i \otimes v_k) = \left(\mu_i^B \lambda_k^B + \mu_i^A \lambda_k^A + (2 - \lambda_k^A) \right) (u_i \otimes v_k).$$

Plugging in for the three cases of μ_i^A and μ_i^B , we get that the distinct eigenvalues of $2nY$ are

$$\begin{cases} 2(g-1)\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2-2a^{(k)}), \\ -2\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2-2a^{(k)}), \\ 2-2a^{(k)}, \end{cases} \tag{4}$$

over $k = 0, \dots, n-1$, as claimed. \square

Claim 12. For $k = 1, \dots, n-1$,

$$b^{(k)} = -\frac{g}{n(g-1)} - \frac{n-g}{n(g-1)}a^{(k)}.$$

Proof. We have that

$$\begin{aligned} b^{(k)} &= \sum_{i=1}^d b_i \cos\left(\frac{2\pi ik}{n}\right) \\ &= \left[\sum_{i=1}^d \frac{2g - (n-g)a_i}{n(g-1)} \cos\left(\frac{2\pi ik}{n}\right) \right] - \frac{g}{n(g-1)} \cos(\pi k). \end{aligned}$$

Using Lemma 2 and the definition of $a^{(k)}$:

$$\begin{aligned} &= \frac{2g}{n(g-1)} \left[\sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) \right] - \frac{n-g}{n(g-1)} \left[\sum_{i=1}^d a_i \cos\left(\frac{2\pi ik}{n}\right) \right] - \frac{g}{n(g-1)} (-1)^k \\ &= \frac{g}{n(g-1)} \left((-1) + (-1)^k \right) - \frac{n-g}{n(g-1)} a^{(k)} - \frac{g}{n(g-1)} (-1)^k \\ &= -\frac{g}{n(g-1)} - \frac{n-g}{n(g-1)} a^{(k)}. \quad \square \end{aligned}$$

Plugging in for the $b^{(k)}$, we can simplify the eigenvalues of $2nY$.

Claim 13. The eigenvalues of $2nY$ are

$$\begin{cases} 0, \\ 2\left(\frac{g}{g-1}\right) + 2\left(\frac{n-g}{g-1}\right)a^{(k)}, \\ 2-2a^{(k)}, \end{cases}$$

over $k = 1, \dots, n - 1$, and

$$\begin{cases} 2n, \\ 0, \end{cases}$$

corresponding to $k = 0$.

Proof. The $k = 0$ follows by simplifying Equation (4) using $a^{(0)} = b^{(0)} = 1$ from Lemmas 4 and 5. Otherwise, notice that

$$\begin{aligned} 2(g-1)\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}) &= -2(g-1)\frac{n}{g}\left(\frac{g}{n(g-1)} + \frac{n-g}{n(g-1)}a^{(k)}\right) + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}) \\ &= 2\left[-1 - \frac{n-g}{g}a^{(k)} + \frac{n}{g}a^{(k)} + 1 - \frac{g}{g}a^{(k)}\right] \\ &= 0. \end{aligned}$$

Similarly,

$$\begin{aligned} -2\frac{n}{g}b^{(k)} + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}) &= 2\frac{n}{g}\left(\frac{g}{n(g-1)} + \frac{n-g}{n(g-1)}a^{(k)}\right) + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}) \\ &= 2\left(\frac{1}{g-1} + \frac{n-g}{g(g-1)}a^{(k)}\right) + 2\frac{n}{g}a^{(k)} + (2 - 2a^{(k)}) \\ &= 2\left(1 + \frac{1}{g-1}\right) + 2\left(\frac{n-g}{g(g-1)} + \frac{n(g-1)}{g(g-1)} - \frac{g(g-1)}{g(g-1)}\right)a^{(k)} \\ &= 2\left(1 + \frac{1}{g-1}\right) + 2\left(\frac{ng - g^2}{g(g-1)}\right)a^{(k)} \\ &= 2\left(\frac{g}{g-1}\right) + 2\left(\frac{n-g}{g-1}\right)a^{(k)}. \quad \square \end{aligned}$$

To complete the proof of Proposition 3, we show that the eigenvalues for the cases $k = 1, \dots, n - 1$ are nonnegative. We use two lemmas.

