Geometric Ramifications of the Lovász Theta Function and Their Interplay with Duality

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

The Lovász theta function and the associated convex sets known as theta bodies are fundamental objects in combinatorial and semidefinite optimization. They are accompanied by a rich duality theory and deep connections to the geometric concept of orthonormal representations of graphs. In this thesis, we investigate several ramifications of the theory underlying these objects, including those arising from the illuminating viewpoint of duality. We study some optimization problems over unit-distance representations of graphs, which are intimately related to the Lovász theta function and orthonormal representations. We also strengthen some known results about dual descriptions of theta bodies and their variants. Our main goal throughout the thesis is to lay some of the foundations for using semidefinite optimization and convex analysis in a way analogous to how polyhedral combinatorics has been using linear optimization to prove min-max theorems.

A unit-distance representation of a graph G maps its nodes to some Euclidean space so that adjacent nodes are sent to pairs of points at distance one. The hypersphere number of G, denoted by $t(G)$, is the (square of the) minimum radius of a hypersphere that contains a unit-distance representation of G. Lovász proved a min-max relation describing $t(G)$ as a function of $\vartheta(\overline{G})$, the theta number of the complement of G. This relation provides a dictionary between unit-distance representations in hyperspheres and orthonormal representations, which we exploit in a number of ways: we develop a weighted generalization of $t(G)$, parallel to the weighted version of ϑ; we prove that $t(G)$ is equal to the (square of the) minimum radius of an Euclidean ball that contains a unit-distance representation of G; we abstract some properties of ϑ that yield the famous Sandwich Theorem and use them to define another weighted generalization of $t(G)$, called ellipsoidal number of G, where the unit-distance representation of G is required to be in an ellipsoid of a given shape with minimum volume. We determine an analytic formula for the ellipsoidal number of the complete graph on n nodes whenever there exists a Hadamard matrix of order n.

We then study several duality aspects of the description of the theta body $\mathrm{TH}(G)$. For a graph G, the convex corner $\mathrm{TH}(G)$ is known to be the projection of a certain convex set, denoted by $\widehat{\mathrm{TH}}(G)$, which lies in a much higher-dimensional matrix space. We prove that the vertices of $\widehat{\mathrm{TH}}(G)$ are precisely the symmetric tensors of incidence vectors of stable sets in G, thus broadly generalizing previous results about vertices of the elliptope due to Laurent and Poljak from 1995. Along the way, we also identify all the vertices of several variants of $\widehat{\mathrm{TH}}(G)$ and of the elliptope. Next we introduce an axiomatic framework for studying generalized theta bodies, based on the concept of diagonally scaling invariant cones, which allows us to prove in a unified way several characterizations of ϑ and the variants ϑ' and ϑ^{+} introduced independently by Schrijver, and by McEliece, Rodemich, and Rumsey in the late 1970's, and by Szegedy in 1994. The beautiful duality equation which states that the antiblocker of $\mathrm{TH}(G)$ is $\mathrm{TH}(\overline{G})$ is extended to this setting. The framework allows us to treat the stable set polytope and its classical polyhedral relaxations as generalized theta bodies, using the completely positive cone and its dual, and it allows us to derive a (weighted generalization of a) copositive formulation for the fractional chromatic number due to Dukanovic and Rendl in 2010 from a completely positive formulation for the stability number due to de Klerk and Pasechnik in 2002. Finally, we study a non-convex constraint for semidefinite programs (SDPs) that may be regarded as analogous to the usual integrality constraint for linear programs. When applied to certain classical SDPs, it specializes to the standard rank-one constraint. More importantly, the non-convex constraint also applies to the dual SDP, and for a certain SDP formulation of ϑ, the modified dual yields precisely the clique covering number. This opens the way to study some exactness properties of SDP relaxations for combinatorial optimization problems akin to the corresponding classical notions from polyhedral combinatorics, as well as approximation algorithms based on SDP relaxations.

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Chapter 1

Introduction

A classical approach for solving a combinatorial optimization problem relies on embedding its finite set of candidate solutions as points in some geometric space and analyzing their convex hull using tools from linear algebra, polyhedral theory, and convex analysis. The past half century of development of this method, epitomized by polyhedral combinatorics [132, 133, 134], has revealed an abundance of pleasant correspondences between combinatorial properties of the problem at hand and geometric and algebraic properties of the associated convex set. Some highlights include:

(i) the equivalence between optimization and separation [59] as a consequence of the far-reaching ellipsoid method;

(ii) the solutions of the "hardest" combinatorial optimization problems known to be tractable, such as submodular function minimization [59, 131, 75], the weighted linear matroid matching problem [74, 115], and the weighted stable set and coloring problems over perfect graphs [59];

(iii) the development of lift-and-project methods [137, 101, 80, 81, 85, 86] for obtaining hierarchies of nested relaxations for arbitrary binary integer programming problems.

A related area of study, not nearly as systematic, is that of regarding graphs essentially as geometric objects, and investigating correspondences between their combinatorial and geometric properties. One very elegant and prototypical correspondence of this kind, and probably one of the first, is Steinitz's Theorem [142, 143] from the early 1920's. Hailed by Grünbaum [60] as "the most important and deepest known result on 3-polytopes," it characterizes the graphs that are skeletons of full-dimensional polytopes in $\mathbb{R}^3$ as precisely the 3-connected planar graphs. Thus, by the planarity criteria of Kuratowski [83] and Wagner [154], we may regard Steinitz's Theorem as identifying, for a given graph, the geometric property of being the skeleton of a full-dimensional polytope in $\mathbb{R}^3$ with the combinatorial property of being 3-connected and having no K_5- or $K_{3,3}$-minor. Subsequently to Steinitz's Theorem, a host of other similarly flavored results have been proved involving a rich variety of interrelated geometric representations of graphs, touching on a broad range of directions, such as:

(i) the Circle Packing Theorem of Koebe [79], Andre'ev [4, 5], and Thurston [148], and its ramifications [128, 18, 110, 157];

(ii) the Tutte [151, 120, 92] method of barycentric representations;

(iii) the *orthonormal representations* of graphs introduced by Lovász [94] to solve a long-standing conjecture of Shannon [135] and further exploited very fruitfully in combinatorial optimization [58, 59, 78] and other areas [99, 100, 118];

(iv) the exploration [141, 43, 146, 113] of the chromatic number of $\mathbb{R}^d$;

(v) the interpretation of graphs as *tensegrity frameworks*, going back to Cauchy (see, e.g., [1, Ch. 13]), with the study of several variations of the concept of rigidity [124, 29, 67, 31], specially in the context of low dimensions [84, 104, 13], as well as in more applied settings [139, 140];

(vi) a spectral graph invariant introduced by Colin de Verdière [28], defined using algebraic geometry concepts, and surprisingly connected to topological properties of graphs, such as planarity and linkless embeddability [102, 70], as well as to Steinitz's Theorem [103, 95];

(vii) the development [127, 152] of algorithmic and complexity results for certain "geometric graphs" and other applications in theoretical computer science [91, 7].

See Lovász's survey [97] for a nice presentation of some of these results.

A centerpiece lying in the intersection of polyhedral combinatorics and the study of geometric representations of graphs is the *Lovász theta function*, often denoted by ϑ. First introduced together with orthonormal representations in the seminal paper by Lovász [94] to solve a problem in information theory, the theta function was further developed in the 1980's, along with applications of the ellipsoid method [58, 59], via a compact semidefinite optimization formulation. This led to a weighted generalization of ϑ that may be approximated to an arbitrary precision in polynomial time and to a semidefinite relaxation of the *stable set polytope* of a graph known as the *theta body*. This relaxation is tight for perfect graphs, and it leads to the only known (strongly) polynomial algorithm for finding optimal stable sets and colorings in such graphs, even after the proof of the Strong Perfect Graph Theorem [27] and the design of a recognition algorithm for perfect graphs [26]. Since then, the theory surrounding the Lovász theta function has been further extended [101, 44, 106], and it has been used in the design of approximation algorithms [76, 77, 23], in complexity theory [147, 42, 10, 9], and in graph entropy [107, 138]. These developments corroborate Goemans' quote [51, p. 147] that "it seems all paths lead to ϑ!"

For a graph $G = (V, E)$, the *theta body* of G may be defined as the set

$$\mathrm{TH}(G) = \left\{ x \in \mathbb{R}^V : \exists X \in \mathbb{S}^V,\, X_{ii} = x_i \,\forall i \in V,\, X_{ij} = 0 \,\forall ij \in E,\, \begin{bmatrix} 1 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathbb{S}_+^{\{0\}\cup V} \right\}. \tag{1.1}$$

Here, $\mathbb{S}^V$ denotes the set of $V \times V$ symmetric matrices and $\mathbb{S}_+^{\{0\}\cup V}$ is the set of symmetric positive semidefinite matrices on the index set $\{0\} \cup V$; we assume that 0 is not an element of V. One of the many possible definitions of the *theta number* $\vartheta(G)$ of G is

$$\vartheta(G) = \max\left\{ \textstyle\sum_{i\in V} x_i : x \in \mathrm{TH}(G) \right\}. \tag{1.2}$$

Equation (1.2) describes $\vartheta(G)$ as the optimal value of a semidefinite program (SDP), that is, a problem of optimizing a linear function over the intersection of an affine subspace and the cone of positive semidefinite matrices [3, 156]. Like linear programs (LPs), every SDP has an associated dual SDP for which Weak

Duality holds. Unlike the case for LPs, it is *not* generally true that an SDP and its dual have equal optimal values, even if both are finite, and even if both primal and dual have optimal solutions (see [150] and references therein). However, under certain so-called regularity conditions, a Strong Duality Theorem holds, so both primal and dual SDPs have optimal solutions and their optimal values coincide. This is the case for the SDPs involving the theta function. As a consequence, the number $\vartheta(G)$ may be approximated to an arbitrary precision in polynomial time by the ellipsoid method in theory [59], and by interior-point methods in theory and in practice [111, 65, 3, 149].

From the SDP formulation (1.2), it is easy to prove that $\alpha(G) \leq \vartheta(G)$, where $\alpha(G)$ denotes the *stability number* of G. In fact, we have $\mathrm{STAB}(G) \subseteq \mathrm{TH}(G)$, where $\mathrm{STAB}(G)$ is the *stable set polytope* of G, i.e., the convex hull of the incidence vectors of the stable sets in G. By inspecting the SDP dual to (1.2), it is also easy to prove that $\vartheta(G) \leq \overline{\chi}(G)$, where $\overline{\chi}(G)$ is the *clique covering number* of G. The combined inequalities

$$\alpha(G) \leq \vartheta(G) \leq \overline{\chi}(G) \tag{1.3}$$

constitute what is known as the Sandwich Theorem [94, 78]. Thus, the number $\vartheta(G)$, which is efficiently computable, lies sandwiched between the graph invariants $\alpha(G)$ and $\overline{\chi}(G)$, which are NP-hard to approximate [105, 6, 63], let alone compute. This sandwich inequality is perhaps the most famous property of the theta function. It has prompted a number computational experiments to approximate these NP-hard quantities (see [35, 36] and references therein). However, the bounds provided by (1.3) are in general rather weak [40, 41].

From a purely theoretical viewpoint, however, the use of the theta function has been very fruitful, as we have previously discussed. This owes to the fact that the theta function and related concepts form very natural objects, worthy of a study of their own, not just as a proxy for the stability or clique covering numbers. This fact is attested by the multitude [94, 59, 44, 106] of characterizations of $\vartheta(G)$. Many of such wealth of interesting characterizations arguably come from SDP Strong Duality. A particularly illuminating manifestation of this duality is the identity [58, Corollary 3.4]

$$\mathrm{abl}(\mathrm{TH}(G)) = \mathrm{TH}(\overline{G}), \tag{1.4}$$

that is, the *antiblocker* of $\mathrm{TH}(G)$ is the theta body of $\overline{G}$, the complement of G.

Some equivalent characterizations of $\vartheta(G)$ rely on the concept of orthonormal representations. An *orthonormal representation* of a graph $G = (V, E)$ is a map from V into the unit vectors of some Euclidean space that sends non-adjacent nodes of G to pairs of orthogonal vectors. That is, an orthonormal representation of G is a map $u\colon V \to \mathbb{R}^d$ for some positive integer d such that u_i has unit norm for each $i \in V$ and the inner product $\langle u_i, u_j \rangle$ is zero whenever i and j are non-adjacent nodes of G. One of the consequences of (1.4) is that

> the members of $\mathrm{TH}(G)$ are precisely the vectors $x \in \mathbb{R}^V$ of the form $x_i = \langle u_0, u_i \rangle^2$ for each $i \in V$, where u is an orthonormal representation of $\overline{G}$ and u_0 is a unit vector of the appropriate dimension. (1.5)

The theory surrounding the Lovász theta function thus involves a rich interplay among combinatorial properties of graphs and their stable sets, the geometric representations of graphs that compose the theta body, and semidefinite optimization duality and the corresponding min-max relations. In this thesis, we investigate some of the ramifications of this theory, focusing mainly on geometric representations of graphs and the descriptions of the theta body, using duality as our guiding viewpoint. Our aim is to lay some foundations for using semidefinite optimization and convex analysis in a way analogous to how polyhedral combinatorics has been using linear optimization to prove min-max theorems. The main tool at our disposal is a Strong Duality Theorem for SDPs, or a similarly flavored Strong Duality Theorem for conic optimization problems.

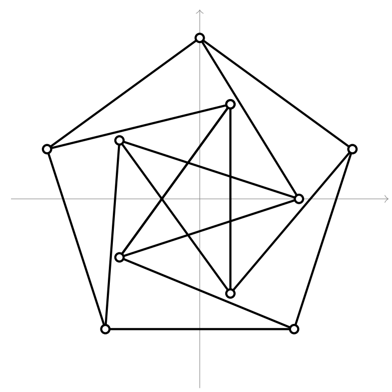

Figure 1.1: A unit-distance representation of the Petersen graph; see [96, Fig. 6.8].

In Chapters 2 and 3, our subject is optimization problems over unit-distance representations of graphs. (A subset of their contents appeared in [22].) A *unit-distance representation* of a graph is a map from its node set to some Euclidean space that sends adjacent nodes to pairs of points at distance one. Figure 1.1 illustrates a unit-distance representation of the Petersen graph on the plane. In Chapter 2, we focus on the problem of finding the smallest radius of a hypersphere that contains a unit-distance representation of a given graph G. The (square of) the radius of such a *hypersphere representation* is called the *hypersphere number* of G, and it was proved by Lovász to be a function of $\vartheta(\overline{G})$. Lovász's result shows that hypersphere representations may be regarded as dual objects to orthonormal representations, and it establishes a dictionary between results involving the theta function and the hypersphere number. We exploit this dictionary in a number of ways:

(i) we define a weighted generalization of the hypersphere number that satisfies some properties parallel to those of the weighted theta number;

(ii) we prove that the hypersphere number of a graph G is equal to the (square of the) smallest radius of an Euclidean ball that contains a unit-distance representation of G, and an analogous equality holds involving representations in hyperspheres and Euclidean balls where we prescribe upper or lower bounds for the length of each edge;

(iii) we define the concept of hom-monotone graph invariants as the invariants that satisfy two axioms that yield sandwich theorems, and argue that such invariants naturally arise from certain geometric representations.

Partially motivated by the notion of hom-monotone graph invariants that yield sandwich theorems, we introduce in Chapter 3 another weighted generalization of the hypersphere number. For a graph G and a positive semidefinite matrix A, the *ellipsoidal number* of G with respect to A, denoted by $\mathcal{E}(G; A)$, is the optimal value of an optimization problem that may be interpreted as finding the smallest ellipsoid of shape given by A that contains a unit-distance representation of G. We prove some basic properties of these optimization problems, which include the existence of an optimal solution and the fact that ellipsoidal numbers yield graph invariants that satisfy the first axiom for hom-monotone graph invariants. Unfortunately, we are not able to prove that the second axiom is satisfied, as it requires us to find analytic formulas for $\mathcal{E}(K_n; A)$, a task that turns out to be surprisingly difficult. We use basic techniques from convex analysis, as well as other weighted variations of the hypersphere number, to prove lower bounds for $\mathcal{E}(K_n; A)$, which we show to be tight for a class of unit-distance representations of complete graphs arising from Hadamard matrices. We are thus able to derive an analytic formula for $\mathcal{E}(K_n; A)$ whenever there is an $n \times n$ Hadamard matrix. We prove in Section A.1 an analytic formula for $\mathcal{E}(K_3; A)$ that differs significantly from the previously mentioned formula, and suggests a possibly erratic behavior of ellipsoidal numbers of complete graphs. Moreover, the non-existence of an $n \times n$ Hadamard matrix may be certified by a lower bound on $\mathcal{E}(K_n; A)$, if the bound lies above the analytic formula we obtain for some positive semidefinite matrix A. We also prove that the problem of computing ellipsoidal numbers is NP-hard in general.

Having studied many variations of hypersphere representations, which have orthonormal representations as dual objects, we move on to study a convex set mainly composed by the latter. Namely, we study the geometric structure of the theta body, whose members arise from orthonormal representations as described in (1.5). In Chapter 4, we undertake the study of the vertices of the lifted theta body. The definition (1.1) describes the theta body $\mathrm{TH}(G)$ as a projection of the set

$$\widehat{\mathrm{TH}}(G) := \Big\{ \hat{X} \in \mathbb{S}_+^{\{0\} \cup V} : \hat{X}_{00} = 1,\, \hat{X}_{ii} = \hat{X}_{i0}\, \forall i \in V,\, \hat{X}_{ij} = 0\, \forall ij \in E \Big\}, \tag{1.6}$$

which we call the *lifted theta body* of G. Recall that a *vertex* of a convex set is an *extreme point* whose *normal cone* is full dimensional, and that the feasible region of an SDP is called a *spectrahedron*. We derive a simple formula for the dimension of the normal cone of a spectrahedron at a given point. *By carefully analyzing this formula, we prove that all vertices of* $\widehat{\mathrm{TH}}(G)$ *have rank one, and thus correspond to the symmetric tensors of incidence vectors of stable sets of* G. This generalizes a result of Laurent and Poljak [87, 88] that characterizes the vertices of the *elliptope*, the feasible region of the famous SDP for MaxCut. Their result is essentially ours applied to graphs with no edges. Our characterization can also be regarded as a lifted counterpart to an observation by Shepherd [136] that the vertices of $\mathrm{TH}(G)$ are precisely the incidence vectors of stable sets in G. We also determine all the vertices of some other SDPs used to formulate $\vartheta(G)$ and some variants.

Some of these variants of $\vartheta(G)$ are usually defined similarly as in (1.2) where the theta body defined in (1.1) is slightly modified to require some sign constraints on entries of the matrix X corresponding to edges or non-edges of the graph. These modified theta bodies yield, for instance, the parameters known as ϑ' and ϑ^+. In Chapter 5, we introduce an axiomatic framework to study these generalized theta bodies, denoted by $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ and their support functions. Besides allowing sign constraints on the off-diagonal entries of the matrix X, which are encoded in the cone $\mathbb{A}$, we also allow the cone $\mathbb{S}_+^{\{0\} \cup V}$ of positive semidefinite matrices to be replaced by a cone $\widehat{\mathbb{K}}$ of matrices. The most important property we require of $\widehat{\mathbb{K}}$ is that it is *diagonally scaling invariant*, i.e., $\widehat{\mathbb{K}}$ must be closed under taking congruences by nonnegative diagonal matrices. Many of the convenient characterizations of theta also hold for the support functions of $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$. We are thus able to derive several characterizations of ϑ, ϑ' and ϑ^+ in a unified manner. Most importantly, we derive the analogue of the antiblocking duality relation (1.4). As a consequence of a result due to de Klerk and Pasechnik [32], the generalized theta body obtained by changing the cone of positive semidefinite matrices with the cone of *completely positive* matrices is precisely the stable set polytope $\mathrm{STAB}(G)$. Combined with antiblocking duality, we obtain as a corollary a description the *fractional stable set polytope*, usually denoted by $\mathrm{QSTAB}(G)$, as a generalized theta body arising from the cone of *copositive matrices*. This yields a weighted generalization of the copositive formulation for the fractional chromatic number described by Dukanovic and Rendl [37].

In Chapter 6, we study a (non-convex) constraint for SDPs which, in some important cases, acts analogously to integrality constraints in LPs. It is well known that the classical SDP relaxations for the maximum cut and stable set problems, with the additional constraint that the matrix variable is rank-one, yields exact formulations for the corresponding problems. However, adding the same rank constraint for, say, the dual SDP for the Lovász theta number, does not yield a formulation for a natural combinatorial problem; the modified problem is in fact infeasible except in trivial cases. This is in contrast to the analogous situation in linear programming, where one may add integrality constraints for both primal and dual LPs arising from combinatorial optimization problems, and in many cases both the modified primal and dual encode sensible combinatorial problems. We introduce a non-convex constraint for SDPs, which satisfy a strong form of primal-dual symmetry, that may play a similar role to integrality constraints in LPs. In many cases, our non-convex constraint reduces to the usual rank-one constraint. When applied to the dual SDP for a formulation of the Lovász theta number, it yields the clique covering problem. We also show how this non-convex constraint generalizes the usual integrality constraint from LPs which are formulated as SDPs via a diagonal embedding. We then study how this non-convex constraint affects the dual SDPs of certain formulations of the maximum cut problem, the vertex cover problem, and formulations arising from the stable set problem via some more general methods.

1.1 Preliminaries and Notation

Our terminology and notation are mostly standard. We collect some of our notation in this section for ease of reference.

The set of real numbers is denoted by $\mathbb{R}$, the set of nonnegative real numbers is denoted by $\mathbb{R}_+$ and the set of positive real numbers is denoted by $\mathbb{R}_{++}$. The set of integers is denoted by $\mathbb{Z}$, and we set $\mathbb{Z}_+ \coloneqq \mathbb{Z} \cap \mathbb{R}_+$ and $\mathbb{Z}_{++} \coloneqq \mathbb{Z} \cap \mathbb{R}_{++}$. The set of natural numbers is denoted by $\mathbb{N} \coloneqq \mathbb{Z}_+$. For any $n \in \mathbb{Z}_+$, we abbreviate $[n] \coloneqq \{1, \dots, n\}$, where by convention we set $[0] \coloneqq \varnothing$. We overload the bracket notation to include the extremely convenient *Iverson bracket*: if P is a predicate, we set

$$[P] \coloneqq \begin{cases} 1 & \text{if } P \text{ holds,} \\ 0 & \text{otherwise.} \end{cases}$$

When the predicate P is false, we consider $[P]$ to be "strongly zero," in the sense that we sometimes write expressions of the form $[x \neq 0](1/x)$ for $x \in \mathbb{R}$, meaning that, if $x = 0$, we take the whole expression to be 0. For a finite set V and $k \in \mathbb{Z}_+$, the set of all subsets of V of size k is denoted by $\binom{V}{k}$. A set of size 2 is usually abbreviated as $ij \coloneqq \{i, j\}$. The *symmetric group* on V is denoted by Sym_V. The composition of functions f and g is denoted by $f \circ g$, so that $(f \circ g)(x) = f(g(x))$ for each x in the domain of g and where $g(x)$ lies in the domain of f. The *restriction* of a function f to a subset S of its domain is denoted by $f\restriction_S$. The set of all functions from a set X to a set Y is denoted by Y^X.

Let V be a finite set. When $V = [n]$, the vector space $\mathbb{R}^{[n]}$ is abbreviated as $\mathbb{R}^n$, and we shall follow this convention with other sets indexed by V whenever $V = [n]$. The standard basis vectors of the vector space $\mathbb{R}^V$ are $\{\, e_i : i \in V \}$. The vector of all ones is denoted throughout simply by $\bar{e}$, its ambient space being easily deduced from the context. The *support* of a vector $x \in \mathbb{R}^V$ is $\operatorname{supp}(x) \coloneqq \{\, i \in V : x_i \neq 0 \}$. For $j \in V$, the jth component of a vector $x \in \mathbb{R}^V$ is usually denoted by x_j. However, we shall deal heavily with functions of the form $x\colon V \to \mathbb{R}^W$, where W is a finite set, and for which we use the notation $x_i \coloneqq x(i) \in \mathbb{R}^W$ for each $i \in V$. In these cases, we refer to the jth component of $x_i \in \mathbb{R}^W$ as $[x_i]_j$. We also use this notation when referring to components of vectors and matrices with subscripts. For instance, the *incidence vector* of a subset $S \subseteq V$ is the vector $\mathbb{1}_S \in \mathbb{R}^V$ defined by $[\mathbb{1}_S]_j \coloneqq [j \in S]$ for every $j \in V$. In all such cases the ground set V shall be clear from the context.

We generally work with finite-dimensional inner product spaces over $\mathbb{R}$, and we denote them by $\mathbb{E}$ and $\mathbb{Y}$. The *inner product* of two points x and y is usually denoted by $\langle x, y \rangle$. The *dual* of $\mathbb{E}$ is denoted by $\mathbb{E}^*$. The *adjoint* of a linear transformation $\mathcal{A}\colon \mathbb{E} \to \mathbb{Y}$ is the linear transformation $\mathcal{A}^*\colon \mathbb{Y}^* \to \mathbb{E}^*$ defined by $\langle x, \mathcal{A}^*(y) \rangle_{\mathbb{E}} \coloneqq \langle \mathcal{A}(x), y \rangle_{\mathbb{Y}}$ for every $x \in \mathbb{E}$ and $y \in \mathbb{Y}^*$. For $\mathscr{C} \subseteq \mathbb{E}$, the *automorphism group* $\operatorname{Aut}(\mathscr{C})$ of $\mathscr{C}$ is the set of all nonsingular linear transformations $T\colon \mathbb{E} \to \mathbb{E}$ such that $T(\mathscr{C}) = \mathscr{C}$. The vector space $\mathbb{R}^V$ is equipped with the standard inner product defined by $\langle x, y \rangle \coloneqq x^\mathsf{T} y = \sum_{i \in V} x_i y_i$ for every $x, y \in \mathbb{R}^V$. The *orthogonal complement* of a subset $\mathscr{C}$ of $\mathbb{E}$ is denoted by $\mathscr{C}^\perp$. If $p \geq 1$ is a real number, the *p-norm* of a vector $x \in \mathbb{R}^V$ is $\|x\|_p \coloneqq (\sum_{i \in V} |x_i|^p)^{1/p}$. Moreover, the ∞-*norm* of $x \in \mathbb{R}^V$ is $\|x\|_\infty \coloneqq \max\{\, |x_i| : i \in V \}$. Unless otherwise specified, the norm of a vector $x \in \mathbb{R}^V$ is its 2-norm $\|x\|_2 = \langle x, x \rangle^{1/2}$, and we always denote $\|x\| \coloneqq \|x\|_2$. A real-valued function f defined on some subset of $\mathbb{E}$ is *coercive* if $\|x_n\| \to \infty$ implies $f(x_n) \to \infty$ for every sequence $(x_n)_{n \in \mathbb{N}}$ in the domain of f.

Let V and W be finite sets. The vector space of all $V \times W$ matrices with real entries is denoted by $\mathbb{R}^{V \times W}$. The *transpose* of a matrix $A \in \mathbb{R}^{V \times W}$ is denoted by A^T. The *trace* of a matrix $X \in \mathbb{R}^{V \times V}$ is $\operatorname{Tr}(X) \coloneqq \sum_{i \in V} X_{ii}$. The vector space $\mathbb{R}^{V \times W}$ is equipped with the *Frobenius inner product* defined by $\langle X, Y \rangle \coloneqq \operatorname{Tr}(X^\mathsf{T} Y) = \sum_{i \in V,\, j \in W} X_{ij} Y_{ij}$. The *identity* matrix is denoted by I. If $S \subseteq V$ and $T \subseteq W$, and $A \in \mathbb{R}^{V \times W}$, then $A[S, T]$ denotes the submatrix of A in $\mathbb{R}^{S \times T}$ indexed by $S \times T$. When $V = W$, we also abbreviate $A[S] \coloneqq A[S, S]$. The linear transformation $\operatorname{diag}\colon \mathbb{R}^{V \times V} \to \mathbb{R}^V$ extracts the diagonal entries of a matrix, and its adjoint is denoted by Diag. Sometimes we abuse the notation and write $\operatorname{Diag}(x_1, \dots, x_n)$ for $\operatorname{Diag}(x)$ when $x \in \mathbb{R}^n$. For $L \in \mathbb{R}^{V \times V}$, the *congruence map* $\operatorname{Congr}_L\colon \mathbb{R}^{V \times V} \to \mathbb{R}^{V \times V}$ is

$$\operatorname{Congr}_L(X) \coloneqq L X L^\mathsf{T} \qquad \forall X \in \mathbb{R}^{V \times V}. \tag{1.7}$$

Note the identity

$$(\operatorname{Congr}_L(X))^\mathsf{T} = \operatorname{Congr}_L(X^\mathsf{T}) \qquad \forall X \in \mathbb{R}^{V \times V}. \tag{1.8}$$

Let V be a finite set. The set of *orthogonal* $V \times V$ matrices is denoted by $\mathbb{O}^V$. The vector subspace of $\mathbb{R}^{V \times V}$ of all *symmetric* $V \times V$ matrices is denoted by $\mathbb{S}^V$. The set of $V \times V$ *positive semidefinite* matrices is denoted by $\mathbb{S}^V_+$, and the set of $V \times V$ *positive definite* matrices is denoted by $\mathbb{S}^V_{++}$. It is well known that every matrix $X \in \mathbb{S}^V$ may be written as $X = Q \operatorname{Diag}(x) Q^\mathsf{T}$ for some $Q \in \mathbb{O}^V$ and $x \in \mathbb{R}^V$. Thus, the columns of Q forms an orthonormal basis of $\mathbb{R}^V$ of eigenvectors of X, with corresponding eigenvalues given by x. The vector in $\mathbb{R}^{|V|}$ obtained from x by sorting its components in non-increasing order is denoted by $\lambda^\downarrow(X)$, i.e., $\lambda^\downarrow_1(X) \geq \cdots \geq \lambda^\downarrow_{|V|}(X)$. The vector $\lambda^\uparrow(X)$ is defined analogously but with the reverse ordering, namely, $\lambda^\uparrow_1(X) \leq \cdots \leq \lambda^\uparrow_{|V|}(X)$. We also set $\lambda_{\max}(X) \coloneqq \lambda^\downarrow_1(X)$ and $\lambda_{\min}(X) \coloneqq \lambda^\uparrow_1(X)$. The *symmetrization map* $\operatorname{Sym}\colon \mathbb{R}^{V \times V} \to \mathbb{S}^V$ denotes the orthogonal projection onto $\mathbb{S}^V$, that is,

$$\operatorname{Sym}(X) \coloneqq \tfrac{1}{2}(X + X^\mathsf{T}) \qquad \forall X \in \mathbb{R}^{V \times V}. \tag{1.9}$$

Note that Sym commutes with any congruence map Congr_L, i.e., if $X, L \in \mathbb{R}^{V\times V}$, then

$$\mathrm{Congr}_L(\mathrm{Sym}(X)) = \mathrm{Sym}(\mathrm{Congr}_L(X)) \qquad \forall X \in \mathbb{R}^{V\times V}. \tag{1.10}$$

1.1.1 Linear Conic Optimization Duality

We use mostly standard terminology of convex analysis and refer the reader to [123].

Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $x, y \in \mathbb{E}$. We use the notation $x \succeq_{\mathbb{K}} y$ to mean that $x - y \in \mathbb{K}$. Similarly, $x \succ_{\mathbb{K}} y$ means that $x - y \in \mathrm{int}(\mathbb{K})$. Note that $\succeq_{\mathbb{K}}$ is a partial order on $\mathbb{E}$. When $\mathbb{K} = \mathbb{R}^n_+$, we write $\succeq_{\mathbb{K}}$ as $\geq$ and when $\mathbb{K} = \mathbb{S}^n_+$, we write $\succeq_{\mathbb{K}}$ as $\succeq$.

Now we describe the basic setting of conic optimization. Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $\mathcal{A}\colon \mathbb{E} \to \mathbb{Y}^*$ be a linear transformation. Let $c \in \mathbb{E}^*$ and $b \in \mathbb{Y}^*$. An optimization problem of the form

$$\sup\{\, \langle c, x\rangle : \mathcal{A}(x) = b,\, x \in \mathbb{K}\} \tag{1.11}$$

is called a *conic optimization problem*. The *dual* of (1.11) is the conic optimization problem

$$\inf\{\, \langle b, y\rangle : y \in \mathbb{Y},\, \mathcal{A}^*(y) \succeq_{\mathbb{K}^*} c\}. \tag{1.12}$$

Here, $\mathbb{K}^* := \{\, s \in \mathbb{E}^* : \langle s, x\rangle \geq 0\, \forall x \in \mathbb{K}\}$ is the *dual cone* of $\mathbb{K}$. It is easy to check that $\langle c, x\rangle \leq \langle b, y\rangle$ whenever x is feasible for (1.11) and y is feasible for (1.12), i.e., Weak Duality holds. Sometimes it is convenient to add an explicit slack variable to (1.12), in which case we rewrite it as

$$\inf\{\, \langle b, y\rangle : y \in \mathbb{Y},\, \mathcal{A}^*(y) - s = c,\, s \in \mathbb{K}^*\}. \tag{1.13}$$

The optimization problem (1.11) is sometimes called the *primal* problem to distinguish it from the dual problem (1.12).

When $\mathbb{K}$ is the direct sum of copies of the nonnegative line $\mathbb{R}_+$ and the full real line $\mathbb{R}$, then the conic optimization problems (1.11) and (1.12) form a routine pair of dual linear programs in some standard format. The Duality Theory for this class of optimization problems is well known. For instance, if any of the values (1.11) or (1.12) is finite, then they both are, the optimal values coincide, and both optimization problems have optimal solutions. This is known as LP Strong Duality; we refer the reader to [130].

In the case of more general cones $\mathbb{K}$, such as when $\mathbb{K} = \mathbb{S}^n_+$, it need not be the case that the optimal values of (1.11) and (1.12) coincide, even if both are finite, and even if additionally both problems have optimal solutions; see, e.g., [150]. However, under certain so-called regularity conditions, a Strong Duality Theorem does hold. One such condition involves the existence of a Slater point for (1.11) or (1.12). A feasible solution $\bar{x}$ for (1.11) such that $\bar{x} \in \mathrm{int}(\mathbb{K})$ is called a *Slater point* for (1.11). A feasible solution $\bar{y}$ for (1.12) such that $\mathcal{A}^*(\bar{y}) \succ_{\mathbb{K}^*} c$ is called a *Slater point* for (1.12), in which case we also say that $\bar{y} \oplus \bar{s}$ is a *Slater point* for (1.13) where $\bar{s} := \mathcal{A}^*(\bar{y}) - c$. Note that, if we rewrite (1.13) in the format of (1.11), the concept of Slater points coincide for both forms. A usual assertion of Strong Duality problems states that, if a conic optimization problem has a Slater point and its optimal value is finite, then its dual has an optimal solution and the optimal values coincide. The latter property is usually referred to as a "zero duality gap."

We shall use a slightly more general setting that allows for explicit linear inequalities in the description of the feasible region, and that uses a weaker variation of the Slater point. Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $\mathcal{A}\colon \mathbb{E} \to \mathbb{R}^p$ and $\mathcal{B}\colon \mathbb{E} \to \mathbb{R}^q$ be linear functions. Let $a \in \mathbb{R}^p$ and $b \in \mathbb{R}^q$. Now our primal takes the form

$$\sup\big\{ \langle c, x\rangle : \mathcal{A}(x) = a,\, \mathcal{B}(x) \leq b,\, x \in \mathbb{K}\big\}. \tag{1.14}$$

In this case the dual of (1.14) is defined to be

$$\inf\big\{ \langle a \oplus b, y \oplus z\rangle : y \in \mathbb{R}^p,\, z \in \mathbb{R}^q_+,\, \mathcal{A}^*(y) + \mathcal{B}^*(z) \succeq_{\mathbb{K}^*} c\big\}. \tag{1.15}$$

Note that (1.14) may be rewritten in the form (1.11) by adding a new slack variable and taking the direct sum of $\mathbb{K}$ with $\mathbb{R}^q_+$. However, in that case, a Slater point for the translated optimization problem would require the inequality $\mathcal{B}(x) \leq b$ to be strict, which is slightly inconvenient. To work around this, we use a variant of the Slater condition. A *restricted Slater point* of (1.14) is a feasible solution $\bar{x}$ for (1.14) such that $\bar{x} \in \operatorname{int}(\mathbb{K})$. A *restricted Slater point* for (1.15) is a feasible solution $\bar{y} \oplus \bar{z}$ for (1.15) such that $\mathcal{A}^*(\bar{y}) + \mathcal{B}^*(\bar{z}) \succ_{\mathbb{K}^*} c$. As before, in the latter case we also say that $\bar{y} \oplus \bar{z} \oplus \bar{s}$ is a *restricted Slater point* for

$$\inf\big\{ \langle a \oplus b, y \oplus z\rangle : y \in \mathbb{R}^p,\, z \in \mathbb{R}^q_+,\, \mathcal{A}^*(y) + \mathcal{B}^*(z) - s = c,\, s \in \mathbb{K}^*\big\}. \tag{1.16}$$

It is well known that the existence of a restricted Slater point and the finiteness of the optimal value for the primal ensure zero duality gap and the existence of an optimal solution for the dual. For the sake of completeness, we include a proof of this result. It assumes some basic properties about linear programming and the Hyperplane Separation Theorem. For those, we refer the reader to [130] and [123].

Theorem 1.1 (A Strong Duality Theorem; see, e.g., [149, Theorem 2.14])**.** *Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $\mathcal{A}\colon \mathbb{E} \to \mathbb{R}^p$ and $\mathcal{B}\colon \mathbb{E} \to \mathbb{R}^q$ be linear functions. Let $a \in \mathbb{R}^p$ and $b \in \mathbb{R}^q$. Suppose the optimization problem (1.15) has a restricted Slater point and its optimal value is finite. Then (1.14) has an optimal solution and the optimal values of (1.14) and (1.15) coincide.*

Proof. Assume that the optimization problem (1.15) has a restricted Slater point and its optimal value is finite. Let $v^* \in \mathbb{R}$ denote the optimal value of (1.15). We may assume that

$$a \oplus b \neq 0 \oplus 0 \tag{1.17}$$

since otherwise $x^* := 0$ is an optimal solution for (1.14) and $v^* = 0$. Define

$$\mathscr{C} := \big\{ \mathcal{A}^*(y) + \mathcal{B}^*(z) - c : y \oplus z \in \mathbb{R}^p \oplus \mathbb{R}^q_+,\, \langle a \oplus b, y \oplus z\rangle \leq v^*\big\}.$$

By definition, there exists a sequence $(y_n \oplus z_n)_{n\in\mathbb{N}}$ in $\mathbb{R}^p \oplus \mathbb{R}^q_+$ with $\langle a \oplus b, y_n \oplus z_n\rangle \to v^*$ as $n \to \infty$. Since the LP $\inf\{ \langle a \oplus b, y \oplus z\rangle : y \oplus z \in \mathbb{R}^p \oplus \mathbb{R}^q_+\}$ has an optimal solution or is unbounded, it follows that

$$\mathscr{C} \neq \varnothing.$$

We claim that

$$\mathscr{C} \cap \operatorname{int}(\mathbb{K}^*) = \varnothing. \tag{1.18}$$

Suppose otherwise, and let $\bar{y} \oplus \bar{z} \in \mathbb{R}^p \oplus \mathbb{R}^q_+$ such that $\langle a \oplus b, \bar{y} \oplus \bar{z}\rangle \leq v^*$ and $\mathcal{A}^*(\bar{y}) + \mathcal{B}^*(\bar{z}) \succ_{\mathbb{K}^*} c$. Then, using (1.17), for some $\varepsilon > 0$ the point $\hat{y} \oplus \hat{z} := (\bar{y} \oplus \bar{z}) - \varepsilon(a \oplus b)$ is feasible in (1.15) and satisfies $\langle a \oplus b, \hat{y} \oplus \hat{z}\rangle < v^*$. This contradicts the definition of v^* and completes the proof of (1.18).

It follows from the Hyperplane Separation Theorem (see, e.g., [123, Theorem 11.3]) and (1.18) that there exists a nonzero $\tilde{x} \in \mathbb{E}$ such that

$$\sup\{ \langle \tilde{x}, s \rangle : s \in \mathscr{C} \} \leq \inf\{ \langle \tilde{x}, s \rangle : s \in \operatorname{int}(\mathbb{K}^*) \}. \tag{1.19}$$

Since $\mathscr{C} \neq \varnothing$, we know that the RHS of (1.19) is bounded from below. Moreover, since $\operatorname{int}(\mathbb{K}^*)$ is a cone, we must have $\langle \tilde{x}, s \rangle \geq 0$ for every $s \in \operatorname{int}(\mathbb{K}^*)$ whence $\tilde{x} \in \mathbb{K}^{**} = \mathbb{K}$ (see, e.g., [123, Theorem 14.1]). By sending $s \in \operatorname{int}(\mathbb{K}^*)$ to 0 in the RHS of (1.19), we find that the RHS is 0. Thus, by the definition of $\mathscr{C}$, for every $y \oplus z \in \mathbb{R}^p \oplus \mathbb{R}^q_+$ such that $\langle a \oplus b, y \oplus b \rangle \leq v^*$, we have $\langle \mathcal{A}^*(y), \tilde{x} \rangle + \langle \mathcal{B}^*(z), \tilde{x} \rangle \leq \langle c, \tilde{x} \rangle$, i.e.,

$$\langle \mathcal{A}(\tilde{x}) \oplus \mathcal{B}(\tilde{x}), y \oplus z \rangle \leq \langle c, \tilde{x} \rangle \text{ for every } y \oplus z \in \mathbb{R}^p \oplus \mathbb{R}^q_+ \text{ such that } \langle a \oplus b, y \oplus z \rangle \leq v^*. \tag{1.20}$$

Thus, by LP Duality there exists $\mu \in \mathbb{R}_+$ such that

$$\mu a = \mathcal{A}(\tilde{x}), \tag{1.21a}$$

$$\mu b \geq \mathcal{B}(\tilde{x}), \tag{1.21b}$$

$$\mu v^* \leq \langle c, \tilde{x} \rangle. \tag{1.21c}$$

We claim that

$$\mu > 0. \tag{1.22}$$

Let $\tilde{y} \oplus \tilde{z}$ be a restricted Slater point for (1.15), so that $\tilde{s} := \mathcal{A}^*(\tilde{y}) + \mathcal{B}^*(\tilde{z}) - c \in \operatorname{int}(\mathbb{K}^*)$. Suppose that $\mu = 0$. Then (1.21) and $\tilde{x} \in \mathbb{K} \setminus \{0\}$ imply

$$0 \leq \langle c, \tilde{x} \rangle = \langle \tilde{y}, \mathcal{A}(\tilde{x}) \rangle + \langle \tilde{z}, \mathcal{B}(\tilde{x}) \rangle - \langle \tilde{s}, \tilde{x} \rangle \leq -\langle \tilde{s}, \tilde{x} \rangle < 0.$$

This proves (1.22).

Set $x^* := \tilde{x}/\mu$. We get from (1.21) that $\mathcal{A}(x^*) = a$ and $\mathcal{B}(x^*) \leq b$ so x^* is feasible for (1.14). Moreover, $\langle c, x^* \rangle \geq v^*$ by (1.21c) so x^* is optimal for (1.14) by Weak Duality. □

1.1.2 Combinatorial Optimization and Graph Theory Notation

Let $G = (V, E)$ be a graph, i.e., V is an arbitrary set, usually finite, and E is a subset of $\binom{V}{2}$. To avoid potential conflicts with the geometric object called vertex, we refer to the elements of V as the *nodes* of G. We assume throughout that 0 is not in the node set of any graph, since we shall constantly need to add a "new" element to V and form the set $\{0\} \cup V$. We sometimes use the notation $V(G)$ to denote the node set of G and $E(G)$ to denote the edge set of G. If $S \subseteq V$, the *set of edges induced by* S is $E[S] := E \cap \binom{S}{2}$ and the *subgraph of* G *induced by* S is $G[S] := (S, E[S])$. The *automorphism group* of G is denoted by $\operatorname{Aut}(G)$. We say that G is *node-transitive* if $\operatorname{Aut}(G)$ acts transitively on V, and G is *edge-transitive* if $\operatorname{Aut}(G)$ acts transitively on E. The *degree* of a node is the number of edges incident to it. A node of G is *isolated* if its degree is zero. We say that G is *regular* if all nodes in G have the same degree, and we call the common degree the *valency* of G. A *coloring* of G is a function from V to some set (whose elements are called colors, and usually has the form $[k]$ for some $k \in \mathbb{Z}_{++}$) that assigns distinct colors to adjacent nodes. The complement of G is the graph $\overline{G} := \left(V, \binom{V}{2} \setminus E\right)$. The *complete graph* on a finite set V is denoted by K_V.

If f is a function on graphs, we use the notation $\overline{f}$ for the function

$$\overline{f}(G) := f(\overline{G}). \tag{1.23}$$

The *stability number* of G, denoted by $\alpha(G)$, is the largest size of a *stable set* in G; the *clique number* of G is $\omega(G) \coloneqq \overline{\alpha}(G)$. The *chromatic number* of G, denoted by $\chi(G)$, is the smallest number of stable sets of G that partitions V; the *clique covering number* of G is $\overline{\chi}(G)$. A graph G is called *perfect* if $\omega(G[S]) = \chi(G[S])$ for every $S \subseteq V(G)$. The stable set polytope of G is

$$\mathrm{STAB}(G) \coloneqq \mathrm{conv}\big\{ \mathbb{1}_S : S \subseteq V(G),\, S \text{ a stable set of } G \big\}. \tag{1.24}$$

All our graphs are *simple*, that is, they have no *loops* nor *parallel edges*, unless explicitly mentioned otherwise.

We include a proof of the following elementary result for the sake of completeness:

Proposition 1.2. Let $u\colon [k] \to \mathbb{R}^d$ and $v\colon [k] \to \mathbb{R}^d$. Then there exists $Q \in \mathbb{O}^d$ such that $Qu_i = v_i$ for every $i \in [k]$ if and only if $\langle u_i, u_j \rangle = \langle v_i, v_j \rangle$ for every $i, j \in [k]$, or, equivalently, if and only if $\|u_i\| = \|v_i\|$ for every $i \in [k]$ and $\|u_i - u_j\| = \|v_i - v_j\|$ for every $ij \in \binom{V}{2}$.

Proof. The equivalence between the latter two conditions is straightforward. We prove the equivalence between the existence of $Q \in \mathbb{O}^d$ such that $Qu_i = v_i$ for every $i \in [k]$ and the equality between the Gram matrices of u and v. Clearly, existence of such an orthogonal matrix implies that the Gram matrices of u and v are equal. We shall prove the converse, so assume the Gram matrices of u and v are equal. The proof is by induction on k, the case $k = 1$ being trivial. Assume that $k > 1$ and $d > 1$. For each $i \in [k]$, set $t_i \coloneqq \|u_i\|$. We may assume that $t_i > 0$ for every i. Since $\mathbb{O}^d$ is a group, by possibly replacing each u_i with $Q_u u_i$ and each v_i with $Q_v v_i$, for some matrices $Q_u, Q_v \in \mathbb{O}^d$, we may assume that $u_k = t_k e_d = v_k$. Set $x_i \coloneqq u_i\restriction_{[d-1]}$ and $y_i \coloneqq v_i\restriction_{[d-1]}$ for each $i \in [k-1]$. Let $i \in [k-1]$. Then $t_k[u_i]_d = \langle u_i, u_k \rangle = \langle v_i, v_k \rangle = t_k[v_i]_d$, so

$$[u_i]_d = [v_i]_d \qquad \forall i \in [k-1]. \tag{1.25}$$

Thus, for $i, j \in [k-1]$, we have $\langle x_i, x_j \rangle = \langle u_i, u_j \rangle - [u_i]_d[u_j]_d = \langle v_i, v_j \rangle - [v_i]_d[v_j]_d = \langle y_i, y_j \rangle$. By induction, there exists $P \in \mathbb{O}^{d-1}$ such that $Px_i = y_i$ for each $i \in [k-1]$. Hence, $Q \coloneqq P \oplus 1 \in \mathbb{O}^d$ is such that $Qu_i = v_i$ for each $i \in [k]$. $\square$

Chapter 2

Hypersphere Representations of Graphs

Let $G = (V, E)$ be a graph. A *unit-distance representation of* G is a map $u \colon V \to \mathbb{R}^d$ for some $d \in \mathbb{Z}_{++}$ such that $\|u_i - u_j\| = 1$ for every $ij \in E$. A unit-distance representation of G contained in a hypersphere centered at the origin is a *hypersphere representation of* G. (Here, by hypersphere, we mean the boundary of an Euclidean ball.) The *radius* of a hypersphere representation u of G is the number $\|u_i\|$ for any $i \in V$. Define the *hypersphere number of* G, denoted by $t(G)$, to be the square of the smallest radius of a hypersphere representation of G; the reason for using the square shall be clear in a moment.

It is easy to see that the hypersphere number of G may be formulated as an SDP. Indeed, let $u \colon V \to \mathbb{R}^d$ be an arbitrary function for some $d \in \mathbb{Z}_{++}$, and form a matrix $U^\mathsf{T} \in \mathbb{R}^{[d] \times V}$ by setting $U^\mathsf{T} e_i := u_i$ for each $i \in V$. Define X to be the Gram matrix $X := UU^\mathsf{T}$ of u. Then we may read off from the entries of X the numbers $\|u_i\|^2 = X_{ii}$ for each $i \in V$ and $\|u_i - u_j\|^2 = X_{ii} - 2X_{ij} + X_{jj}$ for each $ij \in E$. Moreover, since the dimension d is arbitrary, there is no constraint on the rank of the Gram matrix X. We thus have

$$
\begin{aligned}
t(G) = \min \quad & t \\
& t - X_{ii} = 0 && \forall i \in V, \\
& X_{ii} - 2X_{ij} + X_{jj} = 1 && \forall ij \in E, \\
& X \in \mathbb{S}^V_+, \\
& t \in \mathbb{R}.
\end{aligned}
\tag{2.1}
$$

This SDP may be written more compactly by using the *Laplacian* of G, i.e., the linear transformation $\mathcal{L}_G \colon \mathbb{R}^E \to \mathbb{S}^V$ defined by

$$
\mathcal{L}_G(z) := \sum_{ij \in E} z_{ij} (e_i - e_j)(e_i - e_j)^\mathsf{T} \qquad \forall z \in \mathbb{R}^E. \tag{2.2}
$$

Note that the adjoint of $\mathcal{L}_G$ is the linear transformation $\mathcal{L}_G^* \colon \mathbb{S}^V \to \mathbb{R}^E$ such that, for each $ij \in E$, the ijth component of $\mathcal{L}_G^*(X)$ is $\langle \mathcal{L}_G^*(X), e_{ij} \rangle = \langle X, \mathcal{L}_G(e_{ij}) \rangle = \langle X, (e_i - e_j)(e_i - e_j)^\mathsf{T} \rangle = X_{ii} - 2X_{ij} + X_{jj}$. Thus, (2.1) may be rewritten as

$$
t(G) = \min\bigl\{\, t : t\bar{e} - \operatorname{diag}(X) = 0,\ \mathcal{L}_G^*(X) = \bar{e},\ X \in \mathbb{S}^V_+,\ t \in \mathbb{R} \bigr\}. \tag{2.3}
$$

The SDP dual to (2.3) is

$$t(G) = \max\left\{ \bar{e}^{\mathsf{T}} z : y \in \mathbb{R}^V,\, z \in \mathbb{R}^E,\, -\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0,\, \bar{e}^{\mathsf{T}} y = 1 \right\}. \tag{2.4}$$

Note that $X \oplus t = \frac{1}{2}(I \oplus 1)$ is a Slater point for (2.3), whereas $y \oplus z = |V|^{-1}\bar{e} \oplus 0$ is a Slater point for (2.4). (See Figure 2.1.) Thus, by the Strong Duality Theorem, the optimal values of (2.3) and (2.4) coincide and they are both attained.

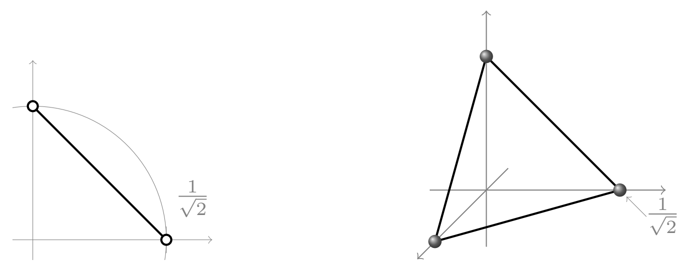

Figure 2.1: Hypersphere representations of K_2 and K_3 corresponding to Slater points.

In this chapter, we undertake a detailed study of the hypersphere number and related objects. Lovász [96] proved a formula that relates the hypersphere number of G and the Lovász theta number of $\overline{G}$. In fact, each of these parameters is a function of the other. This formula may be interpreted as a min-max relation involving hypersphere representations of G and orthonormal representations of $\overline{G}$; the latter is a class of geometric representations closely related to the theta number, as we briefly mentioned in Chapter 1. This intimate relation between hypersphere and theta numbers allows us to get a better understanding of both parameters, as it encodes a dictionary between results involving the corresponding geometric representations. For instance, some basic results about the Lovász theta function seem very naturally proved in the context of hypersphere representations. These include the famous Sandwich Theorem that relates the Lovász theta number to the clique and chromatic numbers, and some formulas describing the behavior of the theta function with respect to some fundamental graph operations. We also rely on the weighted version of the theta number to define a weighted counterpart for the hypersphere number. We shall see that, as in the case for theta, the weighted hypersphere number encodes the unweighted hypersphere number of a certain "blown-up" graph. On the reverse direction, we shall use a "non-convex" property of the theta number to prove that the hypersphere number of a graph G coincides with the square of the smallest radius of an Euclidean ball that contains a unit-distance representation of G. Finally, we shall identify, from the proof of the Sandwich Theorem in the context of hypersphere representations, some sufficient conditions for a graph invariant to yield a sandwich theorem like the one involving the theta number. Naturally, these conditions involve the concept of *graph homomorphisms*.

The main contribution in this chapter is the viewpoint of the presentation. However, Theorem 2.18 seems to be new, along with the content from Section 2.6 on the relation with graph homomorphisms, and they motivate the main object of study in the next chapter. The content from Section 2.4 on the weighted hypersphere number is also new.

2.1 Hypersphere Numbers for Basic Graph Classes

We start by computing the hypersphere number for some basic classes of graphs. We also compute an optimal hypersphere representation in some cases. It is by now a standard technique, going back at least to Lovász [94] in 1979, to use the symmetries of an SDP to decrease its size, sometimes reducing the SDP to an LP; see also [8]. We will use this technique to compute the hypersphere number for a class of very symmetric graphs. (For a generalization to a broader class of symmetric graphs, including distance-regular graphs, we refer the reader to [49, Corollary 5.3] and Theorem 2.4 below.) We shall use the following notation. Recall that Sym_V denotes the symmetric group on a finite set V. If $\sigma \in \mathrm{Sym}_V$, the linear map $P_\sigma \colon \mathbb{R}^V \to \mathbb{R}^V$ is defined as the linear extension of the map $e_i \in \mathbb{R}^V \mapsto e_{\sigma(i)}$. The *adjacency matrix* of a graph G is denoted by A_G, and we extend our notation for eigenvalues to any graph by applying it to the corresponding adjacency matrix; e.g., we set $\lambda_{\min}(G) := \lambda_{\min}(A_G)$.

