On the Dual of the Lovász Theta Prime Number for the Disjunctive Product of Graphs

by

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1 Introduction

The Lovász theta number ϑ was originally defined in [14], where it was used as an upper bound on the *Shannon capacity* of a graph. The Shannon capacity [20] is important in coding theory, as it essentially dictates how efficient information can be sent through a noisy channel, without the possibility of errors. Since there is currently no algorithm known to determine the Shannon capacity of an arbitrary graph, upper bounds, such as the Lovász theta number, are useful for both finding bounds on the Shannon capacity in practical applications, and for investigating properties of the Shannon capacity.

In a more general setting, ϑ is an upper bound on the *independence number* of a graph. Since the independence number is hard to compute [11], and frequently occurs in discrete optimization problems, upper bounds can, again, provide useful information.

ϑ is not the only upper bound on the independence number of a graph. Schrijver, for example, introduced a strengthening of this upper bound, ϑ^-, in [16]. On the other hand, Szegedy introduced a weakened version ϑ^+ of the theta number in [8]. In recent years, these three functions, especially ϑ^-, have been extremely useful in solving hard optimization problems. For example, a similar bound was used to prove upper bounds on the kissing number [15]. Another application is the Cohn-Elkies bound on the sphere packing density [2]. This upper bound shares a remarkable similarity with the bound ϑ^- on the independence number. In 2022, Viazovska was awarded the Fields medal for her proof of the optimal sphere packing density in dimensions 8 and 24. Her proofs [21], [4] made use of the Cohn-Elkies bound.

A reason for the widespread use of the functions ϑ, ϑ^- and ϑ^+, is that they have several useful mathematical properties. In particular, their multiplicity under graph products makes them useful for proving bounds on the independence number for certain, large graphs. In [3], Cohn, de Laat and Salmon used a procedure similar to the multiplicity of ϑ^- under the disjunctive graph product, among other changes, to improve the Cohn-Elkies bound for lattice sphere packings.

Even though it is proven that ϑ^- is multiplicative under the disjunctive graph product, there currently exists no dual construction that attains the optimal value of $\vartheta^-(G * H)$, given optimal solutions to $\vartheta^-(G)$ and $\vartheta^+(G)$. The goal of this thesis is to present such a dual construction. Although the presented construction does not work on all graphs, there is reason to believe that a similar construction will work for the Cohn-Elkies bound.

In **section** 2, the background information needed to work with ϑ and its variants is given. Some basic concepts from semidefinite optimization are treated, and definitions from graph theory are given that will be used in the rest of the thesis.

After that, in **section** 3, the functions ϑ, ϑ^- and ϑ^+ will be defined, and their relationship to the independence number and clique cover number is shown. Then, some properties of ϑ, ϑ^- and ϑ^+ that hold for all vertex-transitive graphs are proved. A new proof is provided for the equation $\vartheta^-(G)\vartheta^+(\overline{G}) = |V_G|$.

Section 4 is dedicated to the multiplicity of ϑ, ϑ^- and ϑ^+. Firstly, some proofs for the multiplicity of ϑ, ϑ^- and ϑ^+ are given. A construction is then given, that under an additional assumption shows the multiplicity of ϑ^- using a minimization formulation. It will subsequently be shown that even though this additional assumption does not hold for arbitrary graphs, all cyclic graphs have solutions that satisfy this condition.

In **section** 5, it will be shown that for abelian graphs, the computation of ϑ, ϑ^- and ϑ^+ reduces to solving a linear program. This linear program is used to prove an upper bound on the spectral gap achievable by optimal solutions to the dual semidefinite program for ϑ^- using Fourier inversion. This lower This is an indication that the construction for the multiplicity of ϑ^- given in section 3 is likely to hold when graphs are sparse, and have abelian automorphism groups.

Lastly, in section 6, the Delsarte linear programming bound [7] is used to show that generally the construction does not work for Hamming graphs, and a conjecture is formulated that asymptotically the construction works if and only if the Hamming graph is defined in a certain way.

2 Background information

2.1 Linear and semidefinite programs

A linear program (LP) is an optimization problem with linear inequalities as constraints.

Definition 1 (LP)**.** *A linear program is an optimization problem, that aims to either maximize, or minimize a linear combination of some variables. These variables have to satisfy some linear inequalities. For each primal maximization LP, as given in equation* (1)*, there is a dual minimization LP, given in equation* (2)*.*

$$\begin{aligned} \max z = c^T x \quad & s.t. \\ A_j x = b_j \; \forall j \in M \\ A_j x \geq b_j \; \forall j \in \overline{M} \\ A_j x \leq b_j \; \forall j \in \tilde{M} \\ x_k \geq 0 \; \forall k \in N \\ x_k \leq 0 \; \forall k \in \tilde{N} \\ x_k \in \mathbb{R} \; \forall k \in \overline{N} \end{aligned} \tag{1}$$

$$\begin{aligned} \min w = b^T y \quad & s.t. \\ y_j \in \mathbb{R} \; \forall j \in M \\ y_j \geq 0 \; \forall j \in \overline{M} \\ y_j \leq 0 \; \forall j \in \tilde{M} \\ (A^T)_k y \leq c_k \; \forall k \in N \\ (A^T)_k y \geq c_k \; \forall k \in \tilde{N} \\ (A^T)_k y = c_k \; \forall k \in \overline{N} \end{aligned} \tag{2}$$

Usually, primal and dual LPs have the same value [1, p. 66]. This is called strong duality.

Theorem 1 (LP duality)**.** *LPs* (1) *and* (2) *have the same optimal value, $z = w$, if this value exists and is finite.*

A way of generalizing LPs is to add constraints that variables have to lie inside some convex cone. Surprisingly, it can be shown that for many such problems duality still holds in a way. One particularly interesting class of convex cones in combinatorial optimization are positive semidefinite (PSD) matrices of a fixed dimension.

Definition 2 (PSD)**.** *Let S^n denote the set of symmetric $n \times n$ matrices. Let S^n_+ denote the set of symmetric matrices A such that $x^T A x \geq 0$ for all $x \in \mathbb{R}^n$. Matrices A such that $x^T A x \geq 0$ for all vectors x are called positive semidefinite (PSD).*

Because of the spectral theorem, symmetric matrices are PSD if and only if all eigenvalues are nonnegative. We are now able to define semidefinite programs.

Definition 3 (SDP)**.** *A semidefinite program (SDP) aims to either maximize, or minimize a linear combination of the entries of a matrix A, provided that the entries satisfy a set of linear equalities, and $A \in S^n_+$. Similar to LPs, for each primal maximization SDP, as given in equation* (3)*, a dual minimization SDP, given by equation* (4)*, can be defined.*

$$\begin{aligned} \sup z = \operatorname{Tr}(CA) \;\; s.t. \\ A \in K, \\ \operatorname{Tr}(B_i A) = b_i \; \forall i \in M. \end{aligned} \tag{3}$$

$$\begin{aligned} \inf w = b^T y \;\; s.t. \\ y \in \mathbb{R}^M, \\ \sum_{j \in M} y_j B_j - C \in S_+^n. \end{aligned} \tag{4}$$

SDPs are a subclass of *conic programs*, a type of optimization problem. Hence, several results from conic optimization can be used. Although a pair of primal and dual SDPs do not have the same optimal value in general, Slater's criterion, as stated in [13, p. 40], gives a sufficient condition for when a pair of primal and dual conic programs have the same optimal value. This theorem can be applied to SDPs.

Theorem 2 (Slater's criterion)**.** *Suppose we have a pair of primal and dual conic program. Let z be the supremum of the primal, and w be the infimum of the dual.*

- *If the dual conic program is bounded from below, and if it is strictly feasible, then the primal conic program attains its supremum, and $z = w$.*
- *If the primal conic program is bounded from above, and if it is strictly feasible, then the dual conic program attains its infimum, and $z = w$.*

To show strict feasibility for primal SDPs, as given in (3), it must be shown that a feasible solution A exists, that has strictly positive eigenvalues. Similarly, to show strict feasibility for dual SDPs, as given in (4), it must be shown that a feasible solution y exists, such that the matrix $\sum_{j \in M} y_j B_j - C$ has strictly positive eigenvalues.

Suppose all values on the i-th row and column of a matrix A, except the value on the diagonal, are 0. Then the value on the diagonal is an eigenvalue, and $A \in S_+^{n+1} \Leftrightarrow A_{ii} \geq 0 \wedge A^{ii} \in S_+^n$, where A^{ii} is the matrix obtained by removing the i-th row and column from A. Because of this, we can add linear inequalities to an SDP by formally adding new variables to the diagonal, and adding constraints to ensure this variable has the same value as the linear combination of the variables in the inequality. It can furthermore be shown that strict inequality in these linear inequalities is not required for Slater's criterion to show that there is no duality gap between the primal and dual SDPs.

There exist algorithms to solve SDPs with polynomial time complexity in both the input size, and the logarithm of the precision. The first of these algorithms was the ellipsoid method [9], but nowadays, much faster algorithms exist, using interior point methods.

2.2 Graph theory preliminaries

We will consider finite, simple graphs $G = (V_G, E_G)$, where V_G is the vertex set, and E_G the edge set. $\overline{E_G}$ is the set of simple edges that are not in E_G. The complement graph of G is defined as $\overline{G} = (V_G, \overline{E_G})$. A graph automorphism is defined as follows.

Definition 4 (Graph automorphisms)**.** *A graph automorphism ρ is a permutation of the vertices V_G such that $(i, j) \in E_G \Leftrightarrow (\rho(i), \rho(j)) \in E_G$. The set of automorphisms of G is denoted* $\mathrm{Aut}(G)$*.*

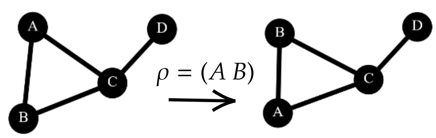
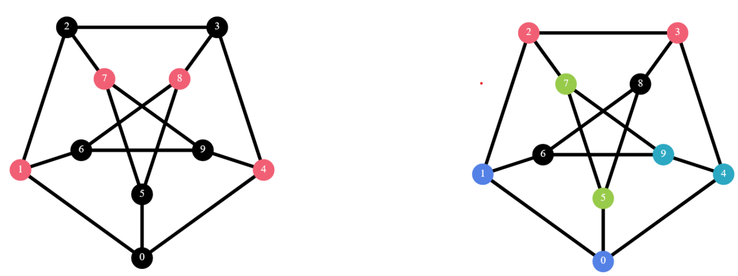


Figure 1: An example of an automorphism ρ, that swaps the vertices A and B.

A special set of graphs are graphs in which for each pair of vertices i, j, there exists an automorphism that maps i onto j. These graphs are called *vertex-transitive*.

Definition 5 (Vertex-transitive graphs)**.** *A graph G is called vertex-transitive, if for all $i, j \in V_G$ there is a $\rho \in$* $\mathrm{Aut}(G)$ *such that $\rho(i) = j$.*

In many optimization problems, the independence number α or the clique cover number $\overline{\chi}$ of a graph are important. These functions $\alpha(G)$ and $\overline{\chi(G)}$ can give meaningful insight into the structure of a graph.



(a) The Petersen graph has independence number 4

(b) The Petersen graph has clique cover number 5

Definition 6 (Independence number)**.** *Let G be a graph. An independent set S of G is a subset of V_G, such that for every pair $i, j \in S$, it holds that $(i, j) \notin E_G$. The independence number $\alpha(G)$ is the maximum cardinality among independent sets of G.*

Definition 7 (Clique cover number)**.** *Let G be a graph. A clique S of G is a subset of V_G, such that for every disjoint pair $i, j \in S$, it holds that $(i, j) \in E_G$. The clique cover number $\overline{\chi}(G)$ is the smallest cardinality of subsets of the cliques of G such that each element of V_G is in precisely one of the selected cliques.*

Computing the independence number of arbitrary graphs, and computing the clique cover number of arbitrary graphs are NP-complete problems, and are thus not practically computable for large graphs [11]. To still get an insight into the structure of large graphs, heuristic algorithms, or approximation algorithms can be used. A mathematically particularly interesting technique for this problem are SDP-based relaxations of the independence number and clique cover number. Since SDPs are continuous optimization problems, instead of discrete optimization problems, and have well-known properties, these relaxations can be useful in mathematical proofs.

3 The Lovász theta function, and its variants

3.1 Definition of ϑ, ϑ^- and ϑ^+

In [14], Lovász introduced the SDP-based function ϑ as an upper bound on the independence number of a graph. He proceeds to show that, due to a remarkable property of this function, ϑ is also an upper bound on the Shannon capacity of a graph. For some graphs, such as the 5-cycle C_5, this bound is equal to the Shannon capacity. Although ϑ is generally not equal to the Shannon capacity, it can be very hard to show that a lower bound on the Shannon capacity exists for an arbitrary graph. Such graphs, for which equality does not hold, were first discovered by Haemers, in [10]. He showed that there exists a graph with 84 vertices, for which the rank-based Haemers bound on the Shannon capacity is lower than the Lovász theta function ϑ. However, the Haemers bound is hard to compute for arbitrary graphs, and does not have some of the useful properties of ϑ.
The Lovász theta function ϑ is defined as follows.

Definition 8. *Suppose G is a (finite) graph. Let $\mathcal{M}_G$ be the set of $|V_G| \times |V_G|$ matrices A satisfying*

$$\begin{aligned} A_{i,j} &= 0 \, \forall (i,j) \in E_G, \\ Tr(A) &= 1. \end{aligned} \tag{5}$$

Then $\vartheta(G)$ is defined as

$$\vartheta(G) := \sup_{A \in S_+^{V_G} \cap \mathcal{M}_G} Tr(JA). \tag{6}$$

The Lovász theta function ϑ can be strengthened by adding additional constraints. This way, better upper bounds on the independence number of a graph can be obtained. In [16], Schrijver introduced such a strengthening ϑ^- of ϑ.

Definition 9. *Suppose G is a (finite) graph. Let $\mathcal{M}_G^-$ be the set of $|V_G| \times |V_G|$ matrices A that satisfy*

$$\begin{aligned} A_{i,j} &= 0 \, \forall (i,j) \in E_G, \\ A_{i,j} &\geq 0 \, \forall (i,j) \in V_G^2, \\ Tr(A) &= 1. \end{aligned} \tag{7}$$

Then $\vartheta^-(G)$ is defined as

$$\vartheta^-(G) := \sup_{A \in S_+^{V_G} \cap \mathcal{M}_G^-} Tr(JA). \tag{8}$$

This strengthened function ϑ^- is still an upper bound on the independence number, but not on the Shannon capacity. On the other hand, the constraints in (5) can also be weakened. To this end, Szegedy introduced the relaxation ϑ^+ of ϑ. While ϑ^+ is a worse upper bound on the independence number, it will prove to be a better bound on the clique cover number. Define ϑ^+ as follows.