Lemma 7. *We have the following trigonometric identity:*

$$\sum_{i=1}^d \cos\left(\frac{\pi ij}{d}\right) \cos\left(\frac{\pi ik}{d}\right) \geq -\mathbb{1}_{j-k \text{ odd}}.$$

Proof. By the product-to-sum identity,

$$\sum_{i=1}^d \cos\left(\frac{\pi ij}{d}\right) \cos\left(\frac{\pi ik}{d}\right) = \frac{1}{2} \left(\sum_{i=1}^d \cos\left(\frac{\pi i(j+k)}{d}\right) + \cos\left(\frac{\pi i(j-k)}{d}\right) \right).$$

Applying Lemma 2 and considering separately the cases where we cannot apply it (those that devolve down to summing $\cos(\theta i)$ over i when θ is an integer multiple of 2π):

$$= \begin{cases} \frac{1}{4}[-1 + (-1)^{j+k} - 1 + (-1)^{j-k}], & j - k, j + k \notin \{0, n\}, \\ \frac{1}{4}[-1 + (-1)^{j+k} + 2d], & j - k \in \{0, n\}, j + k \notin \{0, n\}, \\ \frac{1}{4}[2d - 1 + (-1)^{j-k}], & j - k \notin \{0, n\}, j + k \in \{0, n\}, \\ \frac{1}{4}[2d + 2d], & j - k, j + k \in \{0, n\}. \end{cases}$$

Noting that $(-1)^{j+k} = (-1)^{j-k}$:

$$\begin{aligned} &= (-1)^{j-k} \\ &\geq \frac{1}{2}(-1 + (-1)^{j-k}) \\ &= -\mathbb{1}_{j-k \text{ odd}}. \end{aligned}$$

Note that $j - k, j + k \in \{0, n\}$ requires $j - k = 0$ and $j + k = n$, that is, $j = k = d$. Because j ranges from one to $g - 1$, our final case is irrelevant if each group contains at least two vertices. \square

Lemma 8. For g even,

$$\sum_{j=1}^{g-1} (g - j) \mathbb{1}_{j-k \text{ odd}} = \frac{1}{4}(g(g - 1) + g(-1)^k).$$

Proof. We begin by expanding the left-hand side:

$$\begin{aligned} \sum_{j=1}^{g-1} (g - j) \mathbb{1}_{j-k \text{ odd}} &= -\frac{1}{2} \sum_{j=1}^{g-1} (-1 + (-1)^{j-k})(g - j) \\ &= \frac{1}{2} \sum_{j=1}^{g-1} (g - j) - \frac{1}{2} \sum_{j=1}^{g-1} (-1)^{j-k}(g - j) \\ &= \frac{1}{2}(1 + 2 + \dots + (g - 1)) - \frac{1}{2}(-1)^{-k} \sum_{j=1}^{g-1} (-1)^j (g - j). \end{aligned}$$

Using Lemma 3:

$$\begin{aligned} &= \frac{1}{2} \frac{g(g - 1)}{2} + \frac{1}{2} (-1)^k \frac{g}{2} \\ &= \frac{1}{4}(g(g - 1) + g(-1)^k). \quad \square \end{aligned}$$

Proof of Proposition 3. To complete the proof of Proposition 3, we need only show that the eigenvalues listed in Claim 13 are nonnegative. We thus need to show that

$$2\left(\frac{g}{g-1}\right) + 2\left(\frac{n-g}{g-1}\right)a^{(k)} \geq 0 \text{ and } 2 - 2a^{(k)} \geq 0$$

for $k = 1, \dots, n - 1$. The latter is a direct consequence of Claim 9, because $a_i \geq 0$ implies that

$$a^{(k)} = \sum_{i=1}^d a_i \cos\left(\frac{2\pi i k}{n}\right) \leq \sum_{i=1}^d a_i = 1.$$

Hence, we need only show that $2\left(\frac{g}{g-1}\right) + 2\left(\frac{n-g}{g-1}\right)a^{(k)} \geq 0$. Equivalently, we need to show that

$$a^{(k)} \geq -\frac{g}{n-g}.$$

This result holds because

$$\begin{aligned} a^{(k)} &= \sum_{i=1}^d a_i \cos\left(\frac{2\pi ik}{n}\right) \\ &= \frac{1}{n-g} \left[\left[\sum_{i=1}^d \left(2 + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi ij}{d}\right) \right) \cos\left(\frac{2\pi ik}{n}\right) \right] - \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j) \cos\left(\frac{\pi dj}{d}\right) \right] \cos\left(\frac{2\pi dk}{n}\right) \right] \end{aligned}$$