Proposition 2.1 ([96, Section 6.4.1])**.** *Let $G = (V, E)$ be a node- and edge-transitive graph. Suppose that $E \neq \varnothing$. Let k be the valency of G. Then*

$$t(G) = \frac{k}{2\big(k - \lambda_{\min}(G)\big)}. \tag{2.5}$$

Proof. Set $n := |V|$. The key argument in the proof is to show that

there exists an optimal solution $\bar{y} \oplus \bar{z}$ for the dual SDP (2.4) where $\bar{y} = \frac{1}{n}\bar{e}$ and $\bar{z}$ is a scalar multiple of $\bar{e}$. (2.6)

Define $\pi\colon \mathrm{Aut}(G) \to \mathrm{Sym}_E$ by setting $\pi(\sigma)\colon \{i,j\} \in E \mapsto \{\sigma(i), \sigma(j)\}$. Then,

for a feasible solution $y \oplus z$ of (2.4) and $\sigma \in \mathrm{Aut}(G)$, the point $P_\sigma y \oplus P_{\pi(\sigma)} z$ is also feasible for (2.4) and has the same objective value as $y \oplus z$. (2.7)

Note that $\bar{e}^\mathsf{T} P_\sigma y = \bar{e}^\mathsf{T} y = 1$ and $\bar{e}^\mathsf{T} P_{\pi(\sigma)} z = \bar{e}^\mathsf{T} z$. It is easy to check that $P_\sigma \operatorname{Diag}(y) P_\sigma^\mathsf{T} = \operatorname{Diag}(P_\sigma y)$. Moreover,

$$\begin{aligned} P_\sigma \mathcal{L}_G(z) P_\sigma^\mathsf{T} &= \sum_{ij \in E} \langle e_{ij}, z\rangle P_\sigma (e_i - e_j)(e_i - e_j)^\mathsf{T} P_\sigma^\mathsf{T} \\ &= \sum_{ij \in E} \big\langle e_{\sigma(i)\sigma(j)}, P_{\pi(\sigma)} z\big\rangle \big(e_{\sigma(i)} - e_{\sigma(j)}\big)\big(e_{\sigma(i)} - e_{\sigma(j)}\big)^\mathsf{T} = \mathcal{L}_G(P_{\pi(\sigma)} z). \end{aligned}$$

Thus, $-\operatorname{Diag}(P_\sigma y) + \mathcal{L}_G(P_{\pi(\sigma)} z) = P_\sigma\big(-\operatorname{Diag}(y) + \mathcal{L}_G(z)\big) P_\sigma^\mathsf{T} \preceq 0$. This proves (2.7). We may now prove (2.6). Let $y^* \oplus z^*$ be an optimal solution for (2.4). Then by (2.7) we have that

$$\bar{y} \oplus \bar{z} := \frac{1}{|\mathrm{Aut}(G)|} \sum_{\sigma \in \mathrm{Aut}(G)} \big(P_\sigma y^* \oplus P_{\pi(\sigma)} z^*\big) \tag{2.8}$$

is a convex combination of optimal solutions, and thus is also optimal. Moreover, since $P_\sigma \bar{y} \oplus P_{\pi(\sigma)} \bar{z} = \bar{y} \oplus \bar{z}$ for every $\sigma \in \mathrm{Aut}(G)$ and $\mathrm{Aut}(G)$ acts transitively on V and E, it follows that both $\bar{y}$ and $\bar{z}$ are scalar multiples of $\bar{e}$, whence $\bar{y} = \frac{1}{n}\bar{e}$ since $\bar{e}^\mathsf{T}\bar{y} = 1$. This proves (2.6).

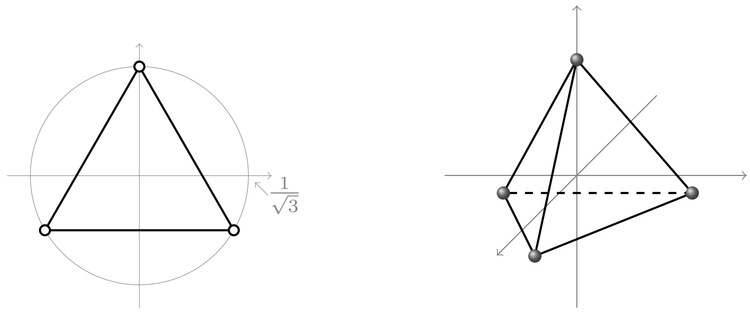

Figure 2.2: Optimal hypersphere representations of K_3 and K_4.

Since $\mathcal{L}_G(\bar{e}) = kI - A_G$, we may use (2.6) to reformulate (2.4) as

$$t(G) = \max\bigl\{\, \beta|E| : \bigl(\tfrac{1}{n} - k\beta\bigr)I + \beta A_G \succeq 0,\, \beta \in \mathbb{R} \bigr\}. \tag{2.9}$$

Note that $\beta \in \mathbb{R}$ is feasible in (2.9) if and only if $1/n \geq \beta\bigl(k - \lambda_i^{\downarrow}(G)\bigr)$ for each $i \in [n]$. Since $k \geq \lambda_i^{\downarrow}(G)$ for each $i \in [n]$ and the inequality is strict for $i = n$ since $E \neq \varnothing$, we find that an optimal solution for (2.9) is

$$\beta^* := \frac{1}{n\bigl(k - \lambda_{\min}(G)\bigr)}$$

with objective value

$$\beta^*|E| = \frac{1}{n\bigl(k - \lambda_{\min}(G)\bigr)} \frac{kn}{2} = \frac{k}{2\bigl(k - \lambda_{\min}(G)\bigr)}. \qquad \square$$

Let us use Proposition 2.1 to compute the hypersphere number for certain natural classes of graphs. We begin with complete graphs. For every $n \in \mathbb{Z}_{++}$, the complete graph K_n is regular with valency $n-1$ and $\lambda_{\min}(K_n) = -1$; in fact, by writing the adjacency matrix of K_n as $\bar{e}\bar{e}^{\mathsf{T}} - I$, it follows that all the eigenvalues of K_n but the largest one are equal to -1. We thus get from (2.5) that

$$t(K_n) = \frac{1}{2}\left(1 - \frac{1}{n}\right). \tag{2.10}$$

An optimal solution for (2.3) is given by $X^* \oplus t(K_n)$ with

$$X^* := \frac{1}{2}\left(I - \frac{1}{n}\bar{e}\bar{e}^{\mathsf{T}}\right). \tag{2.11}$$

It is easy to check that $X^* \oplus t(K_n)$ satisfies the affine constraints in (2.3). For the positive semidefiniteness constraint, note that $2X^*$ is the orthogonal projection onto $\{\bar{e}\}^{\perp}$, and thus its own square. See Figure 2.2.

Complete graphs are important enough that we take the time to describe a slightly different, inductive construction for their optimal hypersphere representations. For K_1, just take $u_1 := 0 \in \mathbb{R}^1$. Now let $n \in \mathbb{Z}_{++}$ with $n \geq 2$. Given an optimal hypersphere representation $v\colon [n-1] \to \mathbb{R}^{n-1}$ of K_{n-1}, we can build an optimal hypersphere representation $u\colon [n] \to \mathbb{R}^n$ of K_n by setting

$$u_i := \begin{bmatrix} \beta \\ v_i \end{bmatrix} \quad \forall i \in [n-1], \quad \text{where } \beta := -\big[2n(n-1)\big]^{-1/2}, \tag{2.12a}$$

$$u_n := \begin{bmatrix} \gamma \\ 0 \end{bmatrix}, \qquad \text{where } \gamma := \left(\frac{n-1}{2n}\right)^{1/2}. \tag{2.12b}$$

Note that here we are embedding the optimal representation of K_{n-1} into the hyperplane $\{\, x \in \mathbb{R}^n : x_1 = \beta \}$ and embedding the new point u_n as a scalar multiple of e_1, and then adjusting the constants β and γ so that this yields a hypersphere representation of K_n.

It is not difficult nor surprising that, by an appropriate relabeling, the hypersphere representation given by (2.12) corresponds to a *Cholesky factorization* of the optimal solution (2.11) for the SDP (2.3) applied to K_n. One just has to make sure that, when forming a matrix with columns $\{\, u_i : i \in [n] \}$, the pattern of zeros arising from (2.12b) yields an upper triangular matrix.

Next we look at cycles. We could use Proposition 2.1 again to compute the hypersphere number of every even cycle, but it is more instructive here to provide a proof for all bipartite graphs:

Proposition 2.2. Let $G = (V, E)$ be a graph. Then $t(G) = 1/4$ holds if and only if G is bipartite and has at least one edge.

Proof. For the 'if' part, the existence of edges implies that $t(G) \geq 1/4$. Equality in the latter is obtained by considering the hypersphere representation $i \in V \mapsto (-1)^{[i \in A]} 1/2$, where $\{A, B\}$ is a partition of V into stable sets of G.

Next we prove the 'only if' part. The existence of an edge follows from $t(G) > 0$. Now suppose we have an optimal hypersphere representation. The hypersphere has radius $1/2$. The only pairs of points at distance 1 in this hypersphere are pairs of antipodal points. Thus, if we consider a great circle in this hypersphere not containing any of the embedded vertices, then the hemispheres of this great circle determine a partition of V into two stable sets of G. ☐

It is easy to see that the proof of the 'if' part in Proposition 2.2 may be further generalized if we consider arbitrary colorings of a graph. Together with an obvious bound for subgraphs, we shall obtain a formula for the hypersphere number of all perfect graphs.

Proposition 2.3. Let G be a graph. Then

$$t(K_{\omega(G)}) \leq t(G) \leq t(K_{\chi(G)}). \tag{2.13}$$

In particular, if $\omega(G) = \chi(G)$, as is the case whenever G is a perfect graph, we have $t(G) = t(K_{\omega(G)})$.

Proof. Clearly, $t(H) \leq t(G)$ for every subgraph H of G. Thus, $t(K_{\omega(G)}) \leq t(G)$. Next let $c\colon V \to [p]$ be a coloring of G for some $p \in \mathbb{Z}_{++}$, and let u be an optimal hypersphere representation of K_p. It is easy to check that the map $i \in V \mapsto u_{c(i)}$ is a hypersphere representation of G. Hence, $t(G) \leq t(K_p)$. Since c is an arbitrary coloring of G, we get $t(G) \leq t(K_{\chi(G)})$. ☐

The proof of Proposition 2.3 already hints at a strong connection with graph homomorphisms. We shall look at it with more detail in Section 2.6.

Let us now consider optimal hypersphere representations of odd cycles. It is well known that the eigenvalues of a cycle C_n on n nodes are $\tau + \tau^{-1}$, where τ ranges over the nth complex roots of unity; this follows from the structure of eigenvalues of circulant matrices and the discrete Fourier transform (see, e.g., Biggs [15, Proposition 3.5]). Thus, if $n = 2k+1$ for some $k \in \mathbb{Z}_{++}$, then $\lambda_{\min}(C_n) = 2\cos(2\pi k/n)$. Hence, by Proposition 2.1, we have

$$t(C_n) = \frac{1}{2\bigl(1 - \cos(2\pi k/n)\bigr)}. \tag{2.14}$$

An optimal representation is given by an n-pointed star in $\mathbb{R}^2$, i.e., the map that sends node j of $V(C_n) = \{0, \dots, n-1\}$ to

$$\sqrt{t(C_n)} \begin{bmatrix} \cos(2\pi kj/n) \\ \sin(2\pi kj/n) \end{bmatrix}.$$

This is illustrated in Figure 2.3.

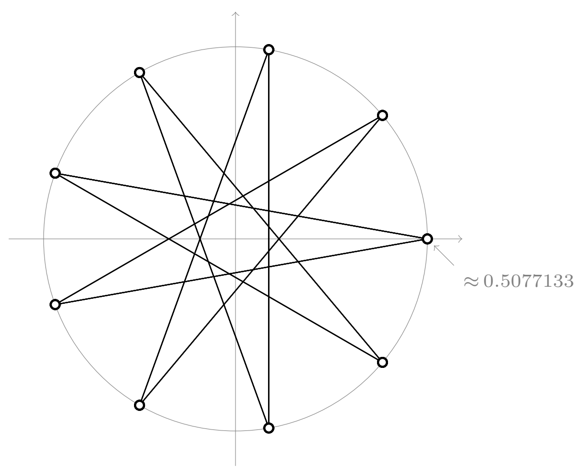

Figure 2.3: An optimal hypersphere representation of the 9-cycle.

We compute the hypersphere number for one final class of very symmetric graphs. Let $n, k \in \mathbb{Z}_{++}$ with $2k \le n$. Define the graph $K_{n:k}$ on node set $\binom{[n]}{k}$ where nodes $S, T \in \binom{[n]}{k}$ are adjacent if $S \cap T = \varnothing$. (Note that one may still take $2k > n$, though the resulting graph will be empty.) Such graphs are known as *Kneser graphs*. Note that $K_{5:2}$ is the *Petersen graph*. Kneser graphs are node- and edge-transitive, so we may indeed apply Proposition 2.1. By using the facts that the valency of $K_{n:k}$ is $\binom{n-k}{k} = \frac{n-k}{k}\binom{n-k-1}{k-1}$ and that $\lambda_{\min}(K_{n:k}) = -\binom{n-k-1}{k-1}$ (see [50, Theorem 9.4.3]), that proposition yields

$$t(K_{n:k}) = \frac{1}{2}\left(1 - \frac{k}{n}\right). \tag{2.15}$$

Thus, the hypersphere number of the Petersen graph $K_{5:2}$ is $3/10$.

2.2 A Min-Max Relation Involving the Lovász Theta Number

We recall one of the many possible definitions of the Lovász theta number. For a finite set V and a subset E of $\binom{V}{2}$, define the linear map $\mathcal{A}_E\colon \mathbb{S}^V \to \mathbb{R}^E$ by setting

$$\mathcal{A}_E^*(e_{ij}) \coloneqq \mathrm{Sym}(e_i e_j^\mathsf{T}) \qquad \forall ij \in E. \tag{2.16}$$

Let $G = (V, E)$ be a graph. The *theta number of* G is

$$\vartheta(G) = \max\bigl\{\, \langle \bar{e}\bar{e}^\mathsf{T}, X\rangle : \langle I, X\rangle = 1,\, \mathcal{A}_E(X) = 0,\, X \in \mathbb{S}^V_+ \bigr\}. \tag{2.17}$$

This graph parameter was first introduced by Lovász in the seminal paper [94], albeit in a different form. We shall still use some other equivalent formulations of the theta number in this chapter. For proofs of their equivalence, we refer the reader to Chapter 5, where we discuss this definition and many other guises of the theta number in depth.

Lovász [96] noted a nonlinear formula relating the numbers $t(G)$ and $\overline{\vartheta}(G)$. We include a proof here for the sake of completeness. Note that the proof essentially describes the dual SDP (2.4) for $t(G)$ as a projectively scaled version of the SDP (2.17) applied to $\overline{G}$.

Theorem 2.4 ([96, Sec. 6.4.1])**.** Let $G = (V, E)$ be a graph. Then

$$2t(G) + \frac{1}{\overline{\vartheta}(G)} = 1. \tag{2.18}$$

Proof. The dual SDP (2.4) can be rewritten as

$$\max\bigl\{\, \bigl\langle \tfrac{1}{2}\bigl(\bar{e}\bar{e}^\mathsf{T} - I\bigr), Y\bigr\rangle : \langle \bar{e}\bar{e}^\mathsf{T}, Y\rangle = 1,\, \mathcal{A}_{\overline{E}}(Y) = 0,\, Y \in \mathbb{S}^V_+ \bigr\} \tag{2.19}$$

by taking $Y \coloneqq \mathrm{Diag}(y) - \mathcal{L}_G(z)$. For any feasible solution Y of (2.19), its objective value is

$$\bigl\langle \tfrac{1}{2}\bigl(\bar{e}\bar{e}^\mathsf{T} - I\bigr), Y\bigr\rangle = \tfrac{1}{2}\bigl[\langle \bar{e}\bar{e}^\mathsf{T}, Y\rangle - \langle I, Y\rangle\bigr] = \tfrac{1}{2}\bigl[1 - \langle I, Y\rangle\bigr]$$

by the first constraint in (2.19). Thus, the optimal value of (2.19) is

$$t(G) = \tfrac{1}{2}\bigl[1 - \tilde{t}(G)\bigr], \tag{2.20}$$

where

$$\tilde{t}(G) \coloneqq \min\bigl\{\, \langle I, Y\rangle : \langle \bar{e}\bar{e}^\mathsf{T}, Y\rangle = 1,\, \mathcal{A}_{\overline{E}}(Y) = 0,\, Y \in \mathbb{S}^V_+ \bigr\}. \tag{2.21}$$

Note that each optimal solution for (2.21) is also an optimal solution for (2.19), and vice-versa. In particular, $\tilde{t}(G)$ is attained. It is clear that

$$\tilde{t}(G)\overline{\vartheta}(G) = 1; \tag{2.22}$$

see, e.g., Lemma A.9. Thus, (2.18) follows from (2.20) and (2.22). □

Theorem 2.4 may be interpreted as a nonlinear min-max relation involving hypersphere and orthonormal representations, as we now describe. Let $G = (V, E)$ be a graph. Recall from Chapter 1 that an orthonormal representation of G is a map from V to the unit vectors of some Euclidean space that sends non-adjacent nodes of G to pairs of orthogonal vectors. That is, an orthonormal representation of G is a map $v\colon V \to \mathbb{R}^d$ for some $d \in \mathbb{Z}_{++}$ such that $\|v_i\| = 1$ for every $i \in V$ and $\langle v_i, v_j\rangle = 0$ for every $ij \in \overline{E}$. Such representations were also introduced by Lovász in [94].

Naturally, hypersphere representations of a graph are intimately related to orthonormal representations of its complement, as described in [96, Section 6.4.1]. Indeed, for a graph $G = (V, E)$, it is easy to check that,

(i) if u is a hypersphere representation of G with squared radius $t \leq 1/2$, then the map $i \in V \mapsto 2^{1/2}\big((\frac{1}{2} - t)^{1/2} \oplus u_i\big)$ is an orthonormal representation of $\overline{G}$; (2.23)

(ii) if $i \in V \mapsto \mu^{-1/2} \oplus \sqrt{2}u_i$ is an orthonormal representation of $\overline{G}$ for some $\mu \in \mathbb{R}_{++}$, then u is a hypersphere representation of G with squared radius $\frac{1}{2}(1 - \frac{1}{\mu})$.

Orthonormal representations are also closely related to the theta body of a graph (see, e.g., [58]). Let $G = (V, E)$ be a graph. An *orthonormal representation constraint of* G is an inequality of the form $\sum_{i\in V} \langle v_0, v_i\rangle^2 x_i \leq 1$ on a variable x in $\mathbb{R}^V$, where $v\colon V \to \mathbb{R}^d$ is an orthonormal representation of G for some $d \in \mathbb{Z}_{++}$ and $v_0 \in \mathbb{R}^d$ is a unit vector. The *theta body of* G may be defined as the set

$$\mathrm{TH}(G) = \big\{\, x \in \mathbb{R}^V_+ : x \text{ satisfies all orthonormal representation constraints of } G\big\}. \tag{2.24}$$

The theta body yields yet another characterization of the theta number of a graph G:

$$\vartheta(G) = \max\big\{\, \langle \bar{e}, x\rangle : x \in \mathrm{TH}(G)\big\}. \tag{2.25}$$

Let us describe Theorem 2.4 as a min-max relation involving the elements of $\mathrm{TH}(\overline{G})$:

Corollary 2.5. Let $G = (V, E)$ be a graph. If t is the squared radius of a hypersphere representation of G and $x \in \mathrm{TH}(\overline{G})$ is nonzero, then

$$2t + \frac{1}{\langle \bar{e}, x\rangle} \geq 1, \tag{2.26}$$

with equality if and only if $t = t(G)$ and $\langle \bar{e}, x\rangle = \overline{\vartheta}(G)$.

Proof. Let $u\colon V \to \mathbb{R}^d$ be a hypersphere representation of G with squared radius t for some $d \in \mathbb{Z}_{++}$. If $t \geq 1/2$, then (2.26) holds, so assume that $t < 1/2$. Let $x \in \mathrm{TH}(\overline{G})$ be nonzero. Define an orthonormal representation $v\colon V \to \mathbb{R} \oplus \mathbb{R}^d$ of $\overline{G}$ from u as in (2.23)(i). Put $v_0 \coloneqq 1 \oplus 0 \in \mathbb{R} \oplus \mathbb{R}^d$. Then

$$(1 - 2t)\langle \bar{e}, x\rangle = \sum_{i\in V} \langle v_0, v_i\rangle^2 x_i \leq 1$$

by the definition of $\mathrm{TH}(\overline{G})$. This proves (2.26). The equality case follows from Theorem 2.4. □

Corollary 2.5 may be read as a purely geometric min-max relation by using the well-known fact [58, Theorem 3.5] that

$x \in \mathbb{R}^V$ lies in $\mathrm{TH}(G)$ if and only if x has the form $x\colon i \in V \mapsto \langle v_0, v_i\rangle^2$ for some orthonormal representation v of $\overline{G}$ and unit vector v_0 of the appropriate dimension. (2.27)

Corollary 2.6. Let $G = (V, E)$ be a graph. If t is the squared radius of a hypersphere representation of G, $v\colon V \to \mathbb{R}^d$ is an orthonormal representation of G for some $d \in \mathbb{Z}_{++}$ and $v_0 \in \mathbb{R}^d$ is a unit vector such that $v_0 \notin \{\, v_i : i \in V \,\}^{\perp}$, then

$$2t + \frac{1}{\sum_{i \in V} \langle v_0, v_i \rangle^2} \geq 1, \tag{2.28}$$

with equality if and only if $t = t(G)$ and $\sum_{i \in V} \langle v_0, v_i \rangle^2 = \overline{\vartheta}(G)$.

Proof. Immediate from Corollary 2.5 via the characterization (2.27) of members of $\mathrm{TH}(\overline{G})$. ☐

Corollary 2.6 has the pleasing feature that both the primal and the dual objects are purely geometric. Indeed, one could argue that the fact that the hypersphere number $t(G)$ may be expressed as the SDP (2.3) immediately yields via the Strong Duality Theorem a min-max relation for $t(G)$. Such min-max relation, however, involves a positive semidefinite constraint on the dual side which seems somewhat unnatural given the original, SDP-free statement of the problem of computing $t(G)$. Moreover, it does not seem easy to interpret the dual SDP (2.4) as an optimization problem over purely geometric objects. This is accomplished by Corollary 2.6.

One may in fact avoid duality entirely and use only the transformations (2.23) to prove an identity that is equivalent to (2.18) via a dual characterization of the theta number. However, as expected, this shall not yield a "good characterization" in the same sense as in Corollary 2.6.

We shall use a fact equivalent to the lower-comprehensiveness of $\mathrm{TH}(G)$. However, for the sake of presenting the proof as purely geometric, we shall prove that fact separately:

Lemma 2.7. Let $G = (V, E)$ be a graph. Let u be an orthonormal representation of G and let u_0 be a unit vector of appropriate dimension. Let $k \in V$ and $\beta \in \mathbb{R}$ such that $0 \leq \beta < \langle u_0, u_k \rangle^2$. Then there exists an orthonormal representation v of G and a unit vector v_0 such that, for each $i \in V$, we have

$$\langle v_0, v_i \rangle^2 = \begin{cases} \beta, & \text{if } i = k, \\ \langle u_0, u_i \rangle^2, & \text{otherwise.} \end{cases}$$

Proof. Set $\mu := \beta^{1/2}/\langle u_0, u_k \rangle \in [0, 1]$ and $\alpha := \sqrt{1 - \mu^2}$. Define $v_k := \mu u_k \oplus \alpha$ and $v_i := u_i \oplus 0$ for every $i \in V \setminus \{k\}$. Finally, set $v_0 := u_0 \oplus 0$. Clearly, $\langle v_i, v_j \rangle = 0$ whenever $\langle u_i, u_j \rangle = 0$, and all images under v have unit norm. So v is an orthonormal representation of G. It is trivial to check that v and v_0 satisfy the desired condition. ☐

Proposition 2.8. Let $G = (V, E)$ be a graph. Then

$$2t(G) + \max_{u, u_0} \min_{i \in V} \langle u_0, u_i \rangle^2 = 1,$$

where u ranges over all orthonormal representations of $\overline{G}$ and u_0 over unit vectors of the appropriate dimension.

Proof. We first prove that

$$t(G) \leq \tfrac{1}{2}\Big(1 - \max_{u,u_0} \min_{i \in V} \langle u_0, u_i \rangle^2\Big). \tag{2.29}$$

It suffices to prove that

$$t(G) \leq \tfrac{1}{2}\Big(1 - \min_{i \in V} \langle u_0, u_i \rangle^2\Big) \tag{2.30}$$

for any orthonormal representation u of $\overline{G}$ and unit vector u_0 of the appropriate dimension. So fix those, and set $\beta \coloneqq \min_{i \in V} \big\{ \langle u_0, u_i \rangle^2 \big\}$. If $\beta = 0$, then the hypersphere representation $i \mapsto 2^{-1/2} e_i \in \mathbb{R}^V$ shows that $t(G) \leq 1/2$ as desired, so assume that $\beta > 0$. Use Lemma 2.7 to get from u and u_0 an orthonormal representation v of $\overline{G}$ and a unit vector v_0 such that $\langle v_0, v_i \rangle^2 = \beta$ for each $i \in V$. By possibly rotating v_0 and the vectors in the image of v, we may assume that $v_0 = e_1$. Moreover, by replacing some vectors v_i's by their opposites if necessary, we may assume that $\langle v_0, v_i \rangle \geq 0$ for every $i \in V$. Thus, we may apply the transformation (2.23)(ii) with $\mu \coloneqq 1/\beta$ to get a hypersphere representation of G with squared radius $\frac{1}{2}(1 - \beta)$. This proves (2.29).

Next we prove that

$$\max_{u,u_0} \min_{i \in V} \langle u_0, u_i \rangle^2 \geq 1 - 2t(G). \tag{2.31}$$

It suffices to find an orthonormal representation v of $\overline{G}$ and a unit vector v_0 such that $\langle v_0, v_i \rangle^2 \geq 1 - 2t(G)$ for every $i \in V$. Let $u \colon V \to \mathbb{R}^d$ be a hypersphere representation of G with squared radius $t(G)$ for some $d \in \mathbb{Z}_{++}$. Build an orthonormal representation $v \colon V \to \mathbb{R} \oplus \mathbb{R}^d$ of $\overline{G}$ as in (2.23)(i) and pick $v_0 \coloneqq 1 \oplus 0 \in \mathbb{R} \oplus \mathbb{R}^d$. Then $\langle v_0, v_i \rangle^2 = 1 - 2t(G)$ for every $i \in V$. This proves (2.31). $\square$

The equivalence between Proposition 2.8 and Theorem 2.4 follows from the following dual characterization of $\vartheta(G)$:

$$\vartheta(G) = \min_{u,u_0} \max_{i \in V} \frac{1}{\langle u_0, u_i \rangle^2}, \tag{2.32}$$

where u ranges over all orthonormal representations of G and u_0 over unit vectors of the appropriate dimension. (In fact, (2.32) was the original definition of $\vartheta(G)$ by Lovász [94].) As we mentioned previously, though, Proposition 2.8 does not yield a good characterization of $t(G)$; it is more akin to the Gallai identities for graphs [98, Lemmas 1.0.1 and 1.0.2].

In this section, we have studied the formula (2.18) relating certain geometric representations of graphs to the reciprocal of the fundamental Lovász theta number via the projective transformation underlying (2.22). A similar formula holds involving other geometric graph embeddings and the reciprocal of a key spectral invariant involving the Laplacian, namely Fiedler's *absolute algebraic connectivity*, also via an analogous projective transformation. This was studied in [55], which also proved connections involving the combinatorial structure of the graph and geometric properties of the corresponding optimal embeddings. Variations on these geometric embedding problems were also studied in [66, 56, 53, 54] which, along with [55], also established somewhat surprising relations with some key concepts in Graph Minors Theory.

2.3 Theta Number Results in Hypersphere Space

We may now use Theorem 2.4 to understand better some known results about the Lovász theta number, by looking at them from the context of hypersphere representations, and the other way around as well. Let us start with two basic properties of the theta number which, albeit simple to prove, fit nicely in the context of hypersphere representations.

Perhaps the most interesting property of the number $\overline{\vartheta}(G)$ is that, although it is possible to approximate it arbitrarily well in polynomial time, it lies sandwiched between two graph invariants which are NP-hard to compute, namely, the clique and chromatic numbers of G.

Theorem 2.9 (The Sandwich Theorem [94, Lemma 3 and Theorem 10])**.** If G is a graph, then

$$\omega(G) \leq \overline{\vartheta}(G) \leq \chi(G).$$

Proof. Immediate from Proposition 2.3 via Theorem 2.4 and (2.10). □

The Sandwich Theorem 2.9 is usually proved by showing that, for every stable set S of G, the point $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^{\mathsf{T}}$ is a feasible solution for (2.17) with objective value $|S|$, and similarly for clique coverings of G and the SDP dual to (2.17). Proposition 2.3, on the other hand, presents it via a clean geometric construction using colorings, and in fact it reveals a simple relation to graph homomorphisms which we shall explore in Section 2.6.

Lovász [96] mentions that a graph G is bipartite if and only if $\overline{\vartheta}(G) \leq 2$. A standard proof relies on showing that $\overline{\vartheta}(C_n) > 2$ for every odd cycle C_n. Indeed, computing $\overline{\vartheta}(C_n)$ is straightforward, e.g., by using the standard technique used in the proof of Proposition 2.1, and we get $\overline{\vartheta}(C_n) = 1 - 1/\cos(2\pi k/n)$ if $n = 2k+1$. (The formula also follows from Theorem 2.4 and (2.14).) While this proof is perfectly fine, the proof of Proposition 2.2, which yields the same characterization via Theorem 2.4, describes a much more pleasing geometric viewpoint:

Proposition 2.10 ([96, Sec. 6.6.1])**.** A graph G is bipartite if and only if $\overline{\vartheta}(G) \leq 2$.

Proof. Immediate from Proposition 2.2 via Theorem 2.4. □

The theta function has a simple behavior with respect to some graph operations; see [94, 78] and references therein. Some of these results also have geometrically attractive proofs in the context of hypersphere representations, which we shall consider in the next subsections.

2.3.1 Graph Sums

We shall consider the sum and cosum of graphs. Let $G = (V, E)$ and $H = (W, F)$ be graphs. By possibly relabeling the nodes, assume that $V \cap W = \varnothing$. The *direct sum of* G *and* H is the graph $G + H := (V \cup W, E \cup F)$. The *direct cosum of* G *and* H is the graph $G \mathbin{\overline{+}} H$ defined by $G \mathbin{\overline{+}} H := \overline{\overline{G} + \overline{H}}$. We shall use the simple fact that,

for every $t \in \mathbb{R}$ such that $t \geq t(G)$, there exists a hypersphere representation of G with squared radius t. (2.33)

Indeed, let $X^* \oplus t^*$ be an optimal solution for the SDP (2.3) and let $X \in \mathbb{S}^V$ such that $X \oplus t$ lies in the line segment joining $X^* \oplus t^*$ to $\frac{1}{2}(I + (2\tilde{t} - 1)\bar{e}\bar{e}^{\mathsf{T}}) \oplus \tilde{t}$, where $\tilde{t} := \max\{t, \frac{1}{2}\}$. Then the columns of $X^{1/2}$ form a hypersphere representation of G with squared radius t.

Proposition 2.11 ([78, Sec. 18 and 19])**.** Let $G = (V, E)$ and $H = (W, F)$ be graphs such that $V \cap W \neq \varnothing$. Then

$$t(G + H) = \max\{t(G), t(H)\}, \tag{2.34a}$$

$$t(G \mp H) = \frac{1 - 4t(G)t(H)}{4(1 - t(G) - t(H))}. \tag{2.34b}$$

Equivalently,

$$\vartheta(G \mp H) = \max\{\vartheta(G), \vartheta(H)\}, \tag{2.35a}$$

$$\vartheta(G + H) = \vartheta(G) + \vartheta(H). \tag{2.35b}$$

Proof. Let us start by proving (2.34a). Clearly '$\geq$' holds. For the reverse inequality, assume that $t(G) \geq t(H)$ and note that there is a hypersphere representation of H with squared radius $t(G)$ by (2.33), which may be glued to a hypersphere representation of G with squared radius $t(G)$.

Next we prove (2.34b). We start with the '$\geq$' part. Let v be an orthonormal representation of G and v_0 a unit vector of the appropriate dimension such that

$$2t(G) + \frac{1}{\sum_{i \in V} \langle v_0, v_i \rangle^2} = 1.$$

Similarly, let w be an orthonormal representation of H and w_0 a unit vector of the appropriate dimension such that

$$2t(H) + \frac{1}{\sum_{j \in W} \langle w_0, w_j \rangle^2} = 1.$$

Such representations exist by Corollary 2.6. We may assume that the images of v and w live in the same space, and by possibly applying a rotation, we may assume that $v_0 = w_0$. Then the map z on $V \cup W$ such that $z\restriction_V = v$ and $z\restriction_W = w$ is an orthonormal representation of $G \mp H$. Hence, by Corollary 2.6, we have

$$2t(G \mp H) \geq 1 - \frac{1}{\sum_{i \in V} \langle v_0, v_i \rangle^2 + \sum_{j \in W} \langle w_0, w_j \rangle^2} = \frac{1 - 4t(G)t(H)}{2(1 - t(G) - t(H))},$$

thus proving '$\geq$' in (2.34b).

For the reverse inequality, let v be an optimal hypersphere representation of G, and let w be an optimal hypersphere representation of H. Define a map u on $V \cup W$ by setting

$$u_i := \begin{bmatrix} v_i \\ \xi(G) \\ 0 \end{bmatrix} \quad \forall i \in V, \qquad u_j := \begin{bmatrix} 0 \\ -\xi(H) \\ w_j \end{bmatrix} \quad \forall j \in W,$$

where

$$\xi(F) := \frac{1 - 2t(F)}{2\big(1 - t(G) - t(H)\big)^{1/2}}$$

for $F \in \{G, H\}$. It is easy to check that u is a hypersphere representation of $G \mp H$ with squared radius given by the RHS of (2.34b). This concludes the proof of (2.34b).

The identities (2.35) are equivalent to (2.34) by Theorem 2.4. $\square$

Note that (2.34a) implies that $t(G) = \max\{\, t(C) : C \text{ a component of } G\}$. In fact, the latter equation generalizes to

$$t(G) = \max\big\{\, t(B) : B \text{ a block of } G\big\}. \tag{2.36}$$

Recall that a *block* of a graph is a maximal subgraph with no cut-node, where a *cut-node* of a graph G is a node whose deletion increases the number of components of G. The formula (2.36) follows from the next result, which describes the behavior of the hypersphere number with respect to clique sums. We shall use the following notation. If $G_i = (V_i, E_i)$ is a graph for each $i \in [2]$, then $G_1 \cup G_2 := (V_1 \cup V_2, E_1 \cup E_2)$ and $G_1 \cap G_2 := (V_1 \cap V_2, E_1 \cap E_2)$.

Proposition 2.12. Let $G = (V, E)$ be a graph, and suppose $G = G_1 \cup G_2$ for graphs G_1 and G_2, where $G_1 \cap G_2$ is a complete graph. Then

$$t(G) = \max\{t(G_1), t(G_2)\}. \tag{2.37}$$

Equivalently,

$$\overline{\vartheta}(G) = \max\{\overline{\vartheta}(G_1), \overline{\vartheta}(G_2)\}. \tag{2.38}$$

Proof. Clearly '$\geq$' holds in (2.37). We may assume that $t(G_1) \geq t(G_2)$. Let u be a hypersphere representation of G_1 with squared radius $t(G_1)$, and let v be a hypersphere representation of G_2 with squared radius $t(G_1)$, which exists by (2.33). We may assume that the images of u and v live in the same space. Since the nodes of $G_1 \cap G_2$ are mapped into points with squared norm $t(G_1)$ and they are pairwise one unit apart, by Proposition 1.2 there exists an orthogonal matrix Q such that $Qu_i = v_i$ for every $i \in V(G_1 \cap G_2)$. Thus, if we take the hypersphere representation $u' \colon i \in V(G_2) \mapsto Qu_i$ of G_2 and glue it with v, we obtain a hypersphere representation of G with squared radius $t(G_1)$. This proves (2.37), which is equivalent to (2.38) by Theorem 2.4. ☐

The behavior of the hypersphere number and $\overline{\vartheta}$ with respect to clique sums described by Proposition 2.12 is shared by many other graph parameters, e.g., the clique and chromatic numbers, the *Hadwiger number* (the size of the largest clique minor), and the graph invariant λ introduced in [69].

2.3.2 Local Graph Operations

We now discuss the behavior of the hypersphere number with respect to edge contraction. For a graph G and an edge e of G, we shall denote by G/e the graph obtained from G by contracting e.

Proposition 2.13. Let $G = (V, E)$ be a graph and let $e \in E$. If $\bar{y} \oplus \bar{z}$ is an optimal solution for the SDP (2.4), then $\bar{z}_e \geq t(G) - t(G/e)$. Equivalently, if $\bar{X}$ is an optimal solution for the SDP (2.17) applied to $\overline{\vartheta}(G)$, then $\overline{\vartheta}(G) \leq (2\bar{X}_{ij} + 1)\overline{\vartheta}(G/e)$.

Proof. Let $\bar{y} \oplus \bar{z}$ be an optimal solution for (2.4). We will construct a feasible solution for (2.4) applied to G/e with objective value $t(G) - \bar{z}_e$. Assume $e = ab$ and $V' := V(G/e) = V \setminus \{b\}$, so we are denoting the contracted node of G/e by a. Let M be the $V' \times V$ matrix defined by $M := e_a e_b^{\mathsf{T}} + \sum_{i \in V'} e_i e_i^{\mathsf{T}}$. Then $M\mathcal{L}_G(\bar{z})M^{\mathsf{T}} = \mathcal{L}_{G/e}(\hat{z})$, where $\hat{z} \in \mathbb{R}^{E(G/e)}$ is obtained from $\bar{z}$ as follows. In taking the contraction G/e from G, immediately after we identify the ends of e, but before we remove resulting parallel edges, there are at most two edges between each pair of nodes of G/e, as we assume that G is simple. If there is exactly one edge between nodes i and j, we just set $\hat{z}_{ij} := \bar{z}_{ij}$. If there are two edges joining nodes i and j, say f and f', we put $\hat{z}_{ij} := \bar{z}_f + \bar{z}_{f'}$. Similarly, if we define $\hat{y}\colon V' \to \mathbb{R}$ by putting $\hat{y}_i := \bar{y}_i$ for $i \in V' \setminus \{a\}$ and $\hat{y}_a := \bar{y}_a + \bar{y}_b$, then $M \operatorname{Diag}(\bar{y}) M^{\mathsf{T}} = \operatorname{Diag}(\hat{y})$. Since $M\,\mathbb{S}_+^V M^{\mathsf{T}} \subseteq \mathbb{S}_+^{V'}$, we see that $\hat{y} \oplus \hat{z}$ is a feasible solution for (2.4) applied to G/e, and its objective value is $\langle \bar{e}, \hat{z}\rangle = \langle \bar{e}, \bar{z}\rangle - \bar{z}_e$.

To prove the inequality involving $\overline{\vartheta}(G)$, we use Theorem 2.4 together with its proof to see that $\bar{X}$ corresponds to an optimal solution $\bar{y} \oplus \bar{z}$ for (2.4) with $\bar{X}/\overline{\vartheta}(G) = \operatorname{Diag}(\bar{y}) - \mathcal{L}_G(\bar{z})$, so $\bar{z}_e = \bar{X}_{ij}/\overline{\vartheta}(G)$ if $e = ij$. $\square$

Finally, we consider a neat geometric proof in the context of hypersphere representations for a result whose counterpart in terms of $\overline{\vartheta}$ is a property also shared by the clique number, the chromatic number, and the fractional chromatic number (see (5.86) for a definition). The property we refer to is the following. Let $G = (V, E)$ be a graph. For each $j \in V$, denote by $N(j)$ the set of neighbors of j. Let $i \in V$ such that $N(i) \neq \varnothing$. If $\beta \in \{\omega, \chi, \chi^*\}$, then $\beta(G) \geq \beta(G[N(i)]) + 1$. The proof is inspired by [76, Lemma 4.3].

Proposition 2.14. Let $G = (V, E)$ be a graph and let $i \in V$ such that $N(i) \neq \varnothing$. Then

$$t(G[N(i)]) \leq 1 - \frac{1}{4t(G)}. \tag{2.39a}$$

Equivalently,

$$\overline{\vartheta}(G) \geq \overline{\vartheta}(G[N(i)]) + 1. \tag{2.39b}$$

Proof. Let $u\colon V \to \mathbb{R}^d$ be a hypersphere representation of G with squared radius $t := t(G)$ for some $d \in \mathbb{Z}_{++}$. By possibly replacing u with the map $i \in V \mapsto Qu_i$ for some $Q \in \mathbb{O}^d$, we may assume that $u_i = t^{1/2} e_d$. For every $j \in N(i)$, we have $1 = \|u_i - u_j\|^2 = \|u_i\|^2 + \|u_j\|^2 - 2\langle u_i, u_j\rangle = 2t - 2t^{1/2}[u_j]_d$. Hence, $[u_j]_d = (2t-1)/(2t^{1/2}) =: \beta$ for every $j \in N(i)$. Define the following hypersphere representation of $G[N(i)]$: for each $j \in N(i)$, set $v_j := u_j\restriction_{[d-1]}$. The squared radius of v is $t - \beta^2$, which is equal to the RHS of (2.39a). This proves (2.39a), which is equivalent to (2.39b) by Theorem 2.4. $\square$

2.4 A Weighted Hypersphere Number

The proof of Theorem 2.4 works by showing that the dual SDP (2.4) for the hypersphere number is a projectively scaled version of the SDP (2.17) for the Lovász theta number. The latter SDP may be generalized to a weighted version of the theta number, so it seems natural to define a corresponding weighted generalization of the hypersphere number. In this section, we shall define the weighted hypersphere number $t(G; w)$ as the optimal value of an SDP by using the proof of Theorem 2.4 as a guide, and we shall show how to interpret geometrically an optimal solution to the corresponding SDP as a compressed encoding of an optimal hypersphere representation of a "blown-up" graph from G.

First, we recall the weighted version of the theta number. Let $G = (V, E)$ be a graph, and let $w \in \mathbb{R}_+^V$. The parameter $\vartheta(G; w)$ is defined by

$$\vartheta(G; w) = \max\Big\{ \big\langle \sqrt{w}\sqrt{w}^{\mathsf{T}}, X \big\rangle : \langle I, X\rangle = 1,\ \mathcal{A}_E(X) = 0,\ X \in \mathbb{S}_+^V \Big\}, \tag{2.40}$$

where $\sqrt{w} \in \mathbb{R}^V$ is defined by

$$[\sqrt{w}\,]_i := \sqrt{w_i} \qquad \forall i \in V. \tag{2.41}$$

We want to define a parameter $t(G;w)$ such that

$$2t(G;w) + \frac{1}{\vartheta(\overline{G};w)} = 1$$

for every graph $G = (V, E)$ and every $w \in \mathbb{R}^V_+$ with $w \neq 0$. Let us start by writing a weighted version of the dual SDP (2.4) for $t(G)$. Following (2.20) and (2.21), define

$$t(G;w) := \tfrac{1}{2}\big[1 - \tilde{t}(G;w)\big],$$

where

$$\tilde{t}(G;w) := \min\Big\{\, \langle I, Y\rangle : \langle \sqrt{w}\sqrt{w}^{\mathsf{T}}, Y\rangle = 1,\ \mathcal{A}_{\overline{E}}(Y) = 0,\ Y \in \mathbb{S}^V_+ \Big\}. \tag{2.42}$$

Let Y be a feasible solution for (2.42). Then Y has the form $Y = \operatorname{Diag}(y) - \mathcal{L}_G(z)$ for a unique $y \oplus z \in \mathbb{R}^V \oplus \mathbb{R}^E$. The constraint $\langle \sqrt{w}\sqrt{w}^{\mathsf{T}}, Y\rangle = 1$ may be written as

$$1 = \big\langle \sqrt{w}\sqrt{w}^{\mathsf{T}}, \operatorname{Diag}(y) - \mathcal{L}_G(z)\big\rangle = \langle w, y\rangle - \big\langle \mathcal{L}^*_G(\sqrt{w}\sqrt{w}^{\mathsf{T}}), z\big\rangle,$$

and we have

$$\begin{aligned}
\tfrac{1}{2}\big[1 - \langle I, Y\rangle\big] &= \tfrac{1}{2}\Big[\big\langle \sqrt{w}\sqrt{w}^{\mathsf{T}} - I, \operatorname{Diag}(y) - \mathcal{L}_G(z)\big\rangle\Big] \\
&= \tfrac{1}{2}\Big[\langle w - \bar{e}, y\rangle + \big\langle 2\bar{e} - \mathcal{L}^*_G(\sqrt{w}\sqrt{w}^{\mathsf{T}}), z\big\rangle\Big].
\end{aligned}$$

So, we shall define $t(G;w)$ as the optimal value of the dual SDP of

$$\begin{aligned}
t(G;w) = \max \quad & \tfrac{1}{2}\langle w - \bar{e}, y\rangle + \big\langle \bar{e} - \tfrac{1}{2}\mathcal{L}^*_G\big(\sqrt{w}\sqrt{w}^{\mathsf{T}}\big), z\big\rangle \\
& y \in \mathbb{R}^V, \\
& z \in \mathbb{R}^E, \\
& -\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0, \\
& \langle w, y\rangle - \big\langle \mathcal{L}^*_G\big(\sqrt{w}\sqrt{w}^{\mathsf{T}}\big), z\big\rangle = 1.
\end{aligned} \tag{2.43}$$

i.e., as

$$\begin{aligned}
t(G,w) = \min \quad & t \\
& tw - \operatorname{diag}(X) = \tfrac{1}{2}(w - \bar{e}), \\
& \mathcal{L}^*_G(X) - t\mathcal{L}^*_G\big(\sqrt{w}\sqrt{w}^{\mathsf{T}}\big) = \bar{e} - \tfrac{1}{2}\mathcal{L}^*_G\big(\sqrt{w}\sqrt{w}^{\mathsf{T}}\big), \\
& X \in \mathbb{S}^V_+.
\end{aligned} \tag{2.44}$$

Note that $\bar{X} \oplus \bar{t} := \frac{1}{2}(I \oplus 1)$ and $\bar{y} \oplus \bar{z} := \bar{e}/\langle \bar{e}, w\rangle \oplus 0$ are Slater points for (2.44) and (2.43), respectively. Thus, the Strong Duality Theorem justifies the use of min and the equation in (2.44).

Before we state a weighted min-max relation corresponding to (2.18), we translate the transformation described in (2.23)(i):

Proposition 2.15. Let $G = (V, E)$ be a graph, and let $w \in \mathbb{R}^V_+$ be nonzero. Let $\bar{X} \oplus \bar{t}$ be a feasible solution for (2.44). If $\bar{t} \leq 1/2$, and $\bar{X}$ is the Gram matrix of the vectors $\{\, u_i : i \in V\}$, then the map

$$v\colon i \in V \mapsto \sqrt{2}\begin{bmatrix} \big((\frac{1}{2} - \bar{t}\,)w_i\big)^{1/2} \\ u_i \end{bmatrix} \tag{2.45}$$

is an orthonormal representation of $\overline{G}$.

Proof. Feasibility of $\bar{X} \oplus \bar{t}$ in (2.44) implies that

$$\begin{aligned} \bar{X}_{ii} &= \tfrac{1}{2} - \left(\tfrac{1}{2} - \bar{t}\right)w_i && \forall i \in V, \\ \bar{X}_{ii} - 2\bar{X}_{ij} + \bar{X}_{jj} &= 1 - \left(\tfrac{1}{2} - \bar{t}\right)[\mathcal{L}_G^*(\sqrt{w}\sqrt{w}^{\mathsf{T}})]_{ij} && \forall ij \in E. \end{aligned}$$

Thus, $\|v_i\|^2 = 2\big((\tfrac{1}{2} - \bar{t})w_i + \bar{X}_{ii}\big) = 1$ for every $i \in V$, and $\langle v_i, v_j\rangle = 2\big((\tfrac{1}{2} - \bar{t})(w_i w_j)^{1/2} + \bar{X}_{ij}\big) = 2(\tfrac{1}{2} - \bar{t})(w_i w_j)^{1/2} + \bar{X}_{ii} + \bar{X}_{jj} - 1 + (\tfrac{1}{2} - \bar{t})[\mathcal{L}_G^*(\sqrt{w}\sqrt{w}^{\mathsf{T}})]_{ij} = 0$ whenever $ij \in E$. $\square$

We now state the weighted version of Corollary 2.5.

Proposition 2.16. Let $G = (V, E)$ be a graph, and let $w \in \mathbb{R}_+^V$ be nonzero. Let $\bar{X} \oplus \bar{t}$ be a feasible solution for the SDP (2.44), and let $\bar{x} \in \mathrm{TH}(\overline{G})$ such that $\langle w, \bar{x}\rangle \neq 0$. Then

$$2\bar{t} + \frac{1}{\langle w, \bar{x}\rangle} \geq 1, \tag{2.46}$$

with equality if and only if $\bar{X} \oplus \bar{t}$ is an optimal solution for (2.44) and $\langle w, \bar{x}\rangle = \vartheta(\overline{G}, w)$.

Proof. We may assume that $\bar{t} < 1/2$. Let $v\colon V \to \mathbb{R} \oplus \mathbb{R}^d$ be an orthonormal representation of $\overline{G}$ arising from $\bar{X} \oplus \bar{t}$ as in Proposition 2.15. Take $v_0 \coloneqq 1 \oplus 0$. Note that $\langle v_0, v_i\rangle^2 = (1 - 2\bar{t})w_i$ for every $i \in V$. Then

$$(1 - 2\bar{t})\langle w, \bar{x}\rangle = \sum_{i \in V}(1 - 2\bar{t})w_i\bar{x}_i = \sum_{i \in V}\langle v_0, v_i\rangle^2\bar{x}_i \leq 1,$$

since $\bar{x} \in \mathrm{TH}(\overline{G})$. This proves (2.46). The assertion about the equality case follows by construction. $\square$

The weighted theta number $\vartheta(G; w)$ for arbitrary $w \in \mathbb{R}_+^V$ is determined by the values of $\vartheta(G; w)$ on $w \in \mathbb{Z}_+^V$, by homogeneity and continuity. The latter values, in turn, are determined combinatorially from G in a well-understood manner: if $w \in \mathbb{Z}_+^V$, then it is well known that $\vartheta(G; w)$ is equal to the theta number of the graph obtained from G by replacing each node i with a stable set of size w_i. Thus, it is expected that optimal solutions for the SDP (2.44) for the weighted hypersphere number encode optimal hypersphere representations of similarly blown up graphs obtained from G. Let us describe the construction precisely.

Let $G = (V, E)$ be a graph, and let $w \in \mathbb{Z}_+^V$. For the remainder of this section, we let G^w denote the graph on node set $\bigcup_{i \in V}\{i\} \times [w_i]$, where nodes (i, p) and (j, q) are adjacent in G^w if $i = j$ or $ij \in E$. Then we have

$$\vartheta(\overline{G}; w) = \overline{\vartheta}(G^w). \tag{2.47}$$

Thus, by Proposition 2.16, we have $t(G; w) = t(G^w)$.

Let $\bar{X} \oplus \bar{t}$ be a feasible solution for the SDP (2.44). Write $\bar{X} = UU^{\mathsf{T}}$ for some $[d] \times V$ matrix U^{T}, and define $u\colon V \to \mathbb{R}^d$ by $u_i \coloneqq U^{\mathsf{T}}e_i$ for $i \in V$. For each $i \in V$ with $w_i > 0$, let $v_i\colon \{i\} \times [w_i] \to \mathbb{R}^{d_i}$ be an optimal hypersphere representation of the complete graph on node set $\{i\} \times [w_i]$. We shall build a hypersphere representation $z\colon V(G^w) \to \mathbb{R}^d \oplus \left(\bigoplus_{i \in V}\mathbb{R}^{d_i}\right)$ with squared radius $\bar{t}$. We may assume that $w_i > 0$ for every $i \in V$. For $(i, k) \in V(G^w)$, with $i \in V$ and $k \in [w_i]$, set

$$z(i, k) \coloneqq w_i^{-1/2}u_i \oplus \left[\bigoplus_{j \in V}[j = i]v_i(i, k)\right].$$

It is easy to check that z is a hypersphere representation of G^w with squared radius $\bar{t}$.

2.5 Unit-Distance Representations in Euclidean Balls

The hypersphere number of a graph G is the smallest (squared) radius of a hypersphere that contains a unit-distance representation of G. A potentially more natural graph invariant is the smallest (squared) radius of an Euclidean ball that contains a unit-distance representation of G. In this section we study this and some other variations of the hypersphere number.

For a graph G, let $t_b(G)$ denote the smallest (squared) radius of an Euclidean ball that contains a unit-distance representation of G. As in the case of hyperspheres, we may restrict our attention to Euclidean balls centered at the origin, and so it is trivial to modify the SDP (2.3) to formulate this graph invariant:

$$t_b(G) = \min\big\{\, t : t\bar{e} - \operatorname{diag}(X) \geq 0,\ \mathcal{L}_G^*(X) = \bar{e},\ X \in \mathbb{S}_+^V,\ t \in \mathbb{R} \big\}. \tag{2.48}$$

Note that the dual of (2.48) is

$$t_b(G) = \max\big\{\, \bar{e}^{\mathsf{T}} z : y \in \mathbb{R}_+^V,\ z \in \mathbb{R}^E,\ -\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0,\ \bar{e}^{\mathsf{T}} y = 1 \big\}, \tag{2.49}$$

i.e., it is obtained from (2.4) by requiring y to be nonnegative. In particular, as for the dual pair of SDPs (2.3) and (2.4), the points $X \oplus t = \frac{1}{2}(I \oplus 1)$ and $y \oplus z = |V|^{-1}\bar{e} \oplus 0$ are restricted Slater points for (2.48) and (2.49), respectively, which justifies the equation in (2.49) and the use of 'min' and 'max'.

It is obvious that $t_b(G) \leq t(G)$ for any graph G. In fact, equality holds, as we proceed to show. We shall mimic the proof of Theorem 2.4 to show that an analogue of the equation (2.18) holds with $t(G)$ replaced with $t_b(G)$ and $\overline{\vartheta}(G)$ replaced with a variant, call it $\overline{\vartheta_b}(G)$. The proof then follows from Theorem 2.4 and the fact that $\vartheta_b(G) = \vartheta(G)$ for every graph G. The proof of this latter fact follows from the following result of Gijswijt's [47], as was pointed out by Oliveira Filho [114].

Proposition 2.17 ([47, Proposition 9])**.** Let $\mathbb{K} \subseteq \mathbb{S}^n$ be a cone such that $\operatorname{Diag}(h) X \operatorname{Diag}(h) \in \mathbb{K}$ whenever $X \in \mathbb{K}$ and $h \in \mathbb{R}_+^n$. Let X^* be an optimal solution of the optimization problem

$$\max\Big\{\, \bar{e}^{\mathsf{T}} X \bar{e} : \operatorname{Tr}(X) = 1,\ X \in \mathbb{S}_+^n,\ X \in \mathbb{K} \Big\}.$$

Then there exists $\mu \in \mathbb{R}_{++}$ such that $\operatorname{diag}(X^*) = \mu X^* \bar{e}$.

Proposition 2.17 is restated in a slightly more general form as Lemma 5.7 in Chapter 5, where we provide a self-contained proof for the sake of completeness. For now, we shall just mention that the proof relies essentially on the *ad hoc*, "non-convex" fact that every local maximizer of the Rayleigh quotient is a global maximizer.

We shall state a slightly more general result in terms of variations of unit-distance representations in hyperspheres and Euclidean balls, where we may change some of the unit-distance constraints to upper or lower bounds on the edge lengths:

Theorem 2.18. Let $G = (V, E)$ be a graph, and let $E^+, E^- \subseteq E$. Define

$$\mathbb{M} := \big\{\, z \in \mathbb{R}^E : z\restriction_{E^+} \geq 0,\ z\restriction_{E^-} \leq 0 \big\}.$$

Then

$$\begin{aligned} &\min\big\{\, t : t\bar{e} - \operatorname{diag}(X) = 0,\ \mathcal{L}_G^*(X) \succeq_{\mathbb{M}} \bar{e},\ X \in \mathbb{S}_+^V,\ t \in \mathbb{R} \big\} \\ &\qquad = \min\big\{\, t : t\bar{e} - \operatorname{diag}(X) \geq 0,\ \mathcal{L}_G^*(X) \succeq_{\mathbb{M}} \bar{e},\ X \in \mathbb{S}_+^V,\ t \in \mathbb{R} \big\}. \end{aligned} \tag{2.50}$$

In particular,

$$t(G) = t_b(G). \tag{2.51}$$

Proof. Denote the LHS of (2.50) by $t_{=}(G)$ and the RHS by $t_{\geq}(G)$. The dual SDPs of the LHS and RHS of (2.50) are, respectively,

$$t_{=}(G) = \max\big\{\, \bar{e}^{\mathsf{T}} z : y \in \mathbb{R}^V,\, z \in \mathbb{M}^*,\, -\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0,\, \bar{e}^{\mathsf{T}} y = 1 \big\}, \tag{2.52a}$$

$$t_{\geq}(G) = \max\big\{\, \bar{e}^{\mathsf{T}} z : y \in \mathbb{R}^V_+,\, z \in \mathbb{M}^*,\, -\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0,\, \bar{e}^{\mathsf{T}} y = 1 \big\}. \tag{2.52b}$$

Thus, $X \oplus t = \frac{1}{2}(I \oplus 1)$ and $y \oplus z = |V|^{-1}\bar{e} \oplus 0$ are respective restricted Slater points for primal and dual in both pairs of SDPs, which justifies the equations in (2.52) and the use of 'min' and 'max'. As in the proof of Theorem 2.4, we have

$$2t_{=}(G) + \frac{1}{\overline{\vartheta_{=}}(G)} = 1, \tag{2.53a}$$

$$2t_{\geq}(G) + \frac{1}{\overline{\vartheta_{\geq}}(G)} = 1, \tag{2.53b}$$

where

$$\overline{\vartheta_{=}}(G) \coloneqq \max\big\{\, \langle \bar{e}\bar{e}^{\mathsf{T}}, X\rangle : \langle I, X\rangle = 1,\, \mathcal{A}_E(X) \in \mathbb{M}^*,\, \mathcal{A}_{\overline{E}}(X) = 0,\, X \in \mathbb{S}^V_+ \big\}, \tag{2.54a}$$

$$\overline{\vartheta_{\geq}}(G) \coloneqq \max\big\{\, \langle \bar{e}\bar{e}^{\mathsf{T}}, X\rangle : X \text{ is feasible in (2.54a) and } \big\langle \operatorname{Sym}(e_i\bar{e}^{\mathsf{T}}), X\big\rangle \geq 0\, \forall i \in V \big\}. \tag{2.54b}$$

Clearly, $\vartheta_{\geq}(G) \leq \vartheta_{=}(G)$. Let X^* be an optimal solution for $\vartheta_{=}(G)$. By Proposition 2.17, we have $\operatorname{diag}(X^*) = \mu X^* \bar{e}$ for some $\mu \in \mathbb{R}_{++}$. Hence, $X^*\bar{e} = \mu^{-1}\operatorname{diag}(X^*) \geq 0$, so $\langle \operatorname{Sym}(e_i\bar{e}^{\mathsf{T}}), X\rangle = e_i^{\mathsf{T}} X^* \bar{e} \geq 0$ for every $i \in V$, i.e., X^* is feasible in the SDP described by the RHS of (2.54b). This proves

$$\vartheta_{=}(G) = \vartheta_{\geq}(G). \tag{2.55}$$

Now (2.50) follows from (2.53) and (2.55). $\square$

2.6 Graph Homomorphisms and Sandwich Theorems

The proof of the Sandwich Theorem 2.9 we presented relies on Proposition 2.3, which in turn displays very simple combinatorial and geometric constructions. They may be summarized by saying that a hypersphere representation of a graph "contains" a hypersphere representation of each of its subgraphs, and that a hypersphere representation of the complete graph K_p "contains" a hypersphere representation of any p-colorable graph. Both constructions may be regarded as the same if we view them in the context of graph homomorphisms.