Definition 10. *Suppose G is a finite graph. Let $\mathcal{M}_G^+$ be the set of $|V_G| \times |V_G|$ matrices A that satisfy*

$$\begin{aligned} A_{ij} &\leq 0 \, \forall (i,j) \in E_G, \\ \mathrm{Tr}(A) &= 1. \end{aligned} \tag{9}$$

Then $\vartheta^+(G)$ is defined as

$$\vartheta^+(G) := \sup_{A \in S_+^{V_G} \cap \mathcal{M}_G^+} \mathrm{Tr}(JA). \tag{10}$$

The following theorem shows that ϑ^-, ϑ and ϑ^+ are indeed bounds on the independence number and the clique covering number.

Theorem 3 (Sandwich theorem)**.** *Suppose G is a finite graph. Then the following inequalities hold.*

$$\alpha(G) \leq \vartheta^-(G) \leq \vartheta(G) \leq \vartheta^+(G) \leq \overline{\chi}(G) \tag{11}$$

Proof. To prove that $\alpha(G) \leq \vartheta(G)$, let $S \subset V_G$ be an arbitrary maximum independent set of G. Let the vector $\mathbb{1}_S$ have values 1 for all indices that are in S, and 0 for all other indices. Then since the matrix $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^T$ is PSD, and satisfies all the properties of $\mathcal{M}_G^-$, we have $\alpha(G) = \mathrm{Tr}(J\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^T) \leq \vartheta^-(G)$. The second and third inequality follow directly from $\mathcal{M}_G^- \subset \mathcal{M}_G \subset \mathcal{M}_G^+$. To prove the last inequality, we use a slightly modified version of Schrijvers proof that $\vartheta \leq \overline{\chi}^*$ in [17, p. 1153]. Let A achieve the optimal objective value in SDP (10). Let $S = \{c_1, \ldots, c_k\}$ be a set of cliques covering V_G, that has the smallest possible cardinality. Let $\mathbb{1}_{c_j}$ be the vector with value 1 for all indices in c_j, and 0 for all other indices. Then since A is PSD, we have

$$\begin{aligned} 0 &\leq \sum_{j=1}^k \left(\overline{\chi}(G)\mathbb{1}_{c_j} - \mathbf{1}\right)^T A \left(\overline{\chi}(G)\mathbb{1}_{c_j} - \mathbf{1}\right) \\ &= \overline{\chi}(G)^2 \sum_{j=1}^k \mathbb{1}_{c_j}^T A \mathbb{1}_{c_j} - 2\overline{\chi}(G) \sum_{j=1}^k \mathbb{1}_{c_j}^T A \mathbf{1} + \overline{\chi}(G)\mathbf{1}^T A \mathbf{1}. \end{aligned} \tag{12}$$

Now per definition we have $\mathbf{1}^T A \mathbf{1} = \mathrm{Tr}(JA) = \vartheta^+(G)$. Furthermore, $\sum_{j=1}^k \mathbb{1}_{c_j}^T = \mathbf{1}^T$ follows from the fact that S covers G. Also, if $u \neq v$, and $u, v \in C_j$, then u and v are connected, so $A_{uv} \leq 0$. Therefore, (12) is less than or equal to

$$\overline{\chi}(G)^2 \mathrm{Tr}(A) - 2\overline{\chi}(G)\mathbf{1}^T A \mathbf{1} + \overline{\chi}(G)\mathbf{1}^T A \mathbf{1} = \overline{\chi}(G)^2 - \overline{\chi}(G)\vartheta^+(G). \tag{13}$$

Since now we have proven that $0 \leq \overline{\chi}(G)^2 - \overline{\chi}(G)\vartheta^+(G)$, it follows that $\vartheta^+(G) \leq \overline{\chi}(G)$. □

3.2 Duality of ϑ, ϑ^- and ϑ^+

Since the functions ϑ, ϑ^- and ϑ^+ are SDPs, they have dual SDPs. Since there are multiple equivalent ways to write the same SDP, due to substitutions, the notation used in existing literature varies. In this thesis, we will use the notation used in lemma 1 to express the dual SDP of (6).

Lemma 1. *The dual formulation of $\vartheta(G)$ is equivalent to*

$$\inf_{A \in \mathcal{L}_G} \Lambda(J + A), \tag{14}$$

where $\Lambda(J+A)$ denotes the largest eigenvalue of $J+A$, and $\mathcal{L}_G$ denotes the set of symmetric $|V_G| \times |V_G|$ matrices A satisfying the constraints

$$A_{i,j} = 0 \, \forall i, j : (i,j) \in \overline{E_G} \vee i = j. \tag{15}$$

Proof. The dual SDP of ϑ is given by definition 3:

$$\begin{aligned} &\inf t \\ \text{s.t. } & y \in \mathbb{R}^{E_G}, \\ tI + \sum_{(i,j) \in E_G} & y_{ij} e_{ij} - J \in S_+^{V_G}, \end{aligned} \tag{16}$$

where e_{ij} is the matrix with value 1 at index i, j, and 0 at all other indices. We can thus view $-\sum_{(i,j)\in E_G} y_{ij} e_{ij}$ as a (symmetric) matrix A, with $A_{ij} = 0$ whenever (i,j) is not in E_G. Since for symmetric $n \times n$ matrices X, $\Lambda(X) \le t$ is equivalent to $tI - X \in S_+^n$, minimizing t is equivalent to minimizing $\Lambda(J+A)$. □

We can also find similar expressions for the dual SDPs of ϑ^- and ϑ^+. These are given without proof in lemmas 2 and 3.

Lemma 2. *The dual formulation of $\vartheta^-(G)$ is equivalent to*

$$\inf_{A \in \mathcal{L}_G^-} \Lambda(J + A), \tag{17}$$

where $\mathcal{L}_G^-$ is the set of symmetric $|V_G| \times |V_G|$ matrices A that satisfy the constraints

$$A_{i,j} \ge 0 \, \forall i, j : (i,j) \in \overline{E_G} \vee i = j. \tag{18}$$

Lemma 3. *The dual formulation of $\vartheta^+(G)$ is equivalent to*

$$\inf_{A \in \mathcal{L}_G^+} \Lambda(J + A), \tag{19}$$

Where $\mathcal{L}_G^+$ is the set of symmetric $|V_G| \times |V_G|$ matrices A such that

$$\begin{aligned} &A_{ij} = 0 \, \forall i, j : (i,j) \in \overline{E_G} \vee i = j, \\ &A_{ij} \le 0 \, \forall (i,j) \in E_G. \end{aligned} \tag{20}$$

The matrix $\frac{1}{|V_G|}I$ is a feasible solution of the primal SDPs of ϑ, ϑ^- as well as ϑ^+, and has strictly positive eigenvalues. Furthermore, $t = |V_G| + 1$ and $y = \mathbf{0}$ is a feasible solution of the dual SDPs of ϑ, ϑ^- and ϑ^+, and the eigenvalues of $(|V_G|+1)I - J$ are strictly positive. Therefore, we know that the primal formulations of ϑ, ϑ^- and ϑ^+ have the same optimal value as their dual formulations, respectively, and this optimal value is attained in both the primal and dual SDP formulations.

Slater's criterion is a rather deep result. Schrijver gives an alternative proof in theorem 67.7 of [17], that does not rely on Slater's criterion. However, an important part of this proof is missing from the book, and the proof is thus not correct. Therefore, a corrected version of this proof is included in theorem 18 of appendix A.

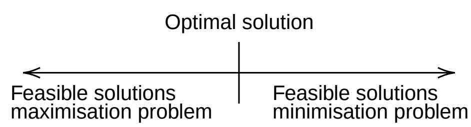


Figure 3: The values of ϑ^-, ϑ and ϑ^+ can be proven, by finding feasible solution to both the primal and dual problem that have the same objective value.

Even though the values of ϑ^-, ϑ and ϑ^+ can be approximated arbitrarily well in polynomial time of the problem size, as well as the logarithm of the accuracy, it can still be hard to prove these values analytically for specific graphs. One way to do this, is by giving a feasible solution for both the primal and dual SDPs that achieve the same objective value λ. Because of strong duality, the optimal objective value of both the maximization and minimization problem have to be λ.

Since often, there is not one single optimal solution to SDPs (14), (17) and (19), not much can be said in general about the entries of optimal solutions to these SDPs. The following result, however, guarantees that there exists a matrix A minimizing (17), of which the values on the diagonal are all 0.

Lemma 4. *Decreasing values on the diagonal of a symmetric matrix A does not increase its largest eigenvalue.*

Proof. Let D be a diagonal matrix with nonnegative entries. Let $v \in \mathrm{R}^{V_G}$ be an arbitrary vector. Then since D is PSD, it follows that

$$v^T(A - D)v = v^T Av - v^T Dv \leq v^T Av, \tag{21}$$

and hence the largest eigenvalue of A can not increase when decreasing values on the diagonal. $\square$

Note that it is in general not required for a matrix A minimizing (17) to have only zeroes on the diagonal, since it might happen that the entries at some indices i of the eigenvector belonging to the largest eigenvalue of A are zero, in which case that eigenvalue does not depend on A_{ii}.

3.3 Vertex-transitive graphs, and some properties of ϑ, ϑ^- and ϑ^+

More can be said about the solutions for ϑ^-, ϑ and ϑ^+ when the graph has a lot of symmetries. For example, in theorem 8 of [14] Lovász proved the following result for vertex-transitive graphs.

Theorem 4. *Suppose G is vertex-transitive, then the following holds:*

$$\vartheta(G)\vartheta(\overline{G}) = |V_G|. \tag{22}$$

This identity in general not true, so the assumption that G is vertex-transitive is necessary. However, Lovász proved in corollary 2 of [14] that

$$\vartheta(G)\vartheta(\overline{G}) \geq |V_G|. \tag{23}$$

ís always true. Remarkably, a similar identity as (22) also holds for $\vartheta^-(G)$ and $\vartheta^+(G)$ whenever G is vertex-transitive. To arrive at the result, we will first need to make some observations about these functions. Firstly, we can show that restricting to solutions A of the primal and dual formulations of ϑ, ϑ^- and ϑ^+ does not affect the optimal value of these SDPs.

Lemma 5 (Automorphism invariant solutions of ϑ, ϑ^-, ϑ^+)**.** *Let $S \subset \mathrm{Aut}(G)$ be a subgroup consisting of automorphisms of G. We can assert that matrices A optimizing SDPs* (6)*,* (8)*,* (10)*,* (14)*,* (17) *and* (19) *are invariant under S without lowering the optimal value.*

Proof. Suppose A is a matrix optimizing either one of these SDPs. Then, by relabeling the vertices using automorphisms, we get other optimal solutions. Because these SDPs are convex optimization problems, the following is also a solution:

$$B := \frac{1}{|S|}\sum_{\rho \in S} \rho(A). \tag{24}$$

Suppose A maximizes one of the primal SDPs. Then

$$\mathrm{Tr}\left(\frac{1}{|S|}\sum_{\rho\in S}\rho(A)\right) = \frac{1}{|S|}\sum_{\rho\in S}\mathrm{Tr}(\rho(A)) = \mathrm{Tr}(A), \tag{25}$$

so the objective value of B is the same as that of A. On the other hand, if A minimizes one of the dual SDPs, then let v be an eigenvector belonging to the largest eigenvalue of $J + B$. Then it follows from the Rayleigh quotient that

$$\Lambda\left(J+B\right) = \frac{v^T\left(J+B\right)v}{v^Tv} = \frac{1}{|S|}\sum_{\rho\in S}\frac{v^T(J+\rho(A))v}{v^Tv} \leq \Lambda(J+A). \tag{26}$$

Therefore, in either case, B is also an optimal solution. Furthermore, B is invariant under the automorphisms in S, since

$$\left[\sum_{\rho\in S}\rho(A)\right]_{ij} = \left[\sum_{\rho\in S}q\rho(A)\right]_{q(i)q(j)} = \left[\sum_{\rho\in S}\rho(A)\right]_{q(i)q(j)} \tag{27}$$

for all automorphisms $q \in S$. $\square$

Since the automorphism group of vertex-invariant graphs is in a sense large enough, the following result shows that the eigenvector belonging to the largest eigenvalue of $J + A$ for any automorphism invariant solution A is the all-ones vector e_G.

Lemma 6. *Let G be a vertex-transitive graph. Suppose A is an automorphism invariant, optimal solution of* (14), (17) *or* (19). *Then the objective value of A is equal to $|V_G| + \sum_{a \in V_G} A_{ba}$.*

Proof. The proofs for ϑ, ϑ^- and ϑ^+ are the same. Therefore, let A, w.l.o.g, minimize (14). We first show that e_G is indeed an eigenvalue of A. Let $a, b \in V_G$ be arbitrary. Let $\rho \in \mathrm{Aut}(G)$ be such that $\rho(a) = b$. Then we have

$$(Ae_G)_b = \sum_{c \in V_G} A_{bc} = \sum_{c \in V_G} A_{\rho(a)\rho(\rho^{-1}(c))} = \sum_{c \in V_G} A_{ac} = (Ae_G)_a. \tag{28}$$

Therefore e_G is an eigenvector of A. Since it is also an eigenvector of J, it is an eigenvector of $J + A$, and all other eigenvectors of $J + A$ are orthogonal to e_G. Now suppose e_G is **not** one of the eigenvectors belonging to the largest eigenvalue of $J + A$. Then let $v \neq e_G$ be an eigenvector of $J + A$. Let us now consider positive scalar multiples of A. Let $0 \leq \lambda < 1$ be arbitrary. We then have

$$\begin{aligned} (J + \lambda A)v &= \lambda A v \\ (J + \lambda A)e_G &= |V_G| + \lambda A e_G \end{aligned} \tag{29}$$

We see that the eigenvalues change linearly with λ. Let w be an eigenvector belonging to the largest eigenvector λ_w of A, and λ_{e_G} be the eigenvalue of A belonging to e_G. Then, if we let $\lambda := \frac{|V_G|}{\lambda_w - \lambda_{e_G}}$. Now since $\lambda_w > |V_G| + \lambda_{e_G}$, it follows that $0 \leq \lambda < 1$. Suppose $v \neq e_G$ is an eigenvector of $J + A$, with eigenvalue λ_v. Then $\lambda_v \leq \lambda\lambda_w = |V_G| + \lambda\lambda_{e_G}$. Hence, we get a solution with a lower objective value. This is a contradiction. Therefore, e_G is an eigenvector belonging to the largest eigenvalue of $J + A$. $\square$

Lemma 6 can be used to prove a relation between ϑ^- and ϑ^+ similar to theorem 4. This relation was first proven in [8]. We, however, propose an alternative proof using substitutions to show equality of $|V_G|\vartheta^-(G)^{-1}$ and $\vartheta^+(\overline{G})$.