By Lemma 2:

$$= \frac{1}{n-g} \left[\left[(-1) + (-1)^k + \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \sum_{i=1}^d \cos\left(\frac{\pi ij}{d}\right) \cos\left(\frac{2\pi ik}{n}\right) \right] - \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right] (-1)^k \right].$$

By Lemma 7:

$$\geq \frac{1}{n-g} \left[\left[(-1) + (-1)^k - \frac{4}{g} \sum_{j=1}^{g-1} (g-j) \mathbb{1}_{j-k \text{ odd}} \right] - \left[1 + \frac{2}{g} \sum_{j=1}^{g-1} (g-j)(-1)^j \right] (-1)^k \right].$$

By Lemmas 3 and 8:

$$\begin{aligned} &= \frac{1}{n-g} \left[\left[(-1) + (-1)^k - \frac{1}{g} (g(g-1) + g(-1)^k) \right] - \left[1 - \frac{2g}{g^2} \right] (-1)^k \right] \\ &= \frac{1}{n-g} [(-1) + (-1)^k - (g-1) - (-1)^k] \\ &= -\frac{g}{n-g}. \quad \square \end{aligned}$$

Proof of Proposition 2. Feasibility of Y follows directly from Claims 6–9 and Proposition 3. \square

We can also compute the objective function value of Y .

Theorem 3. For Y , there exists a constant \tilde{c}_g (depending on g but not n) such that

$$\frac{1}{2} \text{trace}((D \otimes C_1)Y) \leq \frac{\tilde{c}_g}{n}.$$

Proof. Recalling that $D = (J_g - I_g) \otimes J_{n/g}$, we see that $D \otimes C_1$ has blocks of zeros in each of the g major $(n^2/g) \times (n^2/g)$ diagonal blocks of Y . Hence, the only places where $D \otimes C_1$ places a nonzero entry are exactly those where Y has a B block; on each such block, $D \otimes C_1$ has a block C_1 . There are $g(g-1)$ blocks of B matrices, each containing n^2/g^2 copies of B . Accounting for the fact that Y is scaled by $\frac{1}{2n}$, the value of the objective function is thus

$$\frac{1}{2} \text{trace}((D \otimes C_1)Y) = \frac{1}{2} g(g-1) \frac{n^2}{g^2} \frac{1}{2n} \text{trace}(C_1 B).$$

Since $\text{trace}(C_1 B) = 2nb_1$:

$$\begin{aligned} &= \frac{1}{2} g(g-1) \frac{n^2}{g^2} b_1 \\ &= \frac{1}{2} \frac{g-1}{g} n^2 b_1. \end{aligned}$$

Recall that

$$\cos(x) \geq 1 - \frac{1}{2} x^2.$$

Hence,

$$\begin{aligned} b_1 &= \frac{2g - (n - g)a_1}{n(g - 1)} \\ &= \frac{2g - \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g - j) \cos\left(\frac{\pi j}{d}\right)\right]}{n(g - 1)} \\ &\leq \frac{2g - \left[2 + \frac{4}{g} \sum_{j=1}^{g-1} (g - j) \left(1 - \frac{1}{2} \frac{\pi^2 j^2}{d^2}\right)\right]}{n(g - 1)} \\ &= \frac{2(g - 1) - \frac{4}{g} \sum_{j=1}^{g-1} (g - j) + \frac{2\pi^2}{g d^2} \sum_{j=1}^{g-1} (g - j)j^2}{n(g - 1)}. \end{aligned}$$

Define $c_g = \frac{2}{g} \pi^2 \sum_{j=1}^{g-1} (g - j)j^2$, a constant depending on g but not n :

$$\begin{aligned} &= \frac{2(g - 1) - \frac{4}{g} \frac{(g-1)g}{2} + \frac{c_g}{d^2}}{n(g - 1)} \\ &= \frac{c_g}{d^2 n(g - 1)}. \end{aligned}$$

Setting $\hat{c}_g = \frac{4}{g-1} c_g$, a constant depending on g but not n :

$$= \frac{\hat{c}_g}{n^3}.$$

Putting everything together,

$$\frac{1}{2} \text{trace}((D \otimes C_1)Y) = \frac{1}{2} \frac{g-1}{g} n^2 b_1 \leq \frac{1}{2} \frac{g-1}{g} n^2 \frac{\hat{c}_g}{n^3},$$

from which the result follows. \square

We can now prove our main theorem, which we restate as follows.