Let G and H be graphs. A function $\phi\colon V(G) \to V(H)$ is called a *homomorphism* of G to H if it maps edges of G to edges of H, i.e., if $\{i, j\} \in E$ implies $\{\phi(i), \phi(j)\} \in E(H)$. If there exists a homomorphism from G to H, we write $G \to H$, and we use $\phi\colon G \to H$ to denote that ϕ is a homomorphism from G to H. Note that, if G is a subgraph of H, then $G \to H$ via the identity function. Moreover, for a graph G and an integer $p \in \mathbb{Z}_{++}$, we have $G \to K_p$ if and only if G has a coloring with p colors, since the set of homomorphisms from G to K_p is precisely the set of colorings of G with the set of colors $[p]$. We refer the reader to [64, 62, 50] for more properties of graph homomorphisms.

The proof of Proposition 2.3 boils down to the following property of the hypersphere number:

$$\text{if } G \to H \text{ for graphs } G \text{ and } H, \text{ then } t(G) \le t(H). \tag{2.56}$$

Indeed, if $u\colon V(H) \to \mathbb{R}^d$ is a hypersphere representation of H with squared radius t for some $d \in \mathbb{Z}_{++}$ and $\phi\colon V(G) \to V(H)$ is a homomorphism from G to H, then $u \circ \phi$ is a hypersphere representation of G with squared radius t, as is easily checked. This observation completes the proof of Proposition 2.3, since

$$K_{\omega(G)} \to G \to K_{\chi(G)} \text{ for every graph } G. \tag{2.57}$$

Arguably, this monotonicity property of the hypersphere number with respect to graph homomorphisms lies at the root of the Sandwich Theorem 2.9. Based on this, we say that a graph invariant f is *hom-monotone* if it satisfies

(i) $f(G) \le f(H)$ whenever G and H are graphs such that $G \to H$, (2.58)
(ii) there exists a non-decreasing function $g\colon \operatorname{Im}(f) \to \mathbb{R}$ such that $g(f(K_n)) = n$ for every $n \in \mathbb{Z}_{++}$.

In this case, we get from (2.57) and (2.58)(i) that $f(K_{\omega(G)}) \le f(G) \le f(K_{\chi(G)})$ whence

$$\omega(G) \le g\big(f(G)\big) \le \chi(G) \text{ for every graph } G \tag{2.59}$$

by (2.58)(ii). (A similar use of these ideas may be found in [21].)

The second condition in (2.58) may be regarded as a non-degeneracy property of the graph invariant f, since the first condition implies that $f(K_n) \le f(K_{n+1})$ for every $n \in \mathbb{Z}_{++}$. In the case $f = t$, the function g may be taken to be $g(x) := (1 - 2x)^{-1}$ for every $x \in \mathbb{R}$ with $x < 1/2$, by (2.10).

In fact, from the construction given in the proof of (2.56) one might guess that other optimization problems over geometric representations of graphs "should" yield graph invariants that satisfy (2.58)(i). It seems plausible that the only required properties are that all edges and nodes of the graph are treated "uniformly" by the optimization problem. There is a further requirement on the objective function, which is harder to state precisely, that it should not depend additively on quantities associated with individual nodes and edges. To illustrate this, consider the graph invariant $G \mapsto \min\big\{ \langle I, X\rangle : \mathcal{L}_G^*(X) = \bar{e},\, X \in \mathbb{S}_+^{V(G)} \big\}$ and note that it does not satisfy (2.58)(i).

We have already seen one variation of the hypersphere number in Section 2.5, namely, the graph invariant $t_b(G)$. The proof that t_b is hom-monotone is identical to that of (2.56). However, as we have seen from (2.51), this graph invariant is identical to $t(G)$ and we do not gain a new sandwich inequality. We may also try a variation of the hypersphere number where we constrain adjacent nodes to be at least one unit apart, i.e., define for a graph G the number

$$t'(G) := \min\big\{ t : t\bar{e} - \operatorname{diag}(X) = 0,\, \mathcal{L}_G^*(X) \ge \bar{e},\, X \in \mathbb{S}_+^V,\, t \in \mathbb{R} \big\}. \tag{2.60}$$

It is easy to check that the proof of (2.56) carries over for t', and the same for Proposition 2.1. Consequently $t'(K_n) = t(K_n)$ is also given by (2.10). Thus, the function $g(x) := (1-2x)^{-1}$ certifies that property (2.58)(ii) holds. Hence, t' is hom-monotone, and it satisfies the corresponding sandwich inequality (2.59). The proof of Theorem 2.4 also carries over to show that

$$2t'(G) + \frac{1}{\overline{\vartheta'}(G)} = 1, \tag{2.61}$$

where ϑ' is the graph invariant

$$\vartheta'(G) = \max\left\{ \langle \bar{e}\bar{e}^{\mathsf{T}}, X\rangle : \langle I, X\rangle = 1,\, \mathcal{A}_E(X) = 0,\, \mathcal{A}_{\overline{E}}(X) \geq 0,\, X \in \mathbb{S}^V_+ \right\}, \tag{2.62}$$

introduced independently by McEliece, Rodemich, and Rumsey [108] and Schrijver [129]. Thus, $g(t'(G)) = \overline{\vartheta'}(G)$ and the sandwich inequality (2.59) obtained from t' is nothing but $\omega(G) \leq \overline{\vartheta'}(G) \leq \chi(G)$. Similarly, the parameter

$$t^+(G) \coloneqq \min\left\{ t : t\bar{e} - \operatorname{diag}(X) = 0,\, \mathcal{L}^*_G(X) = \bar{e},\, \mathcal{L}^*_{\overline{G}}(X) \leq \bar{e},\, X \in \mathbb{S}^V_+,\, t \in \mathbb{R} \right\} \tag{2.63}$$

is hom-monotone[1], and the corresponding sandwich inequality involves its counterpart

$$\vartheta^+(G) = \max\left\{ \langle \bar{e}\bar{e}^{\mathsf{T}}, X\rangle : \langle I, X\rangle = 1,\, \mathcal{A}_E(X) \leq 0,\, X \in \mathbb{S}^V_+ \right\}, \tag{2.64}$$

introduced by Szegedy [145].

We note that the numbers $t(G)$, $t'(G)$, and $t^+(G)$ are all equal if the graph G is edge-transitive[2]. Indeed, suppose the latter holds. We may assume that G has no isolated nodes. If G is also node-transitive, then the proof of Proposition 2.1 shows that all three numbers are equal and they are given by (2.5). Otherwise, G is bipartite (see [50, Lemma 3.2.1]) and all three numbers are easily seen to equal 1/4. In fact, Godsil proved that the numbers ϑ, ϑ', and ϑ^+ coincide for a more general class of graphs, called 1-homogeneous; see [49, Lemma 5.2].

Let G be graph. Let $\dim(G)$ be the minimum $d \in \mathbb{Z}_+$ such that there is a unit-distance representation of G in $\mathbb{R}^d$. Here we consider $\mathbb{R}^0 \coloneqq \{0\}$. Note that $G \to H$ implies $\dim(G) \leq \dim(H)$. We show later in Lemma 3.9 that $\dim(K_n) = n - 1$. Thus, the function $g(x) \coloneqq x + 1$ shows that dim is hom-monotone, so $\omega(G) \leq \dim(G) + 1 \leq \chi(G)$. However, as was proved in [73, Theorem 2] (and also shown later in Theorem 3.14), computing $\dim(G)$ is NP-hard. (A similar parameter was introduced in [39].)

One may also define some variants of the parameter $\dim(G)$ by requiring extra properties from the unit-distance representation or considering other geometric representations entirely. For instance, define $\dim_h(G)$ as the minimum $d \in \mathbb{Z}_+$ such that there is a hypersphere representation of G in $\mathbb{R}^d$ with squared radius $\leq 1/2$, and define $\dim_o(G)$ as the minimum $d \in \mathbb{Z}_+$ such that there is an orthonormal representation of G in $\mathbb{R}^d$. The parameters $\dim_h$ and $\overline{\dim_o}$ are also hom-monotone.

Clearly $\dim(G) \leq \dim_h(G)$ holds for every graph G, and strict inequality occurs for the Mosers spindle (see Figure 3.2 and the proof of Theorem 3.14). Since (2.23)(i) shows that $\overline{\dim_o}(G) \leq \dim_h(G) + 1$ and [94, Theorem 11] shows that $\overline{\vartheta}(G) \leq \overline{\dim_o}(G)$, these parameters are related by

$$\omega(G) \leq \overline{\vartheta'}(G) \leq \overline{\vartheta}(G) \leq \overline{\dim_o}(G) \leq \dim_h(G) + 1 \leq \chi(G).$$

[1] Roberson [121] noted an error in page 11, line 10 of our paper [22], where we say that t^+ is not hom-monotone.

[2] Roberson [122] pointed out the following typo in page 9, line -2 of our paper [22]: 'node-transitive' should be 'edge-transitive.'

Note that $\dim_h(G) \leq \chi(G) - 1 \leq \Delta(G)$, where $\Delta(G)$ is the maximum degree of G. In fact, by Brooks' Theorem, $\dim_h(G) \leq \Delta(G) - 1$ when G is connected but not complete nor an odd cycle.

One shortcoming in the concept of hom-monotone graph invariants is that it does not include the strongest sandwich inequality known to be satisfied by the Lovász theta number, namely, $\omega(G) \leq \overline{\vartheta}(G) \leq \chi^*(G)$; see [94, Theorem 10] and refer to (5.86) for a definition of χ^*. Indeed, the graph invariant χ is easily checked to be hom-monotone, and the corresponding sandwich inequality is the trivial inequality $\omega(G) \leq \chi(G) \leq \chi(G)$, but it is not the case that $\chi(G)$ lies sandwiched between $\omega(G)$ and $\chi^*(G)$, e.g., for the 5-cycle.

In the next chapter, we shall study another graph invariant arising from geometric representations that could potentially be hom-monotone; see Theorem 3.6.

Chapter 3

Ellipsoidal Representations of Graphs

We have seen in Section 2.5 the hypersphere number of a graph G coincides with the smallest (squared) radius of an Euclidean ball that contains a unit-distance representation of G. In this chapter, we introduce a generalization of the latter problem: find the smallest (squared) radius of an ellipsoid of a given shape that contains a unit-distance representation of G.

The graph invariant $t_b(G)$ may be regarded as the optimal value of the optimization problem over unit-distance representations of $G = (V, E)$ which assigns the objective value $\|(u_i^\mathsf{T} u_i)_{i \in V}\|_\infty$ to each such representation $u\colon V \to \mathbb{R}^V$. Here, $\|(u_i^\mathsf{T} u_i)_{i \in V}\|_\infty$ is the ∞-norm of the vector $(u_i^\mathsf{T} u_i)_{i \in V}$. To generalize this to an ellipsoid of a given shape, let $A \in \mathbb{S}^d_{++}$ for some $d \in \mathbb{Z}_{++}$, and associate with each unit-distance representation $u\colon V \to \mathbb{R}^d$ the objective value $\|(u_i^\mathsf{T} A u_i)_{i \in V}\|_\infty$. If the optimal value of this problem is t and it is attained, then the smallest scalar multiple of the ellipsoid $\{\, x \in \mathbb{R}^d : x^\mathsf{T} A x \leq 1 \}$ that contains a unit-distance representation of G is $\{\, x \in \mathbb{R}^d : x^\mathsf{T} A x \leq t \}$. See Figure 3.1.

It thus makes sense to define, for a graph $G = (V, E)$ and a matrix $A \in \mathbb{S}^d_+$ for some $d \in \mathbb{Z}_{++}$, the *ellipsoidal number of G with respect to A* as

$$\mathcal{E}(G; A) := \inf\Big\{ \big\|\mathrm{diag}(UAU^\mathsf{T})\big\|_\infty : \mathcal{L}_G^*(UU^\mathsf{T}) = \bar{e},\, U^\mathsf{T} \in \mathbb{R}^{[d] \times V} \Big\}. \tag{3.1}$$

(In this setting, we shall call A a "cost matrix.") Note that we allow A to be singular, in which case we are dealing not with ellipsoids, but with elliptic cylinders (see [82] for a related problem). In fact, since it is clear that we are probably dealing with a hard problem, we might as well take the plunge and define an even further generalization. Let $G = (V, E)$ be a graph, and let $A \in \mathbb{S}^d_+$ for some $d \in \mathbb{Z}_{++}$. If $p \in [1, \infty]$, then the *p-norm ellipsoidal number of G with respect to A* is defined as

$$\mathcal{E}_p(G; A) := \inf\Big\{ \big\|\mathrm{diag}(UAU^\mathsf{T})\big\|_p : U^\mathsf{T} \in \mathcal{U}_d(G) \Big\}, \tag{3.2}$$

where the feasible region is

$$\mathcal{U}_d(G) := \big\{ U^\mathsf{T} \in \mathbb{R}^{[d] \times V} : \mathcal{L}_G^*(UU^\mathsf{T}) = \bar{e} \big\}. \tag{3.3}$$

Besides the fact that the parameter $\mathcal{E}(G; A)$ is a natural generalization of the graph invariant $t_b(G)$, a further motivation to study this parameter is the fact that it might lead to new sandwich theorems. This is

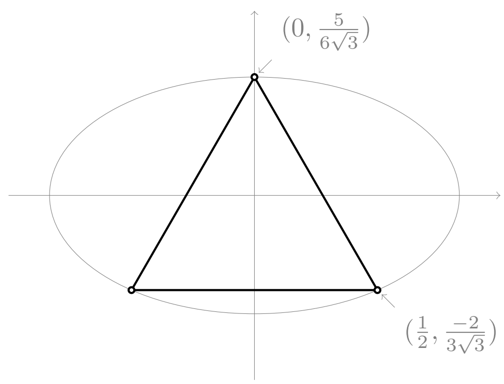

Figure 3.1: A unit-distance representation of K_3 in the ellipsoid $\{\, x \in \mathbb{R}^2 : x_1^2 + 3x_2^2 \leq (5/6)^2 \}$; the ellipsoid corresponding to any smaller RHS does not contain a unit-distance representation of K_3.

not surprising given our discussion about hom-monotone graph invariants in Section 2.6. We shall derive from this parameter a family of graph invariants that satisfy the condition (2.58)(i) of hom-monotonicity; currently we do not know whether the other condition, (2.58)(ii), is satisfied. The main difficulty is that finding an analytic formula for the number $\mathcal{E}(K_n; A)$ for an arbitrary $A \in \mathbb{S}_+^n$ turns out to be quite hard. We shall only be able to provide such a formula for a small but infinite family of complete graphs. For the non-trivial task of proving a lower bound for $\mathcal{E}(K_n; A)$, we rely on the 1-norm variant $\mathcal{E}_1(K_n; A)$, another, weighted variant of the hypersphere number $t(G)$, and, unsurprisingly, on basic tools from convex optimization, namely the Strong Duality Theorem for conic optimization. The tightness of this lower bound for a family of complete graphs will follow from a class of unit-distance representations built from some very remarkable objects: *Hadamard matrices*. The analytic formula for $\mathcal{E}(K_n; A)$ in this infinite family of complete graphs is quite simple. However, we shall provide an analytic formula for $\mathcal{E}(K_n; A)$ for a single complete graph not in this family, namely for $\mathcal{E}(K_3; A)$, and it looks quite different. This seems to indicate a rather intricate parameter. Indeed, we shall prove the unsurprising fact that the problem of computing the ellipsoidal number of an arbitrary graph $G = (V, E)$ and cost matrix $A \in \mathbb{S}_+^V$ is NP-hard.

The main contributions in this chapter are Corollary 3.11, which computes ellipsoidal numbers for complete graphs under the 1-norm, and Theorem 3.12, which shows how certain unit-distance representations built from Hadamard matrices are optimal for ellipsoidal numbers. However, all results in this chapter are new except for Theorem 3.14; we provide a shorter proof for the latter nevertheless.

3.1 Basic Properties

Throughout this chapter, we shall make heavy use of the convenient fact, obvious from the outset, that the feasible region $\mathcal{U}_d(G)$ of $\mathcal{E}_p(G; \cdot)$ is invariant under the action of the orthogonal group. This will allow us to assume almost everywhere that the cost matrix A in $\mathcal{E}_p(G; A)$ is diagonal.

Proposition 3.1. Let $G = (V, E)$ be a graph, and let $d \in \mathbb{Z}_{++}$. Then $\mathbb{O}^d\,\mathcal{U}_d(G) = \mathcal{U}_d(G)$. Consequently, for every $p \in [1, \infty]$, the function $A \in \mathbb{S}_+^d \mapsto \mathcal{E}_p(G; A)$ is spectral, and

$$\mathcal{E}_p(G; A) = \mathcal{E}_p(G; \mathrm{Diag}(\lambda^{\downarrow}(A))) \qquad \forall A \in \mathbb{S}_+^d. \tag{3.4}$$

Proof. If $U^\mathsf{T} \in \mathcal{U}_d(G)$ and $Q \in \mathbb{O}^d$, then $\mathcal{L}_G^*(UQ^\mathsf{T}QU^\mathsf{T}) = \mathcal{L}_G^*(UU^\mathsf{T}) = \bar{e}$, whence $QU^\mathsf{T} \in \mathcal{U}_d(G)$. Thus, $Q\mathcal{U}_d(G) \subseteq \mathcal{U}_d(G)$ for every $Q \in \mathbb{O}^d$, whence $\mathcal{U}_d(G) = Q^\mathsf{T}Q\mathcal{U}_d(G) \subseteq Q^\mathsf{T}\mathcal{U}_d(G) \subseteq \mathcal{U}_d(G)$. Equality throughout proves that $Q\mathcal{U}_d(G) = \mathcal{U}_d(G)$, so $\mathbb{O}^d\mathcal{U}_d(G) = \mathcal{U}_d(G)$. Now let $p \in [1,\infty]$ and $A \in \mathbb{S}_+^d$. For any $Q \in \mathbb{O}^d$, we have

$$\begin{aligned}\mathcal{E}_p(G; QAQ^\mathsf{T}) &= \inf\Big\{ \left\|\operatorname{diag}(UQAQ^\mathsf{T}U^\mathsf{T})\right\|_p : U^\mathsf{T} \in \mathcal{U}_d(G)\Big\}\\ &= \inf\Big\{ \left\|\operatorname{diag}(ZAZ^\mathsf{T})\right\|_p : Z^\mathsf{T} \in Q^\mathsf{T}\mathcal{U}_d(G)\Big\}\\ &= \inf\Big\{ \left\|\operatorname{diag}(ZAZ^\mathsf{T})\right\|_p : Z^\mathsf{T} \in \mathcal{U}_d(G)\Big\} = \mathcal{E}_p(G;A).\end{aligned}$$

Thus, the function $A \in \mathbb{S}_+^d \mapsto \mathcal{E}_p(G;A)$ is spectral. In particular, (3.4) holds. □

Now, we prove that the infimum in (3.2) is attained whenever finite. This is non-trivial since we allow the cost matrix A to be singular. For instance, if $A \in \mathbb{S}_+^d$ is diagonal and all diagonal entries of A are nonzero except for, say, A_{dd}, then it is advantageous to "push a large portion of the representation" $U^\mathsf{T} \in \mathcal{U}_d(G)$ onto its dth row, which has zero cost. That is, by making the entries in the dth row larger and larger relative to the entries on the other rows, while preserving the unit-distance constraint, it is conceivable that the objective function could decrease arbitrarily without attaining its infimum value. We will show that this situation cannot occur by a slightly more careful application of the standard compactness and continuity argument[1].

Theorem 3.2. Let $G = (V,E)$ be a graph. Let $p \in [1,\infty]$ and let $A \in \mathbb{S}_+^d$ for some $d \in \mathbb{Z}_{++}$. If $\mathcal{E}_p(G;A) < +\infty$, then there exists $U^\mathsf{T} \in \mathcal{U}_d(G)$ such that $\mathcal{E}_p(G;A) = \|\operatorname{diag}(UAU^\mathsf{T})\|_p$, i.e., the infimum in the definition (3.2) of $\mathcal{E}_p(G;A)$ is attained.

Proof. By Proposition 3.1, we may assume that $A = \operatorname{Diag}(\lambda)$, where $\lambda := \lambda^{\downarrow}(A)$, and that $\lambda \neq 0$. Let $k \in [d]$ be largest so that $\lambda_k \neq 0$. Throughout this proof, let $P\colon \mathbb{R}^{[d]} \to \mathbb{R}^{[k]}$ denote the projection onto the first k components, and let $Q\colon \mathbb{R}^{[d]} \to \mathbb{R}^{[d]\setminus[k]}$ denote the projection onto the last $d-k$ components, i.e., $x = (Px) \oplus (Qx)$ for every $x \in \mathbb{R}^d$. Note that

$$A = P^\mathsf{T}(A[[k]])P \tag{3.5}$$

and

$$A[[k]] \succeq \lambda_k I. \tag{3.6}$$

The proof relies on modifying the RHS of (3.2) by adding constraints that do not change the optimal value but which make the feasible region compact.

Let $M \in \mathbb{R}$ such that $\mathcal{E}_p(G;A) \leq M$. We claim that adding the constraints

$$\|PU^\mathsf{T}e_i\|_2^2 \leq B := (M+1)/\lambda_k \qquad \forall i \in V, \tag{3.7}$$

does not change the optimal value of the RHS of (3.2), i.e.,

$$\mathcal{E}_p(G;A) = \inf\Big\{ \left\|\operatorname{diag}(UAU^\mathsf{T})\right\|_p : U^\mathsf{T} \in \mathcal{U}_d(G),\, U^\mathsf{T} \text{ satisfies (3.7)}\Big\}. \tag{3.8}$$

[1]The corresponding result in our paper [22], Theorem 5.1, contains an error in the proof, where we say that we may assume that the graph G is connected. This assumption can be made without loss of generality provided $p = \infty$. The proof in this thesis fixes that error.

Suppose $U^\mathsf{T} \in \mathcal{U}_d(G)$ violates (3.7), and let $i \in V$ such that $\|PU^\mathsf{T} e_i\|_2^2 > (M+1)/\lambda_k$. By (3.5) and (3.6), we have

$$\begin{aligned}\left\|\operatorname{diag}(UAU^\mathsf{T})\right\|_p &\geq e_i^\mathsf{T} UAU^\mathsf{T} e_i = e_i^\mathsf{T} UP^\mathsf{T}(A[[k]])PU^\mathsf{T} e_i \\ &\geq e_i^\mathsf{T} UP^\mathsf{T}(\lambda_k I)PU^\mathsf{T} e_i = \lambda_k \|PU^\mathsf{T} e_i\|_2^2 \\ &> M+1 \geq \mathcal{E}_p(G;A)+1,\end{aligned}$$

so U^T may be discarded from the feasible region of the RHS of (3.2) without changing its optimal value. This proves (3.8).

If $k = d$, the proof is complete, since the feasible region of the RHS of (3.8) is compact, so

$$\text{assume that } k < d.$$

Let $\mathcal{H}$ denote the set of components of G. For each $i \in V$, denote by $H(i)$ the component of G which contains i. For each $H \in \mathcal{H}$, choose $i \in H$ arbitrarily and call it $i(H)$. We claim that adding the constraints

$$QU^\mathsf{T} e_{i(H)} = 0 \qquad \forall H \in \mathcal{H}, \tag{3.9}$$

does not change the optimal value in the RHS of (3.8), i.e., that

$$\mathcal{E}_p(G;A) = \inf\Big\{ \left\|\operatorname{diag}(UAU^\mathsf{T})\right\|_p : U^\mathsf{T} \in \mathcal{U}_d(G),\, U^\mathsf{T} \text{ satisfies (3.7) and (3.9)}\Big\}. \tag{3.10}$$

Let $U^\mathsf{T} \in \mathcal{U}_d(G)$ satisfy (3.7). Define a matrix $Z^\mathsf{T} \in \mathbb{R}^{[d]\times V}$ by setting $PZ^\mathsf{T} e_j \coloneqq PU^\mathsf{T} e_j$ and $QZ^\mathsf{T} e_j \coloneqq QU^\mathsf{T}(e_j - e_{i(H(j))})$ for every $j \in V$. Since Z^T is obtained from U^T by applying the same shift to the columns of each component of G, we have $Z^\mathsf{T} \in \mathcal{U}_d(G)$. Since Z^T satisfies (3.7) and (3.9) by construction, Z^T is feasible in the RHS of (3.10). Moreover, by (3.5), we have $ZAZ^\mathsf{T} = ZP^\mathsf{T}(A[[k]])PZ^\mathsf{T} = UP^\mathsf{T}(A[[k]])PU^\mathsf{T} = UAU^\mathsf{T}$, so $\operatorname{diag}(ZAZ^\mathsf{T}) = \operatorname{diag}(UAU^\mathsf{T})$, i.e., Z^T has the same objective value as U^T. Together with (3.8), this completes the proof of (3.10).

To finish the proof, we show that the feasible region $\mathcal{U}$ in the RHS of (3.10) is compact. Clearly $\mathcal{U}$ is closed, so we must only prove that $\mathcal{U}$ is bounded. Let $U^\mathsf{T} \in \mathcal{U}$. Since the columns of U^T form a unit-distance representation of G, the distance between nodes i and j is an upper bound for $\|U^\mathsf{T} e_i - U^\mathsf{T} e_j\|_2$ for any $i, j \in V$. Hence, for every $j \in V$, we have $\|U^\mathsf{T} e_j\|_2 \leq \|U^\mathsf{T} e_{i(H(j))}\|_2 + |V| = \|PU^\mathsf{T} e_{i(H(j))}\|_2 + |V| \leq B^{1/2} + |V|$. Thus, $\mathcal{U}$ is bounded, and thus compact. This concludes the proof, since the objective function is continuous. $\square$

We may refine Theorem 3.2 slightly by ensuring the existence of an optimal solution U^T for (3.2) which is "close to the origin" in the sense that the origin lies in the convex hull of the columns of U^T. It will be convenient in this result to switch to a functional notation for unit-distance representations.

Theorem 3.3. Let $G = (V, E)$ be a graph. Let $p \in [1, \infty]$ and let $A \in \mathbb{S}_+^d$ for some $d \in \mathbb{Z}_{++}$. If $\mathcal{E}_p(G;A) < +\infty$, then there exists a unit-distance representation $u\colon V \to \mathbb{R}^d$ of G such that $\mathcal{E}_p(G;A) = \|(u_i^\mathsf{T} A u_i)_{i \in V}\|_p$ and $0 \in \operatorname{conv}\{\, u_i : i \in V \,\}$.

Proof. We start as in the proof of Theorem 3.2. By Proposition 3.1, we may assume that $A = \operatorname{Diag}(\lambda)$, where $\lambda \coloneqq \lambda^\downarrow(A)$, and that $\lambda \neq 0$. Let $k \in [d]$ be largest so that $\lambda_k \neq 0$. Throughout the proof, let $P\colon \mathbb{R}^{[d]} \to \mathbb{R}^{[k]}$ denote the projection onto the first k components.

Let $u\colon V \to \mathbb{R}^d$ be a unit-distance representation of G. Let $\mathcal{U}$ be the set of all unit-distance representations of G of the form $i \in V \mapsto u_i + r$ for some $r \in \operatorname{Null}(P)$. Note that if $k = d$, then $\mathcal{U}$ is a singleton. Clearly, every element of $\mathcal{U}$ has the same objective value as u. We will show that

$$\text{if } 0 \notin \operatorname{conv}\{\, v_i : i \in V \,\} \text{ for all } v \in \mathcal{U}, \text{ then } \mathcal{E}_p(G; A) < \|(u_i^\top A u_i)_{i\in V}\|_p. \tag{3.11}$$

Suppose that $0 \notin \operatorname{conv}\{\, v_i : i \in V \,\}$ for every $v \in \mathcal{U}$. Since 0 does not lie in the set

$$\bigcup_{v\in\mathcal{U}} \operatorname{conv}\{\, v_i : i \in V \,\} = \bigcup_{r\in\operatorname{Null}(P)} \operatorname{conv}\{\, u_i + r : i \in V \,\} = \operatorname{conv}\{\, u_i : i \in V \,\} + \operatorname{Null}(P),$$

which is a polyhedron, by Farkas' Lemma there exists $h \in \mathbb{R}^d$ and $\alpha \in \mathbb{R}_{++}$ such that $h^\top v_i \geq \alpha$ for every $v \in \mathcal{U}$ and $i \in V$. Note that $h_j = 0$ whenever $j \in [d] \setminus [k]$, since the linear function $h^\top u_i + t h_j = h^\top(u_i + t e_j)$ of t is bounded below by α. Thus,

$$h^\top u_i \geq \alpha > 0 \quad \forall i \in V \qquad \text{and} \qquad h \in \operatorname{Im}(A). \tag{3.12}$$

Let $x \in \mathbb{R}^d$ such that $Ax = h$ and let $s \coloneqq \varepsilon x$, where $\varepsilon > 0$ will be chosen later. Define $z\colon V \to \mathbb{R}^d$ by $z_i \coloneqq u_i - s$ for every $i \in V$. Let $i \in V$. Then

$$z_i^\top A z_i = (u_i - s)^\top A (u_i - s) = u_i^\top A u_i - 2 s^\top A u_i + s^\top A s = u_i^\top A u_i - 2\varepsilon h^\top u_i + \varepsilon^2 x^\top A x.$$

Hence $z_i^\top A z_i < u_i^\top A u_i$ if and only if $2\varepsilon h^\top u_i > \varepsilon^2 x^\top A x$. Thus, we will be done if we can find $\varepsilon > 0$ such that $2 h^\top u_i > \varepsilon x^\top A x$. Since $h^\top u_i \geq \alpha > 0$, such ε exists. Thus, by choosing $\varepsilon > 0$ small enough, we find a unit-distance representation $z\colon V \to \mathbb{R}^d$ of G such that $z_i^\top A z_i < u_i^\top A u_i$ for every $i \in V$. Hence, $\|(z_i^\top A z_i)_{i\in V}\|_p < \|(u_i^\top A u_i)_{i\in V}\|_p$, which shows that z has objective value strictly less than that of u. This proves (3.11).

The result now follows from (3.11) and Theorem 3.2. $\square$

Let $G = (V, E)$ be a graph. Let $p \in [1, \infty]$ and let $A \in \mathbb{S}_+^d$ for some $d \in \mathbb{Z}_{++}$. For the next two results we shall use the fact that the map $A \in \mathbb{S}_+^d \mapsto \mathcal{E}_p(G; A)$ is monotone with respect to the Löwner partial order, i.e.,

$$A \preceq B \text{ implies } \mathcal{E}_p(G; A) \leq \mathcal{E}_p(G; B). \tag{3.13}$$

This follows easily from the fact that p-norms are monotone with respect to the partial order on $\mathbb{R}^n$ induced by $\mathbb{R}_+^n$.

The next result describes a situation in which one may work on a lower dimensional space by dropping some of the most expensive coordinates.

Proposition 3.4. Let $G = (V, E)$ be a graph. Let $p \in [1, \infty]$ and let $A \in \mathbb{S}_+^d$ for some $d \in \mathbb{Z}_{++}$. If $\bar{U}^\top \in \mathcal{U}_d(G)$ is an optimal solution for $\mathcal{E}_p(G; A)$ and k is an integer such that $\operatorname{rank}(\bar{U}) \leq k \leq d$, then

$$\mathcal{E}_p(G; A) = \mathcal{E}_p(G; \operatorname{Diag}(\lambda_1^\uparrow(A), \dots, \lambda_k^\uparrow(A))). \tag{3.14}$$

Proof. Set

$$D \coloneqq \operatorname{Diag}(\lambda_1^\uparrow(A), \dots, \lambda_k^\uparrow(A)).$$

By Proposition 3.1, we may assume that $A = \operatorname{Diag}(\lambda)$, where $\lambda \coloneqq \lambda^{\uparrow}(A)$.

We shall start by proving '$\leq$' in (3.14). Let $U^{\mathsf{T}} \in \mathcal{U}_k(G)$, and set $Z \coloneqq \begin{bmatrix} U & 0 \end{bmatrix} \in \mathbb{R}^{V\times[d]}$, i.e., append $d-k$ zero columns to U. Then $Z^{\mathsf{T}} \in \mathcal{U}_d(G)$ and $\mathcal{E}_p(G; A) \leq \|\operatorname{diag}(ZAZ^{\mathsf{T}})\|_p = \|\operatorname{diag}(UDU^{\mathsf{T}})\|_p$. This proves '$\leq$' in (3.14).

Next we prove '$\geq$' in (3.14). Let $Q \in \mathbb{O}^d$ be such that, for each $i \in V$, the final $d-k$ rows of $Q\bar{U}^{\mathsf{T}}$ are zero; this is possible since $k \geq \operatorname{rank}(\bar{U}^{\mathsf{T}})$. Set $B \coloneqq (QAQ^{\mathsf{T}})[[k]]$. We will be done once we prove that

$$\mathcal{E}_p(G; A) \geq \mathcal{E}_p(G; B) \tag{3.15}$$

and

$$\mathcal{E}_p(G; B) \geq \mathcal{E}_p(G; D). \tag{3.16}$$

Let $Z^{\mathsf{T}} \in \mathbb{R}^{[k]\times V}$ be obtained from $Q\bar{U}^{\mathsf{T}}$ by dropping the final $d-k$ (zero) rows. Clearly, $Z^{\mathsf{T}} \in \mathcal{U}_k(G)$. Then

$$ZBZ^{\mathsf{T}} = \begin{bmatrix} Z & 0 \end{bmatrix} QAQ^{\mathsf{T}} \begin{bmatrix} Z^{\mathsf{T}} \\ 0 \end{bmatrix} = \bar{U}Q^{\mathsf{T}}QAQ^{\mathsf{T}}Q\bar{U}^{\mathsf{T}} = \bar{U}A\bar{U}^{\mathsf{T}},$$

so $\mathcal{E}_p(G; A) = \|\operatorname{diag}(\bar{U}A\bar{U}^{\mathsf{T}})\|_p = \|\operatorname{diag}(ZBZ^{\mathsf{T}})\|_p \geq \mathcal{E}_p(G; B)$. This proves (3.15). Set $\mu \coloneqq \lambda^{\uparrow}(B)$. Since $\lambda = \lambda^{\uparrow}(QAQ^{\mathsf{T}})$, the eigenvalues of B interlace the eigenvalues of A (see, e.g., [72, Theorem 4.3.8]), so $\mu \geq \lambda\restriction_{[k]}$ and $\operatorname{Diag}(\mu) \succeq D$. Thus, by Proposition 3.1 and (3.13) we have $\mathcal{E}_p(G; B) = \mathcal{E}_p(G; \operatorname{Diag}(\mu)) \geq \mathcal{E}_p(G; D)$. This completes the proof of (3.16). $\square$

Corollary 3.5. Let $G = (V, E)$ be a graph. Let $p \in [1, \infty]$ and let $A \in \mathbb{S}^d_+$ for some $d \in \mathbb{Z}_{++}$. If $d \geq |V| - 1$, then

$$\mathcal{E}_p(G; A) = \mathcal{E}_p(G; \operatorname{Diag}(\lambda^{\uparrow}_1(A), \dots, \lambda^{\uparrow}_{|V|-1}(A))). \tag{3.17}$$

Proof. Equation (3.17) holds trivially if $\mathcal{E}_p(G; A) = +\infty$, so assume that $\mathcal{E}_p(G; A) < +\infty$. Let $r \in \mathbb{Z}_{++}$ such that there exists an optimal solution $\bar{U}^{\mathsf{T}} \in \mathcal{U}_d(G)$ of rank r. Then $r \leq |V| - 1 \eqqcolon k$ by Theorem 3.3. Thus, (3.17) follows from Proposition 3.4. $\square$

We can adapt the proof of Proposition 3.4 above to construct some graph invariants from ellipsoidal numbers which satisfy condition (2.58)(i) of hom-monotonicity.

Theorem 3.6. Let $a\colon \mathbb{Z}_{++} \to \mathbb{R}_{++}$ be a non-decreasing sequence of real numbers. Define $A_n \coloneqq \operatorname{Diag}(a_1, \dots, a_n)$ for each $n \in \mathbb{Z}_{++}$. For a graph G on n nodes, set $f(G) \coloneqq \mathcal{E}(G; A_n)$. If G and H are graphs such that $G \to H$, then $f(G) \leq f(H)$.

Proof. Let $\phi\colon G \to H$ be a graph homomorphism. We denote the number of vertices of a graph F by $n(F)$. Let $\bar{U}^{\mathsf{T}} \in \mathcal{U}_{n(H)}(H)$ be a feasible solution for $\mathcal{E}(H; A_{n(H)})$.

Suppose first that $n(H) \leq n(G)$. Define $\bar{Z}^{\mathsf{T}} \in \mathbb{R}^{[n(G)]\times V(G)}$ by setting $\bar{Z}^{\mathsf{T}}e_i \coloneqq \bar{U}^{\mathsf{T}}e_{\phi(i)} \oplus 0$ for each $i \in V(G)$. The fact that ϕ is a homomorphism implies that $\bar{Z}^{\mathsf{T}} \in \mathcal{U}_{n(G)}(G)$. For any $i \in V(G)$, we have $e_i^{\mathsf{T}}\bar{Z}A_{n(G)}\bar{Z}^{\mathsf{T}}e_i = e_{\phi(i)}^{\mathsf{T}}\bar{U}A_{n(H)}\bar{U}^{\mathsf{T}}e_{\phi(i)}$. Thus, $\|\operatorname{diag}(\bar{Z}A_{n(G)}\bar{Z}^{\mathsf{T}})\|_\infty \leq \|\operatorname{diag}(\bar{U}A_{n(H)}\bar{U}^{\mathsf{T}})\|_\infty$, and it follows that $f(G) = \mathcal{E}(G; A_{n(G)}) \leq \mathcal{E}(H; A_{n(H)}) = f(H)$.

Suppose next that $n(H) > n(G)$. Define $\bar{Y}^\mathsf{T} \in \mathbb{R}^{[n(H)]\times V(G)}$ by setting $\bar{Y}^\mathsf{T} e_i \coloneqq \bar{U}^\mathsf{T} e_{\phi(i)}$ for each $i \in V(G)$. The fact that ϕ is a homomorphism implies that $\bar{Y}^\mathsf{T} \in \mathcal{U}_{n(H)}(G)$. Let $Q \in \mathbb{O}^{n(H)}$ such that the final $n(H) - n(G)$ rows of $Q\bar{Y}^\mathsf{T}$ are zero. Set $B \coloneqq (QA_{n(H)}Q^\mathsf{T})[[n(G)]$. We shall be done once we prove

$$\mathcal{E}(H; A_{n(H)}) \geq \mathcal{E}(G; B) \tag{3.18}$$

and

$$\mathcal{E}(G; B) \geq \mathcal{E}(G; A_{n(G)}). \tag{3.19}$$

Let $\bar{Z}^\mathsf{T} \in \mathbb{R}^{[n(G)]\times V(G)}$ be obtained from $Q\bar{Y}^\mathsf{T}$ by dropping the final $n(H) - n(G)$ (zero) rows. Clearly, $\bar{Z}^\mathsf{T} \in \mathcal{U}_{n(G)}(G)$. For $i \in V(G)$, we have

$$e_i^\mathsf{T} \bar{Z} B \bar{Z}^\mathsf{T} e_i = e_i^\mathsf{T} \begin{bmatrix} \bar{Z} & 0 \end{bmatrix} QA_{n(H)}Q^\mathsf{T} \begin{bmatrix} \bar{Z}^\mathsf{T} \\ 0 \end{bmatrix} e_i = e_i^\mathsf{T} \bar{Y} Q^\mathsf{T} Q A_{n(H)} Q^\mathsf{T} Q \bar{Y}^\mathsf{T} e_i = e_{\phi(i)}^\mathsf{T} \bar{U} A \bar{U}^\mathsf{T} e_{\phi(i)},$$

so $\mathcal{E}(G; B) \leq \|\operatorname{diag}(\bar{Z} B \bar{Z}^\mathsf{T})\|_\infty \leq \|\operatorname{diag}(\bar{U} A_{n(H)} \bar{U}^\mathsf{T})\|_\infty$. This proves (3.18). Set $\mu \coloneqq \lambda^\uparrow(B)$. Since $a{\upharpoonright}_{[n(H)]} = \lambda^\uparrow(QA_{n(H)}Q^\mathsf{T})$ and the eigenvalues of B interlace the eigenvalues of $A_{n(H)}$ (see, e.g., [72, Theorem 4.3.8]), we have $\mu \geq a{\upharpoonright}_{[n(G)]}$ and $\operatorname{Diag}(\mu) \succeq A_{n(G)}$. Thus, by Proposition 3.1 and (3.13), we have $\mathcal{E}(G; B) = \mathcal{E}(G; \operatorname{Diag}(\mu)) \geq \mathcal{E}(G; A_{n(G)})$. This completes the proof of (3.19). □

3.2 SDP-based Lower Bound for Complete Graphs

The p-norm variants of the ellipsoidal numbers were not introduced frivolously: inequalities involving p-norms yield inequalities involving the corresponding numbers $\mathcal{E}_p(G; A)$. Thus, they serve as tools for studying our main object, the ellipsoidal number $\mathcal{E}(G; A)$. For instance, since the inequality $\|x\|_\infty \geq \frac{1}{n}\|x\|_1$ holds for every $x \in \mathbb{R}^n$, it follows that

$$\begin{aligned} \mathcal{E}_\infty(G; A) &= \inf\{\, \|\operatorname{diag}(UAU^\mathsf{T})\|_\infty : U^\mathsf{T} \in \mathcal{U}_d(G) \} \\ &\geq \frac{1}{n} \inf\{\, \|\operatorname{diag}(UAU^\mathsf{T})\|_1 : U^\mathsf{T} \in \mathcal{U}_d(G) \} = \frac{1}{n} \mathcal{E}_1(G; A) \end{aligned} \tag{3.20}$$

for every graph G and every $A \in \mathbb{S}^d_+$.

In this section, we shall provide an analytic formula for $\mathcal{E}_1(K_n; A)$, the 1-norm ellipsoidal number of a complete graph. This yields via (3.20) a lower bound for $\mathcal{E}(K_n; A)$, which we shall show in Section 3.3 to be tight for an interesting infinite family of complete graphs. Our main tool is a family of SDPs resembling the hypersphere SDP (2.3).

For every $W \in \mathbb{S}^V$, define

$$t_W(G) \coloneqq \inf\{\, \langle W, X \rangle : \mathcal{L}^*_G(X) = \bar{e},\, X \in \mathbb{S}^V_+ \}, \tag{3.21}$$

and note that its dual is

$$\sup\{\, \bar{e}^\mathsf{T} z : z \in \mathbb{R}^E,\, \mathcal{L}_G(z) \preceq W \}. \tag{3.22}$$

Thus,

$$t(G) = \sup\{\, t_{\operatorname{Diag}(y)}(G) : y \in \mathbb{R}^V,\, \bar{e}^\mathsf{T} y = 1 \} \tag{3.23}$$

by (2.4), so the hypersphere number $t(G)$ of G may be written as a two-stage optimization problem where the inner problem is the SDP (3.21). The same can be said about $\mathcal{E}_1(G; A)$:

Proposition 3.7. Let $G = (V, E)$ be a graph. Let $p \in [1, \infty]$ and $A \in \mathbb{S}^V_+$. Then

$$\mathcal{E}_p(G; A) = \inf\Big\{ \left\|\operatorname{diag}(X^{1/2} Q^\mathsf{T} A Q X^{1/2})\right\|_p : \mathcal{L}^*_G(X) = \bar{e},\ X \in \mathbb{S}^V_+,\ Q \in \mathbb{O}^V \Big\}. \tag{3.24}$$

In particular,

$$\mathcal{E}_1(G; A) = \inf_{Q \in \mathbb{O}^V} t_{Q^\mathsf{T} A Q}(G). \tag{3.25}$$

Proof. Let q^* denote the RHS of (3.24).

We first show that $\mathcal{E}_p(G; A) \leq q^*$. Let (X, Q) be a feasible solution for the RHS. Set $U^\mathsf{T} \coloneqq Q X^{1/2}$. Then $\mathcal{L}^*_G(UU^\mathsf{T}) = \mathcal{L}^*_G(X^{1/2} Q^\mathsf{T} Q X^{1/2}) = \mathcal{L}^*_G(X) = \bar{e}$ and the objective value of U^T in the RHS of (3.2) is $\|\operatorname{diag}(UAU^\mathsf{T})\|_p = \|\operatorname{diag}(X^{1/2} Q^\mathsf{T} A Q X^{1/2})\|_p$, which is the objective value of (X, Q) in the RHS of (3.24).

Next we show that $q^* \leq \mathcal{E}_p(G; A)$. Let $U^\mathsf{T} \in \mathcal{U}_V(G)$, and set $X \coloneqq UU^\mathsf{T}$. By Proposition 1.2, we have $X^{1/2} = QU^\mathsf{T}$ for some $Q \in \mathbb{O}^V$. The objective value of (X, Q^T) in the RHS of (3.24) is $\|\operatorname{diag}(X^{1/2} Q A Q^\mathsf{T} X^{1/2})\|_p = \|\operatorname{diag}(UAU^\mathsf{T})\|_p$, which is the objective value of U^T in the RHS of (3.2). This proves (3.24).

To prove (3.25) note that the objective value of a feasible solution (X, Q) for the RHS of (3.24) is $\|\operatorname{diag}(X^{1/2} Q^\mathsf{T} A Q X^{1/2})\|_1 = \operatorname{Tr}(X^{1/2} Q^\mathsf{T} A Q X^{1/2}) = \operatorname{Tr}(Q^\mathsf{T} A Q X) = \langle Q^\mathsf{T} A Q, X \rangle$. ☐

Before we proceed to compute $t_W(K_n)$, we should inspect whether the optimal value $t_W(G)$ in (3.21) is attained.

Theorem 3.8. Let $G = (V, E)$ be a connected graph and let $W \in \mathbb{S}^V$. If $\bar{e}^\mathsf{T} W \bar{e} > 0$ or $\bar{e} \in \operatorname{Null}(W)$, then the SDP (3.21) has an optimal solution. Otherwise, $t_W(G) = -\infty$.

Proof. Assume throughout that $V = [n]$.

Suppose that $\bar{e}^\mathsf{T} W \bar{e} < 0$. Since $\bar{X}_t \coloneqq \frac{1}{2} I + t\bar{e}\bar{e}^\mathsf{T}$ is feasible for every $t \in \mathbb{R}_+$, then $\lim_{t\to\infty} \langle W, \bar{X}_t \rangle = \frac{1}{2}\langle W, I \rangle + \lim_{t\to\infty} t\bar{e}^\mathsf{T} W \bar{e} = -\infty$ implies that $t_W(G) = -\infty$.

Now we will show that,

$$\text{if } \bar{e}^\mathsf{T} W \bar{e} > 0, \text{ then (3.22) has a Slater point.} \tag{3.26}$$

(In fact, if (3.22) has a Slater point $\bar{z} \in \mathbb{R}^E$, then $\bar{e}^\mathsf{T} W \bar{e} = \bar{e}^\mathsf{T}(W - \mathcal{L}_G(\bar{z}))\bar{e} > 0$.) Let $Q \in \mathbb{O}^n$ such that $Qe_1 = \bar{e}/\|\bar{e}\|_2$. Then $Q^\mathsf{T} \mathcal{L}_G(\bar{e}) Q = 0 \oplus L$ for some matrix $L \in \mathbb{S}^{n-1}_+$. In fact, since G is connected, we have $\operatorname{rank}(\mathcal{L}_G(\bar{e})) = n - 1$ (see, e.g., [50, Lemma 13.1.1]) whence $L \in \mathbb{S}^{n-1}_{++}$. Let $\gamma \in \mathbb{R}$, $b \in \mathbb{R}^{n-1}$, and $A \in \mathbb{S}^{n-1}$ such that

$$Q^\mathsf{T} W Q = \begin{bmatrix} \gamma & b^\mathsf{T} \\ b & A \end{bmatrix}.$$

Note that $\gamma = e_1^\mathsf{T} Q^\mathsf{T} W Q e_1 = \bar{e}^\mathsf{T} W \bar{e}/\|\bar{e}\|_2^2 > 0$. Thus, for any $\lambda \in \mathbb{R}$, the relation $Q^\mathsf{T}(W - \lambda\mathcal{L}_G(\bar{e}))Q \succ 0$ is equivalent to $A - \lambda L \succ \gamma^{-1} bb^\mathsf{T}$ by Schur complement. The latter relation holds if we choose λ negative with $|\lambda|$ sufficiently large, since $L \succ 0$. Thus, $W \succ \mathcal{L}_G(\lambda\bar{e})$ holds for some $\lambda \in \mathbb{R}$ and (3.26) is proved. Since $\frac{1}{2}I$ is feasible in (3.21), the existence of an optimal solution for (3.21) follows from (3.26) and the SDP Strong Duality Theorem.

In the remainder of the proof, we shall deal with the case where $\bar{e}^{\mathsf{T}} W \bar{e} = 0$. We first reduce to the case where $\bar{e} \in \mathrm{Null}(W)$:

$$\text{if } \bar{e}^{\mathsf{T}} W \bar{e} = 0 \text{ and } t_W(G) > -\infty, \text{ then } \bar{e} \in \mathrm{Null}(W). \tag{3.27}$$

The SDP (3.21) has $\frac{1}{2}I$ as a Slater point. Together with the assumption that $t_W(G) > -\infty$, this implies by the Strong Duality Theorem that there is an optimal solution $\bar{z}$ for its dual (3.22). Let $Q \in \mathbb{O}^n$ such that $Qe_1 = \bar{e}/\|\bar{e}\|_2$. Since $Q^{\mathsf{T}}(W - \mathcal{L}_G(\bar{z}))Q \succeq 0$ and $e_1^{\mathsf{T}} Q^{\mathsf{T}}(W - \mathcal{L}_G(\bar{z}))Qe_1 = \bar{e}^{\mathsf{T}}(W - \mathcal{L}_G(\bar{z}))\bar{e}/\|\bar{e}\|_2^2 = 0$, we find that

$$(Qe_k)^{\mathsf{T}} W \bar{e} = e_k^{\mathsf{T}} Q^{\mathsf{T}}(W - \mathcal{L}_G(\bar{z}))\bar{e} = \|\bar{e}\|_2 e_k^{\mathsf{T}} Q^{\mathsf{T}}\big(W - \mathcal{L}_G(\bar{z})\big)Qe_1 = 0$$

for every $k \in [n]$. Thus, $W\bar{e} \in (\mathrm{Im}(Q))^{\perp} = \{0\}$. This proves (3.27).

For the remainder of the proof,

$$\text{assume that } \bar{e} \in \mathrm{Null}(W). \tag{3.28}$$

Let us show that we may add a constraint to (3.21) without changing its optimal value:

$$t_W(G) = \inf\big\{\, \langle W, X\rangle : \mathcal{L}_G^*(X) = \bar{e},\, X \in \mathbb{S}_+^V,\, \langle \bar{e}\bar{e}^{\mathsf{T}}, X\rangle = 0 \big\}. \tag{3.29}$$

Clearly '$\leq$' holds in (3.29). Let $\bar{X}$ be feasible for (3.21). Let $U \in \mathbb{R}^{n\times n}$ such that $\bar{X} = UU^{\mathsf{T}}$. Set $b := \frac{1}{n}U^{\mathsf{T}}\bar{e}$. Note that b is the barycenter of the unit-distance representation of G given by the columns of the matrix U^{T}. Let $Z^{\mathsf{T}} := U^{\mathsf{T}} - b\bar{e}^{\mathsf{T}}$, i.e., each column of Z^{T} is equal to the corresponding column of U^{T} translated by $-b$. Then $Z^{\mathsf{T}}\bar{e} = U^{\mathsf{T}}\bar{e} - \frac{1}{n}U^{\mathsf{T}}\bar{e}\bar{e}^{\mathsf{T}}\bar{e} = 0$. Hence, $\tilde{X} := ZZ^{\mathsf{T}}$ is feasible in (3.21) and $\langle \tilde{X}, \bar{e}\bar{e}^{\mathsf{T}}\rangle = \bar{e}^{\mathsf{T}}ZZ^{\mathsf{T}}\bar{e} = 0$. Moreover, $\tilde{X} = (U - \bar{e}b^{\mathsf{T}})(U^{\mathsf{T}} - b\bar{e}^{\mathsf{T}}) = \bar{X} - 2\,\mathrm{Sym}(Ub\bar{e}^{\mathsf{T}}) + \|b\|^2\bar{e}\bar{e}^{\mathsf{T}}$ so $\langle W, \tilde{X} - \bar{X}\rangle = -2\langle W, \mathrm{Sym}(Ub\bar{e}^{\mathsf{T}})\rangle + \|b\|^2\langle W, \bar{e}\bar{e}^{\mathsf{T}}\rangle = -2\langle W, Ub\bar{e}^{\mathsf{T}}\rangle = -2\bar{e}^{\mathsf{T}}WUb = 0$ by the assumption (3.28). Thus, $\tilde{X}$ is feasible in the RHS of (3.29) and its objective value is the same as that of $\bar{X}$ in (3.21). This concludes the proof of (3.29).

To complete the proof, it is enough to show that the SDP on the RHS of (3.29) has an optimal solution. Its dual is

$$\sup\big\{\, \bar{e}^{\mathsf{T}}z : z \in \mathbb{R}^E,\, \mathcal{L}_G(z) + \mu\bar{e}\bar{e}^{\mathsf{T}} \preceq W,\, \mu \in \mathbb{R}\big\}. \tag{3.30}$$

Since $\bar{e}^{\mathsf{T}}(W + \bar{e}\bar{e}^{\mathsf{T}})\bar{e} > 0$, it follows from (3.26) that there exists $\bar{z} \in \mathbb{R}^E$ such that $\mathcal{L}_G(\bar{z}) \prec W + \bar{e}\bar{e}^{\mathsf{T}}$. Thus, $(\tilde{z}, \tilde{\mu}) := (\bar{z}, -1)$ is a Slater point for (3.30). The existence of an optimal solution for the RHS of (3.29) now follows from the Strong Duality Theorem. $\square$

Next we will derive an analytic formula for $t_W(K_n)$. First, we shall state some convenient properties of the feasible region of the SDP (3.21) for $G = K_n$.