Theorem 5. *Suppose G is vertex-transitive. Then the following equality holds:*

$$\vartheta^-(G)\vartheta^+(\overline{G}) = |V_G|. \tag{30}$$

Proof. As a result of lemma 6, we get the following equivalent formulation of ϑ^-, by enforcing that the eigenvalue belonging to e_G must be the largest eigenvalue:

$$\begin{aligned}\vartheta^-(G) = \min_{A \in S^{V_G}} & |V_G| + \frac{1}{|V_G|}\mathrm{Tr}(JA) \\ \text{s.t. } & \rho(A) = A \,\forall \rho \in \mathrm{Aut}(G), \\ \left(|V_G| + \frac{1}{|V_G|}\mathrm{Tr}(JA)\right) & I - A \in S_+^{V_G}, \\ & A_{ij} \geq 0 \,\forall (i,j) :\in \overline{E_G} \vee i = j.\end{aligned} \tag{31}$$

Define $C := \left(|V_G| + \frac{1}{|V_G|}\mathrm{Tr}(JA)\right) I - A$. Because of lemma 4, we can assume that the sum of the values on the diagonal of A is 0. Therefore $\mathrm{Tr}(C) = |V_G|^2 + \mathrm{Tr}(JA)$. Furthermore, we must have $\mathrm{Tr}(C) = |V_G|^2$. We hence get the following, equivalent LP:

$$\begin{aligned}\vartheta^-(G) = \min_{C \in S^{V_G}} & \frac{1}{|V_G|}\mathrm{Tr}(C) \\ \text{s.t. } & C_{i,j} \leq 0 \,\forall (i,j) \in \overline{E_G}, \\ \rho(C) - C = & \mathbf{0} \,\forall \rho \in \mathrm{Aut}(G), \\ C \in & S_+^{V_G}, \\ \mathrm{Tr}(JC) = & |V_G|^2.\end{aligned} \tag{32}$$

Now, we must notice that $\mathrm{Tr}(JC) = |VG|^2$ is the only constraint with a nonzero factor. Therefore, by scaling the solutions, we get the following equivalent SDP:

$$\begin{aligned}|V_G|\vartheta^-(G)^{-1} = \max_{C \in S^{V_G}} & \mathrm{Tr}(JC) \\ \text{s.t. } & C_{i,j} \leq 0 \,\forall (i,j) \in \overline{E_G}, \\ \rho(C) - C = & \mathbf{0} \,\forall \rho \in \mathrm{Aut}(G), \\ C \in & S_+^{V_G}, \\ \mathrm{Tr}(C) = & 1.\end{aligned} \tag{33}$$

Notice that lemma 5 guarantees that this is the same as $\vartheta^+(\overline{G})$. □

Corollary 1. *Suppose G is vertex-transitive. Then*

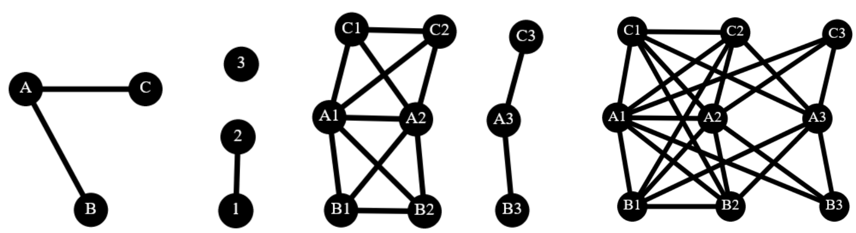
$$\frac{\vartheta^-(G)}{\vartheta(G)} = \frac{\vartheta(\overline{G})}{\vartheta^+(\overline{G})}. \tag{34}$$

Proof. This follows from combining theorem 4 and theorem 5. □

4 Multiplicity of ϑ, ϑ^- and ϑ^+ under the strong and disjunctive graph product

In many applications, the independence number of larger graphs is needed. One example of such a problem is the Shannon capacity of a graph [20], which considers graphs obtained by taking the *strong product* of a graph arbitrarily many times. Another application is sphere packings, where recently Cohn, de Laat and Salmon used an extension of the sphere packing graph, to improve the Cohn-Elkies bound for the lattice sphere packing problem in [3]. Even though the Cohn-Elkies bound and ϑ^- are not the same function, there is plenty of correspondence between the two.

Hence, it is natural to ask ourselves what happens to the functions ϑ^-, ϑ and ϑ^+ when we combine two graphs G, H. We are particularly interested in the *strong graph product* $G \boxtimes H$ and the *disjunctive graph product* $G * H$.



(a) G (b) H (c) $G \boxtimes H$ (d) $G * H$

Figure 4: Strong and disjunctive graph products for two arbitrary graphs G, H.

Definition 11 (Strong graph product)**.** *Suppose G, H are two graphs. Then $G \boxtimes H$ is the graph with vertex set $V_G \times V_H$, and*

$$\begin{aligned}((i_G, i_H), (j_G, j_H)) \in E_{G \boxtimes H} \Leftrightarrow & i_G = j_G \wedge (i_H, j_H) \in E_H \\ & \vee (i_G, j_G) \in E_G \wedge (i_H, j_H) \in E_H \\ & \vee (i_G, j_G) \in E_G \wedge i_H = j_H.\end{aligned} \tag{35}$$

Similarly, we can define the disjunctive graph product.

Definition 12 (Disjunctive graph product)**.** *Suppose G, H are two graphs. Then $G * H$ is the graph with vertex set $V_G \times V_H$, and*

$$((i_G, i_H), (j_G, j_H)) \in E_{G * H} \Leftrightarrow (i_G, j_G) \in E_G \vee (i_H, j_H) \in E_H. \tag{36}$$

The identity $G * H = \overline{\overline{G} \boxtimes \overline{H}}$ relates these graph products. Now it turns out that ϑ is multiplicative under both these graph products.

Theorem 6 (Multiplicity of ϑ)**.** *Let G and H be two arbitrary graphs. Then,*

$$\vartheta(G \boxtimes H) = \vartheta(G)\vartheta(H), \tag{37}$$

as well as

$$\vartheta(G * H) = \vartheta(G)\vartheta(H). \tag{38}$$

Proof. For a proof of (37) refer to theorem 7 of [14]. For a proof of (38), first note that if A_G maximizes (6) for the graph G, and if A_H maximizes (6) for the graph H, then $A_G \otimes A_H$ is a feasible solution of (6) for the graph $G * H$, so $\vartheta(G)\vartheta(H) \leq \vartheta(G * H)$. Furthermore, since $\mathcal{L}_{G\boxtimes H} \subset \mathcal{L}_{G*H}$, it follows that $\vartheta(G * H) \leq \vartheta(G \boxtimes H) = \vartheta(G)\vartheta(H)$. $\square$

It turns out that ϑ^- is not multiplicative under the strong graph product, like ϑ. However, ϑ^- **is** multiplicative under the disjunctive graph product. This was first proved by Cubitt et al. in theorem 25 of [5].

Theorem 7 (Multiplicity of ϑ^-)**.** *Let G and H be two arbitrary graphs. Then*

$$\vartheta^-(G * H) = \vartheta^-(G)\vartheta^-(H). \tag{39}$$

Proof. To show that $\vartheta^-(G*H) \geq \vartheta^-(G)\vartheta^-(H)$, note that if A_G maximizes (8) for G, and A_H maximizes (8) for H, then $A_G \otimes A_H$ is a feasible solution of (8) for the graph $G * H$, and hence $\vartheta^-(G * H) \geq \vartheta^-(G)\vartheta^-(H)$.

To show that $\vartheta^-(G * H) \leq \vartheta^-(G)\vartheta^-(H)$, let A maximize (8) for the graph $G * H$. For every $g \in V_G$, define the $|V_H| \times |V_H|$ matrix A^g as

$$A^g := (e_g \otimes I_H)^T A (e_g \otimes I_H), \tag{40}$$

where $e_g \otimes I_H$ is a $|V_{G*H}| \times |V_H|$ matrix. Then for every choice of g, we have $A^g \in S_+^{V_H}$, and for all $(i,j) \in E_H$ we have $A^g_{ij} = 0$, since in that case $A_{(i_g,i;j_g j)} = 0$ for all $i_g, j_g \in V_G$. Furthermore $A^g_{ij} \geq 0 \, \forall i,j \in V_H$. Therefore $\frac{A^g}{\mathrm{Tr}(A^g)}$ is a feasible solution for (8), for the graph H, and hence $\mathrm{Tr}(J_H A^g) \leq \vartheta^-(H)\mathrm{Tr}(A^g) \forall g \in V_G$. Now define the matrix A^H as

$$A^H := (I_G \times \mathbf{1})^T A (I_G \times \mathbf{1}), \tag{41}$$

where $I_G \times \mathbf{1}$ is a $|V_{G*H}| \times |V_G|$ matrix. Then $A^H_{ij} = 0 \, \forall (i,j) \in E_G$. Furthermore, for all $i,j \in V_G$ we have $A^H_{ij} \geq 0$. Therefore we have $\mathrm{Tr}(J_G A^H) \leq \vartheta^-(G)\mathrm{Tr}(A^H)$. We now have the inequalities

$$\begin{aligned}
\vartheta^-(G * H) &= \mathrm{Tr}\left((J_G \times J_H)A\right) = \mathrm{Tr}(J_G A^H) \\
&\leq \vartheta^-(G)\mathrm{Tr}(A^H) = \vartheta^-(G) \sum_{g \in V_G} \mathrm{Tr}(J_G A^g) \\
&\leq \vartheta^-(G)\vartheta^-(H) \sum_{g \in V_G} \mathrm{Tr}(A^g) \\
&= \vartheta^-(G)\vartheta^-(H)\mathrm{Tr}(A) = \vartheta^-(G)\vartheta^-(H). \qquad (42)
\end{aligned}$$

$\square$

Given theorem 6 and 7, one wound expect ϑ^+ to also be multiplicative under the strong graph product. Even though numerical results indicate that this is true, it is still an unsolved problem to prove this for all graphs G. However, using theorem 5 it is relatively easy to show that ϑ^+ is multiplicative under strong graph products for vertex-transitive graphs.

Theorem 8 (Multiplicity of ϑ^+)**.** *Let G and H be two arbitrary vertex-transitive graphs. Then*

$$\vartheta^+(G \boxtimes H) = \vartheta^+(G)\vartheta^+(H). \tag{43}$$

Proof. By theorem 7 and 5, we have

$$\vartheta^+(G)\vartheta^+(H) = \frac{|V_G||V_H|}{\vartheta^-(\overline{G})\vartheta^-(\overline{H})} = \frac{|V_{G\boxtimes H}|}{\vartheta^-(\overline{G} * \overline{H})} = \vartheta^+\left(\overline{\overline{G} * \overline{H}}\right) = \vartheta^+(G \boxtimes H). \tag{44}$$

□

Even though theorem 7 is proven, current proofs do not reveal what the optimal solutions of the dual formulation (17) of ϑ^- look like for $G * H$. In fact, there are currently no constructions known that give an answer to this question. A computation of $\vartheta^-(G * H)$ for small graphs G, H however suggests that for some graphs, there can be a neat relationship between the solutions of $\vartheta^-(G), \vartheta^-(g)$ and $\vartheta^-(G * H)$. This construction is given in the next subsection.

4.1 A dual construction for the multiplicity of ϑ^-

Theorem 9. *Suppose A is a matrix that minimizes* (17) *for the graph G, and B is a matrix that minimizes the same SDP for the graph H, and suppose*

$$\mathit{Spec}(J + A) \subset [-\vartheta^-(G), \vartheta^-(G)], \tag{45}$$

and $\mathit{Spec}(J + B) \subset [-\vartheta^-(H), \vartheta^-(H)]$. Then the matrix

$$C := A \otimes B + J_G \otimes B + A \otimes J_H \tag{46}$$

minimizes (17) *for the graph $G * H$.*

Proof. We have $(g_1, h_1; g_2, h_2) \notin E_{G*H}$ precisely when $(g_1, g_2) \notin E_G$ and $(h_1, h_2) \notin E_H$. Let $(g_1, h_1; g_2, h_2) \notin E_{G*H}$ be arbitrary. Then

$$C_{g_1,h_1;g_2,h_2} = A_{g1,g_2}B_{h_1,h_2} + A_{g_1,g_2} + B_{h_1,h_2} \geq 0. \tag{47}$$

Furthermore, C is symmetric, since A, B, J_G, J_H are all symmetric. Since

$$\begin{aligned}\mathrm{Spec}\left(J_{G*H} + C\right) &= \mathrm{Spec}\left(J_{G*H} + A \otimes B + J_G \otimes B + A \otimes J_H\right) \\ &= \mathrm{Spec}\left((J_G + A) \otimes (J_H + B)\right) \\ &= \{\lambda_G\lambda_H : \lambda_G \in \mathrm{Spec}(J_G + A), \lambda_H \in \mathrm{Spec}(J_H + B)\}\end{aligned} \tag{48}$$

and $\mathrm{Spec}(J+A) \subset [-\vartheta^-(G), \vartheta^-(G)]$, and $\mathrm{Spec}(J+B) \subset [-\vartheta^-(H), \vartheta^-(H)]$, we have

$$\Lambda\left(J_{G*H} + C\right) = \vartheta^-(G)\vartheta^-(H). \tag{49}$$

We know from theorem 7 that this is optimal. $\square$

Now the question becomes how general this construction is. Note that as a direct consequence of the above construction, if G and H both have optimal solutions to (17) that satisfy (45), then $G*H$ also has such a solution. However, the construction (46) may not work for all possible optimal solutions of two given graphs G, H. Therefore, we have to ask the question

Question 1. *Which graphs have an optimal solution A that satisfies* (45)*?*

4.2 An SDP formulation for validity of the construction

We can numerically check if graphs have a solution that satisfies (45), by adding the additional constraint to (17) that the *smallest* eigenvalue of $J+A$ is at least as large as $-\Lambda(J+A)$. Hence, we define

Definition 13. *The function $t_{\max}(G)$ is defined as*

$$\begin{aligned} t_{\max}(G) = &\min_{A \in \mathcal{L}_G^-} t \\ &s.t.\ tI - J - A \in S_+^{V_G}, \\ &\quad\ \ tI + J + A \in S_+^{V_G}. \end{aligned} \tag{50}$$

Now feasible solutions to (50) are also feasible solutions to (17), and since $t_{\max}$ imposes additional constraints on (17), the inequality $t_{\max}(G) \geq \vartheta^-(G)$ holds. Therefore, we have the following result.