Theorem (Theorem 2). *Let $z \in \mathbb{N}$. Then the integrality gap of SDP (2) is at least z .*

Proof. We again consider the SDP (2) corresponding to an instance on $n + 1$ vertices. Let $s = r = 1$, and consider an instance of the TSP on $n + 1$ vertices with $g = 2z$ groups of vertices. Specifically, let groups $2, \dots, g$ be equally sized, each of size $\frac{n}{g} \in \mathbb{N}$, and let group one have one extra vertex so that group one is of size $\frac{n}{g} + 1$. Note also that

$$\text{OPT}_{\text{TSP}} = g = 2z$$

because each group of vertices must be visited at least once. Set

$$Y = \frac{1}{2n} [(J_g - I_g) \otimes J_{n/g} \otimes B + I_g \otimes J_{n/g} \otimes A + I_g \otimes I_{n/g} \otimes (2I_n - A)],$$

which is feasible for the SDP by our earlier computations. Then the integrality gap is bounded below by

$$\frac{\text{OPT}_{\text{TSP}}}{\text{OPT}_{\text{SDP}}} \geq \frac{2z}{\text{trace}\left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c})\right)Y\right)}.$$

To bound the right-hand side, we note that the linearity of the trace operator implies that

$$\text{trace}\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c})\right)Y = \text{trace}\left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha]\right)Y\right) + \text{trace}(\text{Diag}(\bar{c})Y). \tag{5}$$

We upper bound each term. First note that

$$D[\beta] = D[\{2, \dots, n + 1\}] = (J_g - I_g) \otimes J_{(n/g)}.$$

Similarly,

$$C_1^{(n+1)}[\alpha] = C_1^{(n)} - e_1 e_n^T - e_n e_1^T \leq C_1^{(n)},$$

where \leq is taken entrywise. By nonnegativity,

$$\text{trace}\left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha]\right) Y\right) \leq \frac{1}{2} \text{trace}\left(\left(\left((J_g - I_g) \otimes J_{(n/g)}\right) \otimes \left(C_1^{(n)}\right)\right) Y\right) \leq \frac{\tilde{c}_g}{n} \quad (6)$$

by Theorem 3. As in Theorem 3, \tilde{c}_g remains independent of n .

Second, consider $\text{trace}(\text{Diag}(\bar{c})Y)$. We compute

$$\bar{c} = \text{vec}\left(C_1^{(n)}[\alpha, \{1\}]D[\{1\}, \beta]\right) = \text{vec}\left(\left(e_1^{(n)} + e_n^{(n)}\right)D[\{1\}, \beta]\right) \leq \text{vec}\left(\left(e_1^{(n)} + e_n^{(n)}\right)\left(e^{(n)}\right)^T\right).$$

We note that $\left(e_1^{(n)} + e_n^{(n)}\right)\left(e^{(n)}\right)^T$ is an $n \times n$ matrix with $2n$ ones and the rest of the entries zero. The vec operator stacks the columns of this matrix, creating a vector in \mathbb{R}^{n^2} with $2n$ ones and the remaining entries zero. Finally, $\text{Diag}(\bar{c})$ creates a diagonal matrix with $2n$ ones on the diagonal and the remaining entries zero. Because all diagonal entries of Y are equal to $1/n$, we have that

$$\text{trace}(\text{Diag}(\bar{c})Y) \leq 2n * \frac{1}{n} = 2. \quad (7)$$

Plugging Equations (6) and (7) into Equation (5), we obtain

$$\text{trace}\left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c})\right) Y\right) \leq \frac{\tilde{c}_g}{n} + 2.$$

Hence, the integrality gap is at least

$$\begin{aligned} \frac{\text{OPT}_{\text{TSP}}}{\text{OPT}_{\text{SDP}}} &\geq \frac{2z}{\text{trace}\left(\left(D[\beta] \otimes \frac{1}{2} C_1^{(n+1)}[\alpha] + \text{Diag}(\bar{c})\right) Y\right)} \\ &\geq \frac{2z}{2 + \frac{\tilde{c}_g}{n}} \\ &= \frac{2zn}{2n + \tilde{c}_g} \\ &\rightarrow z, \end{aligned}$$