Lemma 3.9. If $n \in \mathbb{Z}_{++}$, then

$$\big\{\, X \in \mathbb{S}_+^n : \mathcal{L}_{K_n}^*(X) = \bar{e}\big\} = \big\{\, \tfrac{1}{2}I + \tfrac{1}{2}\,\mathrm{Sym}(y\bar{e}^{\mathsf{T}}) : y \in \mathbb{R}^n,\, \|\bar{e}\|\|y\| \leq 2 + \bar{e}^{\mathsf{T}}y\big\} \tag{3.31}$$

and

$$\mathrm{rank}(X) \geq n - 1 \qquad \text{for every } X \in \mathbb{S}_+^n \text{ such that } \mathcal{L}_{K_n}^*(X) = \bar{e}. \tag{3.32}$$

Proof. Let $X \in \mathbb{S}^n$ and set $x := \mathrm{diag}(X)$. Then $\mathcal{L}_{K_n}^*(X) = \bar{e}$ if and only if $X_{ij} = \frac{1}{2}(x_i + x_j - 1)$ for every $ij \in \binom{[n]}{2}$, i.e., if and only if $2X = 2\,\mathrm{Sym}(x\bar{e}^{\mathsf{T}}) - \bar{e}\bar{e}^{\mathsf{T}} + I$. Note that $2\,\mathrm{Sym}(x\bar{e}^{\mathsf{T}}) - \bar{e}\bar{e}^{\mathsf{T}} + I = 2\,\mathrm{Sym}\big((x - \frac{1}{2}\bar{e})\bar{e}^{\mathsf{T}}\big) + I = \mathrm{Sym}(y\bar{e}^{\mathsf{T}}) + I$ for $y := 2x - \bar{e}$. Thus,

$$\big\{\, X \in \mathbb{S}^n : \mathcal{L}_{K_n}^*(X) = \bar{e}\big\} = \big\{\, \tfrac{1}{2}\,\mathrm{Sym}(y\bar{e}^{\mathsf{T}} + I) : y \in \mathbb{R}^n\big\}. \tag{3.33}$$

Let $y \in \mathbb{R}^n$. Since

$$\lambda^{\uparrow}\big(\mathrm{Sym}(y\bar{e}^{\mathsf{T}})\big) = \begin{bmatrix} \frac{1}{2}(\bar{e}^{\mathsf{T}}y - \|\bar{e}\|\|y\|) \\ 0 \\ \vdots \\ 0 \\ \frac{1}{2}(\bar{e}^{\mathsf{T}}y + \|\bar{e}\|\|y\|) \end{bmatrix},$$

we find that

$$\lambda_{\min}\big(\mathrm{Sym}(y\bar{e}^{\mathsf{T}} + I)\big) = \tfrac{1}{2}(\bar{e}^{\mathsf{T}}y - \|\bar{e}\|\|y\|) + 1,$$

which is nonnegative precisely when $\|\bar{e}\|\|y\| \leq 2 + \bar{e}^{\mathsf{T}}y$. Moreover, $\lambda_2^{\uparrow}\big(\mathrm{Sym}(y\bar{e}^{\mathsf{T}} + I)\big) = 1$ shows that $\mathrm{rank}\big(\mathrm{Sym}(y\bar{e}^{\mathsf{T}} + I)\big) \geq n - 1$ for all $y \in \mathbb{R}^n$. ☐

Lemma 3.9 allows us to compute a formula for $t_W(K_n)$ via the Strong Duality Theorem applied to a second-order cone program. The *second-order cone* is defined as

$$\mathrm{SOC}_V \coloneqq \{\, x_0 \oplus x \in \mathbb{R} \oplus \mathbb{R}^V : \|x\|_2 \leq x_0 \}.$$

Note that, like $\mathbb{S}^V_+$ and $\mathbb{R}^V_+$, the closed convex cone SOC_V is *self-dual*, i.e., it is its own dual.

Theorem 3.10. If $n \in \mathbb{Z}_{++}$ and $W \in \mathbb{S}^n$, then

$$2t_W(K_n) = \begin{cases} \langle W, I \rangle - \dfrac{\|W\bar{e}\|^2}{\bar{e}^{\mathsf{T}}W\bar{e}} & \text{if } \bar{e}^{\mathsf{T}}W\bar{e} > 0, \\ \langle W, I \rangle & \text{if } W\bar{e} = 0, \\ -\infty & \text{otherwise.} \end{cases} \tag{3.34}$$

Proof. Let $W \in \mathbb{S}^n$. By Theorem 3.8, we have $t_W(K_n) = -\infty$ unless $\bar{e}^{\mathsf{T}}W\bar{e} > 0$ or $W\bar{e} = 0$, in which case $t_W(K_n)$ has an optimal solution. Assume we are in the latter case.

Let $y \in \mathbb{R}^n$. Set $w \coloneqq W\bar{e}$. Then $\langle W, \frac{1}{2}\,\mathrm{Sym}(y\bar{e}^{\mathsf{T}} + I)\rangle = \frac{1}{2}\langle W, y\bar{e}^{\mathsf{T}}\rangle + \frac{1}{2}\langle W, I\rangle = \frac{1}{2}w^{\mathsf{T}}y + \frac{1}{2}\langle W, I\rangle$. Thus, Lemma 3.9 implies that

$$2t_W(K_n) = \langle W, I \rangle + \min\{\, w^{\mathsf{T}}y : y \in \mathbb{R}^n,\ \|\bar{e}\|\|y\| \leq 2 + \bar{e}^{\mathsf{T}}y \}. \tag{3.35}$$

If $W\bar{e} = 0$, then (3.35) coincides with (3.34), so

$$\text{assume that } \bar{e}^{\mathsf{T}}w = \bar{e}^{\mathsf{T}}W\bar{e} > 0. \tag{3.36}$$

The minimization problem in the RHS of (3.35) may be written as the second-order cone program

$$\min\big\{\, \langle 0 \oplus w, y_0 \oplus y \rangle : \|\bar{e}\|y_0 - \bar{e}^{\mathsf{T}}y = 2,\ y_0 \oplus y \in \mathrm{SOC}_n \big\}, \tag{3.37}$$

which has

$$\tilde{y}_0 \oplus \tilde{y} \coloneqq \left(\frac{2 + \|\bar{e}\|^2}{\|\bar{e}\|}\right) \oplus \bar{e}$$

as a Slater point. The dual of (3.37) is

$$\max\{\, 2\mu : \mu \in \mathbb{R},\ \mu(\|\bar{e}\| \oplus (-\bar{e})) \preceq_{\mathrm{SOC}_n} 0 \oplus w \}. \tag{3.38}$$

By the Strong Duality Theorem, the optimal values of (3.37) and (3.38) coincide. Note that feasibility of $\mu \in \mathbb{R}$ in (3.38) is equivalent to membership of $(-\mu\|\bar{e}\|) \oplus (w + \mu\bar{e})$ in SOC_n, i.e., to the inequalities $\mu \leq 0$ and $\|w + \mu\bar{e}\|^2 \leq \mu^2\|\bar{e}\|^2$. Thus, the feasible region of (3.38) is

$$\left\{ \mu \in \mathbb{R} : \mu \leq -\frac{\|w\|^2}{2\bar{e}^\mathsf{T} w} \right\}.$$

Thus, the optimal value of (3.38) is $-\|w\|^2/(\bar{e}^\mathsf{T} w)$. If follows from (3.35) that $2t_W(K_n) = \langle W, I\rangle - \|w\|^2/(\bar{e}^\mathsf{T} W\bar{e})$, and the proof of (3.34) is complete. $\square$

We can finally derive an analytic formula for $\mathcal{E}_1(K_n; A)$:

Corollary 3.11. Let $n, d \in \mathbb{Z}_{++}$. Let $A \in \mathbb{S}^d_+$. Then

$$\mathcal{E}_1(K_n; A) = \begin{cases} \frac{1}{2}\sum_{i=1}^{n-1} \lambda_i^\uparrow(A) & \text{if } d \geq n-1, \\ +\infty & \text{otherwise.} \end{cases} \tag{3.39}$$

Proof. The key part of the proof is to show that

$$2\mathcal{E}_1(K_n; A) = \mathrm{Tr}(A) - \lambda_{\max}(A) \qquad \forall A \in \mathbb{S}^n_+. \tag{3.40}$$

Let $A \in \mathbb{S}^n_+$. If $A = 0$, then (3.40) holds, so suppose $A \neq 0$. If $Q \in \mathbb{O}^n$ sends $\bar{e}$ to $\mathrm{Null}(A)$, then $2t_{Q^\mathsf{T} AQ}(K_n) = \langle Q^\mathsf{T} AQ, I\rangle = \mathrm{Tr}(A)$ by Theorem 3.10. Thus, by (3.25) and Theorem 3.10, we have

$$\begin{aligned}
2\mathcal{E}_1(G; A) - \mathrm{Tr}(A) &= \inf\left\{ -\frac{\|Q^\mathsf{T} AQ\bar{e}\|^2}{\bar{e}^\mathsf{T} Q^\mathsf{T} AQ\bar{e}} : AQ\bar{e} \neq 0,\, Q \in \mathbb{O}^n \right\} \\
&= -\sup\left\{ \frac{\bar{e}^\mathsf{T} Q^\mathsf{T} A^2 Q\bar{e}}{\bar{e}^\mathsf{T} Q^\mathsf{T} AQ\bar{e}} : AQ\bar{e} \neq 0,\, Q \in \mathbb{O}^n \right\} \\
&= -\sup\left\{ \frac{h^\mathsf{T} A^2 h}{h^\mathsf{T} Ah} : Ah \neq 0,\, \|h\| = \|\bar{e}\|,\, h \in \mathbb{R}^n \right\} \\
&= -\sup\left\{ \frac{h^\mathsf{T} A^2 h}{h^\mathsf{T} Ah} : Ah \neq 0,\, h \in \mathbb{R}^n \right\} \\
&= -\sup\left\{ \frac{x^\mathsf{T} Ax}{x^\mathsf{T} x} : A^{1/2}x \neq 0,\, x \in \mathrm{Im}(A) \right\} \\
&= -\lambda_{\max}(A),
\end{aligned}$$

where we used the change of variables $h := Q\bar{e}$ followed by $x := A^{1/2}h$. The constraint $\|h\| = \|\bar{e}\|$ may be dropped since the numerator and denominator in the objective function are homogeneous in $\|h\|^2$, and the last supremum is attained by any nonzero $x \in \mathbb{R}^n$ such that $Ax = \lambda_{\max}(A)x$. This proves (3.40).

By (3.32), the formula (3.39) is correct when $d < n-1$. So suppose that $d \geq n-1$. By Proposition 3.1, we may assume that $A = \mathrm{Diag}(\lambda)$, where $\lambda := \lambda^\uparrow(A)$. Then by Theorem 3.3, we may apply Proposition 3.4

twice with $k = n-1$ to get

$$\begin{aligned}\mathcal{E}_1(K_n; A) &= \mathcal{E}_1(K_n; \operatorname{Diag}(\lambda_1^{\uparrow}(A), \dots, \lambda_{n-1}^{\uparrow}(A)))\\ &= \mathcal{E}_1(K_n; \operatorname{Diag}(\lambda_1^{\uparrow}(A), \dots, \lambda_{n-1}^{\uparrow}(A)) \oplus \lambda_{n-1}^{\uparrow}(A))\\ &= \frac{1}{2}\sum_{i=1}^{n-1} \lambda_i^{\uparrow}(A),\end{aligned}$$

where the last equation follows from (3.40). $\square$

3.3 Hadamard Representations

Recall that an $n \times n$ matrix H is called a *Hadamard matrix* if all entries of H are in $\{\pm 1\}$ and $H^\mathsf{T} H = nI$. Such matrices are very remarkable objects, and they have applications in quite diverse areas, such as error-correcting codes and pattern recognition; see the survey [71].

It is well known that, if there is an $n \times n$ Hadamard matrix, then either $n \in \{1, 2\}$ or n is divisible by 4. It is a long-standing conjecture that there is an $n \times n$ Hadamard matrix for every integer n which is a multiple of 4. On the positive side, it is well known that if H is an $n \times n$ Hadamard matrix and H_2 is the Hadamard matrix

$$H_2 \coloneqq \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

then $H_2 \otimes H$ is a Hadamard matrix; this is known as Sylvester's construction. Here, $\otimes$ denotes the *tensor product*, also known as *Kronecker product*. It implies that, whenever $n \in \mathbb{Z}_{++}$ is a power of 2, there exists an $n \times n$ Hadamard matrix. This yields a "thin" but infinite family of Hadamard matrices.

Let H be an $n \times n$ Hadamard matrix. By possibly replacing H with $H \operatorname{Diag}(H^\mathsf{T} e_1)$, we may assume that H has the form

$$H = \begin{bmatrix} \bar{e}^\mathsf{T} \\ L^\mathsf{T} \end{bmatrix}$$

for some $L^\mathsf{T} \in \mathbb{R}^{(n-1)\times n}$. Then $LL^\mathsf{T} = H^\mathsf{T} H - \bar{e}\bar{e}^\mathsf{T} = nI - \bar{e}\bar{e}^\mathsf{T}$, so $\mathcal{L}_{K_n}^*(LL^\mathsf{T}) = 2n\bar{e}$. Thus,

$$\bar{L}^\mathsf{T} \coloneqq (2n)^{-1/2} L^\mathsf{T} \in \mathcal{U}_{n-1}(K_n). \tag{3.41}$$

The matrix in (3.41) is called the *Hadamard representation of K_n associated with H*.

Theorem 3.12. Let H be an $n \times n$ Hadamard matrix for some $n \in \mathbb{Z}_{++}$. Suppose that $e_1^\mathsf{T} H = \bar{e}^\mathsf{T}$, and let $\bar{L}^\mathsf{T}$ be the Hadamard representation of K_n associated with H. Then for every $p \in [1, \infty]$ and every diagonal $A \in \mathbb{S}_+^{n-1}$, the matrix $\bar{L}^\mathsf{T}$ is an optimal solution for $\mathcal{E}_p(K_n; A)$.

Proof. Let us start with a p-norm analogue of (3.20). Let $p \in [1, \infty]$, and let $q \in [1, \infty]$ such that $\frac{1}{p} + \frac{1}{q} = 1$. We claim that

$$\mathcal{E}_p(K_n; A) \geq \frac{\operatorname{Tr}(A)}{2n^{1/q}}, \tag{3.42}$$

where we interpret the denominator on the RHS as 2 if $p = 1$. In that case, (3.42) follows from Corollary 3.11, so assume $p > 1$. Note that

$$\|x\|_p \geq \frac{\|x\|_1}{n^{1/q}} \qquad \forall x \in \mathbb{R}^n.$$

We may assume that $x \in \mathbb{R}^n_+$ since the validity of the inequality is invariant under re-signing the components of x. Apply Hölder's inequality to get $\|x\|_1 = x^\mathsf{T}\bar{e} \leq \|x\|_p \|\bar{e}\|_q = \|x\|_p n^{1/q}$. Thus,

$$\begin{aligned}
\mathcal{E}_p(K_n; A) &= \inf\Big\{ \big\|\operatorname{diag}(UAU^\mathsf{T})\big\|_p : U^\mathsf{T} \in \mathcal{U}_d(K_n)\Big\} \\
&\geq \frac{1}{n^{1/q}} \inf\big\{ \|\operatorname{diag}(UAU^\mathsf{T})\|_1 : U^\mathsf{T} \in \mathcal{U}_d(K_n)\big\} \\
&= \frac{1}{n^{1/q}} \mathcal{E}_1(K_n; A) = \frac{\operatorname{Tr}(A)}{2n^{1/q}},
\end{aligned}$$

where the last equation follows from Corollary 3.11. This proves (3.42).

The feasibility of $\bar{L}^\mathsf{T}$ was proved in (3.41). Note that

$$\operatorname{diag}(\bar{L}A\bar{L}^\mathsf{T}) = \frac{\operatorname{Tr}(A)}{2n}\bar{e}. \tag{3.43}$$

Indeed, let $a \in \mathbb{R}^{n-1}$ such that $A = \operatorname{Diag}(a)$. Let $i \in [n]$. Then all entries of $\bar{L}^\mathsf{T}$ lie in $\{\pm(2n)^{-1/2}\}$, so $e_i^\mathsf{T}\bar{L}A\bar{L}^\mathsf{T}e_i = e_i^\mathsf{T}\bar{L}\operatorname{Diag}(a)\bar{L}^\mathsf{T}e_i = \sum_{j=1}^{n-1} a_j \bar{L}_{ij}^2 = \frac{1}{2n}\bar{e}^\mathsf{T}a = \frac{1}{2n}\operatorname{Tr}(A)$. Thus, the objective value of $\bar{L}^\mathsf{T}$ in $\mathcal{E}_p(K_n; A)$ is

$$\frac{\operatorname{Tr}(A)}{2n}\|\bar{e}\|_p = \frac{\operatorname{Tr}(A)}{2n} n^{1/p} = \frac{\operatorname{Tr}(A)}{2n^{1/q}}.$$

Thus, $\bar{L}^\mathsf{T}$ is optimal for $\mathcal{E}_p(K_n; A)$ by (3.42). □

Let $n \in \mathbb{Z}_{++}$ such that there exists an $n \times n$ Hadamard matrix H. Let $\bar{L}^\mathsf{T}$ be the Hadamard representation of K_n associated with H. It seems natural to try to modify $\bar{L}^\mathsf{T}$ to obtain a unit-distance representation of K_{n+1} with a low objective value for $\mathcal{E}_\infty(K_{n+1}; A)$. Let $a \in \mathbb{R}^{n-1}_+$ and $M \geq \|a\|_\infty$, and set $A := \operatorname{Diag}(a)$ and $B := \operatorname{Diag}(a \oplus M)$. We know by Theorem 3.12 that $\bar{L}^\mathsf{T}$ is optimal for $\mathcal{E}_\infty(K_n; A)$, and $\operatorname{conv}\{\bar{L}^\mathsf{T}e_i : i \in [n]\}$ is an $(n-1)$-dimensional simplex Δ_{n-1}. We must add a new vertex v to Δ_{n-1} to form a simplex Δ_n which is a unit-distance representation of K_{n+1}. The shortest distance between the new vertex v and its opposite face Δ_{n-1} is the line segment joining v to the barycenter of Δ_{n-1}. It makes sense to align this line segment with the axis considered most expensive by the cost matrix B. That is, we consider members of $\mathcal{U}_n(K_{n+1})$ of the form

$$U^\mathsf{T} = \begin{bmatrix} \bar{L}^\mathsf{T} & 0 \\ \alpha\bar{e}^\mathsf{T} & \beta \end{bmatrix},$$

where $\alpha, \beta \in \mathbb{R}$.

Note that

$$UU^\mathsf{T} = \begin{bmatrix} \bar{L}\bar{L}^\mathsf{T} + \alpha^2\bar{e}\bar{e}^\mathsf{T} & \alpha\beta\bar{e} \\ \alpha\beta\bar{e}^\mathsf{T} & \beta^2 \end{bmatrix},$$

so

$$\begin{aligned}\mathcal{L}^*_{K_{n+1}}(UU^\mathsf{T}) &= \mathcal{L}^*_{K_n}(\bar{L}\bar{L}^\mathsf{T} + \alpha^2\bar{e}\bar{e}^\mathsf{T}) \oplus \big(\operatorname{diag}(\bar{L}\bar{L}^\mathsf{T} + \alpha^2\bar{e}\bar{e}^\mathsf{T}) + \beta^2\bar{e} - 2\alpha\beta\bar{e}\big)\\ &= \bar{e} \oplus \big(\operatorname{diag}(\bar{L}\bar{L}^\mathsf{T}) + \alpha^2\bar{e} + \beta^2\bar{e} - 2\alpha\beta\bar{e}\big)\\ &= \bar{e} \oplus \left(\frac{n-1}{2n} + (\alpha-\beta)^2\right)\bar{e},\end{aligned}$$

i.e., $U^\mathsf{T} \in \mathcal{U}_n(K_{n+1})$ if and only if $(\alpha-\beta)^2 = \frac{n+1}{2n}$. By symmetry, we shall consider matrices of the form

$$U_\alpha^\mathsf{T} \coloneqq \begin{bmatrix} \bar{L}^\mathsf{T} & 0 \\ \alpha\bar{e}^\mathsf{T} & \beta_\alpha \end{bmatrix}, \tag{3.44a}$$

where

$$\beta_\alpha \coloneqq \alpha + \left(\frac{n+1}{2n}\right)^{1/2}. \tag{3.44b}$$

Note that by our previous discussion, we have

$$U_\alpha^\mathsf{T} \in \mathcal{U}_n(K_{n+1}) \qquad \forall \alpha \in \mathbb{R}. \tag{3.45}$$

The next proposition determines which of these representations of K_{n+1} yields the smallest objective value in $\mathcal{E}_\infty(K_{n+1}; B)$.

Proposition 3.13. Let $n \in \mathbb{Z}_{++}$ be such that there exists an $n \times n$ Hadamard matrix H. Suppose that $e_1^\mathsf{T} H = \bar{e}^\mathsf{T}$. Let $\bar{L}^\mathsf{T}$ be the Hadamard representation of K_n associated with H. For each $\alpha \in \mathbb{R}$, define U_α^T as in (3.44). Let $a \in \mathbb{R}^{n-1}_+$ and $M \in \mathbb{R}_{++}$ such that $M \geq \|a\|_\infty$. Set

$$A \coloneqq \operatorname{Diag}(a), \qquad B \coloneqq \operatorname{Diag}(a \oplus M). \tag{3.46}$$

Then

$$\inf_{\alpha\in\mathbb{R}} \big\|\operatorname{diag}(U_\alpha B U_\alpha^\mathsf{T})\big\|_\infty = \frac{\big(\operatorname{Tr}(B) + Mn\big)^2}{8Mn(n+1)} = \frac{\operatorname{Tr}(B)}{2(n+1)} + \frac{\big(\operatorname{Tr}(B) - Mn\big)^2}{8Mn(n+1)}. \tag{3.47}$$

In particular,

$$\mathcal{E}_\infty(K_{n+1}; B) \leq \frac{\operatorname{Tr}(B)}{2(n+1)} + \frac{\big(\operatorname{Tr}(B) - Mn\big)^2}{8Mn(n+1)}. \tag{3.48}$$

Proof. Let $\alpha \in \mathbb{R}$. We have

$$e_{n+1}^\mathsf{T} U_\alpha B U_\alpha^\mathsf{T} e_{n+1} = M\beta_\alpha^2 = M\alpha^2 + M\frac{(n+1)}{2n} + 2M\alpha\Big(\frac{n+1}{2n}\Big)^{1/2} \eqqcolon f_0(\alpha),$$

and, for every $i \in [n]$, we have

$$e_i^\mathsf{T} U_\alpha B U_\alpha^\mathsf{T} e_i = M\alpha^2 + \sum_{j=1}^{n-1} a_j \bar{L}_{ij}^2 = M\alpha^2 + \frac{\operatorname{Tr}(A)}{2n} \eqqcolon f_1(\alpha),$$

so that $\big\|\operatorname{diag}(U_\alpha B U_\alpha^\mathsf{T})\big\|_\infty = \max\{f_0(\alpha), f_1(\alpha)\}$.

We have

$$f_1(\alpha) \leq f_0(\alpha) \iff \alpha \geq \frac{\mathrm{Tr}(A) - M(n+1)}{4Mn}\left(\frac{n+1}{2n}\right)^{-1/2} =: \bar{\alpha}. \tag{3.49}$$

Hence, $\left\|\mathrm{diag}(U_\alpha^\top B U_\alpha^\top)\right\|_\infty = f_{[\alpha<\bar{\alpha}]}(\alpha)$. Let α^* be a global minimizer of the LHS of (3.47), which exists since the objective function is continuous and coercive. The vertex of the parabola $y = f_1(\alpha)$ lies at $\alpha_1 := 0$, and since $M \geq \|a\|_\infty$, we have $\bar{\alpha} \leq 0$. Thus, $\alpha^* \geq \bar{\alpha}$, and the LHS of (3.47) is $\inf_{\alpha \geq \bar{\alpha}} f_0(\alpha)$. It is easy to check that the vertex of the parabola $y = f_0(\alpha)$ lies at

$$\alpha_0 := -\left(\frac{n+1}{2n}\right)^{1/2}.$$

Since $\alpha_0 < \bar{\alpha}$, it follows that $f_0(\alpha)$ is increasing on $\alpha \geq \bar{\alpha}$, so $\alpha^* = \bar{\alpha}$. It is easy to check that both expressions of (3.47) are equal to $f_0(\alpha^*)$. This completes the proof of (3.47). Now (3.48) follows from (3.47) and (3.45). ☐

The proof of Proposition 3.13 describes a form of local optimality of the representation (3.45) for $\mathcal{E}(K_{n+1};\cdot)$ with $\alpha := \bar{\alpha}$ given in (3.49). The upper bound (3.48) is in fact tight for $n = 2$. The proof of this is a bit long, and not very enlightening. It does not fit well with the usual tools we have been using, so it is presented in Section A.1 in the Appendix, which culminates with Theorem A.8, stating equality in (3.48) for $n = 2$.

3.4 Computational Complexity

The difficulty in proving an analytic formula for $\mathcal{E}(K_n; A)$ even for a "thin" infinite family of complete graphs (Theorem 3.12) and the somewhat erratic behavior for the formula even as n ranges from 2 to 4 (Theorem A.8) indicate how intricate this parameter is. In this section, we prove the unsurprising fact that computing these ellipsoidal numbers for arbitrary graphs is NP-hard. We discuss some further issues related to the computational complexity of geometric representations of graphs in Section 7.1.

For a graph G and a matrix $A \in \mathbb{S}^d_+$ for some $d \in \mathbb{Z}_{++}$, it is clear that $\mathcal{E}_p(G; A) = 0$ if and only if $\dim(G) \leq \dim(\mathrm{Null}(A))$; recall that $\dim(G)$ was defined in Section 2.6. So deciding whether $\dim(G) \leq k$ for any fixed k reduces to computing $\mathcal{E}_p(G; A)$ for any $p \in [1, \infty]$ where A is a matrix of nullity k. It was shown in [73, Theorem 4] that the former decision problem is NP-hard. Below we give a shorter proof.

Theorem 3.14 ([73])**.** The problem of deciding whether $\dim(G) \leq 2$ for a given graph G is NP-hard.

Proof. Let k be a fixed positive integer. Saxe [127, Lemma 4.4] showed that the following problem is NP-hard: given an input graph G and $\ell\colon E \to \mathbb{R}_+$, decide whether there exists $u\colon V \to \mathbb{R}^k$ such that $\|u(i) - u(j)\| = \ell_{ij}$ for every $ij \in E$. Saxe showed that the problem remains NP-hard even if we require $\ell \in \{1, 2\}^E$.

We will show a polynomial-time reduction from the above problem with $k = 2$ and $\ell \in \{1, 2\}^E$ to the problem of deciding whether $\dim(G) \leq 2$. It suffices to show how we can replace any edge of the input graph G which is required to be embedded as a line segment of length 2 by some gadget graph H so

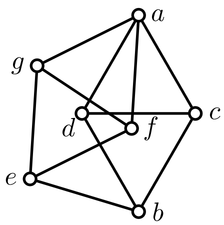

Figure 3.2: The Mosers spindle; see [141].

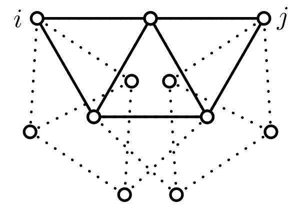

Figure 3.3: The gadget graph H.

that every unit-distance representation of H in $\mathbb{R}^2$ maps two specified nodes of H to a pair of points at distance 2.

Consider the graph M known as the Mosers spindle shown in Figure 3.2. The subgraph of M induced by $\{a, b, c, d\}$ has exactly two unit-distance representations in $\mathbb{R}^2$ modulo rigid motions: one of them as displayed in Figure 3.2, and the other one maps nodes a and b to the same point. We claim that, in any unit-distance representation u of M in $\mathbb{R}^2$, the nodes a and b are not mapped to the same point. Indeed, $\|u(a) - u(b)\|^2, \|u(a) - u(e)\|^2 \in \{0, 3\}$ and $\|u(b) - u(e)\|^2 \in \{0, 1\}$ imply that $u(a), u(b), u(e)$ are distinct points.

Let H be the gadget shown in Figure 3.3, which consists of two copies of M sharing a triangle (some edges of M are drawn in dots for the sake of ease of visualization). Then, every unit-distance representation of H in $\mathbb{R}^2$ maps the nodes i and j to points at distance 2. Thus, if we replace the corresponding edges $\{i, j\}$ of the input graph G by H, we obtain a graph G' such that $\dim(G') \leq 2$ if and only if G can be embedded in $\mathbb{R}^2$ with the prescribed edge lengths. $\square$

Chapter 4

Vertices of Spectrahedra Arising from the Theta Body

In the previous chapters, our focus has been on hypersphere representations of graphs and their variants. From the viewpoint of Theorem 2.4, the hypersphere number may be seen as yet another manifestation of the Lovász theta number, via the intimate connection between hypersphere and orthonormal representations, as exemplified by Corollary 2.6 and the proof of Proposition 2.8. We now turn our attention to orthonormal representations of graphs and the crucial convex set that they describe (cf. (1.5)): the theta body $\mathrm{TH}(G)$. In this chapter and the next, we concern ourselves with various descriptions of $\mathrm{TH}(G)$, again guided by duality. The subject of this chapter is the boundary structure of convex sets.

The study of the boundary structure of polyhedra arising from combinatorial optimization problems has been a very successful undertaking in the field of polyhedral combinatorics. Part of this success relies on a very rich interplay between geometric and algebraic properties of the faces of such polyhedra and corresponding combinatorial structures of the problems they encode. This remains true even in the context of some NP-hard problems, where one is generally resigned to seek partial characterizations of the boundary structure via some families of facets. Interestingly, analogous results for SDPs arising from combinatorial optimization problems are rather scarce [87, 88, 136], despite our somewhat good understanding [24, 93, 90, 12, 116, 117, 11, 2, 112, 14] of the boundary structure of *spectrahedra*, as feasible regions of SDPs are called. This is partially explained by the fact that spectrahedra are much richer in complexity than polyhedra. However, or perhaps owing to that, it is reasonable to presume the existence of a wealth of combinatorial information encoded in the boundary structure of spectrahedra arising from combinatorial optimization problems. Indeed, since semidefinite optimization is a strict generalization of linear optimization, SDPs should in principle encode at least all that is known via polyhedral combinatorics. This is, in fact, our beacon throughout this thesis.

It is instructive to briefly compare some important qualitative differences between polyhedra and spectrahedra. From the viewpoint of linear conic optimization, a (pointed) polyhedron is the intersection of the nonnegative orthant $\mathbb{R}^n_+$ with an affine subspace of $\mathbb{R}^n$, whereas a spectrahedron is the intersection of the positive semidefinite cone $\mathbb{S}^n_+$ with an affine subspace of $\mathbb{S}^n$. By regarding $\mathbb{S}^n$ as $\mathbb{R}^{n(n+1)/2}$ (and thus stripping off the extremely convenient algebraic structure of $\mathbb{S}^n$), one could argue that nothing is gained in terms of ambient space or affine constraints when moving from polyhedra to spectrahedra. On the other hand, the boundary structure of the cone $\mathbb{S}^n_+$, while completely understood (see, e.g., [156]), is far more intricate than that of $\mathbb{R}^n_+$. The latter is in fact separable in that it may be written as the direct sum of n copies of $\mathbb{R}_+$. In this context, one is comparing the rich boundary structure of $\mathbb{S}^n_+$ with the trivial boundary structure of $\mathbb{R}_+$. This difference in complexity goes even further when contrasting the boundary structure of spectrahedra and polyhedra, since the intersection of the affine subspace with $\mathbb{S}^n_+$ can be so pathological that Strong Duality as well as Strict Complementarity may fail for SDPs; see, e.g., [156]. Even the faces of dimension zero of well-behaved spectrahedra have a substantially different structure than that of polyhedra. Recall that an *extreme point* of a convex set is called a *vertex* if its *normal cone* is full-dimensional. For a polyhedron, extreme points and vertices coincide, and there are only finitely many of them. On the other hand, the unit ball $\{ x \in \mathbb{R}^d : \|x\| \leq 1\}$, which is linearly isomorphic to a spectrahedron, has infinitely many extreme points and no vertices whenever $d \geq 2$.

Vertices of a convex set can be regarded as the only likely points to optimize a uniformly chosen linear function, in the following sense. Fix a full-dimensional convex set $\mathscr{C} \subseteq \mathbb{R}^n$ and a point $\bar{x} \in \mathscr{C}$. Now choose a unit vector $c \in \mathbb{R}^n$ uniformly at random. Then the probability that $\bar{x}$ is an optimal solution for the optimization problem $\max_{x \in \mathscr{C}} \langle c, x\rangle$ is positive if and only if $\bar{x}$ is a vertex of $\mathscr{C}$. This property of the vertices may have practical significance in some contexts where one formulates an SDP relaxation to a problem and the vertices of the feasible region correspond *exactly* to the combinatorial (or non-convex) objects from that problem. This kind of situation may be useful in low-rank recovery schemes; see [126]. Other instances occur in combinatorial optimization, in some previous results which suggest that vertices of feasible regions of SDPs play an analogous role to that of for extreme points in polyhedral combinatorics.

In this chapter, we make progress on the relationship between geometric and combinatorial properties of a fundamental spectrahedron related to the Lovász theta function: the lifted theta body $\widehat{\mathrm{TH}}(G)$, defined in (1.6). We prove that the vertices of $\widehat{\mathrm{TH}}(G)$ are precisely the symmetric tensors of (lifted) incidence vectors of stable sets in G. Our result generalizes a characterization due to Laurent and Poljak [87, 88] of the vertices of the elliptope, the spectrahedron arising from the famous SDP relaxation for MaxCut exploited by Goemans and Williamson [52] in their approximation algorithm. Laurent and Poljak's characterization is in fact equivalent to the application of our result to the lifted theta body of a graph with no edges. Our result may also be seen as a lifted version of an observation by Shepherd [136] that the vertices of $\mathrm{TH}(G)$ are precisely the incidence vectors of stable sets in G. All these results state that the vertices of these spectrahedra coincide with the *exact* solutions of the problems of which they are relaxations. We shall also determine the vertices of some relatives of $\widehat{\mathrm{TH}}(G)$ corresponding to the variants ϑ' and ϑ^+ of ϑ described by (2.62) and (2.64), as well as for spectrahedra arising from other characterizations of ϑ.

The remainder of the chapter is organized as follows. After a quick warm-up section on a neat relationship between graph homomorphisms and hypersphere representations corresponding to extreme points, we develop simple formulas for the normal cone of a spectrahedron at a given point and its dimension. We use our formulas to review some of the previous results in the literature, including Laurent and Poljak's [87, 88] characterization of the vertices of the elliptope and Shepherd's [136] characterization of vertices of $\mathrm{TH}(G)$. We then exploit our formula to determine all the vertices of $\widehat{\mathrm{TH}}(G)$ and several related spectrahedra.

The main contribution in this chapter is the content from Section 4.5, especially Theorem 4.16.

We should remark that throughout the chapter we only study spectrahedra in a very special form. In the literature, it is common to define spectrahedra as sets of the form $\{ y \in \mathbb{R}^m : A_0 + \sum_{i=1}^m y_i A_i \in \mathbb{S}^n_+\}$ for given matrices $A_0, \ldots, A_m \in \mathbb{S}^n$; the defining constraint is known as a *linear matrix inequality* (LMI). For the sake of convenience, we shall instead focus only spectrahedra defined as the intersection of the cone $\mathbb{S}^n_+$ with an affine subspace of $\mathbb{S}^n$. The advantage is that, by confining ourselves to subsets of symmetric matrices, we retain the ability to use the simple but powerful algebraic structure of the underlying space $\mathbb{S}^n$. In that sense, to consider other representations of the feasible region which make it harder to exploit the algebraic structure, such as the LMI form, seems akin to just regarding $\mathbb{S}^n$ as $\mathbb{R}^{n(n+1)/2}$.

4.1 Extreme Hypersphere Representations and Homomorphisms

Let $G = (V, E)$ be a graph, and let $t \in \mathbb{R}$. Define

$$\mathscr{R}_t(G) := \{\, X \in \mathbb{S}^V_+ : \operatorname{diag}(X) = t\bar{e},\, \mathcal{L}^*_G(X) = \bar{e}\}, \tag{4.1}$$

so that $\mathscr{R}_t(G)$ is precisely the set of Gram matrices of hypersphere representations of G with squared radius t. Clearly, $\mathscr{R}_t(G) \neq \varnothing$ if and only if $t \geq t(G)$. If $t \geq t(K_n)$, then $\mathscr{R}_t(K_n)$ is a singleton, e.g., by Lemma 3.9. On the other hand, for $t \in \mathbb{R}_{++}$, the set $\mathscr{R}_t(\overline{K_n})$ is the set of all positive semidefinite matrices with constant diagonal, a set which we shall study with more detail later in the chapter.

In this section, we shall look at some simple properties relating some extreme points of $\mathscr{R}_t(G)$ and graph homomorphisms. We briefly recall some basic concepts in convex analysis.

Let $\mathscr{C} \subseteq \mathbb{E}$ be convex. A *face* of $\mathscr{C}$ is a convex subset $\mathscr{F}$ of $\mathscr{C}$ with the following property: if $x, y \in \mathscr{C}$ and $\lambda x + (1 - \lambda)y \in \mathscr{F}$ for some $\lambda \in (0, 1)$, then $x, y \in \mathscr{F}$. That is, a convex subset $\mathscr{F}$ of $\mathscr{C}$ is a face of $\mathscr{C}$ if, whenever the relative interior of some line segment contained in $\mathscr{C}$ meets $\mathscr{F}$, the whole line segment lies in $\mathscr{F}$. A point $x \in \mathscr{C}$ is an *extreme point* of $\mathscr{C}$ if $\{x\}$ is a face of $\mathscr{C}$. The concepts of faces and extreme points are fundamental in convex analysis and polyhedral combinatorics; see, e.g., [123, Section 18] or [132, 133, 134].

The intersection of any set of faces of $\mathscr{C}$ is again a face of $\mathscr{C}$. Therefore, every point $x \in \mathscr{C}$ is contained in a unique minimal face of $\mathscr{C}$, which we denote by $\operatorname{Face}_{\mathscr{C}}(x)$. The minimal face $\operatorname{Face}_{\mathscr{C}}(x)$ is characterized by the fact that x lies in the relative interior of $\operatorname{Face}_{\mathscr{C}}(x)$. When $\mathscr{C}$ is a spectrahedron, the dimension of the set $\operatorname{Face}_{\mathscr{C}}(X)$ for some $X \in \mathscr{C}$ is determined in the following way, as is well known (see, e.g., [90] or [88, Theorem 1.1]):

Theorem 4.1 ([90])**.** Let $\mathscr{C} := \{\, X \in \mathbb{S}^n_+ : \mathcal{A}(X) = b\}$ for some linear map $\mathcal{A}\colon \mathbb{S}^V \to \mathbb{R}^m$ and $b \in \mathbb{R}^m$. Let $\bar{X} \in \mathscr{C}$, set $r := \operatorname{rank}(\bar{X})$, and write $\bar{X} = URU^\mathsf{T}$ for some $U \in \mathbb{R}^{n \times r}$ and $R \in \mathbb{S}^r$. Set $A_i := \mathcal{A}^*(e_i)$ for each $i \in [m]$. Then

$$\dim\bigl(\operatorname{Face}_{\mathscr{C}}(\bar{X})\bigr) = \dim(\mathbb{S}^r) - \dim\bigl(\operatorname{span}\{\, U^\mathsf{T} A_i U : i \in [m]\}\bigr). \tag{4.2}$$

In particular,

$$\bar{X} \text{ is an extreme point of } \mathscr{C} \text{ if and only if } \{\, U^\mathsf{T} A_i U : i \in [m]\} \text{ spans } \mathbb{S}^r. \tag{4.3}$$

Let us use Theorem 4.1 to find out which hypersphere representations of a graph correspond to extreme points of $\mathscr{R}_t(G)$. Let $G = (V, E)$ be a graph, and let $t \geq t(G)$. Let $\bar{X} \in R_t(G)$. Set $r := \operatorname{rank}(\bar{X})$ and write $\bar{X} = UU^\mathsf{T}$ for some $U^\mathsf{T} \in \mathbb{R}^{[r] \times V}$, so that $i \in V \mapsto U^\mathsf{T} e_i =: u_i$ is a hypersphere representation of G with squared radius t. By (4.3), the Gram matrix $\bar{X}$ is an extreme point of $\mathscr{R}_t(G)$ if and only if

$$\{\, u_i u_i^\mathsf{T} : i \in V\} \cup \{\, (u_i - u_j)(u_i - u_j)^\mathsf{T} : ij \in E\} \text{ spans } \mathbb{S}^r. \tag{4.4}$$

We shall thus say that a hypersphere representation $u\colon V \to \mathbb{R}^r$ of a graph $G = (V, E)$ is *extreme* if (4.4) holds.

Proposition 4.2. Let $G = (V, E)$ be a graph, and let $t \in \mathbb{R}$. Let $X \in \mathbb{S}^V$. Then X is an extreme point of $\mathscr{R}_t(G)$ if and only if there is an extreme hypersphere representation $u\colon V \to \mathbb{R}^r$ with squared radius t such that X is the Gram matrix of u.

Proof. The proof is almost immediate by Theorem 4.1 and the previous discussion. The 'only if' part is trivial. For the 'if' part, let X be the Gram matrix of an extreme hypersphere representation $u\colon V \to \mathbb{R}^r$ with squared radius t. By Theorem 4.1, it suffices to show that $L \coloneqq \operatorname{span}\{\, u_i : i \in V\}$ is equal to $\mathbb{R}^r$. Let $d \in L^\perp$. Then $\langle dd^\mathsf{T}, yy^\mathsf{T}\rangle = 0$ for each $y \in \{\, u_i : i \in V\} \cup \{\, u_i - u_j : ij \in E\}$, so that dd^T lies in the orthogonal complement of $\{\, u_i u_i^\mathsf{T} : i \in V\} \cup \{\, (u_i - u_j)(u_i - u_j)^\mathsf{T} : ij \in E\}$. Since u is extreme, it follows that $dd^\mathsf{T} = 0$, so $d = 0$, and $L = \mathbb{R}^r$. ☐

We can use graph homomorphisms to "lift" some extreme hypersphere representations. We refer the reader to Section 2.6 for the definitions and notation concerning graph homomorphisms. Let G and H be graphs, and let $\phi\colon G \to H$. Then ϕ determines a function from $E(G)$ to $E(H)$ by setting $\phi(\{i, j\}) \coloneqq \{\phi(i), \phi(j)\}$ for every $ij \in E(G)$. We say that ϕ is *complete* if $\phi(V(G)) = V(H)$ and $\phi(E(G)) = E(H)$.

Proposition 4.3. Let G be a graph. Let $u\colon V(G) \to \mathbb{R}^r$ be a hypersphere representation of G with squared radius t. Let H be a graph and suppose that $\phi\colon H \to G$ is a homomorphism. If the hypersphere representation $u \circ \phi$ of H is extreme, then u is extreme. Moreover, if the homomorphism ϕ is complete, then the implication above is an equivalence.

Proof. The proof is immediate: $u \circ \phi$ is extreme if and only if

$$\big\{\, u_i u_i^\mathsf{T} : i \in \phi(V(H))\big\} \cup \big\{\, (u_i - u_j)(u_i - u_j)^\mathsf{T} : ij \in \phi(E(H))\big\} \text{ spans } \mathbb{S}^r.$$

The above condition implies that u is extreme, since $\phi(V(H)) \subseteq V(G)$ and $\phi(E(H)) \subseteq E(G)$. If ϕ is complete, then equality holds on both set equations, whence the implication is clearly an equivalence. ☐

We may use this proposition to prove that some hypersphere representations are extreme in case the graph has a large enough clique.

Proposition 4.4. Let $u\colon V \to \mathbb{R}^r$ be a hypersphere representation of a graph $G = (V, E)$ with squared radius t. If $\omega(G) = r + 1$ holds, or if both $\omega(G) = r$ and $t > t(K_r)$ hold, then u is extreme.

Proof. We shall apply Proposition 4.3 with $H \in \{K_r, K_{r+1}\}$ and $\phi \coloneqq \iota\colon H \to G$ as the embedding map. We will set $v \coloneqq u \circ \iota$ and show that v is an extreme hypersphere representation of H. By elementary linear algebra, v is extreme if and only if $\{\, v_i : i \in V(H)\}$ spans $\mathbb{R}^r$. Thus, it suffices to prove that the Gram matrix X of v has rank $\geq r$. If $H = K_{r+1}$, then $\operatorname{rank}(X) \geq r$ by Lemma 3.9. If $H = K_r$ and $t > t(K_r)$, then we also have $\operatorname{rank}(X) \geq r$ by Lemma 3.9. This concludes the proof. ☐

Corollary 4.5. If $u\colon V \to \mathbb{R}^2$ be a hypersphere representation of a nonbipartite graph $G = (V, E)$, then u is extreme.

Proof. If G contains a triangle, then $\omega(G) \geq 2+1$, so equality must hold. If G contains no triangle, then $\omega(G) = 2$ but the squared radius t of u satisfies $t > 1/4 = t(K_2)$ by Proposition 2.2 since G is nonbipartite. In both cases, we are done by Proposition 4.4. □

We know that a graph $G = (V, E)$ satisfies $\chi(G) \leq 3$ if and only if there is a hypersphere representation of G in $\mathbb{R}^2$. This can now be refined to the following statement: a graph $G = (V, E)$ satisfies $\chi(G) = 3$ if and only if there is an extreme hypersphere representation of G in $\mathbb{R}^2$.

For the remainder of the chapter, we shall turn our attention to vertices of spectrahedra related to orthonormal representations of graphs, which may be regarded as dual objects to hypersphere representations by Corollary 2.6.

4.2 Normal Cones of Spectrahedra

In this section, we develop some tools to study normal cones of spectrahedra. We use elementary duality results to obtain formulas for the normal cones of a spectrahedron and their dimensions. These formulas are crucial for our main result in Section 4.5.

Let $\mathscr{C} \subseteq \mathbb{E}$ be a convex set and let $\bar{x} \in \mathscr{C}$. The *normal cone of* $\mathscr{C}$ *at* $\bar{x}$ is defined as

$$\operatorname{Normal}(\mathscr{C}; \bar{x}) := \big\{\, c \in \mathbb{E}^* : \langle c, x\rangle \leq \langle c, \bar{x}\rangle \; \forall x \in \mathscr{C} \big\}.$$

We say that $\bar{x}$ is a *vertex of* $\mathscr{C}$ if $\dim(\operatorname{Normal}(\mathscr{C}; \bar{x})) = \dim(\mathbb{E}^*)$.

The Strong Duality Theorem leads to a dual characterization of normal cones of the feasible region of any conic optimization problem with a restricted Slater point.

Proposition 4.6. Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $\mathcal{A} \colon \mathbb{E} \to \mathbb{R}^p$ and $\mathcal{B} \colon \mathbb{E} \to \mathbb{R}^q$ be linear functions. Let $a \in \mathbb{R}^p$ and $b \in \mathbb{R}^q$. Set $\mathscr{C} := \{\, x \in \mathbb{K} : \mathcal{A}(x) = a,\, \mathcal{B}(x) \leq b \}$. Suppose that $\mathscr{C} \cap \operatorname{int}(\mathbb{K}) \neq \varnothing$. If $\bar{x} \in \mathscr{C}$, then

$$\operatorname{Normal}(\mathscr{C}; \bar{x}) = \operatorname{Im}(\mathcal{A}^*) + \big\{\, \mathcal{B}^*(z) : z \in \mathbb{R}^q_+,\, \operatorname{supp}(z) \cap \operatorname{supp}\big(\mathcal{B}(\bar{x}) - b\big) = \varnothing \big\} - \big(\mathbb{K}^* \cap \{\bar{x}\}^\perp\big). \tag{4.5}$$

Proof. First we prove '$\subseteq$'. Let $c \in \operatorname{Normal}(\mathscr{C}; \bar{x})$. Then $\bar{x}$ is an optimal solution for the conic programming problem

$$\sup\big\{\, \langle c, x\rangle : \mathcal{A}(x) = a,\, \mathcal{B}(x) \leq b,\, x \in \mathbb{K} \big\},$$

which has a restricted Slater point by assumption. By the Strong Duality Theorem, its dual

$$\inf\big\{\, \langle a, y\rangle + \langle b, z\rangle : y \in \mathbb{R}^p,\, z \in \mathbb{R}^q_+,\, \mathcal{A}^*(y) + \mathcal{B}^*(z) \succeq_{\mathbb{K}^*} c \big\}$$

has an optimal solution $\bar{y} \oplus \bar{z} \in \mathbb{R}^p \oplus \mathbb{R}^q_+$ whose slack $\bar{s} := \mathcal{A}^*(\bar{y}) + \mathcal{B}^*(\bar{z}) - c \in \mathbb{K}^*$ satisfies $\langle \bar{s}, \bar{x}\rangle = 0$ by complementarity. (Here we use the usual inner-product $\langle a, b\rangle = a^\mathsf{T} b$ in the dual space.) Again by complementarity, we also have $\langle \mathcal{B}(\bar{x}) - b, \bar{z}\rangle = 0$. Together with $\mathcal{B}(\bar{x}) \leq b$ and $\bar{z} \in \mathbb{R}^q_+$, this implies that $\operatorname{supp}(\bar{z}) \cap \operatorname{supp}\big(\mathcal{B}(\bar{z}) - b\big) = \varnothing$. Since $c = \mathcal{A}^*(\bar{y}) + \mathcal{B}^*(\bar{z}) - \bar{s}$, we find that c lies in the set described by the RHS of (4.5).

Next we prove '$\supseteq$'. Let $\bar{s} \in \mathbb{K}^* \cap \{\bar{x}\}^\perp$, let $\bar{y} \in \mathbb{R}^p$ and $\bar{z} \in \mathbb{R}^q_+$ such that $\operatorname{supp}(\bar{z}) \cap \operatorname{supp}\big(\mathcal{B}(\bar{x}) - b\big) = \varnothing$. Set $c \coloneqq \mathcal{A}^*(\bar{y}) + \mathcal{B}^*(\bar{z}) - \bar{s}$. If $x \in \mathscr{C}$, then

$$\begin{aligned}\langle c, x\rangle &= \langle \mathcal{A}^*(\bar{y}), x\rangle + \langle \mathcal{B}^*(\bar{z}), x\rangle - \langle \bar{s}, x\rangle = \langle \bar{y}, \mathcal{A}(x)\rangle + \langle \bar{z}, \mathcal{B}(x)\rangle - \langle \bar{s}, x\rangle = \langle \bar{y}, a\rangle + \langle \bar{z}, \mathcal{B}(x)\rangle - \langle \bar{s}, x\rangle \\ &\leq \langle \bar{y}, a\rangle + \langle \bar{z}, b\rangle = \langle \bar{y}, a\rangle + \langle \bar{z}, b\rangle - \langle \bar{s}, \bar{x}\rangle = \langle \bar{y}, \mathcal{A}(\bar{x})\rangle + \langle \bar{z}, \mathcal{B}(\bar{x})\rangle - \langle \bar{s}, \bar{x}\rangle \\ &= \langle \mathcal{A}^*(\bar{y}), \bar{x}\rangle + \langle \mathcal{B}^*(\bar{z}), \bar{x}\rangle - \langle \bar{s}, \bar{x}\rangle = \langle c, \bar{x}\rangle.\end{aligned}$$

Thus, $c \in \operatorname{Normal}(\mathscr{C}; \bar{x})$. ☐

Now, we move back to the special case of SDP. In this setting, it is beneficial to exploit the extra algebraic properties of the underlying space $\mathbb{S}^n$. A conspicuous extra feature is the fact that each point in a spectrahedron, as a matrix, has a range, a nullspace, and a rank. We shall use these concepts to massage the identity (4.5) for the normal cone and obtain a simple formula for its dimension.

In what follows, we shall frequently use the following elementary identity. Let $\mathcal{A}\colon \mathbb{E} \to \mathbb{Y}$ be a nonsingular linear map, and let $\mathscr{L} \subseteq \mathbb{E}$ be a linear subspace. Then

$$\big(\mathcal{A}(\mathscr{L})\big)^\perp = \mathcal{A}^{-*}(\mathscr{L}^\perp). \tag{4.6}$$

We start by examining the rightmost term in (4.5), namely $\mathbb{K}^* \cap \{\bar{x}\}^\perp$, known as the conjugate face of $\bar{x}$ in $\mathbb{K}^*$. When $\mathbb{K}$ is the positive semidefinite cone $\mathbb{S}^n_+$, the conjugate face of a point $\bar{X}$ in $\mathbb{S}^n_+$ may be described as a lifted copy of a smaller semidefinite cone, appropriately rotated via a linear automorphism of $\mathbb{S}^n_+$ which depends only on the range of $\bar{X}$. This allows us to associate the dimension of the conjugate face to the rank of $\bar{X}$, as shown by the following well-known result:

Proposition 4.7. Let $\bar{X} \in \mathbb{S}^n_+$. Let $Q \in \mathbb{O}^n$ such that $X = Q \operatorname{Diag}\big(\lambda^\downarrow(\bar{X})\big) Q^\mathsf{T}$, and set $r \coloneqq \operatorname{rank}(\bar{X})$. Then

$$\mathbb{S}^n_+ \cap \{\bar{X}\}^\perp = Q\big(0 \oplus \mathbb{S}^{n-r}_+\big)Q^\mathsf{T}, \tag{4.7}$$

$$\dim\big(\mathbb{S}^n_+ \cap \{\bar{X}\}^\perp\big) = \binom{\dim\big(\operatorname{Null}(\bar{X})\big) + 1}{2}, \tag{4.8}$$

$$\mathbb{S}^n_+ \cap \{\bar{X}\}^\perp = \operatorname{cone}\big\{\, bb^\mathsf{T} : b \in \operatorname{Null}(\bar{X})\big\}. \tag{4.9}$$

Proof. Set $\lambda \coloneqq \lambda^\downarrow(\bar{X})$. Let us prove that

$$\mathbb{S}^n_+ \cap \{\operatorname{Diag}(\lambda)\}^\perp = 0 \oplus \mathbb{S}^{n-r}_+. \tag{4.10}$$

It is clear that '$\supseteq$' holds. For the reverse inclusion, let $Y \in \mathbb{S}^n_+ \cap \{\operatorname{Diag}(\lambda)\}^\perp$. Then $0 = \langle Y, \operatorname{Diag}(\lambda)\rangle = \langle \operatorname{diag}(Y), \lambda\rangle$, which together with $\operatorname{diag}(Y) \geq 0$ and $\lambda \geq 0$ implies that $Y_{ii} = 0$ for each $i \in \operatorname{supp}(\lambda) = [r]$. Since $Y \in \mathbb{S}^n_+$, we find that $Y_{ij} = 0$ for each $i \in [r]$ and $j \in [n]$, so $Y \in 0 \oplus \mathbb{S}^{n-r}_+$. This proves (4.10).

Set $D \coloneqq \operatorname{Diag}(\lambda)$ and apply the linear isomorphism $\operatorname{Congr}_Q = \operatorname{Congr}_Q^{-*}$ to both sides of (4.10) to obtain

$$\begin{aligned}Q\big(0 \oplus \mathbb{S}^{n-r}_+\big)Q^\mathsf{T} &= \operatorname{Congr}_Q\big(\mathbb{S}^n_+ \cap (\operatorname{span}\{D\})^\perp\big) = \operatorname{Congr}_Q(\mathbb{S}^n_+) \cap \operatorname{Congr}_Q\big((\operatorname{span}\{D\})^\perp\big) \\ &= \mathbb{S}^n_+ \cap \big(\operatorname{Congr}_Q^{-*}(\operatorname{span}\{D\})\big)^\perp = \mathbb{S}^n_+ \cap (\operatorname{span}\{\bar{X}\})^\perp.\end{aligned}$$

This proves (4.7).

To prove (4.8), use (4.7) and the fact that the nonsingular map Congr_Q preserves dimension:

$$\begin{aligned}\dim(\mathbb{S}^n_+ \cap \{\bar{X}\}^\perp) &= \dim\bigl(\operatorname{Congr}_Q(0 \oplus \mathbb{S}^{n-r}_+)\bigr) = \dim\bigl(0 \oplus \mathbb{S}^{n-r}_+\bigr)\\ &= \dim\bigl(\mathbb{S}^{n-r}_+\bigr) = \binom{n-r+1}{2} = \binom{\dim\bigl(\operatorname{Null}(\bar{X})\bigr)+1}{2}.\end{aligned}$$

Finally, we prove (4.9). Let $Y \in \mathbb{S}^n_+$ be arbitrary, and write Y as $Y = \sum_{i=1}^k h_i h_i^\mathsf{T}$ where $\{\, h_i : i \in [k]\} \subseteq \mathbb{R}^n$. Since $Y \in \mathbb{S}^n_+$, the equation $\langle X, Y\rangle = 0$ is equivalent to $h_i^\mathsf{T} X h_i = 0$ for each $i \in [k]$. Since $X \in \mathbb{S}^n_+$, the latter is equivalent to $h_i \in \operatorname{Null}(X)$ for each $i \in [k]$. ☐

As the proof of Proposition 4.7 illustrates, it is often helpful to restrict our attention to a specific class of positive semidefinite matrices (e.g., diagonal matrices) for which it is easy to prove a result, and then extend it by changing the basis, e.g., by applying a congruence Congr_Q. We now look at how normal cones behave when we apply such transformations.

Let $\mathscr{C} \subseteq \mathbb{E}$ be a convex set and let $\bar{x} \in \mathscr{C}$. If $T\colon \mathbb{E} \to \mathbb{E}$ is a linear bijection, then

$$\begin{aligned}\operatorname{Normal}\bigl(T(\mathscr{C}); T(\bar{x})\bigr) &= \bigl\{\, c \in \mathbb{E}^* : \langle c, T(x)\rangle \leq \langle c, T(\bar{x})\rangle \;\forall x \in \mathscr{C} \bigr\}\\ &= \bigl\{\, c \in \mathbb{E}^* : \langle T^*(c), x\rangle \leq \langle T^*(c), \bar{x}\rangle \;\forall x \in \mathscr{C} \bigr\}\\ &= \bigl\{\, T^{-*}(d) \in \mathbb{E}^* : \langle d, x\rangle \leq \langle d, \bar{x}\rangle \;\forall x \in \mathscr{C} \bigr\} = T^{-*}\bigl(\operatorname{Normal}(\mathscr{C}; \bar{x})\bigr).\end{aligned} \tag{4.11}$$

The identity (4.11) shows that the coordinate-free properties of normal cones remain invariant under linear bijections. In the case of SDPs, we can say a bit more in terms of the rank of a feasible matrix $\bar{X}$.