Lemma 7. *$t_{\max}(G) = \vartheta^-(G)$ if and only if G permits a solution to SDP 17 that satisfies* (45)*.*

A program was used to check for all possible graphs on $n \leq 7$ vertices if they have solutions that satisfy the condition of lemma 7. This program is listed in appendix B.1, and was cross-verified with known values of ϑ^- for small graphs. For graphs on $1-4$ vertices, it is always the case that $\vartheta^- = t_{\max}$. For graphs on 5 vertices, there are only 6 graphs, up to isomorphisms, for which this condition does not hold.

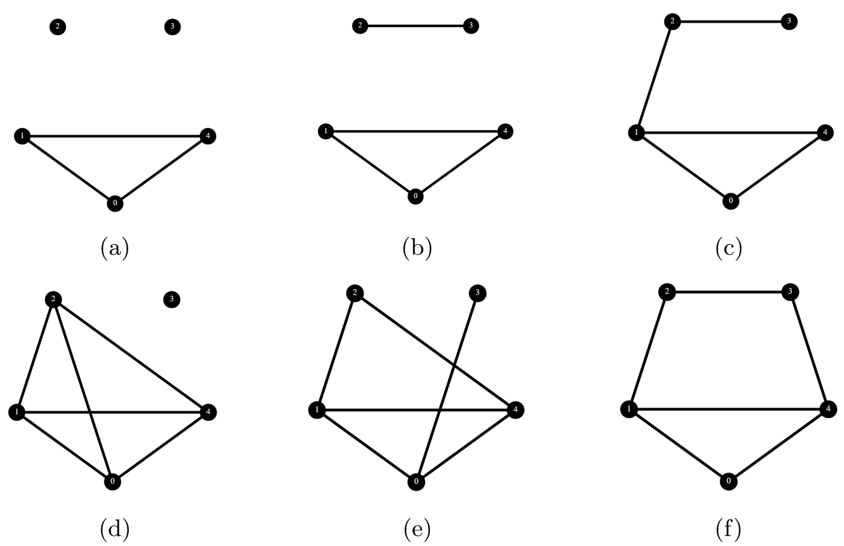


Figure 5: All graphs, up to isomorphisms, on 5 vertices that do not satisfy the conditions of lemma 7.

The number of graphs, up to isomorphisms, for which $\vartheta^- \neq t_{\max}$ is listed in table 1.

n	#Graphs	#Graphs that fail
1	1	0
2	2	0
3	4	0
4	11	0
5	34	6
6	156	33
7	1044	380

Table 1: Number of graphs that fail $t_{\max} = \vartheta^-$, up to isomorphisms.

While it still remains an open question for which graphs in general the construction works, it is possible to find analytic solutions that satisfy (45) for specific sets of graphs. In the next subsection, solutions for cyclic graphs of an arbitrary size are given that satisfy (45).

4.3 ϑ^- for cyclic graphs

The theta number of cyclic graphs is well known. In corollary 5 of [14], Lovász proves that $\vartheta(C_n) = \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$ whenever n is odd. Whenever n is even, this value is $\frac{n}{2}$. It turns out that the value of $\vartheta^-(C_n)$ is the same as $\vartheta(C_n)$ for all n. In theorem 10 and 11, we will prove that this is the case, by giving feasible solutions for both the maximization formulation (8) and the minimization formulation (17) of ϑ^-, that have the same value. Furthermore, the solutions given for the minimisation problems satisfy (45), proving all cyclic graphs have solutions to (17) for which the construction given in theorem (9) works.

Since the automorphism group of a cyclic graph on n vertices contains a cyclic subgroup of size n, we can rearrange the vertices of cyclic graphs in such a way that lemma 5 guarantees that there is an optimal solution A to (17) that is circulant. The following lemma implicates that by restricting the solutions to circulant matrices, the eigenvalues are easier to compute.

Lemma 8. *Suppose an $n \times n$ matrix A is circulant. Then its eigenvalues are equal to the discrete Fourier transform $\widehat{A_1}$ of its first row.*

Proof. Define $v_k = \begin{pmatrix} 1 & e^{\frac{2\pi k i}{n}} & e^{\frac{4\pi k i}{n}} & \dots & e^{\frac{2(n-1)\pi k i}{n}} \end{pmatrix}^T$. Then v_k is an eigenvector of A, since

$$\begin{aligned}
[Av_k]_j &= \sum_{l=1}^{n} A_{jl} e^{\frac{2(l-1)\pi k i}{n}} = e^{\frac{2(j-1)\pi k i}{n}} \sum_{l=1}^{n} A_{jl} e^{\frac{2(l-j)\pi k i}{n}} \\
&= e^{\frac{2(j-1)\pi k i}{n}} \sum_{l=1}^{n} A_{1\,\overline{l-j}+1} e^{\frac{2(l-j)\pi k i}{n}} = e^{\frac{2(j-1)\pi k i}{n}} [Av_k]_1 . \quad (51)
\end{aligned}$$

Therefore, $Av_k = [Av_k]_1 v_k$, and the eigenvalues of A are $\widehat{A_1}(0), \dots, \widehat{A_1}(n-1)$. ☐

Using this lemma, we can calculate ϑ^- of all cyclic graphs on an even number of nodes. It turns out that we can find a solution of the dual program that satisfies (45).

Theorem 10. *For all even n, $\vartheta^-(C_n) = \frac{n}{2}$ and there is an optimal solution to* (2) *that satisfies* (45)*.*

Proof. To show that $\vartheta^-(C_n) \geq \frac{n}{2}$, consider SDP (8). Define the circulant matrix A by

$$A_{1,j} := \begin{cases} \frac{1}{n} \text{ if } j \text{ is odd} \\ 0 \text{ if } j \text{ is even.} \end{cases} \quad (52)$$

Let e_{odd} be the vector with values 1 for all odd indices, and 0 for all odd indices, and let $e_{\text{even}} = \mathbf{1} - e_{\text{odd}}$. Then it is clear that $A \in S_+^n$, because $A = e_{\text{odd}} e_{\text{odd}}^T + e_{\text{even}} e_{\text{even}}^T$. A also satisfies all other constraints of (8), so $\vartheta^-(C_n) \geq \text{Tr}(JA) = \frac{n}{2}$. To show that $\vartheta^-(C_n) \leq \frac{n}{2}$, consider the SDP (17). Define the circulant matrix B by

$$B_{1,j} := \begin{cases} -\frac{n}{4} \text{ if } j \in \{2, n\} \\ 0 \text{ otherwise.} \end{cases} \quad (53)$$

Then B satisfies all the constraints, so

$$\begin{aligned}\vartheta^-(C_n) \le \Lambda(J+B) &= \max_{s\in\{0,\dots,n-1\}} \widehat{J+B}(s) \\ &= \max\left[\frac{n}{2}, \max_{s\in\{1,\dots,n-1\}} -\frac{n}{2}\cos\left(\frac{2\pi s}{n}\right)\right] = \frac{n}{2}, \end{aligned} \tag{54}$$

and B satisfies (45). $\square$

Similarly, can also prove the value of ϑ^- for cyclic graphs on an odd number of vertices, that is at least 3. Again, there is a solution of the dual SDP that satisfies (45). However, this solution is a bit more tricky than that for even n.

Theorem 11. *For all odd $n \ge 3$, $\vartheta^-(C_n) = \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$ and there is an optimal solution to* (2) *that satisfies* (45).

Proof. To show that $\vartheta^-(C_n) \ge \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$, consider the SDP (8). Define the circulant matrix A by

$$A_{1,j} := \frac{\cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{\pi(j-1)(n-1)}{n}\right)}{n\cos\left(\frac{\pi}{n}\right) + n} \tag{55}$$

Then by filling in $j = 2, n$ we verify that $A_{j,k} = 0$ whenever $(j,k) \in E_{C_n}$, and furthermore $\cos\left(\frac{\pi}{n}\right) + \cos\left(\frac{\pi(j-1)(n-1)}{n}\right) \ge 0$ for all j, since n is odd. It is easy to verify that A is symmetric. Since A is circulant, the eigenvalues of A are given by $\widehat{A_1}$, by lemma 8. Let $s \in \{0,\dots,n-1\}$. Then

$$\widehat{A_1}(s) = \begin{cases} \frac{\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)} & \text{if } s = 0, \\ \frac{1}{2+2\cos\left(\frac{\pi}{n}\right)} & \text{if } s = \frac{n\pm1}{2}, \\ 0 & \text{otherwise.} \end{cases} \tag{56}$$

From this it follows that $A \in S_+^n$, and furthermore

$$\mathrm{Tr}(JA) = n\widehat{A_1}(0) = \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}. \tag{57}$$

Therefore $\vartheta^-(C_n) \ge \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$. To show that $\vartheta^-(C_n) \le \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$, consider the SDP (17). Define the circulant matrix B by

$$B_{1,j} = \begin{cases} \frac{-n}{2+2\cos\left(\frac{\pi}{n}\right)} & \text{if } j \in \{2, n\}, \\ 0 & \text{otherwise.} \end{cases} \tag{58}$$

Then B is symmetric, and satisfies all other constraints. Furthermore, by lemma 8, the eigenvalues of $J + B$ are given by $\widehat{e + B_1}$. We find

$$\widehat{e+B_1}(s) = \begin{cases} \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)} \text{ if } s = 0, \\ -\frac{n\cos\left(\frac{2\pi s}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)} \text{ otherwise.} \end{cases} \tag{59}$$

Therefore, we have proven that $\vartheta^-(C_n) = \frac{n\cos\left(\frac{\pi}{n}\right)}{1+\cos\left(\frac{\pi}{n}\right)}$ for odd $n \geq 3$, and B satisfies (45). $\square$

Corollary 2. *All cyclic graphs C_n have a solution to* (17) *that satisfies* (45)*.*

Coincidentally, it turns out that $\vartheta^-(C_n) = \vartheta(C_n)$ for all $n \in \mathbb{N}$. However, lemma 8 is not a coincidence, as we will see in the next section that something similar to happens in general for abelian Cayley graphs.

5 Abelian Cayley graphs

Cayley graphs are defined with group elements as vertices. Therefore, G will from now on denote a group, and $\mathrm{Cay}(G, S)$ will denote a Cayley graph. Similarly to lemma (5), it can be shown that restricting to matrices that are invariant under subgroups of the automorphism group of a graph does not affect the value of $t_{\max}$.

Lemma 9. *Let H be a graph. Let $S \subset \mathrm{Aut}(H)$ be a subgroup. Then there exists an optimal solution of* (50) *that is invariant under S.*

Proof. Let t, A be an optimal solution of (50). Then let

$$B = \frac{1}{|S|} \sum_{\rho \in S} \rho(A). \tag{60}$$

In lemma (5) it was shown that this matrix B is invariant under S. Since SDPs are convex optimization problems, t, B is also a feasible solution of (50), and it is also optimal, since it has objective value t. □

Because of lemmas 5 and 9 the complexity of finding ϑ^-, ϑ and ϑ^+ can be greatly reduced for abelian Cayley graphs, by taking advantage of the group structure.

5.1 Eigenvalues of G-invariant matrices

Definition 14 (Cayley graphs)**.** *For a group G, and a set $S \in G$, the Cayley graph $Cay(G, S)$ is defined to be graph with elements of G as its vertex set, and the edge set consists of all pairs x, y such that $yx^{-1} \in S$.*

Since the functions ϑ^-, ϑ and ϑ^+ are defined for undirected graphs, we must have $g^{-1} \in S$ whenever $g \in S$. This is equivalent to having a symmetric adjacency matrix. Since $G \subset \mathrm{Aut}(\mathrm{Cay}(G, S))$, we may assume that the solution matrices A to both the primal and dual SDPs of ϑ are invariant under G, because of lemma 5. Furthermore, we may assume that the solution matrices A to the SDP (50) are G-invariant, because of lemma 9.

Since the map $f \to A$, defined by $A_{ij} = f(ji^-)$ is an isomorphism between G-invariant, symmetric matrices, and functions $f : G \to \mathbb{R}$ that satisfy $f(g) = f(g^{-1})$ for all $g \in G$, there is a one-to-one correspondence between G-invariant, symmetric matrices A, and functions $f : G \to \mathbb{R}$, for which $f(g) = f(g^{-1})$, for all $g \in G$. This one-to-one correspondence greatly reduces the number of variables in the optimization problems. With some additional algebra, we will be able to further simplify the SDPs belonging to ϑ^- and $t_{\max}$.

Since Cayley graphs are defined on groups, it makes sense to analyze properties of these groups. One way to do this, is to look at *group representations.*

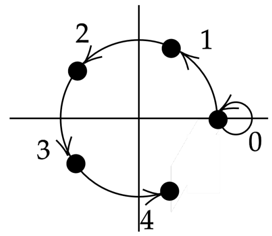


Figure 6: A set of 5 rotation matrices that form a group representation of C_5, acting on the point $1 + 0i$.

These encode the group structure with matrices, which enables us to use tools from linear algebra to study ϑ^- and $t_{\max}$.

Definition 15 (Matrix representations)**.** *A group representation of G is a group homomorphism $\pi : G \to \mathrm{GL}(V)$, where $\mathrm{GL}(V)$ is the group of invertible linear maps on a $\mathbb{C}$-vector space V. Two representations are equivalent if there exists an isomorphism $T : \mathrm{GL}(V_1) \to \mathrm{GL}(V_2)$ such that for all $g \in G$ we have*

$$\pi_1(g)T = T\pi_2(g). \tag{61}$$

Recall that the *trace* of an operator is the sum of its eigenvalues, counting multiplicity. If $\dim(V) = n$, we can furthermore identify V with $\mathbb{C}^n$ by choosing a basis. Let us now define the character of a representation.

Definition 16 (Characters)**.** *The character of a representation π is the map $\chi_\pi : G \to \mathbb{C}$ given by*

$$\chi_\pi(g) = \mathrm{Tr}(\pi(g)). \tag{62}$$

For example, the representation in figure 6 is the map $\pi(x) := \left(e^{\frac{2\pi i x}{5}}\right)$. Its character is trivially $\chi_\pi = e^{\frac{2\pi i x}{5}}$.

It turns out that characters are invariant under the choice of representation: if two representations are equivalent, then their characters are the same. This follows from the fact that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ for all matrices A, B. Suppose π_1 and π_2 are two equivalent representations, and the linear isomorphism T satisfies $\pi_1 T = T\pi_2$. Then

$$\begin{aligned}\chi_{\pi_1}(g) &= \mathrm{Tr}\left(\pi_1(g)\right) = \mathrm{Tr}\left(T\pi_2(g)T^{-1}\right) \\ &= \mathrm{Tr}\left(T\pi_2(g)T^{-1}\right) = \mathrm{Tr}\left(\pi_2(g)T^{-1}T\right) = \mathrm{Tr}\left(\pi_2(g)\right) = \chi_{\pi_2}(g).\end{aligned} \tag{63}$$

Therefore, if π_1 and π_2 are equivalent, their characters are the same. When investigating characters of a representation, we can therefore try to find equivalent representations for which we know more. One of the defining properties of a character is its degree.