as $n \rightarrow \infty$. \square

Gutekunst and Williamson [14] show that the SDPs of Cvetković et al. [5] and de Klerk et al. [10] have a counterintuitive nonmonotonicity property: adding vertices (in a way that retains costs being metric) can arbitrarily decrease the cost of some solutions to the corresponding SDPs. This property contrasts with both TSP and subtour LP solutions: monotonicity of the TSP can be seen through *shortcutting* (see Williamson and Shmoys [28, section 2.4]), whereas Shmoys and Williamson [26] show that the subtour LP is monotonic. Corollary 2 shows that in the $g = 2$ case, the cost of the SDP,

$$\text{OPT}_{\text{SDP}}(D) \leq 1 + \frac{c}{n},$$

decays arbitrarily close to one as the number of vertices in each group grows. Any $g = 2$ instance with cost strictly greater than one thus shows that SDP (2) is nonmonotonic. Moreover, such an instance implies the nonmonotonicity property in \mathbb{R}^1 : the SDP can find a smaller optimal value only by adding more points to visit on the real line.

Corollary 4. *The SDP (2) is nonmonotonic.*

Proof (sketch). It suffices to show a single two-group instance with cost strictly greater than one. Consider such an instance on $n + 1 = 3$ vertices, where the first group has two vertices and the second has one. Explicitly writing down the constraints shows that any feasible solution to the SDP has cost two. \square

Anstreicher [1] gives another SDP relaxation of the QAP, and our simplicial instances also show that its integrality gap is unbounded. In the case where $C = 0$ and e is an eigenvector of either data matrix in the QAP objective function, their SDP is equivalent to the projected eigenvalue bound of Hadley et al. [15]. Because $C_1^{(n)}e^{(n)} = 2e^{(n)}$, it is equivalent to the projected eigenvalue bound when specialized to the TSP. In this case, the SDP is in terms of an $n^2 \times n^2$ matrix, which we give block structure

$$Y = \begin{pmatrix} Y^{(11)} & Y^{(12)} & \dots & Y^{(1n)} \\ Y^{(21)} & Y^{(22)} & \dots & Y^{(2n)} \\ \vdots & \vdots & \ddots & \vdots \\ Y^{(n1)} & Y^{(n2)} & \dots & Y^{(nn)} \end{pmatrix}$$

with $Y^{(ij)} \in \mathbb{R}^{n \times n}$. The SDP is

$$\begin{aligned} \min \quad & \frac{1}{2} \text{trace}\left(\left(D \otimes C_1^{(n)}\right)Y\right) \\ \text{subject to} \quad & \sum_{i=1}^n Y^{(ii)} = I_n, \\ & \left(\text{trace}\left(Y^{(ij)}\right)\right)_{i,j=1}^n = I_n, \\ & \text{trace}(YF^T F) = 2n, \\ & Y - \frac{1}{n^2} J_{n^2} \geq 0, \\ & Y \geq 0, Y \in \mathbb{S}^{n^2 \times n^2}, \end{aligned} \tag{8}$$

where

$$F = \begin{pmatrix} (e^{(n)})^T \otimes I_n \\ I_n \otimes (e^{(n)})^T \end{pmatrix}.$$

Let $Y' = \text{vec}(X)\text{vec}(X)^T$ for any $X \in \Pi_n$; that this is a valid relaxation can be seen by showing that

$$Y' - \frac{1}{n^2}(Y'J_{n^2} + J_{n^2}Y') + \frac{2}{n^2}J_{n^2}$$

is feasible and has the same objective value as Y' . See Anstreicher [1, theorem 3.6] for more details.

Corollary 5. *SDP (8) has an unbounded integrality gap.*

Proof. We show that Y , as defined in Theorem 1, remains feasible. The objective function remains unchanged from SDP (1), so the analysis in Corollary 1 then implies that SDP (8) has an unbounded integrality gap.

By definition of Y , $Y^{(ii)} = \frac{1}{n}I_n$ for $i = 1, \dots, n$, so $\sum_{i=1}^n Y^{(ii)} = I_n$. Moreover, $\text{trace}(Y^{(ii)}) = \frac{1}{n}\text{trace}(I_n) = 1$ for $i = 1, \dots, n$, whereas A and B have zero diagonal, so the trace of any minor off-diagonal block is zero. Hence, $(\text{trace}(Y^{(ij)}))_{i,j=1}^n = I_n$.