Lemma 4.8. Let $\mathcal{A}\colon \mathbb{S}^n \to \mathbb{R}^p$ and $\mathcal{B}\colon \mathbb{S}^n \to \mathbb{R}^q$ be linear functions. Let $a \in \mathbb{R}^p$ and $b \in \mathbb{R}^q$. Let $L \in \mathbb{R}^{n\times n}$ be nonsingular, and define

$$\begin{gathered}\mathcal{A}_L \coloneqq \mathcal{A} \circ \operatorname{Congr}_L^{-1}, \qquad \mathcal{B}_L \coloneqq \mathcal{B} \circ \operatorname{Congr}_L^{-1},\\ \mathscr{C} \coloneqq \{\, X \in \mathbb{S}^n_+ : \mathcal{A}(X) = a,\, \mathcal{B}(X) \leq b\},\\ \mathscr{C}_L \coloneqq \operatorname{Congr}_L(\mathscr{C}) = \{\, Y \in \mathbb{S}^n_+ : \mathcal{A}_L(Y) = a,\, \mathcal{B}_L(Y) \leq b\}.\end{gathered}$$

Then, for any $\bar{X} \in \mathscr{C}$, we have:

(i) $\mathscr{C} \cap \mathbb{S}^n_{++} \neq \varnothing$ if and only if $\mathscr{C}_L \cap \mathbb{S}^n_{++} \neq \varnothing$;

(ii) $\operatorname{Normal}\bigl(\mathscr{C}_L; \operatorname{Congr}_L(\bar{X})\bigr) = \operatorname{Congr}_L^{-*}\bigl(\operatorname{Normal}(\mathscr{C}; \bar{X})\bigr)$ whence $\dim\bigl(\operatorname{Normal}\bigl(\mathscr{C}_L; \operatorname{Congr}_L(\bar{X})\bigr)\bigr) = \dim\bigl(\operatorname{Normal}(\mathscr{C}; \bar{X})\bigr)$;

(iii) $\operatorname{Im}(\mathcal{A}_L^*) = \operatorname{Congr}_L^{-*}\bigl(\operatorname{Im}(\mathcal{A}^*)\bigr)$ whence $\dim\bigl(\operatorname{Im}(\mathcal{A}_L^*)\bigr) = \dim\bigl(\operatorname{Im}(\mathcal{A}^*)\bigr)$; and analogously for $\operatorname{Im}(\mathcal{B}_L^*)$;

(iv) $\operatorname{Null}\bigl(\operatorname{Congr}_L(\bar{X})\bigr) = L^{-\mathsf{T}} \operatorname{Null}(\bar{X})$ whence $\operatorname{rank}\bigl(\operatorname{Congr}_L(\bar{X})\bigr) = \operatorname{rank}(\bar{X})$.

Proof. Most of the proof follows from the fact that the map Congr_L is an automorphism of $\mathbb{S}^n_+$. Note that $\mathscr{C}_L \cap \mathbb{S}^n_{++} = \operatorname{Congr}_L(\mathscr{C}) \cap \mathbb{S}^n_{++} = \operatorname{Congr}_L\bigl(\mathscr{C} \cap \mathbb{S}^n_{++}\bigr)$. This proves (i). Statement (ii) follows from (4.11), whereas (iii) is elementary linear algebra. For (iv), let $h \in \mathbb{R}^n$ and note that $L\bar{X}L^\mathsf{T} h = 0$ is equivalent to $\bar{X}L^\mathsf{T} h = 0$, i.e., $L^\mathsf{T} h \in \operatorname{Null}(\bar{X})$. ☐

Next we derive the principal tool for our main result: a simple algebraic expression for the dimension of the normal cone of a spectrahedron at a given point.

Theorem 4.9. Let $\mathcal{A}\colon \mathbb{S}^n \to \mathbb{R}^p$ and $\mathcal{B}\colon \mathbb{S}^n \to \mathbb{R}^q$ be linear functions. Let $a \in \mathbb{R}^p$ and $b \in \mathbb{R}^q$. Set $\mathscr{C} \coloneqq \{\, X \in \mathbb{S}^n_+ : \mathcal{A}(X) = a,\, \mathcal{B}(X) \le b \}$. Suppose that $\mathscr{C} \cap \mathbb{S}^n_{++} \neq \varnothing$. Let $\bar{X} \in \mathscr{C}$, and let P denote the orthogonal projection onto $\{\, z \in \mathbb{R}^q : \operatorname{supp}(z) \cap \operatorname{supp}(\mathcal{B}(\bar{X}) - b) = \varnothing \}$. Then

$$\dim\bigl(\operatorname{Normal}(\mathscr{C};\bar{X})\bigr) = \dim(\mathbb{S}^n) - \dim\Bigl(\operatorname{Null}(\mathcal{A}) \cap \operatorname{Null}(P\circ\mathcal{B}) \cap \operatorname{span}\bigl\{\operatorname{Sym}(\bar{X}uv^{\mathsf{T}}) : u,v \in \mathbb{R}^n\bigr\}\Bigr). \quad (4.12)$$

In particular, if $\bar{X} = \bar{x}\bar{x}^{\mathsf{T}}$ for some nonzero $\bar{x} \in \mathbb{R}^n$, then

$$\begin{aligned}\dim&\bigl(\operatorname{Normal}(\mathscr{C};\bar{x}\bar{x}^{\mathsf{T}})\bigr)\\ &= \dim(\mathbb{S}^n) - \dim\Bigl(\bigl(\{\, A_i\bar{x} : i \in [p]\} \cup \bigl\{\, B_i\bar{x} : i \in [q] \setminus \operatorname{supp}\bigl(\mathcal{B}(\bar{x}\bar{x}^{\mathsf{T}}) - b\bigr)\bigr\}\bigr)^{\perp}\Bigr), \quad (4.13)\end{aligned}$$

where $A_i \coloneqq \mathcal{A}^*(e_i)$ for all $i \in [p]$ and $B_i \coloneqq \mathcal{B}^*(e_i)$ for all $i \in [q]$; thus,

if $\bar{x}\bar{x}^{\mathsf{T}} \in \mathscr{C}$ for some nonzero $\bar{x} \in \mathbb{R}^n$, then $\bar{x}\bar{x}^{\mathsf{T}}$ is a vertex of $\mathscr{C}$ if and only if $\bigl\{\, A_i\bar{x} : i \in [p]\bigr\} \cup \bigl\{\, B_i\bar{x} : i \in [q] \setminus \operatorname{supp}(\mathcal{B}(\bar{x}\bar{x}^{\mathsf{T}}) - b)\bigr\}$ spans $\mathbb{R}^n$. (4.14)

Proof. We start by proving that

$$\bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \{\bar{X}\}^{\perp}\bigr)\bigr]^{\perp} = \operatorname{span}\bigl\{\operatorname{Sym}(\bar{X}uv^{\mathsf{T}}) : u,v \in \mathbb{R}^n\bigr\}. \quad (4.15)$$

Let $Q \in \mathbb{O}^n$ such that $\bar{X} = Q\operatorname{Diag}(\lambda)Q^{\mathsf{T}}$, where $\lambda \coloneqq \lambda^{\downarrow}(\bar{X})$. Set $D \coloneqq \operatorname{Diag}(\lambda)$ and $r \coloneqq \operatorname{rank}(\bar{X})$. Note that

$$\bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \{D\}^{\perp}\bigr)\bigr]^{\perp} = \operatorname{span}\bigl\{\operatorname{Sym}(Duv^{\mathsf{T}}) : u,v \in \mathbb{R}^n\bigr\}, \quad (4.16)$$

since, by Proposition 4.7, we have

$$\begin{aligned}\bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \{D\}^{\perp}\bigr)\bigr]^{\perp} &= \bigl[\operatorname{span}\bigl(0 \oplus \mathbb{S}^{n-r}_+\bigr)\bigr]^{\perp} = \bigl[0 \oplus \mathbb{S}^{n-r}\bigr]^{\perp}\\ &= \operatorname{span}\bigl\{\operatorname{Sym}(e_ie_j^{\mathsf{T}}) : i \in [r],\, j \in [n]\bigr\}\\ &= \operatorname{span}\bigl\{\operatorname{Sym}(Duv^{\mathsf{T}}) : u,v \in \mathbb{R}^n\bigr\}.\end{aligned}$$

In the latter equality, the inclusion '$\subseteq$' is obvious. For the reverse inclusion, let $u,v \in \mathbb{R}^n$ and note that $\operatorname{Sym}(Duv^{\mathsf{T}}) = \sum_{i=1}^n\sum_{j=1}^n u_iv_j\operatorname{Sym}(De_ie_j^{\mathsf{T}}) = \sum_{i=1}^r\sum_{j=1}^n u_iv_j\operatorname{Sym}(De_ie_j^{\mathsf{T}})$. This proves (4.16).

To prove (4.15), apply Congr_Q to both sides of (4.16) to get

$$\begin{aligned}\bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \{\bar{X}\}^{\perp}\bigr)\bigr]^{\perp} &= \bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \{\operatorname{Congr}_Q(D)\}^{\perp}\bigr)\bigr]^{\perp} = \bigl[\operatorname{span}\bigl(\mathbb{S}^n_+ \cap \operatorname{Congr}_Q^{-*}(\{D\}^{\perp})\bigr)\bigr]^{\perp}\\ &= \bigl[\operatorname{span}\bigl(\operatorname{Congr}_Q^{-*}(\mathbb{S}^n_+ \cap \{D\}^{\perp})\bigr)\bigr]^{\perp} = \bigl[\operatorname{Congr}_Q^{-*}\bigl(\operatorname{span}(\mathbb{S}^n_+ \cap \{D\}^{\perp})\bigr)\bigr]^{\perp}\\ &= \operatorname{Congr}_Q\bigl(\bigl(\operatorname{span}(\mathbb{S}^n_+ \cap \{D\}^{\perp})\bigr)^{\perp}\bigr)\\ &= \operatorname{Congr}_Q\bigl(\operatorname{span}\bigl\{\operatorname{Sym}(Duv^{\mathsf{T}}) : u,v \in \mathbb{R}^n\bigr\}\bigr)\\ &= \operatorname{span}\bigl\{\operatorname{Congr}_Q\bigl(\operatorname{Sym}(Duv^{\mathsf{T}})\bigr) : u,v \in \mathbb{R}^n\bigr\}\\ &= \operatorname{span}\bigl\{\operatorname{Sym}\bigl(\operatorname{Congr}_Q(Duv^{\mathsf{T}})\bigr) : u,v \in \mathbb{R}^n\bigr\}\\ &= \operatorname{span}\bigl\{\operatorname{Sym}\bigl(\bar{X}uv^{\mathsf{T}}\bigr) : u,v \in \mathbb{R}^n\bigr\}.\end{aligned}$$

By Proposition 4.6 and (4.15), we have

$$\begin{aligned}
\Big(\mathrm{span}\big(\mathrm{Normal}(\mathscr{C};\bar{X})\big)\Big)^{\perp} &= \Big(\mathrm{Im}(\mathcal{A}^*)+\mathrm{Im}(\mathcal{B}^*\circ P)-\mathrm{span}\big(\mathbb{S}^n_+\cap\{\bar{X}\}^{\perp}\big)\Big)^{\perp}\\
&= \mathrm{Null}(\mathcal{A})\cap\mathrm{Null}(P\circ\mathcal{B})\cap\Big[\mathrm{span}\big(\mathbb{S}^n_+\cap\{\bar{X}\}^{\perp}\big)\Big]^{\perp}\\
&= \mathrm{Null}(\mathcal{A})\cap\mathrm{Null}(P\circ\mathcal{B})\cap\mathrm{span}\big\{\,\mathrm{Sym}(\bar{X}uv^{\mathsf{T}}) : u,v\in\mathbb{R}^n\big\}.
\end{aligned}$$

This proves (4.12).

For the remainder of the proof, suppose that $\bar{X}=\bar{x}\bar{x}^{\mathsf{T}}$ for some nonzero $\bar{x}\in\mathbb{R}^n$. Note that (4.15) specializes to

$$\big[\mathrm{span}\big(\mathbb{S}^n_+\cap\{\bar{x}\bar{x}^{\mathsf{T}}\}^{\perp}\big)\big]^{\perp}=\big\{\,\mathrm{Sym}(\bar{x}h^{\mathsf{T}}) : h\in\mathbb{R}^n\big\} \tag{4.17}$$

since the RHS of (4.17) is a linear subspace of $\mathbb{S}^n$.

Let $h\in\mathbb{R}^n$. Then $\big[\mathcal{A}(\mathrm{Sym}(\bar{x}h^{\mathsf{T}}))\big]_i=h^{\mathsf{T}}A_i\bar{x}$ for $i\in[p]$ and $\big[\mathcal{B}(\mathrm{Sym}(\bar{x}h^{\mathsf{T}}))\big]_i=h^{\mathsf{T}}B_i\bar{x}$ for $i\in[q]$. Thus, using (4.17), we find that

$$\begin{aligned}
&\mathrm{Null}(\mathcal{A})\cap\mathrm{Null}(P\circ\mathcal{B})\cap\Big[\mathrm{span}\big(\mathbb{S}^n_+\cap\{\bar{X}\}^{\perp}\big)\Big]^{\perp}\\
&\qquad=\Big\{\,\mathrm{Sym}(\bar{x}h^{\mathsf{T}}) : h\in\big(\{\,A_i\bar{x} : i\in[p]\}\cup\{\,B_i\bar{x} : i\in[q]\setminus\mathrm{supp}\big(\mathcal{B}(\bar{x}\bar{x}^{\mathsf{T}})-b\big)\}\big)^{\perp}\Big\},
\end{aligned}$$

which has the same dimension as $\big(\{\,A_i\bar{x} : i\in[p]\}\cup\{\,B_i\bar{x} : i\in[q]\setminus\mathrm{supp}\big(\mathcal{B}(\bar{x}\bar{x}^{\mathsf{T}})-b\big)\}\big)^{\perp}$ since the linear map $h\in\mathbb{R}^n\mapsto\mathrm{Sym}(\bar{x}h^{\mathsf{T}})$ is injective. This concludes the proof of (4.13), from which (4.14) follows immediately. □

4.3 The Elliptope, the Boolean Quadric Body, and Their Variants

Two spectrahedra recur as building blocks for semidefinite relaxations of combinatorial optimization problems: the *elliptope* and the *boolean quadric body*. In this section, we define them and review previous results in the literature about their vertices. These results suggest that vertices of spectrahedra may be regarded as a natural counterpart for extreme points in polyhedral combinatorics.

Let V be a finite set. The set

$$\mathrm{conv}\big\{\,xx^{\mathsf{T}} : x\in\{\pm1\}^V\big\}$$

is sometimes called the *cut polytope*. Since we have

$$\big\{\,xx^{\mathsf{T}} : x\in\{\pm1\}^V\big\}=\big\{\,X\in\mathbb{S}^V_+ : \mathrm{diag}(X)=\bar{e},\ \mathrm{rank}(X)=1\big\},$$

a natural relaxation for the cut polytope is the set

$$\mathscr{E}_V\coloneqq\big\{\,X\in\mathbb{S}^V_+ : \mathrm{diag}(X)=\bar{e}\big\},$$

known as the *elliptope*. This set is the feasible region of the SDP used by Goemans and Williamson [52] in their approximation algorithm for MaxCut.

The set

$$\operatorname{conv}\{\, (1 \oplus x)(1 \oplus x)^{\mathsf{T}} : x \in \{0,1\}^V \,\} \tag{4.18}$$

is a lifting of what is sometimes called the *boolean quadric polytope*. Define the map

$$\mathcal{B}_{\{0\}\cup V} \colon \hat{X} \in \mathbb{S}^{\{0\}\cup V} \mapsto \mathcal{B}_{\{0\}}(\hat{X}) \oplus \mathcal{B}_V(\hat{X}) \in \mathbb{R}^{\{0\}} \oplus \mathbb{R}^V, \tag{4.19a}$$

where $\mathcal{B}_{\{0\}} \colon \mathbb{S}^{\{0\}\cup V} \to \mathbb{R}^{\{0\}}$ and $\mathcal{B}_V \colon \mathbb{S}^{\{0\}\cup V} \to \mathbb{R}^V$ are defined by

$$\mathcal{B}_{\{0\}}^*(e_0) := e_0 e_0^{\mathsf{T}} \qquad \text{and} \qquad \mathcal{B}_V^*(e_i) := \operatorname{Sym}\big(e_i(e_i - e_0)^{\mathsf{T}}\big) \quad \forall i \in V. \tag{4.19b}$$

(Recall that we assume throughout the thesis that $0 \notin V$.) Since we have

$$\{\, (1 \oplus x)(1 \oplus x)^{\mathsf{T}} : x \in \{0,1\}^V \,\} = \{\, \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\, \operatorname{rank}(\hat{X}) = 1 \},$$

a natural relaxation for the boolean quadric polytope is the set

$$\mathrm{BQ}_{\{0\}\cup V} := \{\, \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0 \}. \tag{4.20}$$

Define the square matrix Bool on index set $\{0\} \cup V$ as

$$\mathrm{Bool} := \tfrac{1}{2} \sum_{k \in \{0\}\cup V} e_k (e_0 + e_k)^{\mathsf{T}} = \frac{1}{2} \begin{bmatrix} 2 & 0^{\mathsf{T}} \\ \bar{e} & I \end{bmatrix}. \tag{4.21}$$

Then $\mathrm{Congr}_{\mathrm{Bool}}$ is a linear isomorphism from $\mathscr{E}_{\{0\}\cup V}$ to $\mathrm{BQ}_{\{0\}\cup V}$, i.e.,

$$\mathrm{Congr}_{\mathrm{Bool}}\big(\mathscr{E}_{\{0\}\cup V}\big) = \mathrm{BQ}_{\{0\}\cup V}\,. \tag{4.22}$$

To see this, let $\hat{X} \in \mathbb{S}^{\{0\}\cup V}$, and note that

$$\begin{aligned} \big\langle \mathcal{B}_{\{0\}}^*(e_0), \mathrm{Congr}_{\mathrm{Bool}}(\hat{X}) \big\rangle &= \langle e_0 e_0^{\mathsf{T}}, \hat{X} \rangle, \\ \big\langle \mathcal{B}_V^*(e_i), \mathrm{Congr}_{\mathrm{Bool}}(\hat{X}) \big\rangle &= \tfrac{1}{4} \big\langle (e_i e_i^{\mathsf{T}} - e_0 e_0^{\mathsf{T}}), \hat{X} \big\rangle \qquad \forall i \in V. \end{aligned}$$

Thus, $\operatorname{diag}(\hat{X}) = \bar{e}$ is equivalent to $\mathcal{B}_{\{0\}\cup V}\big(\mathrm{Congr}_{\mathrm{Bool}}(\hat{X})\big) = 1 \oplus 0$. We refer the reader to the papers [33, 89, 45] for more details on the relationship between the cut polytope and the boolean quadric polytope, and their relaxations.

Laurent and Poljak studied the facial structure of the elliptope in the papers [87, 88]. They characterized the vertices of the elliptope as precisely the matrices of the form xx^{T} with $x \in \{\pm 1\}^V$, i.e., they are precisely the extreme points of the cut polytope, of which the elliptope is a relaxation. Thus, by Lemma 4.8, the vertices of the set $\mathrm{BQ}_{\{0\}\cup V}$ are also the matrices of the form $(1 \oplus x)(1 \oplus x)^{\mathsf{T}}$ with $x \in \{0,1\}^V$. In the remainder of the section, we shall go over their proofs for the sake of completeness.

We first state a slightly generalized version of a result by Laurent and Poljak [88].

Theorem 4.10 ([88, Theorem 2.10])**.** Let $\mathcal{A} \colon \mathbb{S}^n \to \mathbb{R}^m$ be a linear map, and let $A_i := \mathcal{A}^*(e_i)$ for each $i \in [m]$. Let $b \in \mathbb{R}^m$ such that $\operatorname{supp}(b) = [m]$. Set $\mathscr{C} := \{\, X \in \mathbb{S}_+^n : \mathcal{A}(X) = b \}$. Suppose that $\mathscr{C} \cap \mathbb{S}_{++}^n \neq \varnothing$ and that $\operatorname{rank}(\sum_{i=1}^m A_i) = \sum_{i=1}^m \operatorname{rank}(A_i)$. Then, for every $\bar{X} \in \mathscr{C}$, we have

$$\dim\big(\operatorname{Normal}(\mathscr{C}; \bar{X})\big) = \dim\big(\operatorname{Im}(\mathcal{A}^*)\big) + \binom{\dim\big(\operatorname{Null}(\bar{X})\big) + 1}{2}. \tag{4.23}$$

Proof. The proof of '$\leq$' in (4.23) follows from Proposition 4.6 and (4.8).

Now we prove the reverse inequality. We shall use the fact that

$$\text{if } L \in \mathbb{R}^{n\times n} \text{ is nonsingular, then the hypotheses and conclusion of the result hold if and only if they also hold if } \mathcal{A} \text{ is replaced with } \mathcal{A}_L \coloneqq \mathcal{A} \circ \operatorname{Congr}_L^{-1} \text{ and } \mathscr{C} \text{ is replaced with } \mathscr{C}_L \coloneqq \operatorname{Congr}_L(\mathscr{C}). \tag{4.24}$$

Note that $\operatorname{rank}\bigl(\sum_{i=1}^m \mathcal{A}_L^*(e_i)\bigr) = \operatorname{rank}\bigl(\sum_{i=1}^m \mathcal{A}^*(e_i)\bigr) = \sum_{i=1}^m \operatorname{rank}\bigl(\mathcal{A}^*(e_i)\bigr) = \sum_{i=1}^m \operatorname{rank}\bigl(\mathcal{A}_L^*(e_i)\bigr)$ since $\operatorname{rank}(\mathcal{A}_L^*(y)) = \operatorname{rank}(L^{-\mathsf{T}}\mathcal{A}^*(y)L^{-1}) = \operatorname{rank}(\mathcal{A}^*(y))$ for each $y \in \mathbb{R}^m$. Together with Lemma 4.8, this proves (4.24).

Let us prove that

$$\text{we may assume that } A_iA_j = 0 \text{ whenever } i,j \in [m] \text{ are distinct.} \tag{4.25}$$

For each $i \in [m]$, set $r_i \coloneqq \operatorname{rank}(A_i)$ and let $B_i \in \mathbb{R}^{n\times r_i}$ have full column-rank such that $\operatorname{Im}(A_i) = \operatorname{Im}(B_i)$. Set $r \coloneqq \sum_{i=1}^m r_i$. Then the $n \times r$ matrix

$$B \coloneqq \begin{bmatrix} B_1 & \cdots & B_m \end{bmatrix}$$

has full column-rank, since our hypothesis and the relation $\operatorname{Im}(\sum_{i=1}^m A_i) \subseteq \sum_{i=1}^m \operatorname{Im}(A_i) = \sum_{i=1}^m \operatorname{Im}(B_i) = \operatorname{Im}(B)$ imply that

$$r = \textstyle\sum_{i=1}^m r_i = \operatorname{rank}\bigl(\sum_{i=1}^m A_i\bigr) = \dim\bigl(\operatorname{Im}\bigl(\sum_{i=1}^m A_i\bigr)\bigr) \leq \dim(\operatorname{Im}(B)) = \operatorname{rank}(B).$$

Thus, there exists a nonsingular $L \in \mathbb{R}^{n\times n}$ such that $LB = \sum_{k=1}^r e_k e_k^{\mathsf{T}}$. If $i,j \in [m]$ are distinct, then $\operatorname{Im}(LB_i) \perp \operatorname{Im}(LB_j)$ holds and so does $\operatorname{Im}(\operatorname{Congr}_L(A_i)) \perp \operatorname{Im}(\operatorname{Congr}_L(A_j))$. Therefore, we have $\operatorname{Congr}_L(A_i)\operatorname{Congr}_L(A_j) = 0$ whenever $i,j \in [m]$ are distinct. Thus, by replacing $\mathcal{A}$ with $\mathcal{A} \circ \operatorname{Congr}_{L^{-\mathsf{T}}}^{-1}$ and applying (4.24), this proves (4.25).

Next we shall refine (4.25) and show that

$$\text{we may assume that } A_i = \operatorname{Diag}(a_i) \text{ for each } i \in [m]\text{, where } a_1,\dots,a_m \in \mathbb{R}^n \text{ are vectors with pairwise disjoint supports.} \tag{4.26}$$

Since the matrices $A_1,\dots,A_m$ pairwise commute by (4.25), there exists $P \in \mathbb{O}^n$ such that $P^{\mathsf{T}}A_iP$ is diagonal for each $i \in [m]$; see, e.g., [72, Theorem 1.3.19]. Let $a_i \in \mathbb{R}^n$ such that $A_i = P\operatorname{Diag}(a_i)P^{\mathsf{T}}$ for each $i \in [m]$. For distinct $i,j \in [m]$, we have $0 = P^{\mathsf{T}}(A_iA_j)P = \operatorname{Diag}(a_i)\operatorname{Diag}(a_j)$, whence $\operatorname{supp}(a_i) \cap \operatorname{supp}(a_j) = \varnothing$. Thus, by replacing $\mathcal{A}$ with $\mathcal{A} \circ \operatorname{Congr}_{P^{-1}}^{-1}$ and applying (4.24), this proves (4.26).

Let $\bar{X} \in \mathscr{C}$, let $\{R_1,\dots,R_p\}$ be a basis of $\mathbb{S}^{n-\operatorname{rank}(\bar{X})}$, and let $Q \in \mathbb{O}^n$ such that $\bar{X} = Q\operatorname{Diag}(\lambda)Q^{\mathsf{T}}$, where $\lambda \coloneqq \lambda^{\downarrow}(\bar{X})$. To prove '$\geq$' in (4.23), it suffices by Proposition 4.6 to show that the set $\{A_1,\dots,A_m\} \cup \{Q(0 \oplus R_1)Q^{\mathsf{T}},\dots,Q(0 \oplus R_p)Q^{\mathsf{T}}\}$ is linearly independent. Let $\alpha \in \mathbb{R}^m$ and $\beta \in \mathbb{R}^p$ such that

$$\sum_{i=1}^m \alpha_i A_i + \sum_{j=1}^p \beta_j Q(0 \oplus R_j)Q^{\mathsf{T}} = 0. \tag{4.27}$$

Let $u \in \operatorname{Null}(\bar{X})^{\perp}$. Then $Q^{\mathsf{T}}u \in Q^{\mathsf{T}}\operatorname{Im}(\bar{X}) = \operatorname{Im}(Q^{\mathsf{T}}\bar{X}) = \operatorname{Im}\bigl(\operatorname{Diag}(\lambda)Q^{\mathsf{T}}\bigr) \subseteq \operatorname{Im}\bigl(\operatorname{Diag}(\lambda)\bigr)$, whence $\operatorname{supp}(Q^{\mathsf{T}}u) \subseteq [\operatorname{rank}(\bar{X})]$. Thus, if we multiply (4.27) on the right by u, we obtain $u \in \operatorname{Null}\bigl(\sum_{i=1}^m \alpha_i A_i\bigr)$. So $\operatorname{Null}(\bar{X})^{\perp} \subseteq \operatorname{Null}\bigl(\sum_{i=1}^m \alpha_i A_i\bigr)$, or, equivalently,

$$\operatorname{Im}\bigl(\textstyle\sum_{i=1}^m \alpha_i A_i\bigr) \subseteq \operatorname{Null}(\bar{X}).$$

Let $k \in [m]$. Then from (4.26) we have $\operatorname{Im}(\alpha_k A_k) \subseteq \operatorname{Im}(\sum_{i=1}^m \alpha_i A_i) \subseteq \operatorname{Null}(\bar{X})$ so $\alpha_k \bar{X} A_k = 0$. Since $0 \neq b_k = \langle A_k, \bar{X} \rangle = \operatorname{Tr}(A_k \bar{X})$, we have $\bar{X} A_k \neq 0$, so it must be the case that $\alpha_k = 0$. This proves that $\alpha = 0$, whence $\beta = 0$. This concludes the proof of (4.23). ☐

By Theorem 4.10, the dimension of a normal cone at matrix $\bar{X}$ of the elliptope is completely determined by the rank of $\bar{X}$. In particular, this leads to a characterization of the vertices of the elliptope:

Corollary 4.11 ([87, Theorem 2.5])**.** Let V be a finite set. Then a point $\bar{X}$ of $\mathscr{E}_V$ is a vertex of $\mathscr{E}_V$ if and only if $\operatorname{rank}(\bar{X}) = 1$. Thus, the vertices of $\mathscr{E}_V$ are precisely the matrices of the form xx^T with $x \in \{\pm 1\}^V$.

Proof. Theorem 4.10 implies that a point $\bar{X} \in \mathscr{E}_V$ is a vertex of $\mathscr{E}_V$ precisely when $\operatorname{Null}(\bar{X})$ has dimension $|V| - 1$. ☐

Corollary 4.12 ([87])**.** Let V be a finite set. Then a point $\bar{X}$ of $\mathrm{BQ}_{\{0\} \cup V}$ is a vertex of $\mathrm{BQ}_{\{0\} \cup V}$ if and only if $\operatorname{rank}(\bar{X}) = 1$. Thus, the vertices of $\mathrm{BQ}_{\{0\} \cup V}$ are precisely the matrices of the form $(1 \oplus x)(1 \oplus x)^\mathsf{T}$ with $x \in \{0,1\}^V$.

Proof. Immediate from Corollary 4.11 and (4.22), via Lemma 4.8. ☐

In the proof of Corollary 4.11 by Laurent and Poljak in the paper [87], the fact that $\bar{x}\bar{x}^\mathsf{T}$ is a vertex of $\mathscr{E}_n$ if $\bar{x} \in \{\pm 1\}^n$ follows from the simple observation that $\{\, (-1)^{[\bar{x}_i \bar{x}_j < 0]} \operatorname{Sym}(e_i e_j^\mathsf{T}) : i, j \in [n] \} \subseteq \operatorname{Normal}(\mathscr{E}_n; \bar{x}\bar{x}^\mathsf{T})$. For the proof that all vertices of $\mathscr{E}_n$ have rank one, Laurent and Poljak give the following argument, which we include for the sake of completeness:

Proposition 4.13 ([87])**.** Let $\mathcal{A} \colon \mathbb{S}^n \to \mathbb{R}^m$ and $b \in \mathbb{R}^m$ and set $\mathscr{C} \coloneqq \{\, X \in \mathbb{S}^n_+ : \mathcal{A}(X) = b \}$. Suppose that $\mathscr{C} \cap \mathbb{S}^n_{++} \neq \varnothing$. Suppose that for some $k \in [n-1]$ there exists a linearly independent subset $\{h_0\} \cup \{\, h_i : i \in [k] \}$ of $\mathbb{R}^n$ such that $\{\operatorname{Sym}(h_0 h_i^\mathsf{T}) : i \in [k] \} \subseteq \operatorname{Null}(\mathcal{A})$. Then every vertex of $\mathscr{C}$ has rank $\leq n - k$.

Proof. We first show that,

> if $L \in \mathbb{R}^{n \times n}$ is nonsingular, then the hypotheses and conclusion of the result hold if and only if they also hold if $\mathcal{A}$ is replaced with $\mathcal{A}_L \coloneqq \mathcal{A} \circ \operatorname{Congr}_L^{-1}$ and $\mathscr{C}$ is replaced with $\mathscr{C}_L \coloneqq \operatorname{Congr}_L(\mathscr{C})$. (4.28)

Note that linear independence of $\{h_0\} \cup \{\, h_i : i \in [k] \} \subseteq \mathbb{R}^n$ is equivalent to that of $\{Lh_0\} \cup \{\, Lh_i : i \in [k] \}$, and the inclusion $\{\operatorname{Sym}(h_0 h_i^\mathsf{T}) : i \in [k] \} \subseteq \operatorname{Null}(\mathcal{A})$ is equivalent to

$$\{\operatorname{Sym}(Lh_0 h_i^\mathsf{T} L^\mathsf{T}) : i \in [k] \} = \operatorname{Congr}_L\big(\{\operatorname{Sym}(h_0 h_i^\mathsf{T}) : i \in [k] \}\big) \subseteq \operatorname{Null}(\mathcal{A} \circ \operatorname{Congr}_L^{-1}) = \operatorname{Null}(\mathcal{A}_L).$$

The proof of (4.28) follows from these facts together with Lemma 4.8.

By applying (4.28) with $L \in \mathbb{R}^{n \times n}$ nonsingular such that $Lh_0 = e_n$ and $Lh_i = e_i$ for $i \in [k]$,

we may assume that $h_0 = e_n$ and $h_i = e_i$ for all $i \in [k]$.

Set $d \coloneqq \dim(\mathrm{Null}(\mathcal{A}))$. Let $P_{\mathrm{Null}(\mathcal{A})} \colon \mathbb{S}^n \to \mathbb{S}^n$ denote the orthogonal projection onto $\mathrm{Null}(\mathcal{A})$. Since the elements of $\{\, \mathrm{Sym}(e_n e_i^{\mathsf{T}}) : i \in [k] \,\} \subseteq \mathrm{Null}(\mathcal{A})$ are pairwise orthogonal, we have

$$P_{\mathrm{Null}(\mathcal{A})}\big(\mathrm{Sym}(e_n e_i^{\mathsf{T}})\big) = \mathrm{Sym}(e_n e_i^{\mathsf{T}}) \qquad \forall i \in [k] \tag{4.29}$$

and

$$\text{there is a linear isomorphism } \varphi\colon \mathrm{Null}(\mathcal{A}) \to \mathbb{R}^d \text{ such that } [\varphi(X)]_i = X_{in} \text{ for all } i \in [k]. \tag{4.30}$$

Let $\bar{X}$ be a vertex of $\mathscr{C}$. By Propositions 4.6 and 4.7, we have

$$\mathrm{Normal}(\mathscr{C}; \bar{X}) = \mathrm{Im}(\mathcal{A}^*) - (\mathbb{S}^n_+ \cap \{\bar{X}\}^{\perp}) = \mathrm{Im}(\mathcal{A}^*) - \mathrm{cone}\big\{\, bb^{\mathsf{T}} : b \in \mathrm{Null}(\bar{X}) \,\big\}.$$

Then

$$P_{\mathrm{Null}(\mathcal{A})}\big(\mathrm{Normal}(\mathscr{C}; \bar{X})\big) = -\,\mathrm{cone}\big\{\, P_{\mathrm{Null}(\mathcal{A})}(bb^{\mathsf{T}}) : b \in \mathrm{Null}(\bar{X}) \,\big\}$$

has dimension d. Hence, there exists a set $\{\, b_j : j \in [d] \,\} \subseteq \mathrm{Null}(\bar{X})$ such that, for $B_j \coloneqq b_j b_j^{\mathsf{T}}$ for $j \in [d]$, the set $\{\, P_{\mathrm{Null}(\mathcal{A})}(B_j) : j \in [d] \,\}$ is linearly independent. So the $d \times d$ matrix M whose jth row is $\varphi(P_{\mathrm{Null}(\mathcal{A})}(B_j))$ is nonsingular, and its submatrix $M_1 \coloneqq M[[d],[k]]$ has k linearly independent rows. By possibly relabeling the set $\{\, B_j : j \in [d] \,\}$, we may assume that the first k rows of M_1 are linearly independent, i.e.,

$$\big\{\, [b_j]_n \big(b_j\restriction_{[k]}\big) : j \in [k] \,\big\} = \big\{\, \varphi(P_{\mathrm{Null}(\mathcal{A})}(B_j))\restriction_{[k]} : j \in [k] \,\big\} \text{ is linearly independent,}$$

where the equation follows from (4.29) and (4.30) since, for every $i, j \in [k]$, we have

$$\begin{aligned} \big[\varphi(P_{\mathrm{Null}(\mathcal{A})}(B_j))\big]_i &= \big[P_{\mathrm{Null}(\mathcal{A})}(B_j)\big]_{in} = \big\langle P_{\mathrm{Null}(\mathcal{A})}(B_j), \mathrm{Sym}(e_i e_n^{\mathsf{T}})\big\rangle \\ &= \big\langle B_j, \mathrm{Sym}(e_i e_n^{\mathsf{T}})\big\rangle = [B_j]_{in} = [b_j]_n [b_j]_i. \end{aligned}$$

In particular, $[b_j]_n \neq 0$ for each $j \in [k]$ and $\{\, b_j : j \in [k] \,\}$ is linearly independent. Since $b_j \in \mathrm{Null}(\bar{X})$ for each $j \in [k]$, we get $\mathrm{rank}(\bar{X}) \leq n - k$. ☐

When Proposition 4.13 is applied to $\mathscr{E}_n$ in the proof of Corollary 4.11 with $h_0 \coloneqq e_n$ and $h_i \coloneqq e_i$ for each $i \in [n-1]$, we find again that each vertex of $\mathscr{E}_n$ is rank-one.

Note, however, that the bound provided by Proposition 4.13 may be quite weak. To see this, consider the set

$$\mathscr{C} \coloneqq \Big\{\, X \in \mathbb{S}^n_+ : \big\langle \mathrm{Sym}(e_i e_j^{\mathsf{T}}), X \big\rangle = 0 \,\forall ij \in \tbinom{[n]}{2} \Big\}.$$

Note that the polyhedral cone $\mathscr{C}$ has a unique vertex (and extreme point) and its rank is 0. Now suppose $\{h_0\} \cup \{\, h_i : i \in [k] \,\} \subseteq \mathbb{R}^n$ is a linearly independent set for some $k \in [n-1]$ such that $\mathrm{Sym}(h_0 h_i^{\mathsf{T}})$ is diagonal for each $i \in [k]$. For $x, y \in \mathbb{R}^n$, the matrix $\mathrm{Sym}(xy^{\mathsf{T}})$ is diagonal if and only if, for each $i \in \mathrm{supp}(x)$, we have $y\restriction_{[n]\setminus\{i\}} = -(y_i/x_i)x\restriction_{[n]\setminus\{i\}}$. Thus, $k \leq 1$. Thus, Proposition 4.13 gives the upper bound $n-1$ for the rank of the vertices of $\mathscr{C}$.

Proposition 4.13 has nonetheless a quite unexpected consequence:

Corollary 4.14. Let $\mathcal{A}\colon \mathbb{S}^n \to \mathbb{R}^m$ be a linear map. Let $b \in \mathbb{R}^m$. Define $\mathscr{C} \coloneqq \{\, X \in \mathbb{S}^n_+ : \mathcal{A}(X) = b \,\}$. Suppose that $\mathscr{C} \cap \mathbb{S}^n_{++} \neq \varnothing$. Then every vertex of $\widehat{\mathscr{C}} \coloneqq \big\{\, \hat{X} \in \mathbb{S}^{\{0\}\cup[n]}_+ : \hat{X}[[n]] \in \mathscr{C} \,\big\}$ has rank one.

Proof. Immediate from Proposition 4.13 applied with $h_i \coloneqq e_i$ for each $i \in \{0\} \cup [n]$. $\square$

Thus, the seemingly innocuous operation of embedding a spectrahedron into a higher-dimensional space completely transforms the boundary structure: the sets $\mathscr{C}$ in Corollary 4.14 could potentially have vertices of all ranks from 1 to n whereas the higher-dimensional set $\widehat{\mathscr{C}}$ can only have vertices of rank one. While one may argue that the transformation described is very easy to detect, upon applying a congruence to the system defining $\widehat{\mathscr{C}}$ this may no longer be the case.

4.4 Vertices of the Theta Body

In the next section, we will determine the vertices of the lifted theta body of a graph $G = (V, E)$, defined as

$$\widehat{\mathrm{TH}}(G) \coloneqq \left\{ \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\ \mathcal{A}_E(\hat{X}[V]) = 0 \right\};$$

recall that the linear map $\mathcal{A}_E$ was defined in (2.16). In this section, we shall present a proof of an observation made by Shepherd [136] that the vertices of the theta body

$$\mathrm{TH}(G) = \left\{ \mathrm{diag}(\hat{X}[V]) : \hat{X} \in \widehat{\mathrm{TH}}(G) \right\} \tag{4.31}$$

are precisely the incidence vectors of stable sets of G.

Theorem 4.15 ([136, p. 281])**.** Let $G = (V, E)$ be a graph. Then a point $\bar{x}$ of $\mathrm{TH}(G)$ is a vertex of $\mathrm{TH}(G)$ if and only if $\bar{x}$ is the incidence vector of a stable set in G.

Proof. For the 'if' part, let $\bar{x}$ be the incidence vector of a stable set in G and note that $\mathrm{TH}(G) \subseteq [0,1]^V$ implies that $\{ (-1)^{[\bar{x}_i = 0]} e_i : i \in V \} \subseteq \mathrm{Normal}(\mathrm{TH}(G); \bar{x})$.

Now we prove the 'only if' part. Set $n \coloneqq |V|$. Let $\bar{x}$ be a vertex of $\mathrm{TH}(G)$. If $n = 1$, then $\mathrm{TH}(G) = [0,1]^V$ so $\bar{x}$ must be the incidence vector of a stable set of G. Assume henceforth that $n > 1$. Then

we may assume that $\bar{x}_i > 0$ for every $i \in V$.

Suppose that $\bar{x}_i = 0$ for some $i \in V$. Then $\bar{x}$ lies in the face $F \coloneqq \{ x \in \mathrm{TH}(G) : x_i = 0 \}$ of $\mathrm{TH}(G)$. Note that $\mathrm{aff}(F) = \bar{x} + \{e_i\}^\perp$ and that $F = \{ y \oplus 0 : y \in \mathrm{TH}(G - i) \}$. It is easy to check that the cone $\{ d \in \{e_i\}^\perp : \langle d, x \rangle \leq \langle d, \bar{x} \rangle\ \forall x \in F \}$ has dimension $n - 1$. Thus, if we form $\bar{y} \in \mathbb{R}^{V \setminus \{i\}}$ by dropping coordinate i from $\bar{x}$, we find that the cone $\left\{ d \in \mathbb{R}^{V\setminus\{i\}} : \langle d, y \rangle \leq \langle d, \bar{y} \rangle\ \forall y \in \mathrm{TH}(G - i) \right\}$ has dimension $n - 1$, i.e., $\bar{y}$ is a vertex of $\mathrm{TH}(G - i)$, and we are done by induction.

We will use the fact that $\mathrm{TH}(G)$ is a convex corner, i.e., a compact, lower-comprehensive convex subset of $\mathbb{R}_+^V$ with nonempty interior. Let $c \in \mathrm{Normal}(\mathrm{TH}(G); \bar{x})$. Then $\langle c, \bar{x} \rangle \geq \langle c, \bar{x} - \bar{x}_i e_i \rangle = \langle c, \bar{x} \rangle - c_i \bar{x}_i$ whence $c_i \bar{x}_i \geq 0$ and $c_i \geq 0$. Hence,

$$\mathrm{Normal}\big(\mathrm{TH}(G); \bar{x}\big) \subseteq \mathbb{R}_+^V. \tag{4.32}$$

Let $c \in \mathrm{Normal}(\mathrm{TH}(G); \bar{x})$ be nonzero. Since $c \geq 0$ by (4.32), we have $\varepsilon c \in \mathrm{TH}(G)$ for some sufficiently small $\varepsilon > 0$, whence $0 < \langle c, \varepsilon c \rangle \leq \langle c, \bar{x} \rangle$. Thus,

$$\langle c, \bar{x} \rangle > 0 \qquad \forall c \in \mathrm{Normal}\big(\mathrm{TH}(G); \bar{x}\big) \setminus \{0\}. \tag{4.33}$$

Let $\{ c_j : j \in [n] \}$ be a linearly independent subset of $\operatorname{Normal}(\operatorname{TH}(G); \bar{x})$. By (4.33), we know that by possibly replacing each c_j with $c_j / \langle c_j, \bar{x} \rangle$, we may assume that $\langle c_j, \bar{x} \rangle = 1$ for each $j \in [n]$. Then $\langle c_j, x \rangle \leq \langle c_j, \bar{x} \rangle = 1$ for all $x \in \operatorname{TH}(G)$, so $\{ c_j : j \in [n] \}$ lies in the antiblocker of $\operatorname{TH}(G)$, which is $\operatorname{TH}(\overline{G})$ by (1.4). Thus,

$$\big\{ c_j : j \in [n] \big\} \subseteq \operatorname{TH}(\overline{G}) \cap \{ x \in \mathbb{R}^V : \langle x, \bar{x} \rangle = 1 \}. \tag{4.34}$$

Since $\operatorname{TH}(\overline{G}) \subseteq \{ x \in \mathbb{R}^V : \langle x, \bar{x} \rangle \leq 1 \}$ and $\dim(\operatorname{aff}(\{ c_j : j \in [n] \})) = n - 1$, it follows from (4.34) that $\langle x, \bar{x} \rangle \leq 1$ is a facet-defining inequality for $\operatorname{TH}(\overline{G})$. By [133, Theorem 67.13], we find that $\bar{x}$ is the incidence vector of some clique of $\overline{G}$. $\square$

4.5 Vertices of the Lifted Theta Body

We have seen in Corollary 4.11 that the vertices of the elliptope are the extreme points of the cut polytope, the set for which the elliptope is a relaxation. Similarly, by Theorem 4.15, the vertices of the theta body $\operatorname{TH}(G)$ of a graph G are the extreme points of the stable set polytope of G, for which $\operatorname{TH}(G)$ is a relaxation. These results also indicate that vertices of these nonpolyhedral convex sets are natural counterparts to the extreme points of polyhedral relaxations often studied in polyhedral combinatorics.

An important qualitative difference between these results is that they deal with quite different classes of sets. The elliptope $\mathscr{E}_V$ is a spectrahedron, whereas the theta body $\operatorname{TH}(G)$ of a graph G is only known to be a projection of a spectrahedron, namely, as a projection of the spectrahedron $\widehat{\operatorname{TH}}(G)$, as defined in (4.31). In a sense, $\operatorname{TH}(G)$ potentially has a more complicated structure than the lifted set $\widehat{\operatorname{TH}}(G)$. Indeed, spectrahedra are in general *facially exposed*, whereas their projections need not be so; see, e.g., [25] for some substantial qualitative differences between spectrahedra and their projections. On the other hand, when solving optimization problems over $\operatorname{TH}(G)$, the latter is represented via $\widehat{\operatorname{TH}}(G)$. Thus, it is very important to understand the facial structure of the lifted representation $\widehat{\operatorname{TH}}(G)$ of the theta body.

In this section, we shall prove that all vertices of $\widehat{\operatorname{TH}}(G)$ have rank one. This result is a generalization of Corollary 4.11 and it may be seen as a lifted version of Theorem 4.15. We shall also discuss analogous results for variants of the lifted set $\widehat{\operatorname{TH}}(G)$, which we introduce next. For a graph $G = (V, E)$, these sets may be defined as

$$\begin{gathered}\widehat{\operatorname{TH}}'(G) := \big\{ \hat{X} \in \mathbb{S}_+^{\{0\} \cup V} : \mathcal{B}_{\{0\} \cup V}(\hat{X}) = 1 \oplus 0,\, \mathcal{A}_E(\hat{X}[V]) = 0,\, \mathcal{A}_{\overline{E}}(\hat{X}[V]) \geq 0 \big\}, \\ \operatorname{TH}'(G) = \Big\{ \operatorname{diag}\big(\hat{X}[V]\big) \in \mathbb{R}^V : \hat{X} \in \widehat{\operatorname{TH}}'(G) \Big\},\end{gathered}$$

and

$$\begin{gathered}\widehat{\operatorname{TH}}^+(G) := \big\{ \hat{X} \in \mathbb{S}_+^{\{0\} \cup V} : \mathcal{B}_{\{0\} \cup V}(\hat{X}) = 1 \oplus 0,\, \mathcal{A}_E(\hat{X}[V]) \leq 0 \big\}, \\ \operatorname{TH}^+(G) = \Big\{ \operatorname{diag}\big(\hat{X}[V]\big) \in \mathbb{R}^V : \hat{X} \in \widehat{\operatorname{TH}}^+(G) \Big\}.\end{gathered}$$

Some well-known variants of the Lovász theta number are the support functions of these sets, i.e., for a graph $G = (V, E)$ and $w \in \mathbb{R}_+^V$, we have

$$\vartheta'(G; w) = \max\big\{ \langle w, x \rangle : x \in \operatorname{TH}'(G) \big\}, \tag{4.35}$$

$$\vartheta^+(G; w) = \max\big\{ \langle w, x \rangle : x \in \operatorname{TH}^+(G) \big\}. \tag{4.36}$$

We refer the reader to [78, 61] and the references therein for more details.

Now the motivation for our main result below should be clear:

Theorem 4.16. Let V be a finite set, and let $E^+, E^- \subseteq \binom{V}{2}$. Set

$$\widehat{\mathscr{C}} \coloneqq \Big\{\, \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\, \mathcal{A}_{E^+}(\hat{X}[V]) \geq 0,\, \mathcal{A}_{E^-}(\hat{X}[V]) \leq 0 \Big\}.$$

Let $\hat{X} \in \widehat{\mathscr{C}}$. Then $\hat{X}$ is a vertex of $\widehat{\mathscr{C}}$ if and only if $\operatorname{rank}(\hat{X}) = 1$.

Proof. Note that

$$\frac{1}{2n}\begin{bmatrix} 2n & \bar{e}^\mathsf{T} \\ \bar{e} & I \end{bmatrix} \in \widehat{\mathscr{C}} \cap \mathbb{S}_{++}^{\{0\}\cup V}$$

for $n \coloneqq |V|$, so we may apply Theorem 4.9.

We first prove the 'if' part. Let $\hat{X} \in \widehat{\mathscr{C}}$ be rank-one, so that $\hat{X}$ is of the form $\hat{X} = (1 \oplus \bar{x})(1 \oplus \bar{x})^\mathsf{T}$ for some $\bar{x} \in \mathbb{R}^V$. Since $\mathcal{B}_V(\hat{X}) = 0$, we have $\bar{x} \in \{0,1\}^V$. Then $[\mathcal{B}_{\{0\}}^*(e_0)](1 \oplus \bar{x}) = e_0 e_0^\mathsf{T}(1 \oplus \bar{x}) = e_0$ and, for $i \in V$, we have $2[\mathcal{B}_V^*(e_i)](1 \oplus \bar{x}) = 2\operatorname{Sym}(e_i(e_i - e_0)^\mathsf{T})(1 \oplus \bar{x}) = (\bar{x}_i - 1)e_i + \bar{x}_i(e_i - e_0) = \big(2\bar{x}_i - 1\big)e_i - \bar{x}_i e_0$. These vectors form a basis for $\mathbb{R}^{\{0\}\cup V}$, whence $\hat{X}$ is a vertex of $\widehat{\mathscr{C}}$ by Theorem 4.9.

Now we prove the 'only if' part. Let $\hat{X}$ be a vertex of $\widehat{\mathscr{C}}$. For each $k \in V$, define

$$\tfrac{1}{2}C_k \coloneqq \operatorname{Sym}(\hat{X}e_k e_0^\mathsf{T}) + \sum\Big\{\, \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}} \operatorname{Sym}\big(\hat{X}e_\ell e_\ell^\mathsf{T}\big) : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \Big\}.$$

For $E \in \{E^+, E^-\}$, denote the orthogonal projection onto $\{\, z \in \mathbb{R}^E : \operatorname{supp}(z) \cap \operatorname{supp}(\mathcal{A}_E(\hat{X}[V])) = \varnothing \}$ by P_E. Let $\mathcal{F} \colon \mathbb{S}^{\{0\}\cup V} \to \mathbb{R}^V \oplus \mathbb{R}^{E+} \oplus \mathbb{R}^{E-}$ be defined as

$$\mathcal{F}(\hat{Y}) \coloneqq \mathcal{B}_V(\hat{Y}) \oplus \big(P_{E^+} \circ \mathcal{A}_{E^+}\big)\big(\hat{Y}[V]\big) \oplus \big(P_{E^-} \circ \mathcal{A}_{E^-}\big)\big(\hat{Y}[V]\big) \quad \forall \hat{Y} \in \mathbb{S}^{\{0\}\cup V}.$$

(Note the absence of $\{0\}$ in the index set of $\mathcal{B}_V$.) Let us prove that

$$C_k \in \operatorname{Null}(\mathcal{F}). \tag{4.37}$$

Let $i, j \in \{0\} \cup V$. Then

$$\begin{aligned} [C_k]_{ij} &= \hat{X}_{ik}[j=0] + [i=0]\hat{X}_{kj} + \sum\Big\{\, \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}}\Big(\hat{X}_{i\ell}[\ell=j] + [\ell=i]\hat{X}_{\ell j}\Big) : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \Big\} \\ &= \hat{X}_{ik}[j=0] + [i=0]\hat{X}_{kj} + \sum\Big\{\, \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}}\Big(\hat{X}_{ij}[\ell=j] + [\ell=i]\hat{X}_{ij}\Big) : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \Big\} \\ &= \hat{X}_{ik}[j=0] + [i=0]\hat{X}_{kj} + \hat{X}_{ij}\sum\Big\{\, \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}}\Big([\ell=j] + [\ell=i]\Big) : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \Big\}. \end{aligned} \tag{4.38}$$

Thus, if $i, j \in V$ are distinct and $\hat{X}_{ij} = 0$, then $[C_k]_{ij} = 0$. Let $i \in V$. Then

$$[C_k]_{ii} = \hat{X}_{ii}\sum\Big\{\, \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}} 2[\ell=i] : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \Big\} = 2[\hat{X}_{ii} > 0]\hat{X}_{ki} = 2\hat{X}_{ki}$$

whereas

$$[C_k]_{i0} = \hat{X}_{ik} + \hat{X}_{i0} \sum \left\{ \frac{\hat{X}_{k\ell}}{\hat{X}_{\ell\ell}} [\ell = i] : \ell \in V,\, \hat{X}_{\ell\ell} > 0 \right\} = \hat{X}_{ik} + [\hat{X}_{ii} > 0] \hat{X}_{ki} = 2\hat{X}_{ki}. \tag{4.39}$$

This concludes the proof of (4.37).

We claim that

$$\text{if } k, \ell \in V \text{ are such that } \hat{X}_{kk} > 0 \text{ and } \hat{X}_{\ell\ell} > 0, \text{then } \hat{X}_{kk} = \hat{X}_{\ell\ell} = \hat{X}_{k\ell}. \tag{4.40}$$

Let $k, \ell \in V$ be distinct such that $\hat{X}_{kk} > 0$ and $\hat{X}_{\ell\ell} > 0$. Set

$$D := \frac{1}{\hat{X}_{kk}} C_k - \frac{1}{\hat{X}_{\ell\ell}} C_\ell.$$

Note that $[C_k]_{00} = 2\hat{X}_{0k} = 2\hat{X}_{kk}$ and $[C_\ell]_{00} = 2\hat{X}_{0\ell} = 2\hat{X}_{\ell\ell}$, whence $D_{00} = 0$. Hence, $D \in \operatorname{Null}(\mathcal{B}_{\{0\}})$. By (4.37), we also have $D \in \operatorname{Null}(\mathcal{F})$. Thus, by Theorem 4.9, we must have $D = 0$. Now from (4.39) we get

$$0 = D_{k0} = \frac{[C_k]_{k0}}{\hat{X}_{kk}} - \frac{[C_\ell]_{k0}}{\hat{X}_{\ell\ell}} = \frac{2\hat{X}_{kk}}{\hat{X}_{kk}} - \frac{2\hat{X}_{\ell k}}{\hat{X}_{\ell\ell}} \implies \hat{X}_{\ell\ell} = \hat{X}_{\ell k}$$

and

$$0 = D_{\ell 0} = \frac{[C_k]_{\ell 0}}{\hat{X}_{kk}} - \frac{[C_\ell]_{\ell 0}}{\hat{X}_{\ell\ell}} = \frac{2\hat{X}_{k\ell}}{\hat{X}_{kk}} - \frac{2\hat{X}_{\ell\ell}}{\hat{X}_{\ell\ell}} \implies \hat{X}_{kk} = \hat{X}_{k\ell}.$$

This concludes the proof of (4.40).