For a group G, suppose $\pi : G \to \mathrm{GL}(V)$ is a representation. Let $\mathrm{Id} \in G$ be the identity element. Then since $\pi(\mathrm{Id})$ has to be an idempotent, invertible matrix, all of its eigenvalues are 1, and hence $\chi_\pi(\mathrm{Id}) = \dim(V)$. This is called the degree of χ_π. Note that the degree must always be a positive integer.

Definition 17. *The degree of a character $\chi_\pi : G \to \mathbb{C}$, belonging to a representation π is defined as*

$$\deg(\chi_\pi) := \chi(\mathrm{Id}) =: \deg(\pi). \tag{64}$$

Since the characters of representations are the same for equivalent representations, we will from now on look at the equivalence classes of representations. This way, it will be possible to decompose some representations into factors. Denote equivalence of representations by $\sim$.

Definition 18 (Reducible representations)**.** *We call a representation π reducible, if there exist representations π_1, π_2, such that*

$$\pi \sim \pi_1 \oplus \pi_2, \tag{65}$$

where $\oplus$ denotes the direct sum. If such representations do not exist, then we call π irreducible.

From this definition, it is immediately clear that if $\pi \sim \pi_1 \oplus \pi_w$, then $\deg(\pi) = \deg(\pi_1) + \deg(\pi_2)$. Hence, if a representation has degree 1, then it must be irreducible. An example of this is the trivial representation.

Example 1. *Each group G has a trivial representation, given by $\pi_{triv}(g) = \begin{bmatrix}1\end{bmatrix}$. Its character, $\chi_{triv} = 1$ is called the trivial character. Since $deg(\chi_{triv}) = 1$, the trivial representation is irreducible.*

For some groups, the reverse implication also holds. If a representation of an abelian group is irreducible, it must have degree 1. To show this, we will use a different, but equivalent way of describing (ir)reducible representations.

Definition 19 (Subrepresentations)**.** *Suppose $\pi : G \to V$ is a representation of G, and $\pi|_W : G \to W$ is another representation, such that*

$$\pi(g)|_W = \pi|_w(g)\; \forall g \in G \tag{66}$$

if the restriction to W, for some linear, proper subspace $W \subsetneq V$, Then $\pi|_W$ is called a subrepresentation.

Finding subrepresentations might at first seem more restrictive than finding two representations π_1 and π_2 such that $\pi \sim \pi_1 \oplus \pi_2$. However, in this case there is a T such that $\pi T = T(\pi_1 \oplus \pi_2)$, and hence w.l.o.g. $T|_{V_1} \pi_1 T|_{V_1}^{-1}$ is a subrepresentation of π, where V_1 is the domain of π_1. Therefore, reducible representations have subrepresentations.

This also works the other way around. The following theorem shows that if π has a subrepresentation, then π is reducible. This is useful, as it implies that reducing representations is the same as finding subrepresentations.

Theorem 12. *Suppose $\pi|_W : G \to W$ is a subrepresentation of $\pi : G \to V$. Then there exists a subrepresentation $\pi|_U : G \to U$ of π such that $V = W \oplus U$.*

Proof. Let $\pi_W : V \to W$ be the projection onto W. Then define

$$p(x) := \frac{1}{\#G} \sum_{g \in G} \left[\pi|_W(g)\pi_W \pi(g^{-1})\right](x). \tag{67}$$

Now suppose $w' \in \ker(p)$, and let $h \in G$ be arbitrary. Then since $\pi(a^{-1}) = \pi(a)^{-1}$, we have

$$\begin{aligned} p(\pi(h)w') &= \pi(h)\pi(h^{-1})\frac{1}{\#G} \sum_{g \in G} \left[\pi|_W(g)\pi_W \pi(g^{-1})\right](\pi(h)w') \\ &= \pi(h)\frac{1}{\#G} \sum_{g \in G} \left[\pi|_W(h^{-1}g)\pi_W \pi(g^{-1}h)\right](w') \\ &= \pi(h)\frac{1}{\#G} \sum_{g \in G} \left[\pi|_W(g)\pi_W \pi(g^{-1})\right](w') = \pi(h)p(w') = 0, \end{aligned} \tag{68}$$

so if $w' \in \ker(p)$, then $\pi(h)w' \in \ker(p)$, for all $h \in G$. Now the restriction of π to $\ker(p)$ is a representation, too. This follows since $\pi(b)$ maps $\ker(p)$ onto $\ker(p)$, and thus

$$\pi(ab)|_{\ker(p)} = \pi(a)\pi(b)|_{\ker(p)} = \pi(a)|_{\ker(p)}\pi(b)|_{\ker(p)}. \tag{69}$$

Furthermore, if $w \in W$, then $p(w) = w$, so $W \perp \ker(p)$. Since p is a projection, $p^2(x) = x \, \forall x \in V$, so $x - p(x) \in \ker(p) \, \forall x \in V$. This implies that

$$x = p(x) + b \, \forall x \in V, \tag{70}$$

where $b \in \ker(p)$, and trivially $p(x) \in W$. Therefore, the identity

$$V = W \oplus \ker(p) \tag{71}$$

holds. □

Now it follows that any representation of G can be decomposed into irreducible representations, and that those are exactly the representations that have no subrepresentations. Schur's lemma [19, p. 13] gives us information about G-linear maps between different irreducible representations:

Lemma 10 (Schur's lemma)**.** *Let $\pi_V : G \to V$, and $\pi_W : G \to W$ be two irreducible representations of G. Let $f : V \to W$ be a G-linear map. That is, $f \circ \pi_V(g) = \pi_W(g) \circ f$ for all $g \in G$. Then the following hold:*

1. *Suppose V, W are not isomorphic. Then $f \equiv \mathbf{0}$.*
2. *Suppose $V = W$, and $\pi_V = \pi_W$. Then f is a scalar multiple of the identity.*

This yields an important result in the case where G is abelian.

Corollary 3 (Irreducible representations of abelian groups)**.** *Suppose G is abelian, and π is an irreducible representation. Then* $\deg(\pi) = 1$.

Proof. Let $x \in G$ be arbitrary. Since G is abelian, we have

$$\pi(x)\pi(g)v = \pi(xg)v = \pi(gx)v = \pi(g)\pi(x)v \, \forall v \in V, g \in G. \tag{72}$$

This means that $v \to \pi(x)v$ is a G-linear map. By Schur's lemma, $\pi(x)v = \lambda_x v$ for some scalar λ_x. Therefore, the restriction of π to any subspace of V is a subrepresentation of π. Since π is irreducible, this implies that the only subspace of V is $\{0\}$, so $\deg(\pi) = 1$. □

Therefore, every irreducible representation of an abelian group G is isomorphic to a homomorphism $\pi : G \to \mathbb{C}^*$, and every irreducible character of an abelian group is a homomorphism $\chi : G \to \mathbb{C}^*$. Subsequently, all possible representations of abelian groups are equivalent to the direct sum of homomorphisms from G to $\mathbb{C}^*$, and all possible characters are the sum of some number of those homomorphisms.

A consequence of the fact that the irreducible representations π of abelian groups have degree 1, is that the characters χ_π of the irreducible representations are multiplicative: $\chi_\pi(gh) = \chi_\pi(g)\chi_\pi(h)$. This would not necessarily be true if the degree were larger than 1. One of the consequences of this property is that the irreducible characters of abelian groups are closely related to the eigenvalues of matrices that are invariant under the group action.

Theorem 13 (Eigenvalues of invariant matrices)**.** *Suppose G is abelian, and the function $f : G \to \mathbb{R}$ defines the matrix A by $A_{ij} = f(ji^{-1})$, and χ is an irreducible character of G. Then the vector $v \in \mathbb{C}^G$, defined by $v_g = \chi(g)$ is an eigenvector of A, and the corresponding eigenvalue is*

$$\lambda_\chi := \sum_{g \in G} f(g)\chi(g). \tag{73}$$

Proof. Since $\deg(\chi) = 1$ by corollary 3, we have

$$(Av)_i = \sum_{j \in G} f(ji^{-1})\chi(j) = \sum_{j \in G} f(j)\chi(ji) = \sum_{j \in G} f(j)\chi(j)\chi(i) = \lambda_\chi v_i, \tag{74}$$

for all $i \in G$. Therefore, v is an eigenvector of A, and λ_χ is its eigenvalue. □

This result is already interesting, but what makes it more interesting, is that we can show that there exist precisely $|G|$ independent eigenvectors of this form. For that, the fundamental theorem of finite abelian groups [12], which classifies all finite, abelian groups, is useful.

Theorem 14 (Fundamental theorem of finite abelian groups)**.** *Let G be an abelian group. Then G is isomorphic to the direct product of cyclic groups*

$$(\mathbb{Z}/n_1\mathbb{Z}) \times \ldots \times (\mathbb{Z}/n_k\mathbb{Z}), \tag{75}$$

where $n_1, \ldots, n_k$ are powers of prime numbers.

This theorem helps us construct $|G|$ different eigenvectors of the G-invariant matrix A.

Corollary 4 (Classification of irreducible characters of abelian groups)**.** *Let G be an abelian group, and*

$$G \overset{\varphi}{\cong} (\mathbb{Z}/n_1\mathbb{Z}) \times \ldots \times (\mathbb{Z}/n_k\mathbb{Z}) \,. \tag{76}$$

Then for all elements $r \in G$, the following is an irreducible character of G:

$$\chi_r(g) := \prod_{j=1}^{k} e^{\frac{2\pi\varphi(r)_j\varphi(g)_j i}{n_j}} \,. \tag{77}$$

Furthermore, all irreducible characters are of this form.

Proof. Let $\pi_r := \big(\chi_r\big)$ be a one-dimensional matrix. Since $\deg(\pi) = 1$, the following holds:

$$\begin{aligned}\pi_r(gh) = \left(\prod_{j=1}^{k} e^{\frac{2\pi\varphi(r)_j\varphi(gh)_j i}{n_j}}\right)& \\ = \left(\prod_{j=1}^{k} e^{\frac{2\pi\varphi(r)_j\varphi(g)_j i}{n_j}}\right)\left(\prod_{j=1}^{k} e^{\frac{2\pi\varphi(r)_j\varphi(h)_j i}{n_j}}\right)& \\ = \pi_r(g)\pi_r(h).&\end{aligned} \tag{78}$$

Therefore, π_r is a one-dimensional matrix representation of G, and is hence irreducible. From Fourier analysis it follows that all π_r defined this way are linearly independent. ◻

We can now combine the above theorems to determine the eigenvalues of G-invariant matrices A, for abelian groups G.

Corollary 5. *Suppose G is abelian, and $f : G \to \mathbb{R}$ is a function that defines A by $A_{ij} = f(ji^{-1})$. By the fundamental theorem of finite abelian groups, there exist prime powers $n_1, \ldots, n_k$, and a function φ such that*

$$G \overset{\varphi}{\cong} (\mathbb{Z}/n_1\mathbb{Z}) \times \ldots \times (\mathbb{Z}/n_k\mathbb{Z}) \,. \tag{79}$$

Now all eigenvalues of A are of the form

$$\lambda_g := \sum_{h\in G} f(h) \prod_{j=1}^{k} e^{\frac{2\pi\varphi(g)_j\varphi(h)_j i}{n_j}} \,, \tag{80}$$

where $g \in G$. Denote the linear map $A \to \big(\lambda_g\big)_{g\in G}$ as $\widehat{A}$, or $\widehat{f}$.

This result is very important, as it shows that the eigenvalues of the G-invariant matrices optimizing the primal and dual formulations of ϑ^-, as well as those optimizing the SDP belonging to $t_{\max}$ depend linearly on the values of the first row of this matrix.

5.2 LP formulation of ϑ^- for abelian Cayley graphs

Since the spectral theorem from linear algebra guarantees that all eigenvalues of symmetric matrices are real, we may take the real part of equation (80). Therefore, if A is symmetric,

$$\widehat{A}(g) = \sum_{h \in G} f(h) \cos\left(\sum_{j=1}^{k} \frac{2\pi\varphi(g)_j\varphi(h)_j i}{n_j}\right). \tag{81}$$

By plugging in $g = \mathrm{Id}$, we see that $\widehat{A}(\mathrm{Id}) = \sum_{h \in G} f(h)$. Because of lemma 6, we thus know the eigenvalue belonging to Id is the largest eigenvalue of $J + A$, whenever A is G-invariant and minimizes (17). We thus can write both the primal and dual formulations of ϑ^- as the linear programs given in lemma 11. It must be noted that an expression similar to (82) was derived in [6, p. 4] by DeCorte, de Laat and Vallentin, although obtained by different means.

Lemma 11. *Let* $\mathrm{Cay}(G, S)$ *be an undirected, abelian graph. Then the primal formulation of* ϑ^- *is equivalent to*

$$\begin{aligned}
\vartheta^-(\mathrm{Cay}(G,S)) &= \max \widehat{f}(\mathrm{Id}) \\
s.t.\ f(g) &= f(g^{-1})\ \forall g \in G, \\
f(\mathrm{Id}) &= 1, \\
f(g) &= 0\ \forall g \in S, \\
f(g) &\geq 0\ \forall g \notin S, \\
\widehat{f}(g) &\geq 0\ \forall g \in G.
\end{aligned} \tag{82}$$

The dual formulation of ϑ^- *is equivalent to*

$$\begin{aligned}
\vartheta^-(\mathrm{Cay}(G,S)) &= \min \widehat{v}(\mathrm{Id}) \\
s.t.\ v(g) &= v(g^{-1})\ \forall g \in G, \\
v(g) &\geq 1\ \forall g \notin S, \\
\widehat{v}(g) - \widehat{v}(\mathrm{Id}) &\leq 0\ \forall g \in G.
\end{aligned} \tag{83}$$

Proof. The first equality follows from (8), and the fact that $\mathrm{Tr}(JA) = |G|\widehat{f}(\mathrm{Id})$, and $A_{ii} = f(0)$ for all $i \in G$. By both rescaling the objective with a factor $\frac{1}{|G|}$, and rescaling the constraints with a factor $|G|$, equality (82) is obtained.
The second equality follows from (31), by substituting $v(g) = A_{\mathrm{Id}g} + 1$. $\square$

Similar to lemma 11, we can express $t_{\max}$ as an LP.