Next, $F^T F = J_n \otimes I_n + I_n \otimes J_n$. Thus, $F^T F$ has a $J_n + I_n$ on each minor diagonal block and an I_n on each minor off-diagonal block. Because A and B have zero diagonal, $\text{trace}(A I_n) = \text{trace}(B I_n) = 0$, and the minor off-diagonal blocks make no contribution to $\text{trace}(Y F^T F)$. Hence,

$$\text{trace}(Y F^T F) = n \times \text{trace}\left(\frac{1}{n}I_n(J_n + I_n)\right) = \text{trace}(I_n(J_n + I_n)) = 2n.$$

By Claim 4 and the definition of Y , Y is nonnegative and symmetric. Hence, it remains to show that $Y - \frac{1}{n^2}J_{n^2} \geq 0$. We note that $e^{(n^2)}$ is an eigenvector of Y . In the notation of Claim 5, it is the eigenvector when $j = 0$

and $i = 1$. In Claim 5, we showed that the corresponding eigenvalue of nY was $2d = n$, so the corresponding eigenvalue of Y is one. Then

$$\left(Y - \frac{1}{n^2}J_{n^2}\right)e^{(n^2)} = Ye^{(n^2)} - \frac{1}{n^2}e^{(n^2)}\left(e^{(n^2)}\right)^T e^{(n^2)} = e^{(n^2)} - \frac{1}{n^2}e^{(n^2)}n^2 = 0e^{(n^2)}.$$

Any other eigenvector v of Y is orthogonal to $e^{(n^2)}$. Letting λ denote the corresponding eigenvalue,

$$\left(Y - \frac{1}{n^2}J_{n^2}\right)v = Yv - \frac{1}{n^2}e^{(n^2)}\left(e^{(n^2)}\right)^T v = \lambda v - 0v = \lambda v.$$

Thus, $Y - \frac{1}{n^2}J_{n^2}$ has the same spectrum as Y except that one eigenvalue (the eigenvalue one corresponding to eigenvector $e^{(n^2)}$) is shifted down by one (to eigenvalue zero). Consequently, all eigenvalues of $Y - \frac{1}{n^2}J_{n^2}$ are nonnegative, and $Y - \frac{1}{n^2}J_{n^2} \geq 0$. \square

Remark 1. De Klerk and Sotirov [9] provide a set of linear inequalities that can be added to SDP relaxations where $Y = \text{vec}(X)\text{vec}(X)^T$ is feasible for any permutation matrix $X \in \Pi_n$, the triangle inequalities. For all distinct r, s, t , these are that

$$0 \leq Y_{rs} \leq Y_{rr}, \quad Y_{rr} + Y_{ss} - Y_{rs} \leq 1, \quad -Y_{tt} - Y_{rs} + Y_{rt} + Y_{st} \leq 0, \quad Y_{tt} + Y_{rr} + Y_{ss} - Y_{rs} - Y_{rt} - Y_{st} \leq 1.$$

We note that these inequalities do not eliminate the feasible solutions defined in Equation (3):

$$Y_{ss} = Y_{rr} = Y_{tt} = \frac{1}{n},$$

while

$$0 \leq Y_{rs}, Y_{rt}, Y_{st} \leq \frac{1}{2n}.$$

The upper bound on off-diagonal entries can be seen directly by noting that $Y_{rs}, Y_{rt}, Y_{st} \in \{0, \frac{a_1}{2n}, \dots, \frac{a_{d-1}}{2n}, \frac{a_d}{n}, \frac{b_1}{2n}, \dots, \frac{b_{d-1}}{2n}, \frac{b_d}{n}\}$; by Lemmas 4 and 5, $0 \leq a_i, b_i \leq 1$, and it is straightforward to directly bound $a_d, b_d \leq \frac{1}{2}$ provided $n/g \geq 3$.

5. Conclusions

In this paper, we introduced simplicial TSP instances to show that the integrality gap of an SDP from de Klerk and Sotirov [8] is unbounded and, moreover, nonmonotonic. The simplicial TSP instances imply the unbounded integrality gap of every SDP relaxation of the TSP mentioned in the survey in Sotirov [27, section 2], as well as the unbounded integrality gap of an SDP from Anstreicher [1]. The simplicial instances thus form a litmus test for new SDP relaxations of the TSP and motivate two questions.

Question 1. Can one find an SDP relaxation of the TSP with finite integrality gap (without directly adding in the subtour elimination constraints of the subtour LP).