From (4.40) we find that there exists $\eta \in \mathbb{R}$ such that

$$\hat{X} = (1 - \eta)\big[(1 \oplus 0)(1 \oplus 0)^\mathsf{T}\big] + \eta\big[(1 \oplus \mathbb{1}_S)(1 \oplus \mathbb{1}_S)^\mathsf{T}\big] \tag{4.41}$$

where $S := \operatorname{supp}(\operatorname{diag}(\hat{X}[V]))$. If $S = \varnothing$, the proof is complete, so assume that $S \neq \varnothing$. Then $\hat{X} \succeq 0$ is equivalent to $\eta \in [0, 1]$. If $\eta = 0$ the proof is complete, so assume $\eta > 0$. Then (4.41) describes the extreme point $\hat{X}$ as a convex combination of two distinct points of $\widehat{\mathscr{C}}$, from which we conclude that $\eta = 1$, whence $\operatorname{rank}(\hat{X}) = 1$. $\square$

We immediately obtain from Theorem 4.16 the vertices of all the lifted theta bodies described above:

Corollary 4.17. Let $G = (V, E)$ be a graph. Let $\widehat{\mathscr{C}} \in \big\{\widehat{\mathrm{TH}}(G), \widehat{\mathrm{TH}'}(G), \widehat{\mathrm{TH}^+}(G)\big\}$. Then a point $\hat{X}$ of $\widehat{\mathscr{C}}$ is a vertex of $\widehat{\mathscr{C}}$ if and only if $\operatorname{rank}(\hat{X}) = 1$. Thus, the vertices of $\widehat{\mathscr{C}}$ are precisely the matrices of the form $(1 \oplus \mathbb{1}_S)(1 \oplus \mathbb{1}_S)^\mathsf{T}$ where $S \subseteq V$ is a stable set of G.

Proof. Immediate from Theorem 4.16: for $\widehat{\mathscr{C}} = \widehat{\mathrm{TH}}(G)$, take $E^+ := E^- := E$; for $\widehat{\mathscr{C}} = \widehat{\mathrm{TH}'}(G)$, take $E^+ := \binom{V}{2}$ and $E^- := E$; for $\widehat{\mathscr{C}} = \widehat{\mathrm{TH}^+}(G)$, take $E^+ := \varnothing$ and $E^- := E$. $\square$

Let V be a finite set. Define

$$\begin{aligned}\mathrm{BQ}'_{\{0\}\cup V} &\coloneqq \bigl\{\, \hat{X} \in \mathrm{BQ}_{\{0\}\cup V} : \hat{X}[V] \geq 0 \bigr\},\\ \mathrm{BQ}''_{\{0\}\cup V} &\coloneqq \bigl\{\, \hat{X} \in \mathrm{BQ}_{\{0\}\cup V} : \bigl\langle \mathrm{Sym}\bigl((e_0 - e_i)(e_0 - e_j)^{\mathsf{T}}\bigr), \hat{X} \bigr\rangle \geq 0,\, \forall ij \in \tbinom{V}{2} \bigr\}.\end{aligned}$$

Like $\mathrm{BQ}_{\{0\}\cup V}$, these sets are also well-known relaxations for the lifting (4.18) of the boolean quadric polytope. Also, define the square matrix Flip on index set $\{0\} \cup V$ as

$$\mathrm{Flip} \coloneqq e_0 e_0^{\mathsf{T}} + \sum_{i\in V} e_i (e_0 - e_i)^{\mathsf{T}} = \begin{bmatrix} 1 & 0^{\mathsf{T}} \\ \bar{e} & -I \end{bmatrix}. \tag{4.42}$$

Note that $\mathrm{Flip}(1 \oplus \mathbb{1}_S) = (1 \oplus \mathbb{1}_{V\setminus S})$ for each $S \subseteq V$. It is easy to check that $\mathrm{Congr}_{\mathrm{Flip}}$ is an automorphism of $\mathrm{BQ}_{\{0\}\cup V}$, and that

$$\mathrm{Congr}_{\mathrm{Flip}}\bigl(\mathrm{BQ}'_{\{0\}\cup V}\bigr) = \mathrm{BQ}''_{\{0\}\cup V}\,. \tag{4.43}$$

Corollary 4.18. Let V be a finite set. Let $\widehat{\mathscr{C}} \in \bigl\{\mathrm{BQ}_{\{0\}\cup V}, \mathrm{BQ}'_{\{0\}\cup V}, \mathrm{BQ}''_{\{0\}\cup V}\bigr\}$. Then a point $\hat{X}$ of $\widehat{\mathscr{C}}$ is a vertex of $\widehat{\mathscr{C}}$ if and only if $\mathrm{rank}(\hat{X}) = 1$. Thus, the vertices of $\widehat{\mathscr{C}}$ are precisely the matrices of the form $(1 \oplus \mathbb{1}_S)(1 \oplus \mathbb{1}_S)^{\mathsf{T}}$ where $S \subseteq V$.

Proof. For $\widehat{\mathscr{C}} \in \bigl\{\mathrm{BQ}_{\{0\}\cup V}, \mathrm{BQ}'_{\{0\}\cup V}\bigr\}$, this follows from Corollary 4.17 via Lemma 4.8, since $\mathrm{BQ}_{\{0\}\cup V} = \widehat{\mathrm{TH}}(\overline{K_V})$ and $\mathrm{BQ}'_{\{0\}\cup V} = \widehat{\mathrm{TH}}'(\overline{K_V})$. For $\widehat{\mathscr{C}} = \mathrm{BQ}''_{\{0\}\cup V}$, this follows from the previous sentence together with (4.43) and Lemma 4.8. $\square$

Currently, we do not know whether all the vertices of the relaxation $\mathrm{BQ}'_{\{0\}\cup V} \cap \mathrm{BQ}''_{\{0\}\cup V}$ of the lifting (4.18) of the boolean quadric polytope have rank one.

Let V be a finite set. Define

$$\begin{aligned}\mathscr{E}'_{\{0\}\cup V} &\coloneqq \bigl\{\, \hat{X} \in \mathscr{E}_{\{0\}\cup V} : \bigl\langle \mathrm{Sym}\bigl((e_0 + e_i)(e_0 + e_j)^{\mathsf{T}}\bigr), \hat{X} \bigr\rangle \geq 0,\, \forall ij \in \tbinom{V}{2} \bigr\},\\ \mathscr{E}''_{\{0\}\cup V} &\coloneqq \bigl\{\, \hat{X} \in \mathscr{E}_{\{0\}\cup V} : \bigl\langle \mathrm{Sym}\bigl((e_0 - e_i)(e_0 - e_j)^{\mathsf{T}}\bigr), \hat{X} \bigr\rangle \geq 0,\, \forall ij \in \tbinom{V}{2} \bigr\}.\end{aligned}$$

Like $\mathscr{E}_{\{0\}\cup V}$, these sets are also relaxations for the set $\mathrm{conv}\bigl\{\, (1 \oplus x)(1 \oplus x)^{\mathsf{T}} : x \in \{\pm 1\}^V \bigr\}$, which is a variant of the cut polytope. It is easy to check that

$$\mathrm{Congr}_{\mathrm{Bool}}(\mathscr{E}_{\{0\}\cup V}) = \mathrm{BQ}_{\{0\}\cup V}, \tag{4.44a}$$

$$\mathrm{Congr}_{\mathrm{Bool}}(\mathscr{E}'_{\{0\}\cup V}) = \mathrm{BQ}'_{\{0\}\cup V}, \tag{4.44b}$$

$$\mathrm{Congr}_{\mathrm{Bool}}(\mathscr{E}''_{\{0\}\cup V}) = \mathrm{BQ}''_{\{0\}\cup V}\,. \tag{4.44c}$$

We thus immediately get the following generalization of Corollary 4.11:

Corollary 4.19. Let V be a finite set. Let $\widehat{\mathscr{C}} \in \bigl\{\mathscr{E}_{\{0\}\cup V}, \mathscr{E}'_{\{0\}\cup V}, \mathscr{E}''_{\{0\}\cup V}\bigr\}$. Then a point $\hat{X}$ of $\widehat{\mathscr{C}}$ is a vertex of $\widehat{\mathscr{C}}$ if and only if $\mathrm{rank}(\hat{X}) = 1$. Thus, the vertices of $\widehat{\mathscr{C}}$ are precisely the matrices of the form $(1 \oplus x_S)(1 \oplus x_S)^{\mathsf{T}}$ where $x_S = \mathbb{1}_S - \mathbb{1}_{V\setminus S}$ for some $S \subseteq V$.

Proof. Immediate from Corollary 4.18 and (4.44) via Lemma 4.8. $\square$

Corollary 4.19 allows us to gauge the extent to which Corollary 4.17 generalizes Corollary 4.11: the latter result characterizes the vertices for one convex set for each positive integer n, whereas the former does the same for each positive integer n and every graph with n nodes.

Kleinberg and Goemans [77] presented SDP relaxations for the vertex cover problem. For a graph $G = (V, E)$, the feasible regions of their relaxations are:

$$\widehat{\mathrm{VC}}(G) \coloneqq \big\{\, \hat{X} \in \mathscr{E}_{\{0\}\cup V} : \big\langle \mathrm{Sym}\big((e_0 - e_i)(e_0 - e_j)^\mathsf{T}\big), \hat{X} \big\rangle = 0,\ \forall ij \in E \big\},$$
$$\widehat{\mathrm{VC}}'(G) \coloneqq \widehat{\mathrm{VC}}(G) \cap \mathscr{E}''_{\{0\}\cup V}.$$

It is easy to verify that

$$\widehat{\mathrm{VC}}(G) = \big(\mathrm{Congr}_{\mathrm{Bool}}^{-1} \circ \mathrm{Congr}_{\mathrm{Flip}}\big)\big(\widehat{\mathrm{TH}}(G)\big), \tag{4.45a}$$
$$\widehat{\mathrm{VC}}'(G) = \big(\mathrm{Congr}_{\mathrm{Bool}}^{-1} \circ \mathrm{Congr}_{\mathrm{Flip}}\big)\big(\widehat{\mathrm{TH}}'(G)\big), \tag{4.45b}$$

i.e., $\widehat{\mathrm{VC}}(G)$ is obtained from $\widehat{\mathrm{TH}}(G)$ by complementing each entry via the map $x \in \mathbb{R}^V \mapsto \bar{e} - x$ and then converting to a $\{\pm 1\}$ formulation.

Corollary 4.20. Let $G = (V, E)$ be a graph. Let $\widehat{\mathscr{C}} \in \big\{\widehat{\mathrm{VC}}(G), \widehat{\mathrm{VC}}'(G)\big\}$. Then a point $\hat{X}$ of $\widehat{\mathscr{C}}$ is a vertex of $\widehat{\mathscr{C}}$ if and only if $\mathrm{rank}(\hat{X}) = 1$. Thus, the vertices of $\widehat{\mathscr{C}}$ are precisely the matrices of the form $(1 \oplus \mathbb{1}_S)(1 \oplus \mathbb{1}_S)^\mathsf{T}$ where $S \subseteq V$ is a vertex cover of G.

Proof. Immediate from Corollary 4.17 and (4.45) via Lemma 4.8. □

Let $G = (V, E)$ be a graph. The Lovász theta number is usually presented in the form

$$\vartheta(G) = \max\big\{\, \langle \bar{e}\bar{e}^\mathsf{T}, X\rangle : \langle I, X\rangle = 1,\ \mathcal{A}_E(X) = 0,\ X \in \mathbb{S}^V_+ \big\}, \tag{4.46}$$

as we have seen in (2.17). Note that, if $S \subseteq V$ is a stable set of G, then $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^\mathsf{T}$ is feasible in (2.17) with objective value $|S|$. Moreover, if we add the constraint $\mathrm{rank}(X) = 1$, then every optimal solution is of the form $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^\mathsf{T}$ for some maximum stable set S of G. Thus, the feasible solutions of the SDP (4.46) which we would consider the exact solutions have the form $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^\mathsf{T}$ for some $S \subseteq V$. Similarly, the variants $\vartheta'(G)$ and $\vartheta^+(G)$ are usually presented as

$$\vartheta'(G) = \max\big\{\, \langle \bar{e}\bar{e}^\mathsf{T}, X\rangle : \mathrm{Tr}(X) = 1,\ \mathcal{A}_E(X) = 0,\ \mathcal{A}_{\overline{E}}(X) \geq 0,\ X \in \mathbb{S}^V_+ \big\}, \tag{4.47}$$
$$\vartheta^+(G) = \max\big\{\, \langle \bar{e}\bar{e}^\mathsf{T}, X\rangle : \mathrm{Tr}(X) = 1,\ \mathcal{A}_E(X) \leq 0,\ S \in \mathbb{S}^V_+ \big\}, \tag{4.48}$$

as we have seen in (2.62) and (2.64). For both of these SDPs, the feasible solutions that are sensible to be called exact also have the form $\frac{1}{|S|}\mathbb{1}_S\mathbb{1}_S^\mathsf{T}$ for some $S \subseteq V$. However, as the next result shows, the vertices of the feasible regions of these SDPs do not coincide with what we consider their exact solutions. We shall denote the degree of a node k in a graph G by $\deg_G(k)$.

Theorem 4.21. Let V be a finite set, and let $E^+, E^- \subseteq \binom{V}{2}$. Let H denote the graph $(V, E^+ \cup E^-)$, and set

$$\mathscr{C} \coloneqq \big\{\, X \in \mathbb{S}^V_+ : \mathrm{Tr}(X) = 1,\ \mathcal{A}_{E^+}(X) \geq 0,\ \mathcal{A}_{E^-}(X) \leq 0 \big\},$$

Then the set of vertices of $\mathscr{C}$ is $\big\{\, e_k e_k^\mathsf{T} : \deg_H(k) = |V| - 1 \big\}$.

Proof. We first show that

$$\text{if } \bar{X} \text{ is a vertex of } \mathscr{C}, \text{ then } \bar{X} = e_k e_k^\mathsf{T} \text{ for some } k \in V. \tag{4.49}$$

Let $\bar{X}$ be a vertex of $\mathscr{C}$. Let $k, \ell \in V$ be distinct. Set

$$\tfrac{1}{2} D \coloneqq \bar{X}_{\ell\ell} \operatorname{Sym}(\bar{X} e_k e_k^\mathsf{T}) - \bar{X}_{kk} \operatorname{Sym}(\bar{X} e_\ell e_\ell^\mathsf{T}).$$

If $i, j \in V$, then

$$\begin{aligned} D_{ij} &= \bar{X}_{\ell\ell}\Big(\bar{X}_{ik}[k=j] + [k=i]\bar{X}_{kj}\Big) - \bar{X}_{kk}\Big(\bar{X}_{i\ell}[\ell=j] + [\ell=i]\bar{X}_{\ell j}\Big) \\ &= \bar{X}_{\ell\ell}\bar{X}_{ij}\big([k=j]+[k=i]\big) - \bar{X}_{kk}\bar{X}_{ij}\big([\ell=j]+[\ell=i]\big) \\ &= \bar{X}_{ij}\Big[\bar{X}_{\ell\ell}\big([k=j]+[k=i]\big) - \bar{X}_{kk}\big([\ell=j]+[\ell=i]\big)\Big]. \end{aligned}$$

For $ij \in \binom{V}{2}$, we clearly have $D_{ij} = 0$ whenever $\bar{X}_{ij} = 0$. We also have

$$\operatorname{Tr}(D) = D_{kk} + D_{\ell\ell} = \big(2\bar{X}_{kk}\bar{X}_{\ell\ell}\big) + \big(-2\bar{X}_{\ell\ell}\bar{X}_{kk}\big) = 0.$$

Note that $|V|^{-1}I$ lies in $\mathscr{C} \cap \mathbb{S}^V_{++}$, so we may apply Theorem 4.9 to get $D = 0$. Thus, $0 = D_{kk} = 2\bar{X}_{kk}\bar{X}_{\ell\ell}$. Since k and ℓ were arbitrary, (4.49) follows from $\operatorname{Tr}(\bar{X}) = 1$.

We will now show that,

$$\text{for } k \in V, \text{ the point } e_k e_k^\mathsf{T} \text{ is a vertex of } \mathscr{C} \text{ if and only if } \deg_H(k) = |V| - 1. \tag{4.50}$$

Let $k \in V$. Set $E \coloneqq E^+ \cup E^-$. By Theorem 4.9, the point $e_k e_k^\mathsf{T}$ is a vertex of $\mathscr{C}$ if and only if $\{e_k\} \cup \{\, 2\operatorname{Sym}(e_i e_j^\mathsf{T}) e_k : ij \in E\}$ spans $\mathbb{R}^V$. The latter set is $\{e_k\} \cup \{\, [j=k]e_i + [i=k]e_j : ij \in E\} = \{e_k\} \cup \{\, e_j : jk \in E\}$, so it spans $\mathbb{R}^V$ precisely when $\deg_H(k) = |V| - 1$.

The result now follows from (4.49) and (4.50). ☐

Corollary 4.22. Let $G = (V, E)$ be a graph. Set $P \coloneqq \{\, k \in V : \deg_G(k) = |V| - 1\}$. Then

(i) the set of vertices of $\{\, X \in \mathbb{S}^V_+ : \operatorname{Tr}(X) = 1, \mathcal{A}_E(X) = 0\}$ is $\{\, e_k e_k^\mathsf{T} : k \in P\}$;
(ii) the set of vertices of $\{\, X \in \mathbb{S}^V_+ : \operatorname{Tr}(X) = 1, \mathcal{A}_E(X) = 0, \mathcal{A}_{\overline{E}}(X) \geq 0\}$ is $\{\, e_k e_k^\mathsf{T} : k \in V\}$;
(iii) the set of vertices of $\{\, X \in \mathbb{S}^V_+ : \operatorname{Tr}(X) = 1, \mathcal{A}_E(X) \leq 0\}$ is $\{\, e_k e_k^\mathsf{T} : k \in P\}$.

Proof. Immediate from Theorem 4.21, as in the proof of Corollary 4.17. ☐

The results in this chapter significantly extend the combinatorially-inspired spectrahedra whose vertices are completely understood. However, we do not know the set of vertices of some of their simplest variants, such as $\mathrm{BQ}'_{\{0\}\cup V} \cap \mathrm{BQ}''_{\{0\}\cup V}$ or even

$$\big\{\, \hat{X} \in \mathrm{BQ}_{\{0\}\cup V} : \big\langle \operatorname{Sym}\big(e_i(e_i - e_j)^\mathsf{T}\big), \hat{X}\big\rangle \geq 0, \forall (i,j) \in V \times V \big\}; \tag{4.51}$$

the constraints of the latter usually appear in spectrahedra arising from the lift-and-project operator of Lovász and Schrijver [101]. This is just a hint of the complexity of the vertex structure of spectrahedra. We roughly discuss some other difficulties next.

When considering sufficient conditions which bound the rank of vertices of a spectrahedron, such as the ones from Theorem 4.10 and Proposition 4.13, ideally one seeks to obtain coordinate-free conditions that are easy to check and that have a built-in detection for a change of basis. Let us use Theorem 4.10 to explain this. Suppose we replace the rank hypothesis from that theorem with the condition that $A_i A_j = 0$ for distinct $i, j \in [n]$. Note that we eventually reach this assumption in (4.25) in its proof. Then the modified theorem would be applicable to the elliptope $\mathscr{E}_{\{0\}\cup V}$, but not to its linear isomorphic image

$$\left\{ \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \left\langle (e_0 - 2e_i)(e_0 - 2e_i)^\mathsf{T}, \hat{X} \right\rangle = 1 \,\forall i \in \{0\} \cup V \right\},$$

which is nothing but $\mathrm{BQ}_{\{0\}\cup V}$. What happened in this case was that we have the following equivalence: there exists a nonsingular $L \in \mathbb{R}^{n\times n}$ such that $\mathrm{Congr}_L(A_i)\,\mathrm{Congr}_L(A_j) = 0$ for distinct $i, j \in [n]$ if and only if the rank condition from Theorem 4.10 holds. That is, a simple algebraic condition subsumes an existential predicate about a convenient basis; the rank condition factors out the trivial congruences. This is in contrast with the existential hypothesis from Proposition 4.13, which is harder to check, and thus harder to apply. However, Theorem 4.10 is not yet entirely coordinate-free; this may be seen from the fact that it does not apply directly to $\mathrm{BQ}_{\{0\}\cup V}$ using its description in (4.20), since the theorem requires the RHS of the defining linear equations to be nonzero everywhere. In this sense, Theorem 4.10 still has room for improvement.

The algebraic aspects just described have a complementary role to geometry in some situations. For instance, it is easy to see how to start with a spectrahedron all of whose vertices have rank one and transform it into one that has all vertices of rank two; one could take a direct sum with a constant nonzero block, and apply a congruence transformation to "hide" the triviality of this transformation. Here the geometric aspect of the transformation is trivial. However, a broad sufficient condition to bound the rank of vertices needs to factor out all these congruences. This seems hard to describe algebraically without an existential hypothesis. On the other direction, Corollary 4.14 describes a transformation of spectrahedra that is trivial in terms of algebra, but geometrically it modifies the boundary structure drastically.

Chapter 5

An Axiomatic Generalization of Theta Bodies

The Lovász theta function may be defined in a number of equivalent forms, that is to say, it has a host of alternative characterizations. Some of these involve the geometric object known as orthonormal representation of a graph, as was already mentioned throughout Chapter 2. The graph invariant $\vartheta(G)$ also admits a weighted generalization $\vartheta(G;w)$ for any nonnegative weight function w on the nodes of G. When w is integral, $\vartheta(G;w)$ is just the theta number of a certain "blown up" graph, as was briefly alluded to in Section 2.4. This weighted theta number also admits numerous characterizations, each of which being more convenient than the others depending on the context. The monograph [59, Sec. 9.3], which develops much of the theory surrounding the theta number, defines weighted parameters $\vartheta_i(G;w)$ for each $i \in [4]$ and shows that they are all equal to $\vartheta(G;w)$ by proving the chain of inequalities

$$\vartheta(G;w) \leq \vartheta_1(G;w) \leq \vartheta_2(G;w) \leq \vartheta_3(G;w) \leq \vartheta_4(G;w) \leq \vartheta(G;w); \tag{5.1}$$

see also [78, Sec. 5]. The proofs of some of these inequalities can be summarized as a change of variables, at the risk of not giving them due justice. Others are deeper and require a more refined tool, namely the Strong Duality Theorem for SDPs, and this leads us immediately to a geometric viewpoint on the theta function.

For a graph $G = (V, E)$, the function $w \in \mathbb{R}^V_+ \mapsto \vartheta(G;w)$ is the support function of the convex subset of $\mathbb{R}^V_+$ known as the theta body of G, denoted by $\mathrm{TH}(G)$. Thus, it can be said that the function $\vartheta(G;\cdot)$ and the convex set $\mathrm{TH}(G)$ encode precisely the same information. The set $\mathrm{TH}(G)$ is in fact a convex corner, that is, it is a compact, lower-comprehensive convex subset of the nonnegative orthant with nonempty interior. In this geometric context, the characterizations of $\vartheta(G;w)$ that involve the Strong Duality Theorem correspond to applications of Antiblocking Duality to $\mathrm{TH}(G)$. It is arguable that all such characterizations are subsumed by the beautiful duality relation

$$\mathrm{abl}(\mathrm{TH}(G)) = \mathrm{TH}(\overline{G}), \tag{5.2}$$

where $\mathrm{abl}(\cdot)$ denotes the antiblocker.

The relation (5.2) is striking in a number of ways. Consider the fact that the set $\mathrm{TH}(G)$ is a nonlinear object in general, since it is known to be non-polyhedral whenever G is not a perfect graph. The boundary structure of $\mathrm{TH}(G)$ is thus expected to be much more complex than that of the objects usually studied in polyhedral combinatorics. Since the boundary of $\mathrm{TH}(G)$ is completely described by its antiblocker, it is quite surprising that $\mathrm{abl}(\mathrm{TH}(G))$ may be obtained from $\mathrm{TH}(G)$ by such a primitive combinatorial operation as taking the complement of G. The simplicity of the latter operation also translates to a simple change in algebraic description, since $\mathrm{TH}(G)$ is given by the following expression:

$$\mathrm{TH}(G) = \left\{ x \in \mathbb{R}^V : \exists X \in \mathbb{S}^V,\, X_{ii} = x_i \,\forall i \in V,\, X_{ij} = 0 \,\forall ij \in E,\, \begin{bmatrix} 1 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathbb{S}_+^{\{0\}\cup V} \right\}. \tag{5.3}$$

To describe another remarkable feature of (5.2), namely its primal-dual symmetry, we shall bring some other similar duality relations into the picture. These relations are

$$\mathrm{abl}(\mathrm{STAB}(G)) = \mathrm{QSTAB}(\overline{G}), \tag{5.4}$$

$$\mathrm{abl}(\mathrm{TH}'(G)) = \mathrm{TH}^+(\overline{G}). \tag{5.5}$$

In (5.4), $\mathrm{STAB}(G)$ is the stable set polytope of G and $\mathrm{QSTAB}(G)$ is the fractional stable set polytope of G; in fact, (5.4) is usually taken to be the definition of the latter. As for (5.5), the convex corners $\mathrm{TH}'(G)$ and $\mathrm{TH}^+(G)$ arise from the weighted variants $\vartheta'(G;\cdot)$ and $\vartheta^+(G;\cdot)$ analogously as $\mathrm{TH}(G)$ arises from $\vartheta(G;\cdot)$, and (5.5) is usually proved in a similar way to (5.2). The duality relations (5.2), (5.4), and (5.5) are equivalent to corresponding Cauchy-Schwarz-type inequalities involving the support functions of the underlying convex corners: for each $w, \bar{w} \in \mathbb{R}_+^V$, we have

$$\langle w, \bar{w} \rangle \leq \vartheta(G; w)\vartheta(\overline{G}; \bar{w}), \tag{5.6}$$

$$\langle w, \bar{w} \rangle \leq \alpha(G; w)\chi^*(\overline{G}; \bar{w}), \tag{5.7}$$

$$\langle w, \bar{w} \rangle \leq \vartheta'(G; w)\vartheta^+(\overline{G}; \bar{w}). \tag{5.8}$$

Here $\alpha(G;\cdot)$ and $\chi^*(G;\cdot)$ are the support functions of $\mathrm{STAB}(G)$ and $\mathrm{QSTAB}(G)$, respectively. Some other inequalities of this type, though in unweighted form, are proved in [61, Theorem 3.1, Proposition 3.5] and in [37, Proposition 8]. By comparing either (5.2) with (5.4) and (5.5), or (5.6) with (5.7) and (5.8), it is clear that (5.2) and (5.6) enjoy a strong form of primal-dual symmetry. Moreover, the striking similarity between the duality relations (5.2), (5.4), and (5.5), involving such fundamental convex sets related to the stable set and clique covering numbers of graphs, seems to demand a common generalization, hopefully shedding some light on the primal-dual symmetry enjoyed by $\mathrm{TH}(G)$.

The weighted variants $\vartheta'(G;\cdot)$ and $\vartheta^+(G;\cdot)$ of the theta function also admit some of the alternative characterizations of $\vartheta(G;\cdot)$. Namely, each of the functions $\vartheta_i(G;\cdot)$ for $i \in [4]$ may be adapted to the contexts of $\vartheta'(G;\cdot)$ so that a chain of inequalities corresponding to (5.1) holds, and similarly for $\vartheta^+(G;\cdot)$. For instance, in [51], after developing some of the functions $\vartheta_i(G;\cdot)$ with $i \in [4]$, Goemans precedes the corresponding functions $\vartheta_i'(G;\cdot)$ for $\vartheta'(G;\cdot)$ by saying: "The validity of these formulations follow easily from the same arguments as before." Thus, to prove the validity of the chain of inequalities for $\vartheta'(G;\cdot)$ corresponding to (5.1), we are led to the error-prone process of adapting each of the corresponding proofs for $\vartheta(G;\cdot)$, rather than applying a black-box result. (And indeed there are errors in the literature concerning the functions $\vartheta_i'(G;\cdot)$, as we pointed out in [22, Sec. 4.1].) This inconvenience is aggravated by the fact that the proofs for $\vartheta(G;\cdot)$ under consideration seem to rely on *ad hoc* properties of orthonormal representations.

It thus seems appropriate to develop a framework that allows each of these proofs to be applied as a black-box to the parameters $\vartheta(G;\cdot)$, $\vartheta'(G;\cdot)$, and $\vartheta^+(G;\cdot)$, and perhaps more. Moreover, by abstracting the most essential parts of the proofs of (5.1), one may gauge the full power of the proof methods involved.

In this chapter, we shall present a framework that achieves some of the aforementioned goals. We will define a family of generalized theta bodies, which include the members $\mathrm{TH}(G)$, $\mathrm{TH}'(G)$, $\mathrm{TH}^+(G)$, $\mathrm{STAB}(G)$, and $\mathrm{QSTAB}(G)$, and we shall prove a generalized antiblocking duality relation which includes (5.2), (5.4), and (5.5). The chain of inequalities corresponding to (5.1) shall also be proved for a generalized theta function ϑ, defined as the support function of the generalized theta body under consideration, and the corresponding variants ϑ_i with $i \in [4]$.

The main contribution in this chapter is Theorem 5.16, which subsumes the antiblocking relations (5.2), (5.4), and (5.5). However, the full significance of that theorem is only revealed by the axiomatic development in the chapter seen as a whole. This includes Theorem 5.9 on the convexity of a certain cone, and the descriptions of some classical relaxations of the stable set polytope as generalized theta bodies, given by Propositions 5.11 and 5.18 and Corollary 5.21.

Some of our results may be regarded as a weighted generalization of part of [37, Sec. 5], and they are quite different from another generalization of theta bodies introduced in [57].

We set the following notation. Throughout the chapter, V shall denote a finite set. For $w \in \mathbb{R}^V_+$, we denote by $\sqrt{w}$ the vector in $\mathbb{R}^V$ defined by

$$[\sqrt{w}\,]_i := \sqrt{w_i} \qquad \forall i \in V. \tag{5.9}$$

The *Hadamard product* $\odot$ is the componentwise product: if $x, y \in \mathbb{R}^V$, then $x \odot y$ denotes the vector in $\mathbb{R}^V$ defined by

$$[x \odot y]_i := x_i y_i \qquad \forall i \in V, \tag{5.10}$$

and if X, Y lies in $\mathbb{R}^{V\times W}$ for some finite set W, then $X \odot Y$ denotes the matrix in $\mathbb{R}^{V\times W}$ defined by

$$[X \odot Y]_{ij} := X_{ij} Y_{ij} \qquad \forall (i,j) \in V \times W. \tag{5.11}$$

If $A \in \mathbb{R}^{V\times W}$, then $A^\dagger$ denotes the Moore-Penrose pseudoinverse of A; see [72] for a definition and basic properties. For $E^+, E^- \subseteq \binom{V}{2}$, set

$$\mathbb{A}_{E^+,E^-} := \{\, X \in \mathbb{S}^V : \mathcal{A}_{E^+}(X) \geq 0,\, \mathcal{A}_{E^-}(X) \leq 0\}, \tag{5.12}$$

where for $E \subseteq \binom{V}{2}$ the linear map $\mathcal{A}_E \colon \mathbb{S}^V \to \mathbb{R}^E$ is defined as in (2.16). We also make use of the linear map $\mathcal{B}_{\{0\}\cup V} \colon \mathbb{S}^{\{0\}\cup V} \to \mathbb{R}^{\{0\}\cup V}$ defined in (4.19). We shall use some basic concepts from convex analysis, and we follow mostly the notation from [123]. Let $\mathscr{C} \subseteq \mathbb{E}$. The *closure* of $\mathscr{C}$ is denoted by $\mathrm{cl}(\mathscr{C})$. The *support function of* $\mathscr{C}$ is the (extended-real-valued) map $\delta^*(\cdot \,|\, \mathscr{C})$ on $\mathbb{E}^*$ defined by

$$\delta^*(w \,|\, \mathscr{C}) := \sup\big\{\, \langle w, x\rangle : x \in \mathscr{C} \big\} \qquad \forall w \in \mathbb{E}^*. \tag{5.13}$$

The *gauge of* $\mathscr{C}$ is the function:

$$\gamma(x \,|\, \mathscr{C}) := \inf\big\{\, \mu : \mu \in \mathbb{R}_+,\, x \in \mu\mathscr{C} \big\} \qquad \forall x \in \mathbb{E}. \tag{5.14}$$

The *polar of* $\mathscr{C}$ is

$$\mathscr{C}^\circ := \big\{\, y \in \mathbb{E}^* : \langle x, y\rangle \leq 1 \,\forall x \in \mathscr{C} \big\}. \tag{5.15}$$

For $\mathscr{C} \subseteq \mathbb{R}^V_+$, the *antiblocker of* $\mathscr{C}$ is

$$\mathrm{abl}(\mathscr{C}) := \mathscr{C}^\circ \cap \mathbb{R}^V_+. \tag{5.16}$$

5.1 Theta Bodies

For each $h \in \mathbb{R}^V$, define the *diagonally scaling* map

$$\mathcal{D}_h \coloneqq \mathrm{Congr}_{\mathrm{Diag}(h)}\,. \tag{5.17}$$

Note that $\mathcal{D}_h(X) = X \odot hh^{\mathsf{T}}$ for every $X \in \mathbb{S}^V$ and $h \in \mathbb{R}^V$. A subset $\mathbb{K}$ of $\mathbb{S}^V$ is called *diagonally scaling-invariant* if $\mathcal{D}_h(\mathbb{K}) \subseteq \mathbb{K}$ for every $h \in \mathbb{R}^V_+$. Some examples of scaling invariants subsets of $\mathbb{S}^V$ are the positive semidefinite cone $\mathbb{S}^V_+$, the set of nonnegative symmetric matrices $\mathbb{S}^V_{\geq 0}$, and sets of the form $\mathbb{A}_{E^+,E^-}$ for some $E^+, E^- \subseteq \binom{V}{2}$. Clearly, every diagonally scaling-invariant set is a cone, and since the map $\mathcal{D}_h$ is self-adjoint, diagonal scaling invariance is preserved under duality. Moreover,

$$\text{if } \mathbb{K} \subseteq \mathbb{S}^V \text{ is diagonally scaling-invariant, then } \{\, \mathcal{D}_h : h \in \mathbb{R}^V_{++} \} \subseteq \mathrm{Aut}(\mathbb{K}). \tag{5.18}$$

For sets $\mathbb{A} \subseteq \mathbb{S}^V$ and $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\}\cup V}$, define

$$\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}}) \coloneqq \Big\{\, \hat{X} \in \widehat{\mathbb{K}} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\ \hat{X}[V] \in \mathbb{A} \Big\} \tag{5.19}$$

and

$$\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}) \coloneqq \Big\{\, \mathrm{diag}(\hat{X}[V]) : \hat{X} \in \widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}}) \Big\}. \tag{5.20}$$

We are interested in sets of the form $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$, where $\mathbb{A}$ and $\widehat{\mathbb{K}}$ are diagonally scaling-invariant convex cones with a few extra properties. The most important examples of sets of this form are the theta body $\mathrm{TH}(G)$ of a graph $G = (V, E)$ and its variants $\mathrm{TH}'(G)$ and $\mathrm{TH}^+(G)$. In fact, we define

$$\mathrm{TH}(G) \coloneqq \mathrm{TH}\big(\mathbb{A}_{E,E}, \mathbb{S}^{\{0\}\cup V}_+\big), \tag{5.21a}$$

$$\mathrm{TH}'(G) \coloneqq \mathrm{TH}\big(\mathbb{A}_{\binom{V}{2},E}, \mathbb{S}^{\{0\}\cup V}_+\big), \tag{5.21b}$$

$$\mathrm{TH}^+(G) \coloneqq \mathrm{TH}\big(\mathbb{A}_{\varnothing,E}, \mathbb{S}^{\{0\}\cup V}_+\big). \tag{5.21c}$$

It thus makes sense to call sets of the form $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ as *theta bodies*. We shall see later that the stable set polytope and some of its classical relaxations are also theta bodies. To avoid confusion, whenever we refer to the specific theta body $\mathrm{TH}(G)$, we shall call it *the* theta body *of* G.

We shall prove that, under certain simple hypotheses, every theta body is a *convex corner*, i.e., a compact, lower-comprehensive convex subset of the nonnegative orthant with nonempty interior. Recall that a subset $\mathscr{C}$ of $\mathbb{R}^V_+$ is called *lower-comprehensive* if, for any $x, y \in \mathbb{R}^V$, the relations $x \in \mathscr{C}$ and $0 \leq y \leq x$ imply $y \in \mathscr{C}$. In what follows, the extra hypotheses (5.22) and (5.23) on $\mathbb{A}$ and $\widehat{\mathbb{K}}$ may be thought of as requiring that $\mathbb{A}$ is not "too small", and that $\widehat{\mathbb{K}}$ is neither "too small" nor "too big."

Proposition 5.1. Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\}\cup V}$ be diagonally scaling-invariant closed convex cones. Suppose that $\mathbb{A}$ satisfies

$$\mathrm{Diag}(\mathbb{R}^V_+) \subseteq \mathbb{A}, \tag{5.22}$$

and suppose that $\widehat{\mathbb{K}}$ satisfies

$$\widehat{\mathbb{K}} \supseteq \big\{\, (e_0 + e_i)(e_0 + e_i)^{\mathsf{T}} : i \in V \big\} \tag{5.23a}$$

and

$$\operatorname{diag}\bigl(\{\, \hat{X} \in \widehat{\mathbb{K}} : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0 \}\bigr) \subseteq [0,1]^{\{0\}\cup V}. \tag{5.23b}$$

Then $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is a convex lower-comprehensive subset of $[0,1]^V$ with nonempty interior. In particular, $\mathrm{cl}\bigl(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})\bigr)$ is a convex corner.

Proof. Convexity follows from the fact that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is a projection of the convex set $\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$. It is clear from (5.23b) that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}) \subseteq [0,1]^V$. To prove that the convex set $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is lower-comprehensive, it suffices to show that if $x \in \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ then $x - x_i e_i \in \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ for each $i \in V$. Let $\hat{X} \in \widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$ such that $x = \operatorname{diag}(\hat{X}[V])$. Let $i \in V$. Set $\hat{Y} := \mathcal{D}_{1\oplus h}(\hat{X}) \in \widehat{\mathbb{K}}$ for $h := \bar{e} - e_i$. Then diagonal scaling invariance of $\mathbb{A}$ and $\widehat{\mathbb{K}}$ imply that $\hat{Y} \in \widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$. Thus, $x - x_i e_i = \operatorname{diag}(\hat{Y}[V]) \in \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$. This proves that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is lower-comprehensive. It remains to show that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ has nonempty interior. Let $i \in V$. By (5.22), we have $e_i e_i^{\mathsf{T}} \in \mathbb{A}$. Thus, $(e_0 + e_i)(e_0 + e_i)^{\mathsf{T}} \in \widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$ by (5.23a) whence $e_i \in \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$. Now convexity of $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ implies that $\frac{1}{n}\bar{e} \in \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$, where $n := |V|$. Since $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is lower-comprehensive, we find that $\frac{1}{2n}\bar{e} \in \operatorname{int}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}))$. □

Under a mild condition on the cone $\widehat{\mathbb{K}}$, already applicable to the descriptions of the sets $\mathrm{TH}(G)$, $\mathrm{TH}'(G)$, and $\mathrm{TH}^{+}(G)$ in (5.21), we can show that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is actually closed, and hence a convex corner:

Corollary 5.2. Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\}\cup V}$ be diagonally scaling-invariant closed convex cones such that (5.22) and (5.23a) hold. If

$$\widehat{\mathbb{K}} \subseteq \Bigl\{\, \hat{X} \in \mathbb{S}^{\{0\}\cup V} : \hat{X}[S] \succeq 0,\ \forall S \in \tbinom{\{0\}\cup V}{2} \Bigr\}, \tag{5.24}$$

then (5.23b) holds and $\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$ is compact. In particular, $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is closed, and hence a convex corner.

Proof. Let $\widehat{\mathbb{M}}$ be the set of all $\hat{X}$ in the RHS of (5.24) such that $\mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0$. Then $\widehat{\mathbb{M}}$ is bounded. To see this, first use sets $S \in \binom{\{0\}\cup V}{2}$ containing 0 to show that $\operatorname{diag}(\widehat{\mathbb{M}}) \subseteq [0,1]^{\{0\}\cup V}$. Note that this already proves (5.23b). Next, use (5.24) with sets $S \in \binom{V}{2}$ to show that all off-diagonal entries of $\hat{X} \in \widehat{\mathbb{M}}$ have absolute value bounded above by 1. Since $\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}}) \subseteq \widehat{\mathbb{M}}$, it follows that $\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$ is compact. Now closedness of $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ follows from the fact that $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ is a linear image of the compact set $\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}})$. The rest follows from Proposition 5.1. □

For many of the theta bodies in this chapter, the cone $\widehat{\mathbb{K}}$ shall be a subset of $\mathbb{S}_{+}^{\{0\}\cup V}$, and hence (5.24) shall be satisfied. An important diagonally scaling-invariant closed convex cone which does not satisfy (5.24) is the cone of copositive matrices. A matrix $X \in \mathbb{S}^V$ is said to be *copositive* if $h^{\mathsf{T}} X h \geq 0$ for every $h \in \mathbb{R}_{+}^{V}$, and the set of all copositive matrices in $\mathbb{S}^V$ is denoted by $\mathcal{C}_V$. Since $\mathbb{S}_{\geq 0}^{\{0\}\cup V} \subseteq \mathcal{C}_{\{0\}\cup V}$, it is clear that $\mathcal{C}_{\{0\}\cup V}$ does not satisfy (5.24). The copositive cone is also an example of a diagonally scaling-invariant closed convex cone with a rather complex facial structure. Namely, if $n \geq 2$, then each ray of $\mathcal{C}_n$ of the form $\mathbb{R}_{+} e_i e_i^{\mathsf{T}}$, with $i \in [n]$, is extreme but not exposed; see [34, Theorem 4.4]. We shall deal with theta bodies arising from the copositive cone in Section 5.7, where we shall prove the closedness of the corresponding theta body directly.

5.2 Polyhedral Diagonally Scaling-Invariant Cones

When studying a theta body $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$, we think of $\mathbb{A}$ as an "easy" cone, while $\widehat{\mathbb{K}}$ is (potentially) a "hard" cone. Here our use of the terms "easy" and "hard" is more similar to their intuitive use in continuous optimization, rather than their precise meaning bestowed by computational complexity. In the most important instances of theta bodies, described in (5.21), the cone $\mathbb{A}$ is polyhedral, whereas $\widehat{\mathbb{K}}$ is the nonlinear cone $\mathbb{S}_+^{\{0\}\cup V}$, whose corresponding membership problem is much harder. In general, it makes sense to focus on the case where $\mathbb{A}$ is polyhedral. At any rate, when defining a theta body $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$, any trace of "non-polyhedrality" may be "pushed" away from $\mathbb{A}$ and into $\widehat{\mathbb{K}}$. We shall show next that requiring a closed convex cone to be both diagonally scaling-invariant and polyhedral severely constrains its structure.

We shall need a family of cones slightly more refined than the cones $\mathbb{A}_{E^+,E^-}$ defined in (5.12). Let $V^+, V^- \subseteq V$ and $E^+, E^- \subseteq \binom{V}{2}$. Define

$$\mathbb{A}_{V^+,V^-,E^+,E^-} := \left\{ X \in \mathbb{S}^V : \operatorname{diag}(X[V^+]) \geq 0,\, \operatorname{diag}(X[V^-]) \leq 0,\, \mathcal{A}_{E^+}(X) \geq 0,\, \mathcal{A}_{E^-}(X) \leq 0 \right\}.$$

Clearly, every set of this form is diagonally scaling-invariant and polyhedral. In fact, every polyhedral diagonally scaling-invariant cone is of this form:

Proposition 5.3. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant closed convex cone. If $\mathbb{A}$ is polyhedral, then $\mathbb{A}$ is of the form $\mathbb{A} = \mathbb{A}_{V^+,V^-,E^+,E^-}$ for some subsets $V^+, V^- \subseteq V$ and $E^+, E^- \subseteq \binom{V}{2}$.

Proof. It suffices to show that

$$\text{every extreme ray of } \mathbb{A}^* \text{ is of the form } \pm\mathbb{R}_+ \operatorname{Sym}(e_i e_j^\mathsf{T}) \text{ for some } i, j \in V. \tag{5.25}$$

We first show that,

$$\text{if } \mathbb{R}_+ X \text{ is an extreme ray of } \mathbb{A}^*, \text{ then } \left|\operatorname{supp}\bigl(\operatorname{diag}(X)\bigr)\right| \leq 1. \tag{5.26}$$

Suppose that $\mathbb{R}_+ X$ is an extreme ray of $\mathbb{A}^*$ such that $X_{ii} \neq 0 \neq X_{jj}$ for distinct $i, j \in V$. Since $\mathbb{A}^*$ is also diagonally scaling-invariant, we have $\{\mathcal{D}_h : h \in \mathbb{R}^V_{++}\} \subseteq \operatorname{Aut}(\mathbb{A}^*)$. For $t \in \mathbb{R}_{++}$, define

$$h(t) := te_i + t^{-1}e_j + \mathbb{1}_{V\setminus\{i,j\}}.$$

Thus, $\{\mathbb{R}_+ \mathcal{D}_{h(t)}(X) : t \in \mathbb{R}_{++}\}$ is an infinite set of extreme rays of $\mathbb{A}^*$. This contradicts the fact that $\mathbb{A}^*$ is polyhedral and thus proves (5.26).

To prove (5.25), let $\mathbb{R}_+ X$ be an extreme ray of $\mathbb{A}^*$. Let us show that

$$X_{ij} \operatorname{Sym}(e_i e_j^\mathsf{T}) \in \mathbb{A}^* \qquad \forall i, j \in V. \tag{5.27}$$

Let $i, j \in V$. If $i = j$ then (5.27) holds by diagonal scaling invariance of $\mathbb{A}$, so assume $i \neq j$. By (5.26), at most one of X_{ii} and X_{jj} is nonzero. We may assume by symmetry that $X_{ii} = 0$. For $t \in \mathbb{R}_{++}$, define $h(t) := te_i + t^{-1}e_j$ and note that $\mathcal{D}_{h(t)}(X) \in \mathbb{A}^*$ for every $t \in \mathbb{R}_{++}$. By driving t to ∞ we find that $2X_{ij} \operatorname{Sym}(e_i e_j^\mathsf{T}) = \lim_{t\to\infty} \mathcal{D}_{h(t)}(X)$ lies in the closed set $\mathbb{A}^*$. This proves (5.27).

Since

$$X = \sum_{i,j\in V} 2^{[i\neq j]} X_{ij} \operatorname{Sym}(e_i e_j^\mathsf{T})$$

and $\mathbb{R}_+ X$ is an extreme ray of $\mathbb{A}^*$, it follows from (5.27) that at most one of the terms in the RHS is nonzero. This proves (5.25) and concludes the proof. ☐

We next show that, under the hypotheses (5.22) and (5.23) on $\mathbb{A}$ and $\widehat{\mathbb{K}}$ from Proposition 5.1 and the additional assumption that $\mathbb{A}$ is polyhedral, the constraints on the diagonal entries of $\mathbb{A}$ are irrelevant in the context of theta bodies. Thus, we shall not lose much when focusing only on cones $\mathbb{A}$ of the form $\mathbb{A}_{E^+,E^-}$.

Corollary 5.4. Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\}\cup V}$ be diagonally scaling-invariant closed convex cones such that (5.22) and (5.23) hold. If the cone $\mathbb{A}$ is polyhedral, then $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}) = \mathrm{TH}(\mathbb{A} + \mathrm{Im}(\mathrm{Diag}), \widehat{\mathbb{K}})$.

Proof. Set $\mathbb{A}' \coloneqq \mathbb{A} + \mathrm{Im}(\mathrm{Diag})$. It suffices to prove that

$$\widehat{\mathrm{TH}}(\mathbb{A}, \widehat{\mathbb{K}}) = \widehat{\mathrm{TH}}(\mathbb{A}', \widehat{\mathbb{K}}) \tag{5.28}$$

The inclusion '$\subseteq$' follows from $\mathbb{A} \subseteq \mathbb{A}'$. For the reverse inclusion, first note that Proposition 5.3 ensures the existence of $V^+, V^- \subseteq V$ and $E^+, E^- \subseteq \binom{V}{2}$ such that $\mathbb{A} = \mathbb{A}_{V^+,V^-,E^+,E^-}$. Then (5.22) implies $V^- = \varnothing$. Let $\hat{X} \in \widehat{\mathrm{TH}}(\mathbb{A}', \widehat{\mathbb{K}})$, and set $X \coloneqq \hat{X}[V]$. Assumption (5.23b) and the inclusion $X \in \mathbb{A}' = \mathbb{A}_{\varnothing,\varnothing,E^+,E^-}$ show that $X \in \mathbb{A}_{V,\varnothing,E^+,E^-} \subseteq \mathbb{A}$. This proves '$\supseteq$' in (5.28). ☐

5.3 Geometric Representations from Theta Bodies

The theta bodies described in (5.21) all have the form $\mathrm{TH}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V})$ for some $E^+, E^- \subseteq \binom{V}{2}$. The elements of these sets arise from certain vectors which may be regarded as geometric representations of graphs:

Proposition 5.5. Let $E^+, E^- \subseteq \binom{V}{2}$. Then $\mathrm{TH}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V})$ consists of all vectors $x \in \mathbb{R}^V$ of the form

$$x_i = \langle u_0, u_i \rangle^2 \qquad \forall i \in V \tag{5.29}$$

for vectors $\{\, u_i : i \in \{0\} \cup V \,\} \subseteq \mathbb{R}^{\{0\}\cup V}$ satisfying the following properties:

$$\begin{aligned}
&\langle u_0, u_i \rangle \geq 0 && \forall i \in V, && (5.30\text{a})\\
&\|u_i\| = 1 && \forall i \in \{0\} \cup V, && (5.30\text{b})\\
&\langle u_i, u_j \rangle \geq 0 && \forall ij \in E^+, && (5.30\text{c})\\
&\langle u_i, u_j \rangle \leq 0 && \forall ij \in E^-. && (5.30\text{d})
\end{aligned}$$

Proof. Set $\mathbb{A} \coloneqq \mathbb{A}_{E^+,E^-}$. Denote by $\mathscr{C}$ the set of all vectors x of the form given by (5.29) for vectors $\{\, u_i : i \in \{0\} \cup V \,\} \subseteq \mathbb{R}^{\{0\}\cup V}$ satisfying (5.30).

We first verify that

$$\mathscr{C} \subseteq \mathrm{TH}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V}). \tag{5.31}$$

Let $\{\, u_i : i \in \{0\} \cup V \,\} \subseteq \mathbb{R}^{\{0\}\cup V}$ satisfy (5.30). Define $U \in \mathbb{R}^{(\{0\}\cup V)\times V}$ by setting $Ue_i \coloneqq u_i$ for every $i \in V$. Next, set

$$Y \coloneqq U \,\mathrm{Diag}(U^\mathsf{T} u_0)$$

and

$$\hat{X} \coloneqq \begin{bmatrix} 1 & x^\mathsf{T} \\ x & X \end{bmatrix} \coloneqq \begin{bmatrix} u_0^\mathsf{T} u_0 & u_0^\mathsf{T} Y \\ Y^\mathsf{T} u_0 & Y^\mathsf{T} Y \end{bmatrix} = \begin{bmatrix} u_0^\mathsf{T} \\ Y^\mathsf{T} \end{bmatrix} \begin{bmatrix} u_0 & Y \end{bmatrix} \in \mathbb{S}_+^{\{0\}\cup V},$$

where we used (5.30b). Let us verify that

$$X \in \mathbb{A}_{E^+,E^-}, \tag{5.32a}$$
$$\operatorname{diag}(X) = x, \tag{5.32b}$$
$$x_i = \langle u_0, u_i\rangle^2 \qquad \forall i \in V. \tag{5.32c}$$

We start with (5.32a). Note that $X = Y^\mathsf{T} Y = \mathcal{D}_{U^\mathsf{T} u_0}\big(U^\mathsf{T} U\big)$ and $U^\mathsf{T} u_0 \geq 0$ by (5.30a). Since $\mathbb{A}_{E^+,E^-}$ is diagonally scaling-invariant, it suffices to show that $U^\mathsf{T} U \in \mathbb{A}_{E^+,E^-}$. But this is immediate from (5.30c) and (5.30d). This proves (5.32a). For (5.32c), note that

$$x = Y^\mathsf{T} u_0 = [\operatorname{Diag}(U^\mathsf{T} u_0) U^\mathsf{T}] u_0 = (U^\mathsf{T} u_0) \odot (U^\mathsf{T} u_0). \tag{5.33}$$

By (5.30b), we have $\operatorname{diag}(U^\mathsf{T} U) = \bar{e}$. Thus, $\operatorname{diag}(X) = \operatorname{diag}\big(\mathcal{D}_{U^\mathsf{T} u_0}(U^\mathsf{T} U)\big) = (U^\mathsf{T} u_0) \odot \operatorname{diag}(U^\mathsf{T} U) \odot (U^\mathsf{T} u_0) = (U^\mathsf{T} u_0) \odot (U^\mathsf{T} u_0) = x$ by (5.33), thus proving (5.32b). It follows that $x \in \operatorname{TH}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V})$, and the proof of (5.31) is complete.

Now we show that

$$\operatorname{TH}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V}) \subseteq \mathscr{C}. \tag{5.34}$$

Let $\hat{X} \in \widehat{\operatorname{TH}}(\mathbb{A}_{E^+,E^-}, \mathbb{S}_+^{\{0\}\cup V})$. Set $X \coloneqq \hat{X}[V]$ and $x \coloneqq \operatorname{diag}(X)$. Let $Y \in \mathbb{R}^{(\{0\}\cup V)\times(\{0\}\cup V)}$ such that $\hat{X} = Y^\mathsf{T} Y$. Set $y_i \coloneqq Y e_i$ for each $i \in \{0\} \cup V$. Let $Z \coloneqq \{\, i \in V : y_i = 0 \}$. Define $u_i \coloneqq y_i / \|y_i\|$ for each $i \in \{0\} \cup (V \setminus Z)$ and let $\{\, u_i : i \in Z \}$ be an orthonormal basis for a subspace of $\{\, u_i : i \in \{0\} \cup (V \setminus Z)\}^\perp$ of appropriate dimension.

We must show that (5.30) holds. Note that (5.30a) for $i \in V \setminus Z$ follows from $x = \operatorname{diag}(X) \geq 0$ and $\mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0$, and for $i \in Z$ it holds by construction. We also know that (5.30b) holds by construction. Let us check (5.30c). Let $ij \in E^+$. If i or j is in Z, then $\langle u_i, u_j\rangle = 0$, so we may assume that $i, j \in V \setminus Z$. Then

$$\langle u_i, u_j\rangle = \frac{\langle y_i, y_j\rangle}{\|y_i\|\|y_j\|} = \frac{X_{ij}}{\|y_i\|\|y_j\|} \geq 0$$

since $X \in \mathbb{A}_{E^+,E^-}$. This completes the proof of (5.30c). The proof of (5.30d) is analogous, so (5.30) holds.

Lastly, we show that x is given by (5.29). Let $i \in V$. Since $\mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0$, we have $x_i = [Y^\mathsf{T} Y]_{0i} = \langle y_0, y_i\rangle = \|y_0\|\|y_i\|\langle u_0, u_i\rangle = X_{ii}^{1/2}\langle u_0, u_i\rangle = x_i^{1/2}\langle u_0, u_i\rangle$. If $x_i > 0$, then $x_i^{1/2} = \langle u_0, u_i\rangle$. Otherwise, $u_i \perp u_0$ by construction, so $x_i = 0 = \langle u_0, u_i\rangle^2$. This proves that x is given by (5.29) and completes the proof of (5.34). ☐

Recall from Section 2.2 that an orthonormal representation of a graph $G = (V, E)$ is a map u that sends V into the unit vectors of some Euclidean space such that $\langle u_i, u_j\rangle = 0$ whenever $ij \in \overline{E}$. If, additionally, $\langle u_i, u_j\rangle \geq 0$ whenever $ij \in E$, then u is called an *acute orthonormal representation of* G. Finally, an *obtuse representation of* G is a map u from V to the unit vectors of some Euclidean space so that $\langle u_i, u_j\rangle \leq 0$ whenever $ij \in \overline{E}$.

Proposition 5.5 immediately leads to the following internal description of the sets in (5.21).

Corollary 5.6. Let $G = (V, E)$ be a graph. Let $\mathscr{C} \in \{\operatorname{TH}(G), \operatorname{TH}'(G), \operatorname{TH}^+(G)\}$. Then $\mathscr{C}$ consists of all vectors $x \in \mathbb{R}^V$ of the form $x_i = \langle u_0, u_i\rangle^2$ for every $i \in V$ for some unit vectors in $\{\, u_i : i \in \{0\} \cup V\} \subseteq \mathbb{R}^{\{0\}\cup V}$ such that

(i) u is an orthonormal representation of $\overline{G}$, if $\mathscr{C} = \mathrm{TH}(G)$;

(ii) u is an acute orthonormal representation of $\overline{G}$ and $\langle u_0, u_i \rangle \geq 0$ for all $i \in V$, if $\mathscr{C} = \mathrm{TH}'(G)$;

(iii) u is an obtuse representation of $\overline{G}$ and $\langle u_0, u_i \rangle \geq 0$ for all $i \in V$, if $\mathscr{C} = \mathrm{TH}^+(G)$.

Proof. Immediate from Proposition 5.5. When $\mathscr{C} = \mathrm{TH}(G)$, the constraint $\langle u_0, u_i \rangle \geq 0$ may be dropped, since for each orthonormal representation u of G and $i \in V$, the map obtained from u by replacing some image u_i by $-u_i$ is also an orthonormal representation of G. □

5.4 Liftings of Cones

After this short interlude, we turn our attention back to the geometric structure of the theta bodies. In the next few sections, we will develop the aspects of duality theory required to generalize the relation (5.2) to a rich family of theta bodies. Preferably, we would like to have the antiblocker of a theta body in this family to be another theta body in the same family, so that the family is closed under antiblocking duality. As in the case of the Lovász theta function, our investigation encodes the complete structure of theta bodies via their support functions. A careful study of alternative formulations for such functions will lead to the desired generalization of (5.2).