Lemma 12. *Let* $\mathrm{Cay}(G, S)$ *be an undirected, abelian graph. Then the following equation holds.*

$$
\begin{aligned}
t_{\max}(Cay(G,S)) &= \min \widehat{v}(\mathrm{Id}) \\
s.t.\ v(g) &= v(g^{-1})\,\forall g \in G, \\
v(g) &\geq 1\,\forall g \notin S, \\
\widehat{v}(g) - \widehat{v}(\mathrm{Id}) &\leq 0\,\forall g \in G, \\
\widehat{v}(g) + \widehat{v}(\mathrm{Id}) &\geq 0\,\forall g \in G.
\end{aligned} \tag{84}
$$

A program, which was cross-verified with the program in B.1, and is included in appendix B.2, was used to check for all abelian Cayley graphs on at most 31 vertices whether they satisfy $t_{\max} = \vartheta^-$. This was done by calculation LPs (82) and (84) for all symmetric subsets S of G, for all groups G of size $n \leq 31$, that are of the form given in theorem 14. If we let

$$G = (\mathbb{Z}/n_1\mathbb{Z}) \times (\mathbb{Z}/n_1\mathbb{Z}) \times \ldots \times (\mathbb{Z}/n_k\mathbb{Z}),$$

then the cardinality of G is $|G| = \prod_{j=1}^{k} n_j$. Because of this, we can generate all possible abelian groups G of size n from the prime factorization of n. Suppose

$$n = 2^{a_1} 3^{a_2} 5^{a_3} \ldots p_{l-1}^{a_{l-1}} p_l^{a_l}$$

is the prime factorization of n. We may assume that whenever $n_i = p_x^{b_x}$, and $n_j = p_y^{b_y}$, and $p < q$ are both primes, then $i < j$, so that the values of $n_1, \ldots, n_k$ are sorted by prime base. We may furthermore assume that whenever $n_i = p^{b_x}$, and $n_j = p^{b_y}$, and $b_x < b_y$, then $i < j$. Therefore, it suffices to look at all partitions of $a_1, a_2, \ldots, a_l$. For example, all possible abelian groups with cardinality 36 are isomorphic to either one of the following:

1. $(\mathbb{Z}/4\mathbb{Z}) \times (\mathbb{Z}/9\mathbb{Z})$,
2. $(\mathbb{Z}/2\mathbb{Z}) \times (\mathbb{Z}/2\mathbb{Z}) \times (\mathbb{Z}/9\mathbb{Z})$,
3. $(\mathbb{Z}/4\mathbb{Z}) \times (\mathbb{Z}/3\mathbb{Z}) \times (\mathbb{Z}/3\mathbb{Z})$,
4. $(\mathbb{Z}/2\mathbb{Z}) \times (\mathbb{Z}/2\mathbb{Z}) \times (\mathbb{Z}/3\mathbb{Z}) \times (\mathbb{Z}/3\mathbb{Z})$.

It turns out that for $n \in \{1, 2, 3, 4, 5, 7\}$, there are no abelian Cayley graphs for which $t_{\max} \neq \vartheta^-$. For $n = 6$, there are exactly two abelian Cayley graphs for which this is the case. These are shown in figure 7.

(a) (b)

Figure 7: All abelian Cayley graphs on 6 vertices, for which there exists no optimal solution A to (17) that satisfies (45).

While it is therefore impossible to prove that for all Cayley graphs there exists an optimal solution to (17) that satisfies (45), it is possible to show that an optimal solution must exist for which the smallest eigenvalue of $J + A$ is bounded from below by some number, using Fourier inversion.

Theorem 15. *Let* $\mathrm{Cay}(G, S)$ *be an arbitrary abelian Cayley graph. Then there exists an optimal solution* A *to* (17) *such that all eigenvalues of* $J + A$ *are at least* $\vartheta^- - |G|$.

Proof. We can make a LP to maximize the smallest eigenvalue, provided that the largest eigenvalue is equal to ϑ^-. This value will be called λ_{min}.

$$\begin{aligned} \lambda_{min} &:= \max t \\ \text{s.t. } v_g &= v_{g^{-1}} \, \forall g \in G, \\ \widehat{v}(\mathrm{Id}) &= \vartheta^- - |G|, \\ \widehat{v}(g) &\leq \vartheta^- \, \forall g \in G \backslash \{\mathrm{Id}\}, \\ \widehat{v}(g) &\geq t \, \forall g \in G \backslash \{\mathrm{Id}\}, \\ v_g &\geq 0 \, \forall g \notin S, \\ v_g &\in \mathbb{R} \, \forall g \in S. \end{aligned} \tag{85}$$

Now substitute $w = \widehat{v}$. Fourier inversion gives us $\sum_{g \in G \backslash \{\mathrm{Id}\}} w_g \geq |G| - \vartheta^-$, since $w_{\mathrm{Id}} = \vartheta^- - |G|$, and $v_{\mathrm{Id}} \geq 0$. This way, we can eliminate the variable w_{Id} from the LP.

$$\begin{aligned} \lambda_{min} &= \max t \\ \text{s.t. } w_g &= w_{g^{-1}} \, \forall g \in G \backslash \{\mathrm{Id}\}, \\ w_g &\leq \vartheta^- \, \forall g \in G \backslash \{\mathrm{Id}\}, \\ w_g &\geq t \, \forall g \in G \backslash \{\mathrm{Id}\}, \\ w_{\mathrm{Id}} &= 0, \\ \widehat{w}(g) &\geq |G| - \vartheta^- \, \forall g \notin S. \end{aligned} \tag{86}$$

We now take the dual LP of this LP.

$$
\begin{aligned}
\lambda_{min} &= \min\ \vartheta^{-}\widehat{c_1}(\mathrm{Id}) + (|G|-\vartheta^{-})\widehat{c_3}(\mathrm{Id}) \\
\text{s.t. } c_1^g &= c_1^{g^{-1}}\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_2^g &= c_2^{g^{-1}}\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_3^g &= c_3^{g^{-1}}\ \forall g \in G\backslash S, \\
c_1^g &\geq 0\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_2^g &\leq 0\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_3^g &\leq 0\ \forall g \notin S, \\
c_1^{\mathrm{Id}} &= c_2^{\mathrm{Id}} = 0, \\
c_3^g &= 0\ \forall g \in S, \\
\widehat{c_2}(\mathrm{Id}) &= -1, \\
c_1^g + c_2^g + \widehat{c_3}(g) &= 0\ \forall g \in G\backslash\{\mathrm{Id}\}.
\end{aligned} \tag{87}
$$

Since this is a minimisation problem, we get a lower bound by relaxing the constraints. To this end, substitute $R_g = 1 + c_1^g + c_2^g$. Then it follows that $R^g \geq 0\ \forall g \in G\backslash\{\mathrm{Id}\}$. Furthermore, $\sum_{g\in G\backslash\{\mathrm{Id}\}} R_g = |G| - 2 + \sum_{g\in G\backslash\{\mathrm{Id}\}} c_1^g$. Therefore,

$$
\begin{aligned}
\lambda_{min} &\geq \vartheta^{-}(2-|G|) + \min \vartheta^{-}\widehat{R}(\mathrm{Id}) + (|G|-\vartheta^{-})\widehat{c_3}(g) \\
\text{s.t. } R_g &= R_{g^{-1}}\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_3^g &= c_3^{g^{-1}}\ \forall g \in G\backslash S, \\
R_g &\geq 0\ \forall g \in G\backslash\{\mathrm{Id}\}, \\
c_3^g &\leq 0\ \forall g \in G\backslash S, \\
c_3^g &= 0\ \forall G \in S, \\
R_{\mathrm{Id}} &= 0, \\
\widehat{R}(\mathrm{Id}) &\geq |G| - 2, \\
R_g + \widehat{c_3}(g) &= 1\ \forall g \in G\backslash\{\mathrm{Id}\}.
\end{aligned} \tag{88}
$$

Now since summing the last equation yields $\widehat{R}(\mathrm{Id}) - \widehat{c_3}(\mathrm{Id}) = |G|-1$, by the fourier inversion theorem, inequality (88) reduces to

$$\begin{aligned}
\lambda_{min} &\geq \vartheta^-(2-|G|) + (|G|-\vartheta^-)(1-|G|) + |G| \min \widehat{R}(\mathrm{Id}) \\
\text{s.t. } R_g &= R_{g^{-1}} \, \forall g \in G \backslash \{\mathrm{Id}\}, \\
c_3^g &= c_3^{g^{-1}} \, \forall g \in G \backslash S, \\
R_g &\geq 0 \, \forall g \in G \backslash \{\mathrm{Id}\}, \\
c_3^g &\leq 0 \, \forall g \in G \backslash S, \\
c_3^g &= 0 \, \forall G \in S, \\
R_{\mathrm{Id}} &= 0, \\
\widehat{R}(\mathrm{Id}) &\geq |G| - 2, \\
R_g + \widehat{c_3}(g) &= 1 \, \forall g \in G \backslash \{\mathrm{Id}\}.
\end{aligned} \tag{89}$$

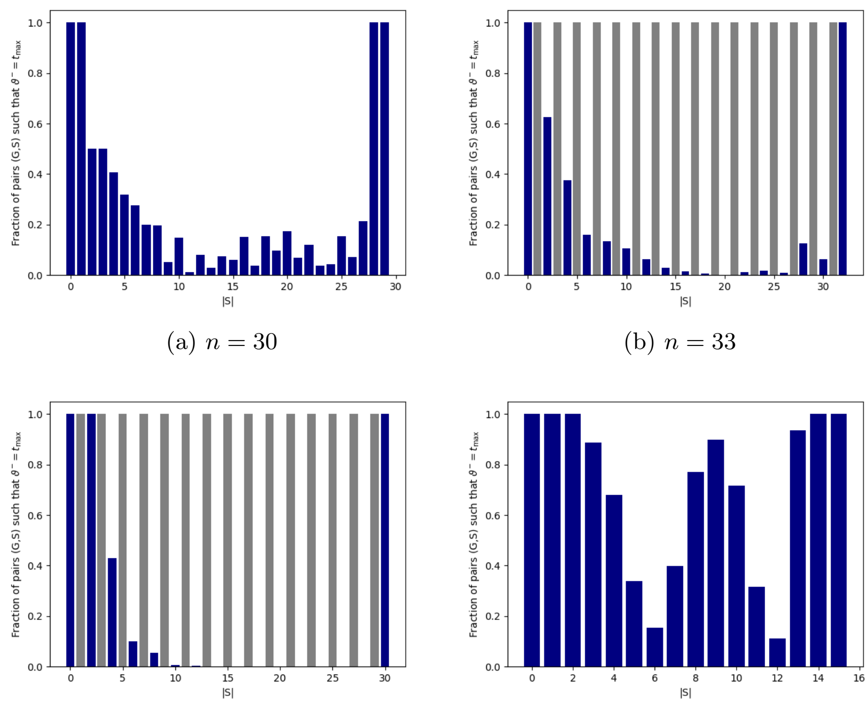
From this, it immediately follows that

$$\lambda_{min} \geq \vartheta^-(2-|G|) + (|G|-\vartheta^-)(1-|G|) + |G|(|G|-2) = \vartheta^- - |G|. \tag{90}$$

□

We have thus proven that for abelian Cayley graphs, there always exists an optimal solution to (17) for which the gap between the largest and least eigenvalue of $J + A$ is at most $|G|$. This is an indication that when $|S|$ is smaller, (17) is more likely to have solutions that satisfy (45), since ϑ^- is larger for those graphs, and the bound proven in theorem 15 is hence closer to $-\vartheta^-$.

This observation is reflected by numerical results, obtained by partitioning the pairs (G, S) consisting of abelian groups of cardinality n and symmetric sets S by the cardinality of S, and counting what fraction of such pairs satisfy $\vartheta^-(\mathrm{Cay}(G,S)) = t_{\max}(\mathrm{Cay}(G,S))$. Bar plots showing these fractions are depicted in figures



(a) $n = 30$

(b) $n = 33$

(c) $n = 31$

(d) $n = 16$

Figure 8: Some representative bar plots for the fraction of pairs (G, S) for which $\vartheta^-(\mathrm{Cay}(G, S)) = t_{\max}(\mathrm{Cay}(G, S))$, split by $|S|$. The gray bars represent those values of $|S|$, for which no abelian Cayley graph exists on n vertices.

In figure 8a, the blue bar at $|S| = 0$ is the empty graph. The bar at $|S| = 1$ are graphs that are the disjoint union of 2-cycles C_2. The bar at $|S| = 28$ are the complements of graphs that are the disjoint union of 2-cycles. Finally, the bar at $|S| = 29$ represents the complete graph K_{30}. These four bars occur for all even n. In figure 8b, n is odd, so all group elements $g \neq \mathrm{Id}$ of G are not equal to their own inverse: $g \neq g^{-1}$. For this reason, there are no graphs which $|S|$ is odd, when n is odd. Figure 8c is indicative of what happens if n is prime. In this case, all graphs for which $|N| = 2$ are cyclic, and we know by corollary 2 that $\vartheta^- = t_{\max}$. It is now clear that this is generally not true for the complement of a cyclic graph. Lastly, figure 8d is indicative of what happens when n has many divisors. Since whenever two smaller graphs G_1, G_2 both have an optimal solution to (17) that satisfies (45), $G_1 * G_2$ also has such a solution, as discussed in section 4.1. In each case, a significant portion of the sparse graphs has a solution to (8) that satisfies (45), as predicted by theorem 15.

6 Association schemes and Hamming graphs

While the complexity of the problem is already greatly reduced for abelian Cayley graphs, it might happen that the automorphism group of a graph gives even more information, and the complexity of calculating ϑ^- can be reduced even further. One way to obtain such graphs, is through *association schemes.* These, for example, play a role in determining upper bounds on how efficiently messages can be transmitted in coding theory. The first person to use association schemes to this end was Delsarte, in [7]. Symmetric association schemes are defined as follows [7, p. 8]:

Definition 20 (Symmetric association schemes)**.** *A symmetric association scheme consists of a finite set X and a partition $\mathcal{R} = \{R_0, \ldots, R_n\}$ of $X \times X$, such that the following properties hold:*

- $R_0 = \{(x, x) : x \in X\}$,
- $(x, y) \in R_i \implies (y, x) \in R_i$ *for all* $i \in \{0, \ldots, n\}$,
- *For all* $0 \leq i, j, h \leq n$ *there is a number* p_{ij}^h *such that the number of elements* x *of* X *that satisfy* $(y, x) \in R_i$ *and* $(x, z) \in R_j$ *is* p_{ij}^h, *for all choices of* $(y, z) \in R_h$.

One example of a symmetric association schemes are Hamming schemes. Consider an alphabet consisting of q letters. The Hamming distance $d_H(x, y)$ between two words x and y of equal length is the number of characters in which the word differs. This allows us to define the Hamming scheme.