It would suffice, for example, to find SDP constraints that implied that scaled solutions lie in the minimum-spanning-tree polytope. It is also known that at some level of the Lasserre, Sherali–Adams, or Lovász–Schrijver hierarchies (Lasserre [21], Lovász and Schrijver [22], Sherali and Adams [25]), the corresponding SDPs give the convex hull of tours. It would be of interest to know if a constant integrality gap can be obtained at some constant level of the hierarchy.

Question 2. What are the integrality gaps of any of the TSP SDP relaxations when the subtour elimination constraints are added? Can any be shown to beat $\frac{3}{2}$?

To our knowledge, the only SDP for which Question 2 has been answered is for the SDP of Cvetković et al. [5]: Goemans and Rendl [11] show that any feasible solution to the subtour LP gives an equivalent feasible to their SDP of the same cost; adding the subtour elimination constraints to this SDP thus effectively is the same as just solving the subtour LP.

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Appendix. Proofs of Trigonometric and Algebraic Identities

In this appendix, we sketch pertinent results from Gutekunst and Williamson [14].

Lemma (Gutekunst and Williamson [14, lemma 4.8]). *Let n be even and $0 < k < n$ be an integer. Then*

$$\sum_{j=1}^d \cos\left(\frac{2\pi jk}{n}\right) = \frac{-1 + (-1)^k}{2}.$$

Proof. Our identity is a consequence of Lagrange’s trigonometric identity (see Jeffrey and Dai [18, identity 14 in section 2.4.1.6]), which states, for $0 < \theta < 2\pi$, that

$$\sum_{j=1}^m \cos(j\theta) = -\frac{1}{2} + \frac{\sin\left((m + \frac{1}{2})\theta\right)}{2 \sin\left(\frac{\theta}{2}\right)}.$$

Taking $\theta = \frac{2\pi k}{n}$ and using $n = 2d$, we obtain

$$\begin{aligned} \sum_{j=1}^d \cos\left(\frac{2\pi k}{n} j\right) &= -\frac{1}{2} + \frac{\sin\left(\pi k + \frac{\pi k}{n}\right)}{2 \sin\frac{\pi k}{n}} \\ &= -\frac{1}{2} + (-1)^k \frac{1}{2}, \end{aligned}$$

where we recall that $\sin(\pi + \theta) = -\sin(\theta)$. □

Notice that when $k = 0$ or $k = n$, the sum is d .

Proposition (Gutekunst and Williamson [14, proposition 3.2]). *We have that, (a) $\sum_{i=1}^d a_i = \sum_{i=1}^d b_i = 1$. Equivalently, $a^{(0)} = b^{(0)} = 1$. We have that: (b) $b^{(k)} = -(1 - \frac{2}{n}) a^{(k)} - \frac{2}{n}$. (c) For $k = 1, \dots, d$,*

$$a^{(k)} = \begin{cases} \frac{d-2}{n-2}, & \text{if } k = 1, \\ -\frac{2}{n-2}, & \text{otherwise.} \end{cases}$$

We have that: (d) $b_1 \leq \frac{4\pi^2}{n^3}$.

Proof. For the first result, we use the identity

$$\sum_{j=1}^d \cos\left(\frac{2\pi jk}{n}\right) = \frac{-1 + (-1)^k}{2}$$

with $k = 1$. Then

$$\sum_{i=1}^d a_i = \frac{2}{n-2} \sum_{i=1}^d \left(\cos\left(\frac{\pi i}{d}\right) + 1 \right) = \frac{2}{n-2} (-1 + d) = 1.$$

Similarly,

$$\sum_{i=1}^d b_i = \sum_{i=1}^{d-1} \left(\frac{4}{n} - \left(1 - \frac{2}{n}\right) a_i \right) + \left(\frac{2}{n} - \left(1 - \frac{2}{n}\right) a_d \right) = (d-1) \frac{4}{n} + \frac{2}{n} - \left(1 - \frac{2}{n}\right) \sum_{i=1}^d a_i = 1.$$

For the second result,

$$\begin{aligned} b^{(k)} &= \sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) b_i \\ &= \left(\sum_{i=1}^{d-1} \cos\left(\frac{2\pi ik}{n}\right) \left(\frac{4}{n} - \left(1 - \frac{2}{n}\right) a_i \right) \right) + \cos\left(\frac{2\pi dk}{n}\right) \left(\frac{2}{n} - \left(1 - \frac{2}{n}\right) a_d \right) \\ &= \frac{4}{n} \left(\sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) \right) - \left(1 - \frac{2}{n}\right) \left(\sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) a_i \right) - \cos(\pi k) \left(\frac{2}{n} \right). \end{aligned}$$