We briefly outline our approach to motivate the upcoming concepts. We follow to a degree the development from [59, Sec. 9.3]. We start by fixing a theta body $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ from a restricted but sufficiently rich family, with the goal of computing its antiblocker as another theta body. The theta function $\vartheta(\mathbb{A}, \widehat{\mathbb{K}}; \cdot)$ is defined simply as the support function of $\mathrm{abl}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}))$ on the nonnegative orthant. We then define several new functions, call them $\vartheta_i(\mathbb{A}, \widehat{\mathbb{K}}; \cdot)$ for each $i \in [4]$, all of which will turn out to be equal to the original theta function $\vartheta(\mathbb{A}, \widehat{\mathbb{K}}; \cdot)$. The function $\vartheta_4(\mathbb{A}, \widehat{\mathbb{K}}; \cdot)$ shall be defined as the support function of another theta body, which is then the antiblocker of $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ by standard Duality Theory.

In [59, Theorem 9.3.12] (and in [78, Sec. 12]), the proof that the functions ϑ and $\vartheta_1, \dots, \vartheta_4$ are all equal is obtained by proving the chain of inequalities (5.1), which corresponds in our setting to

$$\vartheta(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta_1(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta_2(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta_3(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta_4(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta(\mathbb{A}, \widehat{\mathbb{K}}; w) \quad \forall w \in \mathbb{R}^V_+. \tag{5.35}$$

The proof of some of these inequalities boil down to a change of variable, while others make an essential use of duality. In fact, Grötschel, Lovász, and Schrijver [59] identify the proof of the inequality $\vartheta_2(G; w) \leq \vartheta_3(G; w)$, corresponding to

$$\vartheta_2(\mathbb{A}, \widehat{\mathbb{K}}; w) \leq \vartheta_3(\mathbb{A}, \widehat{\mathbb{K}}; w), \tag{5.36}$$

as "the heart of the proof," where an application of the Strong Duality Theorem is paramount to prove that the parameters $\vartheta_2(\mathbb{A}, \widehat{\mathbb{K}}; w)$ and $\vartheta_3(\mathbb{A}, \widehat{\mathbb{K}}; w)$, defined as the optimal values of certain optimization problems, are equal.

Our development is similar, though our proof does not prove the chain (5.35) directly, rather, each inequality is proved separately as an equation. (Not all of the new functions ϑ_i's are needed, but we include them to generalize the chain (5.1) completely to our setting.) Most importantly, a difficulty arises at the proof of the critical inequality (5.36): the corresponding pair of dual problems in [59] involves optimization over a cone $\mathbb{K}$ in the space $\mathbb{S}^V$ rather than over the "lifted" cone $\widehat{\mathbb{K}}$, which lives in $\mathbb{S}^{\{0\}\cup V}$. In there, this is not a problem since no lifted space $\mathbb{S}^{\{0\}\cup V}$ is even mentioned, and $\mathrm{TH}(G)$ is defined purely in terms of the *ad hoc* concept of orthonormal representations of G, in a way related to the previous section.

To work around this difficulty, we shall prove that certain optimization problems involving a lifted cone $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\}\cup V}$ may be reformulated to involve only a lower-dimensional cone $\mathbb{K} \subseteq \mathbb{S}^V$. It does not seem reasonable to expect that all cones $\widehat{\mathbb{K}}$ in $\mathbb{S}^{\{0\}\cup V}$ may be crammed into a lower-dimensional cone $\mathbb{K}$ in $\mathbb{S}^V$ while preserving all the information we need. Thus, rather than allowing for arbitrary (though always diagonally scaling-invariant) closed convex cones $\widehat{\mathbb{K}}$ to define our theta bodies, we shall instead start with a given cone $\mathbb{K} \subseteq \mathbb{S}^V$ and build a lifting $\widehat{\mathbb{K}}$ of $\mathbb{K}$ in the space $\mathbb{S}^{\{0\}\cup V}$. That is, we focus on theta bodies that have the form $\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})$ where $\widehat{\mathbb{K}}$ is a function of a cone $\mathbb{K}$, which lives in the space $\mathbb{S}^V$. (In view of this, to keep our outline accurate, all occurrences of the functions $\vartheta(\mathbb{A}, \widehat{\mathbb{K}}; w)$ and $\vartheta_i(\mathbb{A}, \widehat{\mathbb{K}}; w)$ in our previous discussion should be replaced with $\vartheta(\mathbb{A}, \mathbb{K}; w)$ and $\vartheta_i(\mathbb{A}, \mathbb{K}; w)$, since $\widehat{\mathbb{K}}$ is built from $\mathbb{K}$.) In fact, on each side of the inequality (5.36), we shall use a different lifting of the cone $\mathbb{K}$. In the next subsections, we shall define these liftings and the basic properties we shall need to prove from them a generalization of (5.2).

5.4.1 PSD Liftings of Cones

Let $\mathbb{K} \subseteq \mathbb{S}^V$. Define the *PSD lifting of* $\mathbb{K}$ as

$$\mathrm{Psd}(\mathbb{K}) := \Big\{ \hat{X} \in \mathbb{S}_+^{\{0\}\cup V} : \hat{X}[V] \in \mathbb{K} \Big\}. \tag{5.37}$$

Note that if $\mathbb{K}$ is diagonally scaling-invariant, then so is $\mathrm{Psd}(\mathbb{K})$. Moreover,

$$\mathrm{Psd}(\mathbb{S}_+^V) = \mathbb{S}_+^{\{0\}\cup V}. \tag{5.38}$$

Before using PSD liftings, we shall need the following straightforward weighted generalization of [47, Proposition 9], a special case of which was already stated as Proposition 2.17.

Lemma 5.7. Let $\mathbb{M} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant closed convex cone. Suppose that

$$\mathrm{diag}(\mathbb{M}) \subseteq \mathbb{R}_+^V, \tag{5.39a}$$
$$\text{if } X_{ii} = 0 \text{ for some } X \in \mathbb{M} \text{ and } i \in V, \text{ then } X_{ij} = 0 \text{ for all } j \in V, \tag{5.39b}$$
$$\{\, X \in \mathbb{M} : \mathrm{Tr}(X) = 1 \} \text{ is compact.} \tag{5.39c}$$

Let $w \in \mathbb{R}_+^V$. Let X^* be an optimal solution of

$$\max\Big\{ \sqrt{w}^{\mathsf{T}} X \sqrt{w} : \mathrm{Tr}(X) = 1,\ X \in \mathbb{M} \Big\}, \tag{5.40}$$

and suppose that $\sqrt{w}^{\mathsf{T}} X^* \sqrt{w} > 0$. Set

$$d := \mathrm{diag}(X^*),$$
$$\bar{X} := \mathrm{Diag}(\sqrt{d})^\dagger X^* \,\mathrm{Diag}(\sqrt{d})^\dagger,$$
$$\lambda := \lambda_{\max}(\mathcal{D}_{\sqrt{w}}(\bar{X})).$$

Then

$$\mathcal{D}_{\sqrt{w}}(\bar{X})\sqrt{d} = \lambda\sqrt{d}, \tag{5.41a}$$

$$\lambda = \sqrt{w}^{\mathsf{T}} X^* \sqrt{w}, \tag{5.41b}$$

$$X^*\sqrt{w} = \lambda \operatorname{Diag}(\sqrt{w})^{\dagger} d. \tag{5.41c}$$

Proof. We first show that

$$\operatorname{supp}(d) \subseteq \operatorname{supp}(w). \tag{5.42}$$

Let $i \in \operatorname{supp}(d)$, so that $X^*_{ii} > 0$. Suppose that $w_i = 0$. If $X^*_{ii} = 1$, then $X^* = e_i e_i^{\mathsf{T}}$ by (5.39a) and (5.39b) whence $\sqrt{w}^{\mathsf{T}} X^* \sqrt{w} = 0$. If $X^*_{ii} < 1$, then $(1 - X^*_{ii})^{-1}\mathcal{D}_{\bar{e}-e_i}(X^*)$ is feasible for (5.40) with objective value $(1 - X^*_{ii})^{-1}\sqrt{w}^{\mathsf{T}} X^* \sqrt{w}$, hence strictly larger than the objective value of X^*. In either case, we get a contradiction. This proves (5.42).

If $d_i = 0$ for some $i \in V$, we are done by induction on $|V|$; the verification of this fact is long and tedious but straightforward. Thus, from (5.42) we may assume that

$$\operatorname{supp}(d) = \operatorname{supp}(w) = V. \tag{5.43}$$

Set $d^{-1/2} := \operatorname{diag}\big(\operatorname{Diag}(\sqrt{d})^{-1}\big)$ so that $\bar{X} = \mathcal{D}_{d^{-1/2}}(X^*) \in \mathbb{M}$ and $\operatorname{diag}(\bar{X}) = \bar{e}$. For every $h \in \mathbb{R}^V_+$ with $\|h\| = 1$, the point $\mathcal{D}_h(\bar{X})$ is feasible for (5.40) with objective value $\sqrt{w}^{\mathsf{T}}\mathcal{D}_h(\bar{X})\sqrt{w} = h^{\mathsf{T}}\mathcal{D}_{\sqrt{w}}(\bar{X})h$. Since $X^* = \mathcal{D}_{\sqrt{d}}(\bar{X})$ is optimal for (5.40), it follows that $\sqrt{d}$ is an optimal solution for

$$\max\big\{\, h^{\mathsf{T}}\mathcal{D}_{\sqrt{w}}(\bar{X})h : h \in \mathbb{R}^V_+,\ \|h\| = 1 \big\}.$$

In fact, since $[\sqrt{d}\,]_i > 0$ for all $i \in V$, we find that $\sqrt{d}$ is a local optimal solution for

$$\max\big\{\, h^{\mathsf{T}}\mathcal{D}_{\sqrt{w}}(\bar{X})h : h \in \mathbb{R}^V,\ \|h\| = 1 \big\},$$

hence also a global one; see Theorem A.10. Thus, $\mathcal{D}_{\sqrt{w}}(\bar{X})\sqrt{d} = \lambda\sqrt{d}$. This proves (5.41a). Now we unroll:

$$\begin{aligned}
\lambda d &= \lambda \operatorname{Diag}(\sqrt{d})\sqrt{d} = \operatorname{Diag}(\sqrt{d})\mathcal{D}_{\sqrt{w}}(\mathcal{D}_{d^{-1/2}}(X^*))\sqrt{d} = \operatorname{Diag}(\sqrt{d})\mathcal{D}_{d^{-1/2}}\big(\mathcal{D}_{\sqrt{w}}(X^*)\big)\sqrt{d} \\
&= \operatorname{Diag}(\sqrt{d}) \operatorname{Diag}(d^{-1/2})\mathcal{D}_{\sqrt{w}}(X^*) \operatorname{Diag}(d^{-1/2})\sqrt{d} = \operatorname{Diag}(\sqrt{w})X^* \operatorname{Diag}(\sqrt{w})\bar{e} \\
&= \operatorname{Diag}(\sqrt{w})X^*\sqrt{w}.
\end{aligned}$$

This proves (5.41c). Finally, $\lambda = \lambda \operatorname{Tr}(X^*) = \lambda \bar{e}^{\mathsf{T}} d = \bar{e}^{\mathsf{T}} \operatorname{Diag}(\sqrt{w})X^*\sqrt{w} = \sqrt{w}^{\mathsf{T}} X^* \sqrt{w}$ so (5.41b) is proved. ◻

We can now show that the support function of some theta bodies of the form $\operatorname{TH}(\mathbb{A}, \operatorname{Psd}(\mathbb{K}))$ may be formulated as a conic optimization problem over the cones $\mathbb{A}$ and $\mathbb{K}$. Note that the next result does not make use of Duality Theory.

Theorem 5.8. Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\mathbb{K} \subseteq \mathbb{S}^V_+$ be diagonally scaling-invariant closed convex cones. Let $w \in \mathbb{R}^V_+$. Suppose that $\operatorname{Diag}(\mathbb{R}^V_+) \subseteq \mathbb{A} \cap \mathbb{K}$. Then

$$\delta^*(w \mid \operatorname{TH}(\mathbb{A}, \operatorname{Psd}(\mathbb{K}))) = \max\Big\{\, \langle \sqrt{w}\sqrt{w}^{\mathsf{T}}, X\rangle : \langle I, X\rangle = 1,\ X \in \mathbb{A},\ X \in \mathbb{K} \Big\}. \tag{5.44}$$

Proof. We begin by proving '$\leq$'. Let $y \in \mathrm{TH}(\mathbb{A}, \mathrm{Psd}(\mathbb{K}))$ and let $\hat{Y} \in \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Psd}(\mathbb{K}))$ such that $y = \mathrm{diag}(Y)$ for $Y := \hat{Y}[V]$. We will show that there exists a feasible solution X for the RHS of (5.44) with objective value $\geq \langle w, y \rangle$. We may assume that $\langle w, y \rangle > 0$; otherwise, take $X = e_i e_i^\mathsf{T}$ for any $i \in V$. Set

$$\begin{aligned} h &:= \langle w, y \rangle^{-1/2} \sqrt{w} \geq 0, \\ X &:= \mathcal{D}_h(Y) \in \mathbb{A} \cap \mathbb{K}. \end{aligned}$$

Then

$$\mathrm{Tr}(X) = \frac{1}{\langle w, y \rangle} \mathrm{Tr}(\mathcal{D}_{\sqrt{w}}(Y)) = \frac{1}{\langle w, y \rangle} \langle \sqrt{w} \odot \sqrt{w}, \mathrm{diag}(Y) \rangle = 1,$$

whence X is feasible on the RHS of (5.44). Moreover,

$$\begin{bmatrix} 1 & (h \odot y)^\mathsf{T} \\ h \odot y & X \end{bmatrix} = \mathcal{D}_{1 \oplus h}\left(\begin{bmatrix} 1 & y^\mathsf{T} \\ y & Y \end{bmatrix} \right) \in \mathcal{D}_{1 \oplus h}(\mathrm{Psd}(\mathbb{K})) \subseteq \mathrm{Psd}(\mathbb{K}) \subseteq \mathbb{S}_+^{\{0\} \cup V}.$$

Thus, by Schur complement, we get $X \succeq \langle w, y \rangle^{-1} (\sqrt{w} \odot y)(\sqrt{w} \odot y)^\mathsf{T}$ and

$$\sqrt{w}^\mathsf{T} X \sqrt{w} \geq \frac{1}{\langle w, y \rangle} \sqrt{w}^\mathsf{T} \big(\mathrm{Diag}(\sqrt{w}) y\big) \big(\mathrm{Diag}(\sqrt{w}) y\big)^\mathsf{T} \sqrt{w} = \frac{1}{\langle w, y \rangle} \langle w, y \rangle^2.$$

This completes the proof of '$\leq$'.

Now we prove '$\geq$'. For that, we will show that,

$$\text{if } X \in \mathbb{A} \cap \mathbb{K} \text{ and } X\sqrt{w} \geq 0, \text{ then } \sqrt{w}^\mathsf{T} X \sqrt{w} \leq [\mathrm{Tr}(X)] \langle w, y \rangle \text{ for some } y \in \mathrm{TH}(\mathbb{A}, \mathrm{Psd}(\mathbb{K})). \tag{5.45}$$

So, let $X \in \mathbb{A} \cap \mathbb{K}$ such that $X\sqrt{w} \geq 0$. We may assume that $\sqrt{w}^\mathsf{T} X \sqrt{w} > 0$; otherwise take $y = 0$. Since $X \in \mathbb{K} \subseteq \mathbb{S}_+^V$, there exists $B \in \mathbb{R}^{V \times V}$ such that $X = B^\mathsf{T} B$. Define

$$\begin{aligned} c &:= \big(\sqrt{w}^\mathsf{T} X \sqrt{w}\big)^{-1/2} B \sqrt{w}, \\ d &:= \mathrm{diag}(X), \\ \tilde{B} &:= B \big[\mathrm{Diag}(\sqrt{d})\big]^\dagger, \\ \bar{B} &:= \tilde{B}\, \mathrm{Diag}(\tilde{B}^\mathsf{T} c), \\ y &:= \bar{B}^\mathsf{T} c = \mathrm{Diag}(\tilde{B}^\mathsf{T} c) \tilde{B}^\mathsf{T} c = (\tilde{B}^\mathsf{T} c) \odot (\tilde{B}^\mathsf{T} c). \end{aligned}$$

We will show that

$$y \in \mathrm{TH}(\mathbb{A}, \mathrm{Psd}(\mathbb{K})). \tag{5.46}$$

Set $Y := \bar{B}^\mathsf{T} \bar{B}$ and note that

$$\hat{Y} := \begin{bmatrix} 1 & y^\mathsf{T} \\ y & Y \end{bmatrix} = \begin{bmatrix} 1 & c^\mathsf{T} \bar{B} \\ \bar{B}^\mathsf{T} c & \bar{B}^\mathsf{T} \bar{B} \end{bmatrix} = \begin{bmatrix} c^\mathsf{T} \\ \bar{B}^\mathsf{T} \end{bmatrix} \begin{bmatrix} c & \bar{B} \end{bmatrix} \in \mathrm{Psd}(\mathbb{K}); \tag{5.47}$$

to see that $Y = \bar{B}^\mathsf{T} \bar{B} \in \mathbb{K}$, note that $Y = \mathcal{D}_h(X)$ for some $h \geq 0$ since

$$\tilde{B}^\mathsf{T} c \geq 0, \tag{5.48}$$

which follows from $(\sqrt{w}^{\mathsf{T}} X \sqrt{w})^{1/2} \tilde{B}^{\mathsf{T}} c = \big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger} B^{\mathsf{T}} B \sqrt{w} = \big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger} X \sqrt{w} \geq 0$. We also get that

$$Y = \mathcal{D}_h(X) \in \mathcal{D}_h(\mathbb{A}) \subseteq \mathbb{A}.$$

Thus, $\hat{Y} \in \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Psd}(\mathbb{K}))$. Finally,

$$\begin{aligned}
\mathrm{diag}(Y) &= \mathrm{diag}(\bar{B}^{\mathsf{T}} \bar{B}) = \mathrm{diag}\Big(\mathrm{Diag}(\tilde{B}^{\mathsf{T}} c) \tilde{B}^{\mathsf{T}} \tilde{B} \, \mathrm{Diag}(\tilde{B}^{\mathsf{T}} c)\Big) \\
&= (\tilde{B}^{\mathsf{T}} c) \odot \mathrm{diag}(\tilde{B}^{\mathsf{T}} \tilde{B}) \odot (\tilde{B}^{\mathsf{T}} c) \\
&= (\tilde{B}^{\mathsf{T}} c) \odot \mathrm{diag}\Big(\big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger} B^{\mathsf{T}} B \big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger}\Big) \odot (\tilde{B}^{\mathsf{T}} c) \\
&= (\tilde{B}^{\mathsf{T}} c) \odot \mathbb{1}_{\mathrm{supp}(d)} \odot (\tilde{B}^{\mathsf{T}} c) = (\tilde{B}^{\mathsf{T}} c) \odot (\tilde{B}^{\mathsf{T}} c) = y,
\end{aligned}$$

where we used for the second-to-last equation the fact that $d_j = 0$ implies that $(\tilde{B}^{\mathsf{T}} c)_j = e_j^{\mathsf{T}} \tilde{B}^{\mathsf{T}} c = e_j^{\mathsf{T}} \big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger} B^{\mathsf{T}} c = 0^{\mathsf{T}} B^{\mathsf{T}} c = 0$. This proves (5.46).

We also have $\tilde{B}\, \mathrm{Diag}(\sqrt{d}) = B \big[\mathrm{Diag}(\sqrt{d})\big]^{\dagger} \mathrm{Diag}(\sqrt{d}) = B \, \mathrm{Diag}(\mathbb{1}_{\mathrm{supp}(d)}) = B$ since $d_i = 0$ implies $Be_i = 0$. Thus,

$$\begin{aligned}
\sqrt{w}^{\mathsf{T}} X \sqrt{w} &= \left(\frac{\sqrt{w}^{\mathsf{T}} B^{\mathsf{T}} B \sqrt{w}}{(\sqrt{w}^{\mathsf{T}} X \sqrt{w})^{1/2}} \right)^2 = \Big(\sqrt{w}^{\mathsf{T}} B^{\mathsf{T}} c \Big)^2 \\
&= \Big(\sqrt{w}^{\mathsf{T}} \mathrm{Diag}(\sqrt{d}) \tilde{B}^{\mathsf{T}} c \Big)^2 = \Big(\sqrt{d}^{\mathsf{T}} \mathrm{Diag}(\sqrt{w}) \sqrt{y} \Big)^2 \\
&\leq \big\|\sqrt{d}\big\|^2 \big\|\mathrm{Diag}(\sqrt{w}) \sqrt{y}\big\|^2 = [\mathrm{Tr}(X)] \langle w, y \rangle.
\end{aligned}$$

This completes the proof of (5.45).

Let X be an optimal solution for the RHS of (5.44). By Lemma 5.7, we have $X\sqrt{w} \geq 0$. Thus, $\delta^*(w \mid \mathrm{TH}(\mathbb{A}, \mathrm{Psd}(\mathbb{K}))) \geq \sqrt{w}^{\mathsf{T}} X \sqrt{w}$ by (5.45) and the proof of '$\geq$' is complete. □

5.4.2 Schur Liftings of Cones

Let $\mathbb{K} \subseteq \mathbb{S}^V$. Define the *Schur lifting of* $\mathbb{K}$ as

$$\mathrm{Schur}(\mathbb{K}) := \left\{ \begin{bmatrix} x_0 & x^{\mathsf{T}} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\} \cup V} : X \in \mathbb{K},\, x_0 \in \mathbb{R}_+,\, x_0 X \succeq_{\mathbb{K}} x x^{\mathsf{T}} \right\}. \tag{5.49}$$

Note that $\mathrm{Schur}(\mathbb{S}_+^V) = \mathbb{S}_+^{\{0\} \cup V}$. It is instructive to rewrite the PSD lifting $\mathrm{Psd}(\mathbb{K})$ in the following format similar to $\mathrm{Schur}(\mathbb{K})$:

$$\text{if } \mathbb{K} \subseteq \mathbb{S}_+^V, \text{ then } \mathrm{Psd}(\mathbb{K}) = \left\{ \begin{bmatrix} x_0 & x^{\mathsf{T}} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\} \cup V} : X \in \mathbb{K},\, x_0 \in \mathbb{R}_+,\, x_0 X \succeq x x^{\mathsf{T}} \right\}; \tag{5.50}$$

note the difference in the last (conic) inequality.

Whereas the expression (5.37) makes it clear that the PSD lifting of a closed convex cone is convex, the same can not be said about the Schur lifting. We shall now show that, under certain simple conditions, the Schur lifting of a convex cone is also convex, and in fact it may be used as the cone $\widehat{\mathbb{K}}$ in Proposition 5.1:

Theorem 5.9. Let $\mathbb{K} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant closed convex cone such that $\mathbb{K} \supseteq \mathbb{S}^V_+$ and $\operatorname{diag}(\mathbb{K}) \subseteq \mathbb{R}^V_+$. Then $\operatorname{Schur}(\mathbb{K})$ is a diagonally scaling-invariant closed convex cone that satisfies (5.23). In particular, if $\mathbb{A} \subseteq \mathbb{S}^V$ is a diagonally scaling-invariant polyhedral cone such that (5.22) holds, then $\operatorname{cl}\big(\operatorname{TH}(\mathbb{A}, \operatorname{Schur}(\mathbb{K}))\big)$ is a convex corner contained in $[0,1]^V$.

Proof. To see that $\operatorname{Schur}(\mathbb{K})$ is closed, note that $x_0 X \succeq_{\mathbb{K}} xx^\mathsf{T}$ is equivalent to $\langle H, x_0X - xx^\mathsf{T}\rangle \geq 0$ for each $H \in \mathbb{K}^*$, and the function

$$\begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \mapsto x_0X - xx^\mathsf{T}$$

is continuous.

Set

$$\widehat{\mathbb{M}} := \left\{ \begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\}\cup V} : X \in \mathbb{K},\, x_0 \in \mathbb{R}_{++},\, x_0X \succeq_{\mathbb{K}} xx^\mathsf{T} \right\}.$$

We start by noting that

$$\operatorname{Schur}(\mathbb{K}) = \operatorname{cl}(\widehat{\mathbb{M}}\,). \tag{5.51}$$

The inclusion '$\supseteq$' follows from the closedness of $\operatorname{Schur}(\mathbb{K})$. For the reverse inclusion, let

$$\hat{X} := \begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \operatorname{Schur}(\mathbb{K}).$$

If $x_0 > 0$, then obviously $\hat{X} \in \widehat{\mathbb{M}}$. If $x_0 = 0$, then $0 = x_0X \succeq_{\mathbb{K}} xx^\mathsf{T}$ and $\operatorname{diag}(\mathbb{K}) \subseteq \mathbb{R}^V_+$ imply that $x = 0$. Thus, $X \in \mathbb{K}$ implies that $\hat{X}$ is clearly the limit of a sequence that lies in $\widehat{\mathbb{M}}$ with x_0 converging to 0 from above. This proves (5.51).

It is obvious that $\operatorname{Schur}(\mathbb{K})$ is a cone. We shall prove that $\operatorname{Schur}(\mathbb{K})$ is convex by showing that

$$\widehat{\mathbb{M}} \text{ is convex.} \tag{5.52}$$

Since

$$\widehat{\mathbb{M}} = \left\{ \begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\}\cup V} : X \in \mathbb{K},\, x_0 \in \mathbb{R}_{++},\, \langle H, x_0X - xx^\mathsf{T}\rangle \geq 0\, \forall H \in \mathbb{K}^* \right\},$$

it suffices to show that, for each $H \in \mathbb{K}^*$, the set

$$\left\{ \begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\}\cup V} : x_0 \in \mathbb{R}_{++},\, \frac{x^\mathsf{T}Hx}{x_0} - \langle H, X\rangle \leq 0 \right\}$$

is convex. Thus, it suffices to show that, for each $H \in \mathbb{K}^*$,

$$\text{the function } f_H \colon x_0 \oplus x \in \mathbb{R}_{++} \oplus \mathbb{R}^V \mapsto \frac{x^\mathsf{T}Hx}{x_0} \text{ is convex.} \tag{5.53}$$

Let $H \in \mathbb{K}^*$. The gradient of f_H is

$$\nabla f_H(x_0 \oplus x) = -\frac{x^\mathsf{T}Hx}{x_0^2} \oplus \frac{2Hx}{x_0}$$

and its Hessian is

$$\nabla^2 f_H(x_0 \oplus x) = \frac{2}{x_0^2}\begin{bmatrix} x^\mathsf{T} Hx/x_0 & -(Hx)^\mathsf{T} \\ -Hx & x_0 H \end{bmatrix}.$$

From the hypothesis that $\mathbb{K} \supseteq \mathbb{S}_+^V$ we get $\mathbb{K}^* \subseteq \mathbb{S}_+^V$ whence $H \succeq 0$, so we may write $H = \sum_{h\in\mathscr{H}} hh^\mathsf{T}$ for a finite subset $\mathscr{H}$ of $\mathbb{R}^V$. For $u := x_0^{1/2} \oplus x_0^{-1/2}\bar{e} \in \mathbb{R}_{++}^{\{0\}} \oplus \mathbb{R}_{++}^V$, we have

$$\begin{aligned}\frac{x_0^2}{2}\mathcal{D}_u\big(\nabla^2 f_H(x_0\oplus x)\big) &= \begin{bmatrix} x^\mathsf{T} Hx & -(Hx)^\mathsf{T} \\ -Hx & H \end{bmatrix} = \sum_{h\in\mathscr{H}} \begin{bmatrix} \langle h,x\rangle^2 & -\langle h,x\rangle h^\mathsf{T} \\ -\langle h,x\rangle h & hh^\mathsf{T} \end{bmatrix} \\ &= \sum_{h\in\mathscr{H}} \mathcal{D}_{\langle h,x\rangle\oplus\bar{e}}\left(\begin{bmatrix} 1 & -h^\mathsf{T} \\ -h & hh^\mathsf{T} \end{bmatrix}\right) = \sum_{h\in\mathscr{H}} \mathcal{D}_{\langle h,x\rangle\oplus\bar{e}}\Big((-1\oplus h)(-1\oplus h)^\mathsf{T}\Big) \succeq 0.\end{aligned}$$

This concludes the proof of (5.53), whence (5.52) is proved. Therefore, $\mathrm{Schur}(\mathbb{K})$ is convex by (5.51).

To see that $\mathrm{Schur}(\mathbb{K})$ is diagonally scaling-invariant, let

$$\hat{X} := \begin{bmatrix} x_0 & x^\mathsf{T} \\ x & X \end{bmatrix} \in \mathrm{Schur}(\mathbb{K}),$$

and let $h_0 \oplus h \in \mathbb{R}_+^{\{0\}} \oplus \mathbb{R}_+^V$. The condition $\mathcal{D}_{h_0\oplus h}(\hat{X}) \in \mathrm{Schur}(\mathbb{K})$ is equivalent to $\mathcal{D}_h(X) \in \mathbb{K}$ and $h_0^2 x_0 \mathcal{D}_h(X) \succeq_{\mathbb{K}} h_0^2 (h\odot x)(h\odot x)^\mathsf{T} = h_0^2\mathcal{D}_h(xx^\mathsf{T})$, both of which follow from the diagonal scaling invariance of $\mathbb{K}$. It is easy to check that $\mathrm{Schur}(\mathbb{K})$ satisfies (5.23a). For (5.23b), let $\hat{X} \in \mathrm{Schur}(\mathbb{K})$ and set $X := \hat{X}[V]$ and $x := \mathrm{diag}(X)$. Then $x - (x\odot x) = \mathrm{diag}(X - xx^\mathsf{T}) \geq 0$ since $\mathrm{diag}(\mathbb{K}) \subseteq \mathbb{R}_+^V$ whence $x \subseteq [0,1]^V$. This completes the proof that (5.23) holds.

Now, if $\mathbb{A} \subseteq \mathbb{S}^V$ is a diagonally scaling-invariant polyhedral cone such that (5.22) holds, then Proposition 5.1 implies that $\mathrm{cl}\big(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}))\big)$ is a convex corner contained in $[0,1]^V$. $\square$

The hypothesis that $\mathbb{K} \supseteq \mathbb{S}_+^V$ holds cannot be dropped from Theorem 5.9. Consider the cone $\mathcal{C}_V^*$ of completely positive matrices, dual to the cone $\mathcal{C}_V$ of copositive matrices. A matrix $X \in \mathbb{S}^V$ is said to be *completely positive* if $X = \sum_{i=1}^k h_i h_i^\mathsf{T}$ for some $h_1,\dots,h_k \in \mathbb{R}_+^V$. Now take $V := [n]$ for some $n \geq 2$ and note that both $\mathbb{1}_{\{0,1\}}\mathbb{1}_{\{0,1\}}^\mathsf{T} + \mathbb{1}_{\{2\}}\mathbb{1}_{\{2\}}^\mathsf{T}$ and $\mathbb{1}_{\{0,2\}}\mathbb{1}_{\{0,2\}}^\mathsf{T} + \mathbb{1}_{\{1\}}\mathbb{1}_{\{1\}}^\mathsf{T}$ lie in $\mathrm{Schur}(\mathcal{C}_V^*)$, whereas their midpoint does not.

As we hinted in the discussion in Section 5.4, PSD and Schur liftings of cones are in a sense dual to each other. In the next result, we make the picture a bit clearer by stating a containment relation between theta bodies defined using these two liftings. The relation may be regarded as a form of Weak Duality, and we shall later prove that equality, and hence a form of Strong Duality, holds.

Proposition 5.10. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant polyhedral cone such that (5.22) holds. Let $\mathbb{K} \subseteq \mathbb{S}_+^V$ be a diagonally scaling-invariant closed convex cone such that $\mathbb{K} \supseteq \mathrm{Diag}(\mathbb{R}_+^V)$. Then

$$\mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})) \subseteq \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))). \tag{5.54}$$

Proof. By continuity, it suffices to show that $\langle x,y\rangle \leq 1$ if $x \in \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K}))$ and $y \in \mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))$. Let $x \in \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K}))$, and let $\hat{X} \in \widehat{\mathrm{TH}}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K}))$ such that $x = \mathrm{diag}(X)$ for $X := \hat{X}[V]$. Let $y \in \mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))$, and let $\hat{Y} \in \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))$ such that

$y = \operatorname{diag}(Y)$ for $Y := \hat{Y}[V]$. Write $X = \operatorname{Diag}(u) - B$ where $B \in \mathbb{A}^*$. By Corollary 5.4, we may assume that $\operatorname{Im}(\operatorname{Diag}) \subseteq \mathbb{A}$ whence $u = x$. Then

$$\begin{aligned} 0 &\leq \langle X, Y - yy^{\mathsf{T}} \rangle = \langle \operatorname{Diag}(x) - B, Y \rangle - y^{\mathsf{T}} X y = \langle x, y \rangle - \langle B, Y \rangle - y^{\mathsf{T}} X y \\ &\leq \langle x, y \rangle - y^{\mathsf{T}} (x x^{\mathsf{T}}) y = \langle x, y \rangle - \langle x, y \rangle^2. \end{aligned}$$

Hence, $\langle x, y \rangle \leq 1$. □

A result analogous to Theorem 5.8 holds for Schur liftings, i.e., a certain optimization problem over $\operatorname{Schur}(\mathbb{K})$ may be reformulated as an optimization problem over $\mathbb{K}$. We postpone its presentation to the next section, where we can give a better motivation for the corresponding optimization problems. For now, we shall show that another classical polyhedral relaxation for the stable set polytope is a theta body defined via a Schur lifting.

Let $G = (V, E)$ be a graph. The *weak fractional stable set polytope of* G is the polytope

$$\operatorname{FRAC}(G) := \{\, x \in [0,1]^V : B_G^{\mathsf{T}} x \leq \bar{e} \}, \tag{5.55}$$

where B_G denotes the $V \times E$ *incidence matrix* of G.

Proposition 5.11. Let $G = (V, E)$ be a graph such that $|V| \geq 2$. Set

$$\mathbb{K}_2 := \left\{ X \in \mathbb{S}^V : X[e] \succeq 0 \, \forall e \in \tbinom{V}{2} \right\}. \tag{5.56}$$

Then

$$\operatorname{FRAC}(G) = \operatorname{TH}(\mathbb{A}_{E,E}, \operatorname{Schur}(\mathbb{K}_2)). \tag{5.57}$$

Proof. We first prove '$\supseteq$'. Let $x \in \operatorname{TH}(\mathbb{A}_{E,E}, \operatorname{Schur}(\mathbb{K}_2))$, and let $\hat{X} \in \widehat{\operatorname{TH}}(\mathbb{A}_{E,E}, \operatorname{Schur}(\mathbb{K}_2))$ such that $x = \operatorname{diag}(X)$ for $X := \hat{X}[V]$. By Theorem 5.9, we have $x \in [0,1]^V$. Let $e = ij \in E$. Set $Y := X[e]$ and $y := x\restriction_e$. Then $X \succeq_{\mathbb{K}_2} xx^{\mathsf{T}}$ implies $Y \succeq yy^{\mathsf{T}}$ so

$$\begin{bmatrix} 1 & x_i & x_j \\ x_i & x_i & 0 \\ x_j & 0 & x_j \end{bmatrix} \succeq 0 \implies \begin{bmatrix} 1 & -x_i & -x_j \\ -x_i & x_i & 0 \\ -x_j & 0 & x_j \end{bmatrix} \succeq 0 \implies 1 - x_i - x_j = \left\langle \begin{bmatrix} 1 & -x_i & -x_j \\ -x_i & x_i & 0 \\ -x_j & 0 & x_j \end{bmatrix}, \bar{e}\bar{e}^{\mathsf{T}} \right\rangle \geq 0.$$

Thus $x \in \operatorname{FRAC}(G)$, and '$\supseteq$' is proved.

For the reverse inclusion, it suffices by Theorem 5.9 to show that $\operatorname{TH}(\mathbb{A}_{E,E}, \operatorname{Schur}(\mathbb{K}_2))$ contains all the extreme points of $\operatorname{FRAC}(G)$. So let x be an extreme point of $\operatorname{FRAC}(G)$. By [133, Theorem 64.7], all coordinates of x lie in $\{0, \frac{1}{2}, 1\}$. Define

$$\hat{X} := \begin{bmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{bmatrix} \in \mathbb{S}^{\{0\} \cup V}$$

by setting $\operatorname{diag}(X) := x$ and $X_{ij} := \left[ij \in \overline{E} \right] \left[x_i + x_j > 1 \right] x_i x_j$ for every $ij \in \binom{V}{2}$. Note that $X \in \mathbb{A}_{E,E} \cap \mathbb{K}_2$ holds, and that $X \succeq_{\mathbb{K}_2} xx^{\mathsf{T}}$ is equivalent to

$$Y^{ij} := \begin{bmatrix} 1 & x_i & x_j \\ x_i & x_i & X_{ij} \\ x_j & X_{ij} & x_j \end{bmatrix} \in \mathbb{S}_+^{\{0\} \cup \{i,j\}}.$$

for each $ij \in \binom{V}{2}$. So let $ij \in \binom{V}{2}$. If $x_i + x_j \leq 1$, then $X_{ij} = 0$ and either $0 \in \{x_i, x_j\}$ or $x_i = x_j = \frac{1}{2}$, so $Y^{ij} \succeq 0$ is easily verified. So assume $x_i + x_j > 1$. If $x_i = x_j = 1$, then $ij \in \overline{E}$, so $X_{ij} = x_i x_j$, and $Y^{ij} = \bar{e}\bar{e}^\mathsf{T} \succeq 0$. If $x_i = 1$ and $x_j = \frac{1}{2}$, then

$$Y^{ij} = \begin{bmatrix} 1 & 1 & \frac{1}{2} \\ 1 & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \mathcal{D}_{\bar{e}-e_2/2}\big(\bar{e}\bar{e}^\mathsf{T} + e_2 e_2^\mathsf{T}\big) \succeq 0.$$

Thus, $\hat{X} \in \mathrm{Schur}(\mathbb{K}_2)$ and the proof of '$\subseteq$' is complete. $\square$

5.5 Reformulations of Antiblocking Duality

In this section, we study some reformulations of optimization problems leading up to a problem over the Schur lifting of a cone $\mathbb{K}$ which may be reformulated over $\mathbb{K}$ itself. We shall use these results in the next section to prove a generalization of (5.2).

In the next result, we shall follow the rules set for [59, Eq. (9.3.6)] to interpret the quotient w_i/x_i^*:

> if $w_i = 0$, then we take the fraction to be 0, even if the denominator is 0; if $w_i > 0$ but the denominator is 0, we take the fraction to be $+\infty$. (5.58)

Proposition 5.12. Let $\mathscr{C} \subseteq \mathbb{R}^V$ be a convex corner. Let $w \in \mathbb{R}^V_+$. Then

$$\delta^*(w \,|\, \mathscr{C}) = \min_{s \in \mathrm{abl}(\mathscr{C})} \max_{i \in V} \frac{w_i}{s_i}. \tag{5.59}$$

In particular,

$$\delta^*(w \mid \mathrm{abl}(\mathscr{C})) = \min_{x \in \mathscr{C}} \max_{i \in V} \frac{w_i}{x_i}. \tag{5.60}$$

Proof. If $w = 0$, then (5.59) is trivially true, so suppose $w \neq 0$.

Let us prove '$\leq$'. Let $s \in \mathrm{abl}(\mathscr{C})$. We may assume the max on the RHS is finite so that, by following the rules from (5.58), we have $\mathrm{supp}(w) \subseteq \mathrm{supp}(s)$. Let $x \in \mathscr{C}$. Set $W \coloneqq \mathrm{supp}(w)$ and $S \coloneqq \mathrm{supp}(s)$. Then

$$\langle w, x\rangle = \sum_{i \in W} w_i x_i = \sum_{i \in S} \frac{w_i}{s_i} s_i x_i \leq \left(\max_{i \in S} \frac{w_i}{s_i}\right) \sum_{i \in V} s_i x_i \leq \max_{i \in V} \frac{w_i}{s_i},$$

where (5.58) is only used in the rightmost term. This proves '$\leq$' in (5.59).

Let $\vartheta \coloneqq \delta^*(w \,|\, \mathscr{C}) > 0$. Then $\langle w, x\rangle \leq \vartheta$ for all $x \in \mathscr{C}$ implies that $s \coloneqq \frac{1}{\vartheta} w \in \mathrm{abl}(\mathscr{C})$. Since $\max_{i \in V} w_i/s_i = \vartheta$, we find that the RHS of (5.59) is bounded above by $\vartheta = \delta^*(w \,|\, \mathscr{C})$. This proves '$\geq$' in (5.59), as well as attainment for its RHS.

Equation (5.60) follows from (5.59) by antiblocking duality, i.e., $\mathrm{abl}(\mathrm{abl}(\mathscr{C})) = \mathscr{C}$. $\square$

We shall later formulate the parameter ϑ_1 (see the discussion at the beginning of Section 5.4) essentially as the optimization problem on the RHS of (5.60) applied to a theta body. In a way, that formulation is unnecessary for the proof of the generalization of (5.2), and it may be further simplified as a line-search, i.e., by a gauge function:

Proposition 5.13. Let $\mathscr{C} \subseteq \mathbb{R}^V$ be a convex corner. Let $w \in \mathbb{R}^V_+$. Then

$$\min_{x\in\mathscr{C}} \max_{i\in V} \frac{w_i}{x_i} = \min\{\, \lambda \in \mathbb{R}_+ : w \in \lambda\mathscr{C} \}. \tag{5.61}$$

Proof. If $w = 0$, then (5.61) is easily seen to hold, so assume $w \neq 0$.

First we show '$\leq$'. Let $\lambda \in \mathbb{R}_+$ such that $w \in \lambda\mathscr{C}$. Then $\lambda > 0$ since $w \neq 0$ and $\mathscr{C}$ is bounded. Set $x := \frac{1}{\lambda} w \in \mathscr{C}$. Then $w_i/x_i = [w_i \neq 0]\lambda$ for every $i \in V$, according to the rules from (5.58), so that $\max_{i\in V} w_i/x_i = \lambda$, whence the LHS of (5.61) is $\leq \lambda$. This proves '$\leq$'.

For the reverse inequality, let $x \in \mathscr{C}$ attain the LHS of (5.61), and let $\lambda := \max_{i\in V} w_i/x_i$. Since $w \neq 0$, we have $\lambda > 0$. Set $y := \frac{1}{\lambda} w$. We claim that $y \leq x$. Indeed, if $w_i = 0$ then $y_i = 0 \leq x_i$. If $w_i > 0$, then $\lambda < \infty$ implies $x_i > 0$, whence $w_i/x_i \leq \lambda$ implies $y_i = w_i/\lambda \leq x_i$. Since $0 \leq y \leq x \in \mathscr{C}$ and $\mathscr{C}$ is lower-comprehensive, we find that $y \in \mathscr{C}$, i.e., $w \in \lambda\mathscr{C}$. This proves '$\geq$' on (5.61), as well as attainment on its RHS. $\square$

The RHS of (5.61) is the gauge function $\gamma(w \,|\, \mathscr{C})$ of $\mathscr{C}$ at w. From Propositions 5.12 and 5.13, we recover the fact that

$$\text{for a convex corner } \mathscr{C} \subseteq \mathbb{R}^V_+, \text{ we have } \delta^*(\cdot \mid \operatorname{abl}(\mathscr{C})) = \gamma(\cdot \,|\, \mathscr{C}) \text{ on } \mathbb{R}^V_+; \tag{5.62}$$

see [123, Theorem 14.5].

A gauge function is oblivious to the upper surface of a set which is "almost" a convex corner:

Proposition 5.14. Let $\mathscr{C} \subseteq \mathbb{R}^V_+$ be a lower-comprehensive convex set with nonempty interior. Then

$$\gamma(w \,|\, \mathscr{C}) = \gamma(w \mid \operatorname{cl}(\mathscr{C})) \qquad \forall w \in \mathbb{R}^V_+. \tag{5.63}$$

Proof. The proof of '$\geq$' is obvious. For the reverse inequality, let $w \in \mathbb{R}^V_+$ and let $\lambda \in \mathbb{R}_+$ such that $w \in \lambda \operatorname{cl}(\mathscr{C})$. If $\lambda = 0$, then $w = 0$ and $\gamma(w \,|\, \mathscr{C}) = 0 = \gamma(w \mid \operatorname{cl}(\mathscr{C}))$, so assume $\lambda > 0$. We will show that $w \in (\lambda + \varepsilon)\mathscr{C}$ for every $\varepsilon > 0$. Let $\varepsilon > 0$. Since $\mathscr{C}$ is lower-comprehensive and has nonempty interior, there exists $M \in \mathbb{R}_{++}$ such that $\bar{e}/M \in \operatorname{int}(\mathscr{C})$. Thus, for every $\mu \in \mathbb{R}$ such that $0 < \mu \leq 1$, we have

$$\frac{\mu}{M}\bar{e} + \frac{1-\mu}{\lambda} w \in \operatorname{int}(\mathscr{C}).$$

For $\mu := \varepsilon/(\lambda + \varepsilon)$, this gives

$$\frac{\varepsilon}{M(\lambda+\varepsilon)}\bar{e} + \frac{1}{\lambda+\varepsilon} w \in \operatorname{int}(\mathscr{C}),$$

and since $\mathscr{C}$ is lower-comprehensive, we get $w \in (\lambda + \varepsilon)\mathscr{C}$. Since $\varepsilon > 0$ was arbitrary, this proves '$\leq$' in (5.63). $\square$

We are now ready to show how an optimization problem over $\operatorname{Schur}(\mathbb{K})$ may sometimes be reduced to an optimization problem over $\mathbb{K}$. We shall use the following simple fact:

$$\text{if } \mathbb{K} \supseteq \mathbb{S}^V_+, \text{ then } \begin{bmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{bmatrix} \in \operatorname{Schur}(\mathbb{K}) \text{ if and only if } X \succeq_{\mathbb{K}} xx^{\mathsf{T}}. \tag{5.64}$$

Proposition 5.15. Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\widehat{\mathbb{K}} \subseteq \mathbb{S}^{\{0\} \cup V}$ be diagonally scaling-invariant closed convex cones such that (5.22) and (5.23) hold. Let $w \in \mathbb{R}^V_+$ be nonzero. Then

$$\delta^*(w \mid \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})))) = \inf\left\{ \lambda \in \mathbb{R}_+ : W \in \mathbb{A},\ \mathrm{diag}(W) = \lambda \bar{e},\ \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & W \end{bmatrix} \in \widehat{\mathbb{K}} \right\}. \tag{5.65}$$

In particular, if $\mathbb{A}$ is polyhedral, then

$$\delta^*(w \mid \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})))) = \inf\left\{ \lambda \in \mathbb{R}_+ : Y \in -\mathbb{A} \cap \mathrm{Null}(\mathrm{diag}),\ \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & \lambda I - Y \end{bmatrix} \in \widehat{\mathbb{K}} \right\}, \tag{5.66}$$

and if $\mathbb{K} \subseteq \mathbb{S}^V$ is a diagonally scaling-invariant closed convex cone such that $\mathbb{K} \supseteq \mathbb{S}^V_+$ and $\mathrm{diag}(\mathbb{K}) \subseteq \mathbb{R}^V_+$ then

$$\delta^*(w \mid \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}))))) = \inf\left\{ \lambda : \lambda I \succeq_{\mathbb{K}} Y + \sqrt{w}\sqrt{w}^\mathsf{T},\ Y \in -\mathbb{A} \cap \mathrm{Null}(\mathrm{diag}) \right\}. \tag{5.67}$$

Proof. From Propositions 5.1 and 5.14 and from (5.62), we have

$$\begin{aligned} \delta^*(w \mid \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})))) &= \gamma(w \mid \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})) = \inf\left\{ \lambda \in \mathbb{R}_{++} : w \in \lambda\, \mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}}) \right\} \\ &= \inf\left\{ \lambda \in \mathbb{R}_{++} : W \in \mathbb{A},\ \mathrm{diag}(W) = \tfrac{1}{\lambda} w,\ \begin{bmatrix} 1 & \frac{1}{\lambda} w^\mathsf{T} \\ \frac{1}{\lambda} w & W \end{bmatrix} \in \widehat{\mathbb{K}} \right\}. \end{aligned}$$

Using the diagonal scaling invariance of $\mathbb{A}$ and $\widehat{\mathbb{K}}$ and the change of variable

$$\hat{X} = \mathcal{D}_{1 \oplus \lambda w^{-1/2}}\left(\begin{bmatrix} 1 & \frac{1}{\lambda} w^\mathsf{T} \\ \frac{1}{\lambda} w & W \end{bmatrix} \right) = \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & \mathcal{D}_{\lambda w^{-1/2}}(W) \end{bmatrix},$$

where

$$[w^{-1/2}]_i := \begin{cases} w_i^{-1/2} & \text{if } w_i > 0, \\ 1 & \text{otherwise}, \end{cases}$$

we get

$$\delta^*(w \mid \mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \widehat{\mathbb{K}})))) = \inf\left\{ \lambda \in \mathbb{R}_{++} : X \in \mathbb{A},\ \mathrm{diag}(X) = \lambda \mathbb{1}_{\mathrm{supp}(w)},\ \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & X \end{bmatrix} \in \widehat{\mathbb{K}} \right\}, \tag{5.68}$$

since

$$\mathrm{diag}(\mathcal{D}_{\lambda w^{-1/2}}(W)) = (\lambda w^{-1/2}) \odot \mathrm{diag}(W) \odot (\lambda w^{-1/2}) = \lambda \mathbb{1}_{\mathrm{supp}(w)}$$

if $\mathrm{diag}(W) = \frac{1}{\lambda} w$.

Note that the constraint $\lambda \in \mathbb{R}_{++}$ in (5.68) may be relaxed to $\lambda \in \mathbb{R}_+$. For suppose there exists $X \in \mathbb{A}$ such that $\mathrm{diag}(X) = 0$ and

$$\begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & X \end{bmatrix} \in \widehat{\mathbb{K}}.$$

By the diagonal scaling invariance of $\widehat{\mathbb{K}}$ and assumptions (5.22) and (5.23a), we find that $X + \varepsilon\, \mathrm{Diag}(\mathbb{1}_{\mathrm{supp}(w)})$ is feasible on the RHS of (5.68) for each $\varepsilon > 0$, so the RHS of (5.68) is 0.

To prove (5.65), it suffices by (5.68) to show that

$$\inf\left\{ \lambda \in \mathbb{R}_+ : W \in \mathbb{A},\, \operatorname{diag}(W) = \lambda\bar{e},\, \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & W \end{bmatrix} \in \widehat{\mathbb{K}} \right\}$$
$$= \inf\left\{ \lambda \in \mathbb{R}_+ : X \in \mathbb{A},\, \operatorname{diag}(X) = \lambda \mathbb{1}_{\operatorname{supp}(w)},\, \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & X \end{bmatrix} \in \widehat{\mathbb{K}} \right\}. \quad (5.69)$$

If $\lambda \oplus W$ is a feasible solution for the LHS of (5.69), then $\lambda \oplus \mathcal{D}_{\mathbb{1}_{\operatorname{supp}(w)}}(W)$ is feasible for the RHS. Conversely, if $\lambda \oplus X$ is feasible for the RHS of (5.69), then $\lambda \oplus [X + \lambda \operatorname{Diag}(\bar{e} - \mathbb{1}_{\operatorname{supp}(w)})]$ is feasible for the LHS by diagonal scaling invariance of $\mathbb{A}$ and $\mathbb{K}$ together with assumptions (5.22) and (5.23a). This completes the proof of (5.65).

Suppose that $\mathbb{A}$ is polyhedral, and set $\mathbb{A}' := \mathbb{A} + \operatorname{Im}(\operatorname{Diag})$. Then by Corollary 5.4 and (5.65), we have

$$\delta^*(w \mid \operatorname{abl}(\operatorname{cl}(\operatorname{TH}(\mathbb{A}, \widehat{\mathbb{K}})))) = \delta^*(w \mid \operatorname{abl}(\operatorname{cl}(\operatorname{TH}(\mathbb{A}', \widehat{\mathbb{K}}))))$$
$$= \inf\left\{ \lambda \in \mathbb{R}_+ : W \in \mathbb{A}',\, \operatorname{diag}(W) = \lambda\bar{e},\, \begin{bmatrix} 1 & \sqrt{w}^\mathsf{T} \\ \sqrt{w} & W \end{bmatrix} \in \widehat{\mathbb{K}} \right\}. \quad (5.70)$$

Let $\lambda \in \mathbb{R}_+$ and $W \in \mathbb{S}^V$. We claim that

> $W \in \mathbb{A}'$ and $\operatorname{diag}(W) = \lambda\bar{e}$ hold if and only if there exits $Y \in -\mathbb{A} \cap \operatorname{Null}(\operatorname{diag})$ such that $W = \lambda I - Y$. (5.71)

The proof of the 'if' part is clear. For the 'only if' part, suppose that $W \in \mathbb{A}'$ and $\operatorname{diag}(W) = \lambda\bar{e}$ hold. Then $Y := \lambda I - W \in \operatorname{Im}(\operatorname{Diag}) - \mathbb{A}' \subseteq -\mathbb{A}'$, whence $Y \in -\mathbb{A}' \cap \operatorname{Null}(\operatorname{diag})$. By Proposition 5.3, we have $-\mathbb{A}' \cap \operatorname{Null}(\operatorname{Diag}) = -\mathbb{A} \cap \operatorname{Null}(\operatorname{Diag})$; see the proof of Corollary 5.4. This completes the proof of (5.71), from which (5.66) follows. Finally, (5.67) follows from (5.66) and Theorem 5.9, using the equivalence (5.64). The constraint $\lambda \in \mathbb{R}_+$ may be dropped since $\operatorname{diag}(\mathbb{K}) \subseteq \mathbb{R}^V_+$. □

5.6 A Plethora of Theta Functions

We are now ready to carry out the plan outlined in the beginning of Section 5.4.

Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\mathbb{K} \subseteq \mathbb{S}^V$. For each $w \in \mathbb{R}^V_+$, define:

$$\vartheta(\mathbb{A}, \mathbb{K}; w) := \delta^*(w \mid \operatorname{abl}(\operatorname{cl}(\operatorname{TH}(\mathbb{A}, \operatorname{Schur}(\mathbb{K}^*))))),$$
$$\vartheta_1(\mathbb{A}, \mathbb{K}; w) := \inf\left\{ \max_{i \in V} \frac{w_i}{x_i} : x \in \operatorname{cl}(\operatorname{TH}(\mathbb{A}, \operatorname{Schur}(\mathbb{K}^*))) \right\},$$
$$\vartheta_2(\mathbb{A}, \mathbb{K}; w) := \inf\left\{ \lambda : \lambda I \succeq_{\mathbb{K}^*} Y + \sqrt{w}\sqrt{w}^\mathsf{T},\, Y \in -\mathbb{A} \cap \operatorname{Null}(\operatorname{Diag}) \right\},$$
$$\vartheta_3(\mathbb{A}, \mathbb{K}; w) := \sup\left\{ \sqrt{w}^\mathsf{T} X \sqrt{w} : \operatorname{Tr}(X) = 1,\, X \in \mathbb{K},\, X \in \operatorname{Im}(\operatorname{Diag}) - \mathbb{A}^* \right\},$$
$$\vartheta_4(\mathbb{A}, \mathbb{K}; w) := \delta^*(w \mid \operatorname{TH}(\operatorname{Im}(\operatorname{Diag}) - \mathbb{A}^*, \operatorname{Psd}(\mathbb{K}))).$$

Theorem 5.16. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant polyhedral cone such that (5.22) holds. Let $\mathbb{K} \subseteq \mathbb{S}^V_+$ be a diagonally scaling-invariant closed convex cone such that $\mathbb{K} \supseteq \mathrm{Diag}(\mathbb{R}^V_+)$. Let $w \in \mathbb{R}^V_+$. Then

$$\vartheta(\mathbb{A}, \mathbb{K}; w) = \vartheta_1(\mathbb{A}, \mathbb{K}; w) = \vartheta_2(\mathbb{A}, \mathbb{K}; w) = \vartheta_3(\mathbb{A}, \mathbb{K}; w) = \vartheta_4(\mathbb{A}, \mathbb{K}; w). \tag{5.72}$$

In particular,

$$\mathrm{abl}(\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))) = \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})). \tag{5.73}$$

Proof. Equation $\vartheta_2(\mathbb{A}, \mathbb{K}; w) = \vartheta_3(\mathbb{A}, \mathbb{K}; w)$ follows by Conic Programming Strong Duality. Although the conic formulation for $\vartheta_3(\mathbb{A}, \mathbb{K}; w)$ may not have a Slater point, the assumptions that $\mathbb{A}$ is polyhedral and $\mathbb{K}^* \supseteq \mathbb{S}^V_+$ show that, by taking λ large enough and Y set to 0, we get a restricted Slater point for the conic program $\vartheta_2(\mathbb{A}, \mathbb{K}; w)$. Equation (5.72) follows from $\vartheta_2(\mathbb{A}, \mathbb{K}; w) = \vartheta_3(\mathbb{A}, \mathbb{K}; w)$, Propositions 5.12 and 5.15, and Theorem 5.8 since $\mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))$ is a convex corner by Theorem 5.9. Now (5.73) follows from conjugate duality applied to $\vartheta(\mathbb{A}, \mathbb{K}; w) = \vartheta_4(\mathbb{A}, \mathbb{K}; w)$ for every $w \in \mathbb{R}^V_+$. □

Theorem 5.16 implies (5.2) using the descriptions (5.21), and also that

$$\mathrm{abl}(\mathrm{TH}'(G)) = \mathrm{TH}^+(\overline{G}) \tag{5.74}$$

for every graph G, which is also a well-known result. Theorem 5.16 and Proposition 5.11 also yield a description of $\mathrm{abl}(\mathrm{FRAC}(G)) = (\mathrm{conv}\{\, \mathbb{1}_{ij} : ij \in E\} - \mathbb{R}^V_+) \cap \mathbb{R}^V_+$, for a graph $G = (V, E)$ with no isolated nodes, as

$$\mathrm{abl}(\mathrm{FRAC}(G)) = \mathrm{TH}(\mathbb{A}_{\overline{E},\overline{E}},, \mathbb{K}_2^*),$$

where

$$\mathbb{K}_2^* = \sum \Big\{ \mathbb{S}^e_+ \oplus 0 : e \in \tbinom{V}{2} \Big\} \subseteq \mathbb{S}^V.$$

Note also that we could have mimicked the proof of the chain (5.1) as in [59] and [78]; the proof that $\vartheta_4(\mathbb{A}, \mathbb{K}; w) \leq \vartheta(\mathbb{A}, \mathbb{K}; w)$ is essentially contained in Proposition 5.10.