Definition 21 (Hamming scheme)**.** *For positive integers n, q, let $X = q^{\times n}$ be the set of words of length n, with an alphabet consisting of q symbols. Furthermore, for $i = 0, \ldots, n$, define the set R_i as*

$$R_i = \{(x, y) \in X \times X : d_H(x, y) = i\}, \tag{91}$$

and $\mathcal{R} = \{R_0, \ldots, R_n\}$. The graphs with edge set $\cup_{i \in M} R_i$, for $M \subset \{1, \ldots, n\}$ are called Hamming graphs.

It is easily verifiable that Hamming schemes are indeed symmetric association schemes.

Given a symmetric association scheme, we can define *associate matrices*, which encode information about the scheme.

Definition 22 (Associate matrices)**.** *Suppose $(X, \mathcal{R})$ is a symmetric association scheme, and $\mathcal{R} = \{R_0, \ldots, R_n\}$. Then we define its associate matrices $D_0, \ldots, D_n$ as follows:*

$$[D_i]_{xy} = \begin{cases} 1 & \text{if } (i, j) \in R_i, \\ 0 & \text{otherwise.} \end{cases} \tag{92}$$

These associate matrices are clearly all symmetric. Hence they commute: $D_iD_j = (D_iD_j)^T = D_j^T D_i^T = D_jD_i$. Therefore, the span $\mathcal{S}$ of all these matrices is a vector space of dimension $n+1$. Furthermore, we have $D_0 = I$, and from the definition of (symmetric) association schemes it follows that

$$D_iD_j = \sum_{h=0}^{n} p_{ij}^h D_h. \tag{93}$$

Therefore, all linear combinations of the D_i are linear operators. Since a set of diagonisable matrices commute if and only if they are simultaneously diagonisable, and the $n+1$ operators D_i commute, There are $n+1$ common orthogonal unit eigenvectors $v_0, \dots v_n$ of $D_0, \dots, D_n$ in $\mathcal{S}$. Therefore $\mathcal{S}$ has an orthogonal, idempotent and symmetric basis $E_i := v_i v_i^T$, where i ranges over $\{0, \dots, n\}$. Now define the unique $n+1 \times n+1$ matrix P by

$$D_i = \sum_{j=0}^{n} P_{ji} E_j, \tag{94}$$

and the unique $n+1 \times n+1$ matrix Q by

$$|X| E_i = \sum_{j=0}^{n} Q_{ji} D_j. \tag{95}$$

It hence follows that $P_{ij} : j = 0, \dots, n$ are the eigenvalues of the $|X| \times |X|$ matrix D_i, and each such eigenvalue has multiplicity $\mathrm{Tr}(E_j)$, since the eigenvalues of E_j are all either 0 or 1. We furthermore know that $\sum_{i=0}^{n} E_i = I$, since

$$M = \sum_{i=0}^{n} M E_i = M \sum_{i=0}^{n} E_i \tag{96}$$

Delsarte found a way of using these matrices to bound the size of independent sets of graphs obtained from association schemes. Suppose $Y \subset X$. Then we define the inner distribution of Y as

Definition 23 (Inner distribution)**.** *The inner distribution* $(a_0, \dots, a_n)$ *of* Y *is defined as*

$$a_i = \frac{|R_i \cap (Y \times Y)|}{|Y|}. \tag{97}$$

It is clear that $\sum_{i=0}^{n} a_i = |Y|$. Delsarte used the inner distribution to bound the independence number of graphs with edge set $\cup_{i \in M} R_i$, for some subset $M \subset \{1, \dots, n\}$, in [7, p. 27].

Theorem 16 (Delsarte bound)**.** *Let* $M \subset \{1, \dots n\}$. *Suppose* $Y \subset X$ *satisfies*

$(x,y) \notin R_i\ \forall i \in M$, for all $x,y \in Y$. Then the following inequality holds.

$$
\begin{aligned}
|Y| \leq \mathcal{L}(X, \mathcal{R}, M) := \max_{a \in \mathbb{R}^{n+1}} \sum_{i=0}^{n} a_i \\
s.t.\ a \geq \mathbf{0}, \\
a_i = 0\ \forall i \in M, \\
a_0 = 1, \\
aQ \geq \mathbf{0}.
\end{aligned}
\tag{98}
$$

Proof. The inner distribution a of Y is nonnegative, and is 0 for all R_{m_i}. Furthermore, $a_0 = \frac{|Y|}{|Y|} = 1$. Lastly, since all E_i are idempotent and symmetric, their eigenvalues are a subset of $\{0,1\}$, and thus nonnegative. Let e_Y be the vector with values 1 for all indices in Y, and 0 for all other indices. We have

$$
\begin{aligned}
0 \leq e_Y^T E_i e_Y = e_Y^T \frac{1}{|X|} \sum_{j=0}^{n} Q_{ji} D_j e_Y \\
= \frac{|Y|}{|X|} \sum_{j=0}^{n} Q_{ji} \frac{e_Y^T D_j e_Y}{|Y|} = \frac{|Y|}{|X|} \sum_{j=0}^{n} Q_{ji} a_j,
\end{aligned}
\tag{99}
$$

and hence $aQ \geq \mathbf{0}$. a thus satisfies all constraints. Therefore the maximum objective value is at least as large as $|Y|$. □

It turns out that for a hamming scheme, the graph with edge set $\bigcup_{i \in M} R_i$ is an abelian Cayley graph.

Lemma 13. *The graph $(\{1,\dots,q\}^{\times d}, \bigcup_{i \in M} R_i)$ is an abelian Cayley graph on the group $(\mathbb{Z}/q\mathbb{Z})^{\times d}$.*

Proof. Let $\rho \in (\mathbb{Z}/q\mathbb{Z})^{\times d}$ be arbitrary. Suppose $d_H(x,y) = r$. Then $d_H(\rho(x), \rho(y)) = d_H(x,y)$, since the number of characters that differ remains the same after applying ρ. □

In [16], Schrijver discovered that this upper bound on the independence number of the graph with edge set $R_{m_1} \cup \dots R_{m_r}$ has the same value as ϑ^- has. To show this, we need the dual LP formulation of Delsarte's bound.

Lemma 14 (Dual Delsarte bound)**.** *The LP dual of the Delsarte bound is*

$$
\begin{aligned}
\mathcal{L}(X, \mathcal{R}, M) = \min \sum_{i=0}^{n} b_i \\
s.t.\ b \geq \mathbf{0}, \\
b_0 = 1, \\
\sum_{j=0}^{n} b_j P_{ij} \leq 0\ \forall i \in \{1,\dots,n\} \backslash M.
\end{aligned}
\tag{100}
$$

It can be shown that $\text{Tr}(E_i)P_{ij} = p^0_{jj}Q_{ji}$ [18]. With this, Schrijver constructed an optimal solution of (17) in theorem 3 of [16], using the dual Delsarte bound.

Theorem 17. *Suppose b attains the minimum in* (100) *with objective value λ. Then the matrix*

$$A := \lambda I - \sum_{k=0}^{n} \left(\sum_{u=0}^{n} \frac{b_u}{\text{Tr}(E_u)} Q_{ku} \right) D_k \tag{101}$$

attains the minimum of the dual formulation of ϑ^-, and $\vartheta^- = \lambda$.

The eigenvalues of the matrix A can be easily computed since we know the eigenvalues of each D_k. They hence are

$$\lambda - \sum_{k=0}^{n} \left(\sum_{u=0}^{n} \frac{b_u}{\text{Tr}(E_u)} Q_{ku} \right) P_{ik} = \lambda - \frac{b_i}{\text{Tr}(E_i)} |X| \tag{102}$$

for $i = 0, \ldots, n$. Since we know that $\sum_{i=0}^{n} E_i = I = D_0$, the trivial eigenvalue corresponds to $i = 0$.

We are interested in finding a solution such that all eigenvalues of $J + A$ are bounded between λ and $-\lambda$. To this end, we can add the constraint that for all $i \neq 0$ it must hold that $b_i \leq \frac{2\text{Tr}(E_i)\lambda}{|X|}$. Thus, we define the following LP:

Lemma 15. *Define $t^{\mathcal{L}}_{\min}$ as*

$$\begin{aligned} t^{\mathcal{L}}_{\min}(X, \mathcal{R}, M) := \min_{b \in \mathbb{R}^{n+1}} &\sum_{i=0}^{n} b_i \\ s.t.\ &b \geq \mathbf{0}, \\ &b_0 = 1, \\ \sum_{j=0}^{n} b_j P_{ij} &\leq 0\ \forall i \in \{1, \ldots, n\} \setminus M \\ b_i - \frac{2\text{Tr}(E_i)}{|X|} \sum_{j=0}^{n} b_j &\leq 0\ \forall i \in \{1, \ldots, n\}. \end{aligned} \tag{103}$$

Suppose $t^{\mathcal{L}}_{\min}(X, \mathcal{R}, M) = \mathcal{L}(X, \mathcal{R}, M)$, then the graph with vertex set X, and edge set $\bigcup_{i \in M} R_i$ has an optimal solution to (17) *that satisfies* (45).

For Hamming schemes, the matrices P and Q are known, and determined by the Krawtchouk polynomials of degree n, as proven in theorem 4.2 of [7]:

$$P_{ku} = \sum_{j=0}^{k} \binom{n-j}{k-j} \binom{u}{j} (-q)^j (q-1)^{k-j}, \tag{104}$$

and

$$\text{Tr}(E_i) = \binom{n}{i} (q-1)^i. \tag{105}$$

Using these polynomials, lemma 15 was checked numerically using the program listed in appendix B.3, for several Hamming graphs. The values of $\mathcal{L}(n, q, M)$ were cross-verified with some known values of the Delsarte bound. It turns out that not all Hamming graphs satisfy the conditions of lemma 15. For example, when $n = 2, q = 5$ and $M = \{1\}$ it follows that $\mathcal{L}(n, q, M) = 5$, but $t^{\mathcal{L}}_{\min}(n, q, M) \approx 6.82$.

A count of several small Hamming graphs suggest that when either n or q becomes large, the proportion of all possible $M \subset \{1, \ldots, n\}$ such that $t^{\mathcal{L}}_{\min}(n, q, M) = \mathcal{L}(n, q, M)$ approaches 0.

	q=2	q=3	q=4	q=5	q=6	q=7	q=8	q=9
n=1	1	1	1	1	1	1	1	1
n=2	3	3	3	2	2	2	2	2
n=3	5	5	5	3	3	3	3	3
n=4	11	5	6	5	4	4	4	4
n=5	14	8	8	6	5	5	5	5
n=6	22	11	11	7	10	6	6	6
n=7	40	17	12	8	9	8	10	6

Table 2: Number of sets M such that $t^{\mathcal{L}}_{\min}(n, q, M) = \mathcal{L}(n, q, M)$

Furthermore, when $q \to \infty$, this seems to only holds for $n + 1$ different, specific sets M, although this is not yet proven.

Conjecture 1. *For Hamming schemes, for any n, there exists a number N such that for all $q \geq N$, only the sets $M = \emptyset, \{n\}, \{n-1, n\}, \ldots, \{1, 2, \ldots, n\}$ satisfy $t^{\mathcal{L}}_{\min}(n, q, M) = \mathcal{L}(n, q, M)$.*

Since the Hamming distance between two words is preserved under both the permutations of an arbitrary letter in the words, and the permutations of the letters in the words, it follows that for every two pairs of words with the same Hamming distance i there is an automorphism of the graph induced by R_i that maps the first pair onto the second pair. Therefore, lemmas 5 and 9 guarantee that checking if $t^{\mathcal{L}}_{\min}(n, q, M) = \mathcal{L}(n, q, M)$ is sufficient for checking if there exists an optimal solution to (17) for the induced graph that satisfies (45). Generally, the construction given in section 4.1 does not work for Hamming graphs.

7 Conclusion

In this thesis, the multiplicity of Schrijvers variant ϑ^- of the Lovász theta number ϑ under the disjunctive graph product was investigated. Firstly, a few key properties of the functions ϑ, ϑ^- and ϑ^+ were proven, and a new proof of the equation $\vartheta^-(G)\vartheta^+(\overline{G}) = |V_G|$ for vertex-transitive graphs was given. Then a novel construction of an optimal dual solution for $\vartheta^-(G * H)$, given optimal dual solutions of $\vartheta^-(G)$ and $\vartheta^-(H)$ was presented, which makes use of an additional assumption on the spectrum of these optimal solutions. After that, it was investigated for which graphs there are solutions to the dual formulation of ϑ^-, that satisfy this additional assumption. It is proven that this holds for all cyclic graphs, and an upper bound on the minimal gap between the eigenvalues belonging to optimal solutions of the dual formulation of ϑ^- was proven for abelian Cayley graphs. Lastly, it was shown that the complexity of the problem is greatly reduced for abelian Cayley graphs, and in particular for graphs induced by Association schemes.

While the construction presented in this thesis does not work in general, it does work for many sparse, abelian Cayley graphs. These frequently occur in problems, such as the optimal sphere packing density.

Future research into the dual multiplicity of ϑ^- can focus on finding more general constructions than the one presented in this thesis. Furthermore, a continuous extension of this construction should be investigated for infinite extensions of ϑ^-, such as the Cohn-Elkies bound. Lastly, asymptotic properties of the eigenmatrices P and Q of Hamming schemes might be used to prove conjecture 1.