Using Lemma 2:

$$\begin{aligned} &= \frac{4}{n} \left(\frac{-1 + (-1)^k}{2} \right) - \left(1 - \frac{2}{n} \right) a^{(k)} - (-1)^k \left(\frac{2}{n} \right) \\ &= - \left(1 - \frac{2}{n} \right) a^{(k)} - \frac{2}{n}. \end{aligned}$$

For the third result, we use the product-to-sum identity for cosines and then do casework using Lemma 2. We have

$$\begin{aligned} a^{(k)} &= \sum_{i=1}^d \cos\left(\frac{2\pi ik}{n}\right) a_i, \\ &= \frac{2}{n-2} \sum_{i=1}^d \left(\cos\left(\frac{2\pi ik}{n}\right) + \cos\left(\frac{2\pi ik}{n}\right) \cos\left(\frac{\pi i}{d}\right) \right), \\ &= \frac{2}{n-2} \sum_{i=1}^d \left(\cos\left(\frac{2\pi ik}{n}\right) + \frac{1}{2} \cos\left(\frac{2\pi i(k+1)}{n}\right) + \frac{1}{2} \cos\left(\frac{2\pi i(k-1)}{n}\right) \right). \end{aligned}$$

We cannot apply Lagrange’s trigonometric identity only when $k = 1$, so

$$\begin{aligned} &= \begin{cases} \frac{2}{n-2} \left(\frac{-1+(-1)^k}{2} + \frac{-1+(-1)^{k+1}}{4} + \frac{-1+(-1)^{k-1}}{4} \right), & \text{if } k > 1 \\ \frac{2}{n-2} \left(-1 + 0 + \frac{1}{2}d \right), & \text{if } k = 1 \end{cases} \\ &= \begin{cases} -\frac{2}{n-2}, & \text{if } k > 1 \\ \frac{d-2}{n-2}, & \text{if } k = 1. \end{cases} \end{aligned}$$

Finally, the fourth result follows from Taylor series with remainder,

$$\cos\left(\frac{\pi}{d}\right) = 1 - \frac{\pi^2}{2d^2} + \frac{1}{4!} \frac{\pi^4}{d^4} \cos(\xi_{1/d}) \geq 1 - \frac{\pi^2}{2d^2},$$

where $\xi_{1/d} \in [0, \frac{1}{d}]$. Hence,

$$b_1 = \frac{2}{n} \left(1 - \cos\left(\frac{\pi}{d}\right) \right) \leq \frac{2}{n} \frac{\pi^2}{2d^2} = \frac{4\pi^2}{n^3}. \quad \square$$

Endnotes

¹To find this shared set of eigenvectors, note that $J_m = e^{(m)}(e^{(m)})^T$ is a rank-one matrix and that

$$J_m e^{(m)} = e^{(m)}(e^{(m)})^T e^{(m)} = m e^{(m)}.$$

The only nonzero eigenvector of J_m is thus $e^{(m)}$ with corresponding eigenvalue m . All other eigenvectors have corresponding eigenvalue zero, and a convenient basis for them is $e_1^{(m)} - e_i^{(m)}$ for $i = 2, \dots, m$. Then

$$J_m (e_1^{(m)} - e_i^{(m)}) = e^{(m)} - e^{(m)} = 0 (e_1^{(m)} - e_i^{(m)}).$$

The vectors $e^{(m)}, e_1^{(m)} - e_2^{(m)}, \dots, e_1^{(m)} - e_m^{(m)}$ are linearly independent and so form an eigenbasis for J_m . To extend these to find eigenvectors of $(I_2 \otimes J_d) - I_n, (J_2 - I_2) \otimes J_d,$ and $2I_n,$ we use (1) the spectral properties of Kronecker products noted in the Introduction and (2) the fact that if v is an eigenvector of a matrix M with corresponding eigenvalue λ , then v is also an eigenvector of $M - I$ with corresponding eigenvalue $\lambda - 1$:

$$(M - I)v = \lambda v - v = (\lambda - 1)v.$$

²These values come from assuming that

$$\left(\frac{n}{g} - 1 \right) a_i + \frac{g-1}{g} n b_i = \begin{cases} 2, & i < d, \\ 1, & i = d. \end{cases}$$

The intuition for choosing these values of b_i is to impose an analogue of the degree constraints from Gutekunst and Williamson [14].

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