A Duality of ϑ, without use of Slater's criterion

Lemma 16. *Suppose $m \in \mathbb{R}^n$ maximizes $\langle l, \cdot\rangle$ over all values in $A \cap C \subset \mathbb{R}^n$, where A is affine, and C convex. Then there exist $c, d \in \mathbb{R}^n$, and $\gamma, \delta \in \mathbb{R}$ such that the following hold.*

$$\begin{aligned} \langle c, A\rangle &\subset (-\infty, \gamma] \\ \langle d, C\rangle &\subset (-\infty, \delta] \\ \langle c, m\rangle &= \gamma \\ \langle d, m\rangle &= \delta \\ c + d &= l \end{aligned} \tag{106}$$

Proof. Since we can shift all variables by a factor m, assume that $m = \mathbf{0}$, and A is linear. Define $n := \pi_A l$. Since $\mathbf{0}$ maximizes $\langle l, \cdot\rangle$ on $A \cap C$, $\mathbf{0}$ also maximizes $\langle n, \cdot\rangle$ on $A \cap C$, so $\langle n, A\rangle \subset (-\infty, 0]$. Let $T_A := A \cap n^\perp$. Since C is convex, $\pi_{T_A^\perp} C \subset T_A^\perp$ is also convex. Furthermore, $\mathbf{0}$ lies on the boundary of $\pi_{T_A^\perp} C$ inside $T_A^\perp$. Hence, there is a vector $p \in T_A^\perp$ such that $\langle p, \pi_{T_A^\perp} C\rangle \subset (-\infty, 0]$, and since $p \in T_A^\perp$ we have $\langle p, C\rangle = \langle p, \pi_{T_A^\perp} C\rangle \subset (-\infty, 0]$. Since $p \in T_A^\perp$, it follows that there is a $\lambda > 0$ such that $\pi_A p = \lambda n$. Therefore, we have $p = \frac{\|\pi_A p\|}{\|n\|} n + \pi_{A^\perp} p$, and hence $n = \frac{\|n\|}{\|\pi_A p\|} p - \frac{\|n\|}{\|\pi_A p\|} \pi_{A^\perp} p$. Consequently, the identity

$$l = \left[l - n - \frac{\|n\|}{\|\pi_A p\|} \pi_{A^\perp} p\right] + \left[\frac{\|n\|}{\|\pi_A p\|} p\right] \tag{107}$$

holds. As $l - n \perp A$, $c := l - n - \frac{\|n\|}{\|\pi_A p\|} \pi_{A^\perp} p \perp A$, and hence $\langle c, A\rangle = 0 \subset (-\infty, 0]$. Since furthermore $\langle \frac{\|n\|}{\|\pi_A p\|} p, C\rangle \subset (-\infty, 0]$, the values c and $d := \frac{\|n\|}{\|\pi_A p\|} p$ satisfy the conditions in (106). By taking the original, non-zero value of m, we obtain the values $\gamma := \langle c, m\rangle$ and $\delta := \langle d, m\rangle$. $\square$

Using the results from lemma 16, Schrijver gives an alternative proof of duality of ϑ in theorem 67.7 of [17].

Theorem 18. *The optimal values in* (6) *and* (14) *are the same.*

Proof. Let the matrix M maximize (6), and $m = \mathrm{Tr}(JM)$. Let the matrix A minimize (14), and $a = \Lambda(J + A)$. To prove that $m \leq a$, consider the matrix $Y := aI - J - A$. Since Y is PSD, it follows that

$$0 \leq \mathrm{Tr}(YM) = \mathrm{Tr}\left((aI - J - A)M\right) = a\mathrm{Tr}(M) - \mathrm{Tr}(JM), \tag{108}$$

since For all (i, j), either $M_{ij} = 0$ or $A_{ij} = 0$, and hence $\mathrm{Tr}(AM) = 0$. Therefore,

$$0 \leq a - m. \tag{109}$$

Proving $a \leq m$ is a bit more tricky. Since $S_+^{V_G}$ is convex, and $\mathcal{M}_G$ is affine, there are $C, D \in \mathrm{R}^{V_G^2}$ and $\gamma, \delta \in \mathbb{R}$ such that $\mathrm{Tr}(CX) \leq \gamma$ for all $X \in \mathcal{M}_G$, and $\mathrm{Tr}(DX) \leq \delta$ for all $X \in S_+^{V_G}$, with equality for $X = M$, and $C + D = J$. Assume C, D are symmetric, by replacing them with $\frac{1}{2}(C+C^T)$ and $\frac{1}{2}(D+D^T)$. This works, since $S_+^{V_G}$ and $\mathcal{M}_G$ consist of symmetric matrices. Since $S_+^{V_G}$ is a cone, $\delta = 0$. Now $-D \in S_+^{V_G}$, since $xx^T \in S_+^{V_G}$ for all $x \in \mathbb{R}^{V_G}$, and hence $x^T Dx = \mathrm{Tr}(xx^t D) \leq 0$. Since $\mathcal{M}_G \subset \{X | \mathrm{Tr}(CX) = \gamma\}$, there is a matrix $B \in \mathcal{L}_G$ such that $C = \gamma I - B$. Therefore, since $-D \in S_+^{V_G}$, it follows that $\gamma I - J - B \in S_+^{V_G}$. Therefore, $a = \Lambda(j + A) \leq \Lambda(J + B) \leq \gamma = \mathrm{Tr}(CM) = m$. By combining both inequalities, we have shown that $a = m$. □

B Code

B.1 Program for checking which graphs satisfy $\vartheta^- = t_{\max}$

The following Julia code was used to determine which graphs satisfy the condition of lemma 7, for all graphs with $n = 1 - 7$ vertices.

```
using LinearAlgebra, COSMO, JuMP, Plots, GraphRecipes, Distributions,
    Combinatorics
max_err = 1e-3
iter=1

function theta_prime(G)
    n = size(G)[1]
    model = JuMP.Model(COSMO.Optimizer)
    set_silent(model)
    @variable(model, X[1:n, 1:n], PSD)
    @objective(model, Max, sum(X))
    @constraint(model, tr(X)==1)
    for i in 1:n
        for j in 1:n
            if (G[i,j]==1)
                @constraint(model, X[i,j] == 0)
            else
                @constraint(model, X[i,j] >= 0)
            end
        end
    end
    JuMP.optimize!(model)
    return JuMP.objective_value(model)
end

function theta_prime_dual_conjecture(G)
    n = size(G)[1]
    Ig = Matrix(1I, n, n)
    Jg = ones(n,n)
    model = JuMP.Model(COSMO.Optimizer)
    set_silent(model)
    @variable(model, l)
    @variable(model, X[1:n, 1:n])
    @objective(model, Min, l)
    @constraint(model, (l*Ig - Jg - X) in PSDCone())
    @constraint(model, (l*Ig + Jg + X) in PSDCone())
    for i in 1:n
```

```
        for j in 1:n
            if (G[i,j]==0)
                @constraint(model, X[i,j] >= 0)
            end
        end
    end
    JuMP.optimize!(model)
    return JuMP.objective_value(model)
end

function validate_conjecture(G)
    t = theta_prime(G)
    c = theta_prime_dual_conjecture(G)
    return (abs(t-c)<max_err)
end

function check_if_done(R,S)
    return in(R,S)
end

function add_to_done(R,S,n)
    R2 = copy(R)
    perms = permutations(collect(1:n))
    for p in perms
        for i in 1:n
            for j in 1:n
                R2[p[i],p[j]] = R[i,j]
            end
        end
        push!(S,copy(R2))
    end
end

function validate_all_m(n,m,from,fixedset,S,iter,coll)
    r = length(fixedset)
    if (m==0)
        R = zeros(n,n)
        cnt=0
        pos=1
        i=2
        while pos<=r
            if (fixedset[pos]-cnt<=i-1)
                R[i,fixedset[pos]-cnt] = 1
                R[fixedset[pos]-cnt,i] = 1
                pos+=1
            else
                cnt+=i-1
                i+=1
            end
        end
        if check_if_done(R,S)
            return
        end
        good = validate_conjecture(R)
        if (!good)
            push!(coll,R)
        end
```

```
        add_to_done(R,S,n)
        return
    end
    for i in from:trunc(Int,(n*(n-1)/2 -m + 1))
        push!(fixedset,i)
        validate_all_m(n,m-1,i+1,fixedset,S,iter,coll)
        pop!(fixedset)
    end
end

function get_fails_size_n(n)
    S = Set()
    iter=[1,1]
    coll = []
    for m in 0:trunc(Int,n*(n-1)/2)
        L=[]
        iter[2]=1
        validate_all_m(n,m,1,L,S,iter,coll)
    end
    return coll
end
```

B.2 Program for comparing ϑ^{-} and $t_{\max}$ for abelian Cayley graphs

The following Python code was used to check which of the abelian Cayley graphs on n vertices satisfy the conditions of lemma 7, for $n = 1 - 31, 33$.

```
from scipy.optimize import linprog
from math import *
import numpy as np

eps = 1e-6
partitions = [[], [[1]], [[2],[1,1]], [[3],[2,1],[1,1,1]],
     [[4],[3,1],[2,2],[2,1,1],[1,1,1,1]],
     [[5],[4,1],[3,2],[3,1,1],[2,2,1],[2,1,1,1],[1,1,1,1,1]]]

def solve_Cayley_2(S, A, b, obj_func):
    var_bounds = [(None,None) if p else (1,None) for p in S]
    res = linprog(obj_func, A_ub = A, b_ub = b, bounds = var_bounds)
    return res.fun

def solve_Cayley_conjecture_2(S, A_conj, b_conj, obj_func):
    var_bounds = [(None,None) if p else (1,None) for p in S]
    res = linprog(obj_func, A_ub = A_conj, b_ub = b_conj, bounds = var_bounds)
    return res.fun

def prime_decomposition(n):
    m = n
    pfact = []
    curp = 2
    while (m>1):
        if (m%curp==0):
            pfact.append([curp,0])
        while (m%curp==0):
            pfact[-1][1] += 1
```

```
            m//=curp
        curp+=1
    return pfact

def advance_partition_set(numbers, current):
    for i in range(len(numbers)):
        current[i] += 1
        if current[i] == numbers[i]:
            current[i] = 0
        else: break

def get_pairs(n, cycles, rs):
    pairs = []
    id_seen = [True for i in range(n)]
    for p in range(n):
        if (id_seen[p]):
            id_seen[p] = False
            p_inv, tmp = 0, 1
            for perm in range(len(cycles)):
                p_inv += tmp*(cycles[perm] - rs[p][perm]) if rs[p][perm]>0 else 0
                tmp *= cycles[perm]
            if (p == p_inv):
                pairs.append([p])
            else:
                id_seen[p_inv] = False
                pairs.append([p,p_inv])
    return pairs

def verify_conjecture_size(n):
    numgood, numbad, numnone, numerror = 0, 0, 0, 0
    pfact = prime_decomposition(n)
    number_parts = [len(partitions[p[1]]) for p in pfact]
    current_partition_set = [0 for p in pfact]
    times = np.prod(number_parts)

    for _ in range(times):
        cycles = [pfact[i][0]**c for i in range(len(pfact)) for c in partitions[pfact[i][1]][current_partition_set[i]]]
        rs = [[0 for i in range(len(cycles))]]
        for c in range(len(cycles)):
            curlen = len(rs)
            for j in range(1,cycles[c]):
                for perm in range(curlen):
                    rs.append([rs[perm][i] if i!= c else j for i in range(len(cycles))])

        pairs = get_pairs(n, cycles, rs)

        A = [[(cos(sum(2*pi*rs[perm][j]*rs[p[0]][j]/cycles[j] for j in range(len(cycles))))-1)*len(p) for p in pairs] for perm in range(1,n)]
        b = [0 for perm in range(1,n)]

        A_conj = [[(cos(sum(2*pi*rs[perm][j]*rs[p[0]][j]/cycles[j] for j in range(len(cycles))))-1)*len(p) for p in pairs] for perm in range(1,n)] + [[-(cos(sum(2*pi*rs[perm][j]*rs[p[0]][j]/cycles[j] for j in range(len(cycles))))+1)*len(p) for p in pairs] for perm in range(1,n)]
        b_conj = [0 for perm in range(1,n)] + [0 for perm in range(1,n)]
```

```

        obj_func = [len(p) for p in pairs]

        numgood += 1

        for S_bitmask in range(1,1<<(len(pairs)-1)):
            S = [True if (((S_bitmask<<1)>>j)&1)==1 else False for j in range(len
    (pairs))]
            theta = solve_Cayley_2(S,A,b,obj_func)
            t_{\mathrm{max}} = solve_Cayley_conjecture_2(S,A_conj,b_conj,obj_func
    )
            if (theta == None):
                numerror += 1
            elif (t_{\mathrm{max}} == None):
                numnone += 1
            elif (abs(theta-t_{\mathrm{max}}) < eps):
                numgood += 1
            else:
                numbad += 1

        advance_partition_set(number_parts, current_partition_set)

    return [numgood, numbad, numnone, numerror]
```

B.3 Program for comparing ϑ^- and $t_{\max}$ for Hamming graphs

The following code was used to check which Hamming graphs satisfy the conditions of lemma 7, for several small values of n, q, and all subsets $M \subset \{1, \ldots, n\}$.

```
    from scipy.optimize import linprog
from math import *
import numpy as np

facts = [1]
for i in range(1,30): facts.append(facts[-1]*i)
print(facts)

def binom(a,b):
    return (facts[a])//(facts[b]*facts[a-b])

def getKrawchouk(d,q):
    pow_min_q = [1]
    pow_q_min_1 = [1]
    for i in range(1,d+1): pow_min_q.append(-pow_min_q[-1]*q)
    for i in range(1,d+1): pow_q_min_1.append(pow_q_min_1[-1]*(q-1))
    return [[sum(binom(d-j,k-j)*binom(u,j)*pow_min_q[j]*pow_q_min_1[k-j] for j in
      range(d+1)) for k in range(d+1)] for u in range(d+1)]

def getTracesE(d,q):
    pow_q_min_1 = [1]
    for i in range(1,d+1): pow_q_min_1.append(pow_q_min_1[-1]*(q-1))
    return [binom(d,u)*pow_q_min_1[u] for u in range(d+1)]

def Delsarte_dual_ordinary(d,q,M):
    P = getKrawchouk(d,q)
    obj_fun = [1 for i in range(d+1)]
```

```
    var_bounds = [(1,1)] + [(0,None) for i in range(d)]
    A = [[P[j][i] for j in range(d+1)] for i in range(1,d+1) if M[i]==1]
    b = [0 for i in range(1,d+1) if M[i]==1]
    res = linprog(obj_fun, A_ub = A, b_ub = b, bounds = var_bounds)
    return res.fun

def Delsarte_dual_test(d,q,M):
    P = getKrawchouk(d,q)
    mu = getTracesE(d,q)
    q_pow_d = q**d
    obj_fun = [1 for i in range(d+1)]
    var_bounds = [(1,1)] + [(0,None) for i in range(d)]
    A = [[P[j][i] for j in range(d+1)] for i in range(1,d+1) if M[i]==1] + [[(i==j) - 2*mu[i]/q_pow_d for j in range(d+1)] for i in range(1,d+1)]
    b = [0 for i in range(1,d+1) if M[i]==1] + [0 for i in range(1,d+1)]
    res = linprog(obj_fun, A_ub = A, b_ub = b, bounds = var_bounds)
    return res.fun

for d in range(1,8):
    for q in range(2,10):
        cnt = 0
        cnt2 = 0
        for m in range((1<<d)+1, (1<<(d+1))):
            M = [(m>>i)&1 for i in range(d,-1,-1)]
            reg = Delsarte_dual_ordinary(d,q,M)
            test = Delsarte_dual_test(d,q,M)
            if (abs(reg-test) > 0.00001):
                # print(d,q,M,reg,test)
                cnt += 1
            else:
                cnt2 += 1
        print(cnt2, end=" & ")
    print("\n \\hline \\\\")
```

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