In the context of Theorem 5.16, the support functions of the two theta bodies that appear in (5.73) are gauges polar to each other[1]; see [123, Sec. 15]. The corresponding polar inequality (that is, the corresponding Cauchy-Schwarz inequality) for these gauges is stated next; compare it to [37, Proposition 8 and Theorem 18]. We recall that the symmetric group on V is denoted by Sym_V and that, for each $\sigma \in \mathrm{Sym}_V$, the linear map $P_\sigma \colon \mathbb{R}^V \to \mathbb{R}^V$ is defined as the linear extension of the map $e_i \in \mathbb{R}^V \mapsto e_{\sigma(i)}$.

Corollary 5.17. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant polyhedral cone such that (5.22) holds. Let $\mathbb{K} \subseteq \mathbb{S}^V_+$ be a diagonally scaling-invariant closed convex cone such that $\mathbb{K} \supseteq \mathrm{Diag}(\mathbb{R}^V_+)$. If $w, \bar{w} \in \mathbb{R}^V_+$, then

$$\langle w, \bar{w} \rangle \leq \delta^*(w \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))\delta^*(\bar{w} \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))). \tag{5.75}$$

Moreover, if there exists a subgroup Γ of Sym_V acting transitively on V and such that

$$\{\, \mathrm{Congr}_{P_\sigma} : \sigma \in \Gamma\} \subseteq \mathrm{Aut}(\mathbb{A}) \cap \mathrm{Aut}(\mathbb{K}), \tag{5.76}$$

then

$$n = \delta^*(\bar{e} \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))\delta^*(\bar{e} \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))), \tag{5.77}$$

where $n := |V|$.

[1]To be completely precise: if $\mathscr{C}, \mathscr{D} \subseteq \mathbb{R}^V_+$ are convex corners such that $\mathrm{abl}(\mathscr{C}) = \mathscr{D}$, then the support functions $\delta^*(\cdot \mid \mathscr{C})$ and $\delta^*(\cdot \mid \mathscr{D})$ are equal to the gauges $\gamma(\cdot \mid \mathscr{C}^\circ)$ and $\gamma(\cdot \mid \mathscr{D}^\circ)$, respectively, when restricted to $\mathbb{R}^V_+$, by (5.62). Under this restriction to $\mathbb{R}^V_+$, we also have $\gamma(\cdot \mid \mathscr{D}^\circ) = \gamma(\cdot \mid \mathrm{abl}(\mathscr{D}))$, and the gauge $\gamma(\cdot \mid \mathrm{abl}(\mathscr{D})) = \gamma(\cdot \mid \mathscr{C})$ is polar to $\gamma(\cdot \mid \mathscr{C}^\circ)$.

Proof. By Theorem 5.9, we know that $\mathrm{cl}(\mathrm{TH}(\mathbb{A},\mathrm{Schur}(\mathbb{K}^*)))$ is a convex corner. By (5.62) and Theorem 5.16, the gauge function $\gamma(\cdot \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A},\mathrm{Schur}(\mathbb{K}^*))))$ is the support function $\delta^*(\cdot \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))$. Hence, the support functions $\delta^*(\cdot \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A},\mathrm{Schur}(\mathbb{K}^*))))$ and $\delta^*(\cdot \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag})-\mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))$ are gauges polar to each other; see [123, Corollary 15.1.2]. Now (5.75) follows immediately.

Next, we prove that '$\geq$' holds in (5.77) if $w = \bar{w} = \bar{e}$ and (5.76) holds. Assume the latter, and set $\widehat{\Gamma} \coloneqq \{\, \hat{\sigma} \in \mathrm{Sym}_{\{0\}\cup V} : \hat{\sigma}(0) = 0,\ \hat{\sigma}\restriction_V \in \Gamma \}$. It is clear that

$$\{\, \mathrm{Congr}_{P_{\hat{\sigma}}} : \hat{\sigma} \in \widehat{\Gamma} \} \subseteq \mathrm{Aut}(\widehat{\mathbb{K}}) \qquad \forall \widehat{\mathbb{K}} \in \{\mathrm{Psd}(\mathbb{K}), \mathrm{Schur}(\mathbb{K}^*)\}.$$

Together with $\{\, \mathrm{Congr}_{P_\sigma} : \sigma \in \Gamma \} \subseteq \mathrm{Aut}(\mathbb{A})$, this yields

$$\{\, \mathrm{Congr}_{P_{\hat{\sigma}}} : \hat{\sigma} \in \widehat{\Gamma} \} \subseteq \mathrm{Aut}(\widehat{\mathscr{C}}) \qquad \forall \widehat{\mathscr{C}} \in \{\widehat{\mathrm{TH}}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})), \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))\},$$

whence

$$\{\, P_\sigma : \sigma \in \Gamma \} \subseteq \mathrm{Aut}(\mathscr{C}) \qquad \forall \mathscr{C} \in \{\mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})), \mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))\}.$$

Thus, each support function on the RHS of (5.77) is attained by a fixed point of the map

$$x \in \mathbb{R}^V \mapsto \frac{1}{|\Gamma|} \sum_{\sigma \in \Gamma} P_\sigma x.$$

Since Γ acts transitively on V, there exist $\mu, \nu \in \mathbb{R}$ such that $\mu\bar{e}$ attains $\delta^*(\bar{e} \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))$ and $\nu\bar{e}$ attains $\delta^*(\bar{e} \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*))))$. By (5.73) from Theorem 5.16, we get $\langle \mu\bar{e}, \nu\bar{e} \rangle \leq 1$ so $\mu\nu n \leq 1$. Thus,

$$\delta^*(\bar{e} \mid \mathrm{TH}(\mathrm{Im}(\mathrm{Diag}) - \mathbb{A}^*, \mathrm{Psd}(\mathbb{K})))\delta^*(\bar{e} \mid \mathrm{cl}(\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathbb{K}^*)))) = \langle \bar{e}, \mu\bar{e} \rangle \langle \bar{e}, \nu\bar{e} \rangle = \mu\nu n^2 \leq n. \qquad \square$$

The preceding results apply to the Lovász theta number and the variants ϑ' and ϑ^+ as follows. Let $G = (V, E)$ be a graph. We may now finally define, for each $w \in \mathbb{R}^V_+$, the parameters

$$\vartheta(G; w) \coloneqq \vartheta(\mathbb{A}_{\overline{E},\overline{E}}, \mathbb{S}^V_+; w), \tag{5.78}$$

$$\vartheta'(G; w) \coloneqq \vartheta(\mathbb{A}_{\varnothing,\overline{E}}, \mathbb{S}^V_+; w), \tag{5.79}$$

$$\vartheta^+(G; w) \coloneqq \vartheta(\mathbb{A}_{\binom{V}{2},\overline{E}}, \mathbb{S}^V_+; w). \tag{5.80}$$

5.7 The Stable Set Polytope as a Theta Body

In this section, we show that the stable set polytope of a graph and one of its classical fractional versions are theta bodies. The key result we use to prove this is a completely positive formulation for the stability number of a graph, due to de Klerk and Pasechnik [32]. As a consequence of the antiblocker duality relation from Theorem 5.16, we shall derive a weighted generalization of a copositive formulation for the fractional chromatic number of a graph, due to Dukanovic and Rendl [37].

We shall use the cone $\mathcal{C}_V$ of copositive matrices and its dual $\mathcal{C}^*_V$, the cone of completely positive matrices. Recall that a matrix $X \in \mathbb{S}^V$ is said to be *copositive* if $h^\mathsf{T} X h \geq 0$ for every $h \in \mathbb{R}^V_+$, and X is said to be *completely positive* if $X = \sum_{h \in H} hh^{\mathsf{T}}$ for some finite subset H of $\mathbb{R}^V_+$. There has been much interest around these cones recently; see, for instance, [19, 119, 17, 20].

Let $G = (V, E)$ be a graph. For each $w \in \mathbb{R}^V_+$, we set

$$\alpha(G; w) \coloneqq \delta^*(w \mid \mathrm{STAB}(G)); \tag{5.81}$$

recall that the stable set polytope $\mathrm{STAB}(G)$ was defined in (1.24).

The key argument of the next result comes from [32, Theorem 2.2]:

Proposition 5.18. If $G = (V, E)$ is a graph, then

$$\mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Psd}(\mathcal{C}^*_V)) = \mathrm{STAB}(G). \tag{5.82}$$

Proof. If $S \subseteq V$ is a stable set of G, then $\mathbb{1}_S \in \mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Psd}(\mathcal{C}^*_V))$ since $(1 \oplus \mathbb{1}_S)(1 \oplus \mathbb{1}_S)^{\mathsf{T}} \in \mathrm{Psd}(\mathcal{C}^*_V)$ and $\mathbb{1}_S \mathbb{1}_S^{\mathsf{T}} \in \mathbb{A}_{E,E}$. This proves that $\mathrm{STAB}(G) \subseteq \mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Psd}(\mathcal{C}^*_V))$.

For the reverse inclusion it suffices by conjugate duality and Corollary 5.2 to show that, for $w \in \mathbb{R}^V_+$, we have $\alpha(G; w) \geq \delta^*(w \mid \mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Psd}(\mathcal{C}^*_V)))$. Thus, it suffices by Theorem 5.8 to show that, for $w \in \mathbb{R}^V_+$, we have

$$\alpha(G; w) \geq \max\Big\{ \sqrt{w}^{\mathsf{T}} X \sqrt{w} : \mathrm{Tr}(X) = 1,\ X \in \mathbb{A}_{E,E},\ X \in \mathcal{C}^*_V \Big\}. \tag{5.83}$$

Let $w \in \mathbb{R}^V_+$. If $w = 0$ then (5.83) holds trivially, so assume $w \neq 0$. The extreme rays of the cone $\mathcal{C}^*_V \cap \mathbb{A}_{E,E}$ are of the form $\mathbb{R}_+ xx^{\mathsf{T}}$ with $x \in \mathbb{R}^V_+$ and $\mathrm{supp}(x)$ stable in G. So there exists an optimal solution for the RHS of (5.83) of the form $\bar{x}\bar{x}^{\mathsf{T}}$ for some $\bar{x} \in \mathbb{R}^V_+$ such that $\|\bar{x}\|^2 = \mathrm{Tr}(\bar{x}\bar{x}^{\mathsf{T}}) = 1$ and $\mathrm{supp}(\bar{x})$ is a stable set in G. In fact, for any $y \in \mathbb{R}^V_+$ such that $\|y\|^2 = 1$ and $\mathrm{supp}(y) \subseteq \mathrm{supp}(\bar{x})$, the point yy^{T} is feasible in the RHS of (5.83) with objective value $\langle \sqrt{w}, y \rangle^2$ whence

$$\begin{aligned} &\max\Big\{ \sqrt{w}^{\mathsf{T}} X \sqrt{w} : \mathrm{Tr}(X) = 1,\ X \in \mathbb{A}_{E,E},\ X \in \mathcal{C}^*_V \Big\} \\ &\qquad = \max\Big\{ \langle \sqrt{w}, y \rangle^2 : y \in \mathbb{R}^V_+,\ \|y\|^2 = 1,\ \mathrm{supp}(y) \subseteq \mathrm{supp}(\bar{x}) \Big\}. \end{aligned} \tag{5.84}$$

The optimality conditions for the RHS of (5.84) (i.e., Cauchy-Schwarz) show that an optimal solution is given by $\bar{y} \coloneqq \frac{\sqrt{u}}{\|\sqrt{u}\|}$ where $u \coloneqq w \odot \mathbb{1}_{\mathrm{supp}(\bar{x})}$, and its objective value is

$$\frac{\langle \sqrt{w}, \sqrt{u} \rangle^2}{\|\sqrt{u}\|^2} = \frac{\langle \sqrt{u}, \sqrt{u} \rangle^2}{\|\sqrt{u}\|^2} = \|\sqrt{u}\|^2 = \langle w, \mathbb{1}_{\mathrm{supp}(\bar{x})} \rangle.$$

Since $\mathrm{supp}(\bar{x})$ is stable, this concludes our proof of (5.83). $\square$

Let $G = (V, E)$ be a graph. The *fractional stable set polytope of* G is defined as

$$\mathrm{QSTAB}(G) \coloneqq \mathrm{abl}(\mathrm{STAB}(\overline{G})), \tag{5.85}$$

and for $w \in \mathbb{R}^V_+$, we set

$$\chi^*(G; w) \coloneqq \delta^*(w \mid \mathrm{QSTAB}(\overline{G})). \tag{5.86}$$

Proposition 5.18 yields immediately a weighted generalization of [37, Corollary 5]:

Corollary 5.19. Let $G = (V, E)$ be a graph. Let $w \in \mathbb{R}^V_+$. Then

$$\chi^*(G; w) = \inf\left\{ \lambda : Y \in \mathbb{A}^{\perp}_{\overline{E},\overline{E}},\ \begin{bmatrix} 1 & \sqrt{w}^{\mathsf{T}} \\ \sqrt{w} & \lambda I - Y \end{bmatrix} \in \mathrm{Psd}(\mathcal{C}^*_V) \right\}. \tag{5.87}$$

Proof. By Proposition 5.18 and (5.66) from Proposition 5.15, we have

$$\begin{aligned} \chi^*(G; w) &= \delta^*(w \mid \mathrm{QSTAB}(\overline{G})) = \delta^*(w \mid \mathrm{abl}(\mathrm{STAB}(G))) = \delta^*(w \mid \mathrm{abl}(\mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Psd}(\mathcal{C}^*_V)))) \\ &= \inf\left\{ \lambda \in \mathbb{R}_+ : Y \in -\mathbb{A}_{E,E} \cap \mathrm{Null}(\mathrm{diag}),\ \begin{bmatrix} 1 & \sqrt{w}^{\mathsf{T}} \\ \sqrt{w} & \lambda I - Y \end{bmatrix} \in \mathrm{Psd}(\mathcal{C}^*_V) \right\} \\ &= \inf\left\{ \lambda : Y \in \mathbb{A}^{\perp}_{\overline{E},\overline{E}},\ \begin{bmatrix} 1 & \sqrt{w}^{\mathsf{T}} \\ \sqrt{w} & \lambda I - Y \end{bmatrix} \in \mathrm{Psd}(\mathcal{C}^*_V) \right\}. \end{aligned}$$

The constraint $\lambda \in \mathbb{R}_+$ may be dropped since $\mathrm{diag}(\mathcal{C}^*_V) \subseteq \mathbb{R}^V_+$. $\square$

By the antiblocker relation from Theorem 5.16, we know that $\mathrm{QSTAB}(G)$ is the closure of a theta body. Unlike in the cases presented so far, the fact that the latter theta body is actually closed does not follow from our previous results. Thus, we proceed to prove the closedness separately. We shall use an argument from [46, Theorem 5] (more specifically, in the proof of (5.94) below).

Theorem 5.20. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant polyhedral cone. Then

$$\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathcal{C}_V)) = \left\{ \mathrm{diag}(\hat{X}[V]) : \hat{X} \in \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Schur}(\mathcal{C}_V)),\ \|\hat{X}\|_\infty \leq 1 \right\}. \tag{5.88}$$

Consequently, $\mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathcal{C}_V))$ is a convex corner.

Proof. The inclusion '$\supseteq$' in (5.88) is trivial. For the reverse inclusion, let $x \in \mathrm{TH}(\mathbb{A}, \mathrm{Schur}(\mathcal{C}_V))$, and let $\hat{Y} \in \widehat{\mathrm{TH}}(\mathbb{A}, \mathrm{Schur}(\mathcal{C}_V))$ such that $x = \mathrm{diag}(Y)$ for $Y \coloneqq \hat{Y}[V]$. We shall use (5.64) throughout the proof without further mention. Note that $Y - xx^{\mathsf{T}} \in \mathcal{C}_V$ implies that $x - (x \odot x) = \mathrm{diag}(Y - xx^{\mathsf{T}}) \geq 0$ so

$$x \in [0, 1]^V. \tag{5.89}$$

Let us prove that

$$\text{we may assume that } Y \in \mathbb{S}^V_{\geq 0} \text{ and } Y = Y[\mathrm{supp}(x)] \oplus 0. \tag{5.90}$$

Indeed, the principal submatrix $Y = \hat{Y}[V]$ from $\hat{Y}$ may possibly be replaced with

$$Y - 2\sum\left\{ [Y_{ij} < 0] Y_{ij}\, \mathrm{Sym}(e_i e_j^{\mathsf{T}}) : ij \in \tbinom{V}{2} \right\}$$

without affecting the relations $\hat{Y}[V] \in \mathbb{A}$ or $\hat{Y}[V] \succeq_{\mathcal{C}_V} xx^{\mathsf{T}}$, by Proposition 5.3 and the trivial fact that $\mathcal{C}_V + \mathbb{S}^V_{\geq 0} = \mathcal{C}_V$. Clearly, for $S \coloneqq \mathrm{supp}(x)$ and $\bar{x} \coloneqq x\restriction_S$, we have $Y[S] \succeq_{\mathcal{C}_S} \bar{x}\bar{x}^{\mathsf{T}}$. Thus, by possibly replacing $\hat{Y}[V]$ with $\hat{Y}[S] \oplus 0$, we shall have $Y = Y[\mathrm{supp}(x)] \oplus 0$, and the proof of (5.90) is complete. Thus, by possibly restricting our attention to the index set $\mathrm{supp}(x)$,

$$\text{we may assume that } \mathrm{supp}(x) = V. \tag{5.91}$$

Write $D \coloneqq \operatorname{Diag}(x)$ and $B \coloneqq Y - D$. Let G be the graph on V where $ij \in \binom{V}{2}$ is an edge if $B_{ij} > 0$. Define $A \in \mathbb{A}$ by setting $A_{ij} \coloneqq \frac{1}{2}[ij \in E]\big(1/x_i + 1/x_j\big)$ for each $ij \in \binom{V}{2}$. We claim that

$$D^{-1} + A - \bar{e}\bar{e}^{\mathsf{T}} \in \mathcal{C}_V. \tag{5.92}$$

We shall need to consider the following optimization problem in our proof:

$$\min\big\{\, h^{\mathsf{T}}(D^{-1} + A)h : h \in \mathbb{R}^V_+,\ \langle \bar{e}, h\rangle = 1 \big\}. \tag{5.93}$$

Let us show that

$$\text{there exists an optimal solution } \bar{h} \text{ for (5.93) whose support is a stable set in } G. \tag{5.94}$$

Indeed, let $\bar{h}$ be an optimal solution for (5.93) with minimal support. Note that an optimal solution exists by continuity and compactness. Suppose that $ij \subseteq \operatorname{supp}(\bar{h})$ for some $ij \in E$. For each $t \in \mathbb{R}$, define $h_t \coloneqq \bar{h} + t(e_i - e_j)$, and note that h_t is feasible for (5.93) whenever $t \in [-\bar{h}_i, \bar{h}_j]$. The objective value of h_t in (5.93) is, $h_t^{\mathsf{T}}(D^{-1} + A)h_t = \bar{h}^{\mathsf{T}}(D^{-1} + A)\bar{h} + 2t(e_i - e_j)^{\mathsf{T}}(D^{-1} + A)\bar{h} = \bar{h}^{\mathsf{T}}(D^{-1} + A)\bar{h}$, where the final equation follows from the optimality of $\bar{h} = h_0$. Since $h_{\bar{t}}$ is feasible in (5.93) for $\bar{t} \coloneqq \bar{h}_i$ and $\operatorname{supp}(h_{\bar{t}}) \subsetneq \operatorname{supp}(\bar{h})$, the proof of (5.94) is complete.

It follows from (5.94) that $\bar{h}^{\mathsf{T}} A\bar{h} = 0$ and $\bar{h}^{\mathsf{T}} D^{-1}BD^{-1}\bar{h} = 0$. Thus, since $D^{-1}YD^{-1} \succeq_{\mathcal{C}_V} D^{-1}xx^{\mathsf{T}}D^{-1}$ by the diagonal scaling invariance of $\mathcal{C}_V$, we get

$$\begin{aligned}\bar{h}^{\mathsf{T}}(D^{-1} + A)\bar{h} &= \bar{h}^{\mathsf{T}}D^{-1}\bar{h} = \bar{h}^{\mathsf{T}}(D^{-1}DD^{-1})\bar{h} = \bar{h}^{\mathsf{T}}(D^{-1}(D+B)D^{-1})\bar{h}\\ &\geq \bar{h}^{\mathsf{T}}D^{-1}xx^{\mathsf{T}}D^{-1}\bar{h} = \bar{h}^{\mathsf{T}}\bar{e}\bar{e}^{\mathsf{T}}\bar{h} = 1.\end{aligned}$$

Thus, $\min\{\, h^{\mathsf{T}}(D^{-1} + A - \bar{e}\bar{e}^{\mathsf{T}})h : h \in \mathbb{R}^V_+,\ \bar{e}^{\mathsf{T}}h = 1\} \geq 0$ and (5.92) is proved. Set $X \coloneqq \mathcal{D}_x(D^{-1} + A)$. Then (5.92) implies $X \succeq_{\mathcal{C}_V} \mathcal{D}_x(\bar{e}\bar{e}^{\mathsf{T}}) = xx^{\mathsf{T}}$. Moreover, $\operatorname{diag}(X) = x$ and, for $ij \in E$, we have

$$X_{ij} = \big[\mathcal{D}_x(A)\big]_{ij} = \frac{x_i x_j}{2}\left(\frac{1}{x_i} + \frac{1}{x_j}\right) = \frac{x_j + x_i}{2} \leq 1$$

by (5.89). Since $X_{ij} = 0$ for $ij \in \overline{E}$, it follows that

$$\hat{X} \coloneqq \begin{bmatrix} 1 & x^{\mathsf{T}} \\ x & X \end{bmatrix} \in \widehat{\mathrm{TH}}(\mathbb{A}, \operatorname{Schur}(\mathcal{C}_V))$$

and $\|\hat{X}\|_\infty \leq 1$. This completes the proof of (5.88). It follows that the set $\mathrm{TH}(\mathbb{A}, \operatorname{Schur}(\mathcal{C}_V))$ is closed, since it is described by (5.88) as the linear image of a compact set. Thus, $\mathrm{TH}(\mathbb{A}, \operatorname{Schur}(\mathcal{C}_V))$ is a convex corner by Theorem 5.9. ☐

Corollary 5.21. Let $G = (V, E)$ be a graph. Then

$$\mathrm{QSTAB}(G) = \mathrm{TH}(\mathbb{A}_{E,E}, \operatorname{Schur}(\mathcal{C}_V)). \tag{5.95}$$

In particular, for every $w \in \mathbb{R}^V_+$, we have

$$\chi^*(G; w) = \max\Big\{\, \langle w, x\rangle : X \in \mathbb{A}_{\overline{E},\overline{E}},\ \operatorname{diag}(X) = x,\ X \succeq_{\mathcal{C}_V} xx^{\mathsf{T}} \Big\}. \tag{5.96}$$

Proof. By Theorems 5.16 and 5.20 and Proposition 5.18, we get

$$\operatorname{abl}(\mathrm{TH}(\mathbb{A}_{E,E}, \mathrm{Schur}(\mathcal{C}_V))) = \mathrm{TH}(\mathbb{A}_{\overline{E},\overline{E}}, \mathrm{Psd}(\mathcal{C}_V^*)) = \mathrm{STAB}(\overline{G}).$$

Thus, (5.95) follows from antiblocking duality. Now (5.96) follows from (5.95) and (5.64) since, for each $w \in \mathbb{R}^V_+$, we have

$$\chi^*(G; w) = \delta^*(w \mid \mathrm{QSTAB}(\overline{G})) = \delta^*(w \mid \mathrm{TH}(\mathbb{A}_{\overline{E},\overline{E}}, \mathrm{Schur}(\mathcal{C}_V))). \qquad \square$$

5.8 Hoffman Bounds

The Lovász theta number $\vartheta(G)$ may be regarded as the "best" lower bound for the clique covering number of G from a family of bounds inspired by a result of Hoffman. In this section, we shall generalize this observation to our framework.

Hoffman [68] proved the following classical lower bound for the chromatic number of a graph $G = (V, E)$:

$$\chi(G) \geq 1 - \frac{\lambda_{\max}(A_G)}{\lambda_{\min}(A_G)}. \tag{5.97}$$

Here, A_G denotes the adjacency matrix of G. Lovász [94, Theorem 6] proved that the lower bound (5.97) on $\chi(G)$ remains valid if the adjacency matrix A_G is replaced with any matrix in $\mathbb{A}^{\perp}_{E,E}$, and that the tightest lower bound on $\chi(G)$ arising in this manner is precisely $\overline{\vartheta}(G)$. Knuth [78, Sec. 33] defined another graph parameter, denoted by $\vartheta_6(G; w)$, which is in fact equal to $\vartheta(G; w)$. The parameter $\vartheta_6(G; w)$ is defined as an optimization problem, and the objective value corresponding to $\vartheta_6(\overline{G}; \bar{e})$ yields precisely the expression of the RHS of (5.97) when applied to an arbitrary matrix $A \in \mathbb{A}^{\perp}_{E,E}$. We shall partially extend our framework in this direction.

Let $\mathbb{A} \subseteq \mathbb{S}^V$ and $\mathbb{K} \subseteq \mathbb{S}^V$. Following Knuth [78, Sec. 33], we define

$$\vartheta_6(\mathbb{A}, \mathbb{K}; w) := \sup\big\{\, \lambda_{\max}(B) : \operatorname{diag}(B) = w,\ B \in \mathbb{K},\ B \in \operatorname{Im}(\mathrm{Diag}) - \mathbb{A}^* \big\} \tag{5.98}$$

for every $w \in \mathbb{R}^V_+$. Note that the optimization problem on the RHS above is not convex. The next result relates $\vartheta_6(\mathbb{A}, \mathbb{K}; w)$ to $\vartheta_3(\mathbb{A}, \mathbb{K}; w)$.

Proposition 5.22. Let $\mathbb{M} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant closed convex cone such that (5.39) holds. Suppose that $\mathrm{Diag}(\mathbb{R}^V_+) \subseteq \mathbb{M}$, and that either $\mathcal{D}_h(\mathbb{M}) \subseteq \mathbb{M}$ for every $h \in \mathbb{R}^V$ or $\mathbb{M} \subseteq \mathbb{S}^V_{\geq 0}$. Let $w \in \mathbb{R}^V_+$. Then

$$\max\Big\{\, \sqrt{w}^{\mathsf{T}} X \sqrt{w} : \operatorname{Tr}(X) = 1,\ X \in \mathbb{M} \Big\} = \max\Big\{\, \lambda_{\max}(B) : B \in \mathbb{M},\ \operatorname{diag}(B) = w \Big\}. \tag{5.99}$$

Proof. It is easy to check that (5.99) holds if $w = 0$ by using (5.39b). Thus, we may assume that $w \neq 0$. Together with the assumption that $\mathrm{Diag}(\mathbb{R}^V_+) \subseteq \mathbb{M}$ we know that the LHS of (5.99) is positive, whence Lemma 5.7 may be applied.

We start by proving '$\leq$' in (5.99). Let X^* be an optimal solution for the LHS of (5.99). Define d and $\bar{X}$ as in Lemma 5.7. Then $\bar{B} := \mathcal{D}_{\sqrt{w}}(\bar{X}) + \mathrm{Diag}\big(w \odot \mathbb{1}_{V \setminus \operatorname{supp}(d)}\big)$ is feasible for the RHS and its objective value is $\lambda_{\max}(\bar{B}) \geq \lambda_{\max}\big(\mathcal{D}_{\sqrt{w}}(\bar{X})\big) = \sqrt{w}^{\mathsf{T}} X^* \sqrt{w}$ by (5.41b).

Next we prove '$\geq$' in (5.99). Let $\bar{B}$ be an optimal solution for the RHS of (5.99). (An optimal solution exists by continuity and compactness, where compactness is an easy consequence of (5.39c).) Let $\lambda \coloneqq \lambda_{\max}(\bar{B})$ and let $b \in \mathbb{R}^V$ be a unit vector such that $\bar{B}b = \lambda b$. Note that $\operatorname{supp}(b) \subseteq \operatorname{supp}(w)$ by (5.39b). The matrix $\tilde{X} \coloneqq \operatorname{Diag}(\sqrt{w})^\dagger \bar{B} \operatorname{Diag}(\sqrt{w})^\dagger$ satisfies $\operatorname{diag}(\tilde{X}) = \mathbb{1}_{\operatorname{supp}(w)}$, whence $\bar{X} \coloneqq \mathcal{D}_b(\tilde{X})$ satisfies $\operatorname{Tr}(\bar{X}) = 1$. If $\mathcal{D}_h(\mathbb{M}) \subseteq \mathbb{M}$ for each $h \in \mathbb{R}^V$, then $\bar{X} \in \mathbb{M}$ follows from $\bar{B} \in \mathbb{M}$. If $\mathbb{M} \subseteq \mathbb{S}^V_{\geq 0}$, then $\bar{X} \in \mathbb{M}$ follows from $\bar{B} \in \mathbb{M}$ and by the diagonal scaling invariance of $\mathbb{M}$, since we may assume that $b \geq 0$ by the Perron-Frobenius Theorem; see, e.g., [72, Theorem 8.3.1] or [50, Theorem 8.8.1]. In either case, we find that $\bar{X} \in \mathbb{M}$, whence $\bar{X}$ is feasible in the LHS of (5.99). Finally, its objective value in the LHS of (5.99) is

$$\sqrt{w}^\mathsf{T} \bar{X} \sqrt{w} = \sqrt{w}^\mathsf{T} \mathcal{D}_b(\tilde{X}) \sqrt{w} = b^\mathsf{T} \mathcal{D}_{\sqrt{w}}(\tilde{X}) b = b^\mathsf{T} \bar{B} b = \lambda,$$

where we used (5.39b) to get $\bar{B} = \mathcal{D}_{\sqrt{w}}(\tilde{X})$. This completes the proof of (5.99). ☐

Next we shall show that, when applied to $w = \bar{e}$, the objective value of the RHS of (5.99) has the same form as the RHS of (5.97), and thus generalizes it:

Proposition 5.23. Let $\mathbb{A} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant polyhedral cone. Let $\mathbb{K} \subseteq \mathbb{S}^V$ be a diagonally scaling-invariant closed convex cone. Suppose that $I \in \mathbb{K}$. Then

$$\begin{aligned} &\max\left\{\, \lambda_{\max}(B) : B \in \mathbb{A} \cap \mathbb{K},\ \operatorname{diag}(B) = \bar{e} \right\} \\ &\qquad = \max\left\{\, 1 - [\mu \neq 0] \frac{\lambda_{\max}(A)}{\mu} : A \in \mathbb{A} \cap \operatorname{Null}(\operatorname{diag}),\ \mu \in -\mathbb{R}_+,\ A \succeq_{\mathbb{K}} \mu I \right\}. \end{aligned} \tag{5.100}$$

Proof. We have

$$\begin{aligned} \max&\left\{\, \lambda_{\max}(B) : B \in \mathbb{A} \cap \mathbb{K},\ \operatorname{diag}(B) = \bar{e} \right\} \\ &= \max\left\{\, \lambda_{\max}(I + A) : I + A \in \mathbb{A} \cap \mathbb{K},\ \operatorname{diag}(A) = 0 \right\} \\ &= \max\left\{\, 1 + [\nu \neq 0] \nu \lambda_{\max}(A) : A \in \mathbb{A} \cap \operatorname{Null}(\operatorname{diag}),\ \nu \in \mathbb{R}_+,\ \nu A \succeq_{\mathbb{K}} -I \right\} \\ &= \max\left\{\, 1 - [\mu \neq 0] \frac{\lambda_{\max}(A)}{\mu} : A \in \mathbb{A} \cap \operatorname{Null}(\operatorname{diag}),\ \mu \in -\mathbb{R}_+,\ A \succeq_{\mathbb{K}} \mu I \right\}. \end{aligned}$$

Note that we used Proposition 5.3 on the second equation. ☐

Let $G = (V, E)$ be a graph. Then we have

$$\begin{aligned} \max\left\{\, 1 - [A \neq 0] \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} : A \in \mathbb{A}^\perp_{E,E} \right\} &= \vartheta_6(\mathbb{A}_{E,E}, \mathbb{S}^V_+; \bar{e}) && \text{by Proposition 5.23,} \\ &= \vartheta_3(\mathbb{A}_{E,E}, \mathbb{S}^V_+; \bar{e}) && \text{by Proposition 5.22,} \\ &= \delta^*(\bar{e} \mid \operatorname{TH}(\mathbb{A}_{\overline{E},\overline{E}}, \mathbb{S}^V_+)) && \text{by Theorem 5.16,} \\ &\leq \delta^*(\bar{e} \mid \operatorname{TH}(\mathbb{A}_{\overline{E},\overline{E}}, \mathcal{C}_V)) && \text{since } \mathbb{S}^V_+ \subseteq \mathcal{C}_V, \\ &= \delta^*(\bar{e} \mid \operatorname{QSTAB}(\overline{G})) && \text{by Corollary 5.21,} \\ &= \chi^*(G; \bar{e}) \leq \chi(G). \end{aligned}$$

This proves that the best bound from this family of lower bounds for $\chi(G)$ is $\vartheta(\overline{G})$, as was already shown by Lovász [94, Theorem 6].

Chapter 6

Integrality Constraints for SDPs

In polyhedral combinatorics, one usually considers a chain of inequalities of the form

$$
\begin{aligned}
&\max\{\, c^{\mathsf{T}}x : Ax \le b,\ x \ge 0,\ x \in \mathbb{Z}^n \} && (6.1a)\\
&\quad \le \max\{\, c^{\mathsf{T}}x : Ax \le b,\ x \ge 0,\ x \in \mathbb{R}^n \} && (6.1b)\\
&\qquad \le \min\{\, b^{\mathsf{T}}y : y \ge 0,\ A^{\mathsf{T}}y \ge c,\ y \in \mathbb{R}^m \} && (6.1c)\\
&\qquad\quad \le \min\{\, b^{\mathsf{T}}y : y \ge 0,\ A^{\mathsf{T}}y \ge c,\ y \in \mathbb{Z}^m \}, && (6.1d)
\end{aligned}
$$

where the feasible region of (6.1a) is contained in $\{0,1\}^n$, and some optimal solution of (6.1d) lies in $\{0,1\}^m$. In many interesting cases, equality holds throughout in (6.1), and a combinatorial min-max theorem follows. For instance, if A is the $E \times V$ incidence matrix of a graph $G = (V, E)$ with no isolated nodes, $b = \bar{e}$, and $c = \bar{e}$, then (6.1a) is a formulation for the stable set problem and (6.1d) yields a formulation for the minimum edge-cover problem. Equality throughout holds in (6.1) if G is bipartite. Alternatively, if A is the $\mathcal{K} \times V$ incidence matrix of G, where $\mathcal{K}$ is the set of all cliques of G, then (6.1a) still formulates the stable set problem, but (6.1c) formulates the fractional clique-covering number, and (6.1d) is a formulation for the clique-covering number. Equality throughout holds in (6.1) if G is perfect, even if we allow c to be an arbitrary vector in $\mathbb{Z}^V_+$. However, even when we do not have equality throughout in (6.1), the conceptual framework provided by this chain of inequalities is quite valuable theoretically, e.g., in the design of primal-dual approximation algorithms [153, 155].

In the context of SDPs, the following partial analogue of the chain (6.1) is usually considered:

$$
\begin{aligned}
&\sup\big\{\, \langle C, X\rangle : \mathcal{A}(X) \le b,\ X \in \mathbb{S}^n_+,\ \operatorname{rank}(X) = 1 \big\} && (6.2a)\\
&\quad \le \sup\big\{\, \langle C, X\rangle : \mathcal{A}(X) \le b,\ X \in \mathbb{S}^n_+ \big\} && (6.2b)\\
&\qquad \le \inf\big\{\, \langle a, y\rangle : y \in \mathbb{R}^m_+,\ \mathcal{A}^*(y) \succeq C \big\}. && (6.2c)
\end{aligned}
$$

The (non-convex) optimization problem (6.2a) usually models a combinatorial optimization problem exactly, so its role is similar to that of (6.1a). Analogously, (6.2b) is an SDP relaxation of (6.2a) and (6.2c) is its dual, so they correspond to the LPs (6.1b) and (6.1c) from the chain (6.1). It is desirable to extend the chain of inequalities (6.2) to be as complete as (6.1), so that new concepts of exactness of SDP formulations may be studied, akin to classical polyhedral combinatorics concepts such as *total dual integrality* (see, e.g., [38] or [130, Chapter 22]). We regard the integrality constraints of the endpoints of (6.1), as well as the rank constraint from (6.2a), as non-convex constraints used to formulate combinatorial problems exactly. Similarly, we would like to have a non-convex constraint that, when added to the dual SDP (6.2c), yields a sensible problem, much like the integrality constraint in (6.1d) usually yields sensible combinatorial problems for a wide class of combinatorial optimization problems formulated in the format of (6.1a).

It is easy to add a non-convex constraint to the dual (6.2c) so as to extend the chain of inequalities (6.2) to match (6.1) in a way that "generalizes" the latter. For instance, suppose the problem (6.1b) is embedded into an SDP in the format of (6.2b) as

$$\begin{aligned} \sup\quad & \langle \mathrm{Diag}(0 \oplus c), \hat{X} \rangle \\ & \langle e_0 e_0^{\mathsf{T}}, \hat{X} \rangle = 1, \\ & \langle 2\,\mathrm{Sym}(e_j (e_j - e_0)^{\mathsf{T}}), \hat{X} \rangle = 0 \quad \forall j \in [n], \\ & \langle -b_i \oplus \mathrm{Diag}(A^{\mathsf{T}} e_i), \hat{X} \rangle \leq 0 \qquad \forall i \in [m], \\ & \hat{X}[[n]] \geq 0, \\ & \hat{X} \in \mathbb{S}_+^{\{0\} \cup [n]}. \end{aligned} \tag{6.3}$$

(The reasons for using slightly differently constants multiplying the constraint matrices, compared to previous chapters, shall be explained later; for now, just note that each constraint matrix has only integral components if A and b are integral.) The dual SDP, written with an explicit slack, is

$$\begin{aligned} \inf\quad & \eta \\ & \eta \in \mathbb{R},\ u \in \mathbb{R}^n,\ y \in \mathbb{R}^m_+,\ Z \in \mathbb{S}^n_{\geq 0}, \\ & \begin{bmatrix} \eta & -u^{\mathsf{T}} \\ -u & \mathrm{Diag}(2u) - Z \end{bmatrix} + \sum_{i \in [m]} y_i \begin{bmatrix} -b_i & 0^{\mathsf{T}} \\ 0 & \mathrm{Diag}(A^{\mathsf{T}} e_i) \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^{\mathsf{T}} \\ 0 & \mathrm{Diag}(c) \end{bmatrix}, \\ & \hat{S} \in \mathbb{S}_+^{\{0\} \cup [n]}. \end{aligned} \tag{6.4}$$

Suppose we add the constraint $\mathrm{rank}(\hat{S}) \leq 1$ to (6.4). Then each feasible solution y for (6.1d) yields a feasible solution for the modification of problem (6.4), with the same objective value: just take $\eta \oplus u \oplus Z := \langle b, y \rangle \oplus 0 \oplus \mathrm{Diag}(A^{\mathsf{T}} y - c)$, so that the corresponding dual slack is $\hat{S} = 0$. In fact, if A, b, and c are integral, we may even add integrality constraints on the variable $\eta \oplus u \oplus y \oplus Z$. The resulting extension of the chain (6.2) is then at least as tight as (6.1).

However, when trying to extend the chain (6.2), we want to include not only the chain (6.1) arising from binary integer linear programs, but also some important SDP relaxations not arising as (6.3). In this respect, the rank constraint on the dual slack seems quite unsatisfactory, since it does not meet one crucial minimum requirement, namely, it does yield an "adequate" modified dual when applied to the SDP for the Lovász theta number. Indeed, let $G = (V, E)$ be a graph, and let $w \in \mathbb{Z}^V_{++}$. Let us consider the formulation for $\vartheta(G; w)$ given by:

$$\begin{aligned} \vartheta(G; w) = \max\quad & \langle \mathrm{Diag}(0 \oplus w), \hat{X} \rangle \\ & \langle e_0 e_0^{\mathsf{T}}, \hat{X} \rangle = 1, \\ & \langle 2\,\mathrm{Sym}(e_i (e_i - e_0)^{\mathsf{T}}), \hat{X} \rangle = 0 \quad \forall i \in V, \\ & \langle 2\,\mathrm{Sym}(e_i e_j^{\mathsf{T}}), \hat{X} \rangle = 0 \qquad\quad\ \forall ij \in E, \\ & \hat{X} \in \mathbb{S}_+^{\{0\} \cup V}. \end{aligned} \tag{6.5}$$

Its dual, written with an explicit slack, is

$$\begin{aligned} \inf \quad & \eta \\ & \eta \in \mathbb{R},\, u \in \mathbb{R}^V,\, z \in \mathbb{R}^E, \\ & \begin{bmatrix} \eta & -u^\mathsf{T} \\ -u & 2\operatorname{Diag}(u) \end{bmatrix} + \sum_{ij\in E} z_{ij} \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & 2\operatorname{Sym}(e_i e_j^\mathsf{T}) \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & \operatorname{Diag}(w) \end{bmatrix}, \\ & \hat{S} \in \mathbb{S}_+^{\{0\}\cup V}. \end{aligned} \tag{6.6}$$

Suppose we add the constraint $\operatorname{rank}(\hat{S}) \leq 1$ to (6.6). Since $\eta > 0$ for any feasible solution by Weak Duality, the constraint $\operatorname{rank}(\hat{S}) \leq 1$ is equivalent to

$$\operatorname{Diag}(2u - w) + 2\sum_{ij\in E} z_{ij} \operatorname{Sym}(e_i e_j^\mathsf{T}) = \tfrac{1}{\eta} u u^\mathsf{T}.$$

Moreover, $\operatorname{supp}(w) = V$ implies that $\operatorname{supp}(u) = V$, since $\operatorname{diag}(\hat{S}) \geq 0$ whenever $\hat{S}$ is a feasible dual slack. However, then either $E = \binom{V}{2}$ or the modified dual is infeasible.

In this chapter, we present a non-convex constraint for the dual SDP that achieves our minimum requirements, i.e., it generalizes the chain (6.1) and yields sensible modified duals for the SDP formulation of the Lovász theta number. The "mirror image" of this non-convex constraint for the primal SDP reduces in many cases to the rank constraint from (6.2a). In this sense, the new constraint enjoys a form of primal-dual symmetry. We describe the modified duals for SDP formulations for the maximum cut and the vertex cover problems. We also use general methods for obtaining SDP relaxations of binary integer linear programs and examine the effect of the non-convex constraint on the dual SDPs, with a focus on the stable set problem.

Throughout the chapter, we shall state some SDP formulations using slightly different constraint matrices than in previous chapters; see the observation following (6.3). Up to this chapter in the thesis, all of our considerations were essentially of a geometric nature, so that equality and inequality constraints could be freely rescaled without changing the corresponding feasible regions. From now on, since we are concerned about integrality, and in fact mostly about $\{0,1\}$ solutions, the scale has been fixed. This is no different than the analogous situation in LP relaxations in the context of Integer Programming. For instance, any rational system of inequalities can be made *totally dual integral*[1] by multiplying it by a "large" natural number; see [48] or [130, Ch. 22, Eq. (36)]. In the current context, it seems natural to require the constraint matrices of an SDP to have only integral entries, and similarly for the right-hand sides. This is why some constraints on the SDPs (6.3) and (6.5) were rescaled when compared to previous formulations.

The main contributions in this chapter are the primal-dual symmetric integrality constraints (6.10) and (6.11), which provide the basis for Theorem 6.3, and their preliminary study when applied to some important SDP formulations, given by Propositions 6.1 and 6.6.

6.1 A Rank-Constrained SDP Formulation for Clique Covering Number

Let us start by considering the dual SDP for a formulation of the theta number and a sensible integrality constraint for it. As in previous chapters, we shall first derive a more general result which we then specialize

[1] A rational system $Ax \leq b$ of linear inequalities is called *totally dual integral* if the LP $\min\{\, b^\mathsf{T} y : A^\mathsf{T} y = c,\, y \geq 0\}$ has an integral optimal solution for each integral vector c for which the minimum is finite.

to statements concerning formulations for ϑ and the variants ϑ' and ϑ^+.

Let V be a finite set, and let $w \in \mathbb{Z}^V_+$. Let $E^+, E^- \subseteq \binom{V}{2}$. Set $E \coloneqq E^-$ and $G \coloneqq (V, E)$. Consider the optimization problem

$$\begin{array}{lll} \max & \langle \mathrm{Diag}(0 \oplus w), \hat{X} \rangle & \\ & \langle e_0 e_0^\mathsf{T}, \hat{X} \rangle = 1, & \\ & \langle 2\,\mathrm{Sym}(e_i(e_i - e_0)^\mathsf{T}), \hat{X} \rangle = 0 & \forall i \in V, \\ & \langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle \geq 0 & \forall ij \in E^+, \\ & \langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle \leq 0 & \forall ij \in E^-, \\ & \hat{X} \in \mathbb{S}^{\{0\} \cup V}_+. & \end{array} \tag{6.7}$$

The SDP (6.7) plays the role of (6.2b). When we add the constraint $\mathrm{rank}(\hat{X}) = 1$ to (6.7), the resulting optimization problem corresponds to (6.2a) and it is an exact formulation for $\alpha(G; w)$; recall the definition of the latter from (5.81). The dual of (6.7), written with an explicit slack, is:

$$\begin{array}{ll} \inf & \eta \\ & \eta \in \mathbb{R},\ u \in \mathbb{R}^V,\ z^+ \in \mathbb{R}^{E^+}_+,\ z^- \in \mathbb{R}^{E^-}_+, \\ & \begin{bmatrix} \eta & -u^\mathsf{T} \\ -u & 2\,\mathrm{Diag}(u) \end{bmatrix} - \displaystyle\sum_{ij \in E^+} z^+_{ij} \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}) \end{bmatrix} \\ & \qquad + \displaystyle\sum_{ij \in E^-} z^-_{ij} \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}) \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & \mathrm{Diag}(w) \end{bmatrix}, \\ & \hat{S} \in \mathbb{S}^{\{0\} \cup V}_+. \end{array} \tag{6.8}$$

If we were working with the LP relaxation $\max\{\, \langle w, x \rangle : x \in \mathrm{QSTAB}(G) \}$, then the addition of integrality constraints for the variables of the dual LP would yield an exact formulation for the weighted clique covering number $\overline{\chi}(G; w)$; in fact, this may be taken as the definition of $\overline{\chi}(G; w)$. We would like to add a non-convex constraint to (6.8) to emulate the same behavior in the lifted space of that formulation. Our previous observation actually guides us in that direction. If $K \subseteq V$ is a clique of G, then the inequality $\langle \mathbb{1}_K, x \rangle \leq 1$, valid for $\mathrm{QSTAB}(G)$, is embedded into the positive semidefiniteness constraint of SDP (6.7) in the form

$$\begin{aligned} 0 &\leq (1 \oplus -\mathbb{1}_K)^\mathsf{T} \begin{bmatrix} 1 & x^\mathsf{T} \\ x & X \end{bmatrix} (1 \oplus -\mathbb{1}_K) = 1 - 2\langle \mathbb{1}_K, x \rangle + \mathbb{1}_K^\mathsf{T} X \mathbb{1}_K \\ &= 1 - 2\langle \mathbb{1}_K, x \rangle + \langle \mathbb{1}_K, x \rangle + \sum_{ij \in \binom{V}{2}} X_{ij} [i \in K][j \in K] \\ &\leq 1 - 2\langle \mathbb{1}_K, x \rangle + \langle \mathbb{1}_K, x \rangle. \end{aligned} \tag{6.9}$$

Thus, it makes sense to require the following constraint for the dual slack $\hat{S}$ in (6.8):

> $\hat{S}$ is a sum $\hat{S} = \sum_{k=1}^N \hat{S}^{(k)}$ of rank-one matrices $\hat{S}^{(1)}, \ldots, \hat{S}^{(N)} \in \mathbb{S}^{\{0\} \cup V}_+$ such that, for each $k \in [N]$, we have $\langle e_0 e_0^\mathsf{T}, \hat{S}^{(k)} \rangle = 1$ and $\langle \mathrm{Sym}(e_i(e_i + e_0)^\mathsf{T}), \hat{S}^{(k)} \rangle = 0$ for every $i \in V$. (6.10)

The constraint (6.10) is equivalent to requiring that $\hat{S}$ has the form $\hat{S} = \sum_{K\in\mathcal{K}}(-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ for some family $\mathcal{K}$ of subsets of V. By *family* we mean a set in which each element may occur more than once; the number of occurrences of an element is its *multiplicity* in the family.

The "mirror image" of this constraint on the primal space of (6.7) is:

$$\hat{X} \text{ is a sum } \hat{X} = \sum_{k=1}^{N} \hat{X}^{(k)} \text{ of rank-one matrices } \hat{X}^{(1)}, \dots, \hat{X}^{(N)} \in \mathbb{S}_+^{\{0\}\cup V} \text{ such that, for each } k \in [N], \text{ we have } \langle e_0 e_0^{\mathsf{T}}, \hat{X}^{(k)} \rangle = 1 \text{ and } \langle \mathrm{Sym}(e_i(e_i - e_0)^{\mathsf{T}}), \hat{X}^{(k)} \rangle = 0 \text{ for every } i \in V. \tag{6.11}$$

Note that, since the SDP (6.7) also has the constraint $\langle e_0 e_0^{\mathsf{T}}, \hat{X} \rangle = 1$, the non-convex constraint (6.11) specializes to $\mathrm{rank}(\hat{X}) = 1$.

Now we prove that the addition of the non-convex constraint (6.10) to the SDP (6.8) yields a formulation for the clique covering number:

Proposition 6.1. Let V be a finite set, and let $w \in \mathbb{Z}_+^V$. Let $E^+, E^- \subseteq \binom{V}{2}$. Set $E \coloneqq E^-$ and $G \coloneqq (V, E)$. If the constraint (6.10) is added to the SDP (6.8), then the optimal value of the resulting optimization problem is $\overline{\chi}(G; w)$.

Proof. Suppose we add the non-convex constraint (6.10) to (6.8), so that the dual slack $\hat{S}$ is required to have the form $\hat{S} = \sum_{K\in\mathcal{K}}(-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ for some family $\mathcal{K}$ of subsets of V. Then the affine constraints from (6.8) translate to:

$$\begin{aligned}
|\mathcal{K}| &= \hat{S}_{00} = \eta, \\
-\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \hat{S}[V,0] = -u, \\
\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \mathrm{diag}(\hat{S}[V]) = 2u - w, \\
\sum_{K\in\mathcal{K}} [i \in K][j \in K] &= \hat{S}_{ij} = -[ij \in E^+]z_{ij}^+ + [ij \in E^-]z_{ij}^- \qquad \forall ij \in \tbinom{V}{2}.
\end{aligned}$$

Thus, in every feasible solution, we have $z^+\restriction_{E^+\setminus E^-} = 0$ and each $K \in \mathcal{K}$ is a clique of G. Thus, the problem (6.8) with the additional constraint (6.10) may be restated as

$$\begin{array}{ll}
\min & |\mathcal{K}| \\
 & \mathcal{K} \text{ a family of subsets of } V, \\
 & G[K] \text{ is complete for each } K \in \mathcal{K}, \\
 & w = \sum_{K\in\mathcal{K}} \mathbb{1}_K.
\end{array} \tag{6.12}$$

This is precisely the formulation of the clique covering problem for G with weights given by w. $\square$

We now specialize Proposition 6.1 to the formulations of ϑ, ϑ', and ϑ^+. In this chapter, we formulate these parameters as

$$
\vartheta(G;w) = \max \quad \langle \mathrm{Diag}(0 \oplus w), \hat{X} \rangle \\
\langle e_0 e_0^\mathsf{T}, \hat{X} \rangle = 1, \\
\langle 2\,\mathrm{Sym}(e_i (e_i - e_0)^\mathsf{T}), \hat{X} \rangle = 0 \quad \forall i \in V, \\
\langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle = 0 \quad \forall ij \in E, \\
\hat{X} \in \mathbb{S}_+^{\{0\} \cup V}, \tag{6.13}
$$

$$
\vartheta'(G;w) = \max \quad \langle \mathrm{Diag}(0 \oplus w), \hat{X} \rangle \\
\langle e_0 e_0^\mathsf{T}, \hat{X} \rangle = 1, \\
\langle 2\,\mathrm{Sym}(e_i (e_i - e_0)^\mathsf{T}), \hat{X} \rangle = 0 \quad \forall i \in V, \\
\langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle = 0 \quad \forall ij \in E, \\
\langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle \geq 0 \quad \forall ij \in \overline{E}, \\
\hat{X} \in \mathbb{S}_+^{\{0\} \cup V}, \tag{6.14}
$$

$$
\vartheta^+(G;w) = \max \quad \langle \mathrm{Diag}(0 \oplus w), \hat{X} \rangle \\
\langle e_0 e_0^\mathsf{T}, \hat{X} \rangle = 1, \\
\langle 2\,\mathrm{Sym}(e_i (e_i - e_0)^\mathsf{T}), \hat{X} \rangle = 0 \quad \forall i \in V, \\
\langle 2\,\mathrm{Sym}(e_i e_j^\mathsf{T}), \hat{X} \rangle \leq 0 \quad \forall ij \in E, \\
\hat{X} \in \mathbb{S}_+^{\{0\} \cup V}. \tag{6.15}
$$

Corollary 6.2. Let $G = (V, E)$ be a graph. Let $w \in \mathbb{Z}_+^V$. For each of the SDPs (6.13), (6.14), and (6.15), if the constraint (6.10) is added to its dual, then the optimal value of the resulting optimization problem is $\overline{\chi}(G;w)$.

Proof. Immediate from Proposition 6.1. □

Note that Proposition 6.1 remains true even if the constraint that "$\eta \oplus u \oplus z^+ \oplus z^-$ is integral" is added to (6.8).

We further note that the paper [109] describes an integrality constraint for the dual of an SDP formulation of the theta number, yielding the chromatic number of a graph. That approach, however, is *ad hoc* and thus not widely applicable.

6.2 Primal and Dual SDPs with Integrality Constraints

The non-convex constraints (6.10) and (6.11) for dual pairs of SDPs extends the chain of inequalities (6.2) and yields a generalization of (6.1) to the context of SDPs:

Theorem 6.3. Let $\mathcal{A}\colon \mathbb{S}^{\{0\}\cup[n]} \to \mathbb{R}^m$ be a linear function. Let $b \in \mathbb{R}^m$ and $\hat{C} \in \mathbb{S}^{\{0\}\cup[n]}$. Then

$$
\begin{aligned}
&\sup\bigl\{\, \langle \hat{C}, \hat{X}\rangle : \mathcal{A}(\hat{X}) \leq b,\ \hat{X} \in \mathbb{S}_+^{\{0\}\cup[n]},\ \hat{X} \text{ satisfies (6.11)} \bigr\} && \text{(6.16a)}\\
&\quad\leq \sup\bigl\{\, \langle \hat{C}, \hat{X}\rangle : \mathcal{A}(\hat{X}) \leq b,\ \hat{X} \in \mathbb{S}_+^{\{0\}\cup[n]} \bigr\} && \text{(6.16b)}\\
&\qquad\leq \inf\bigl\{\, \langle b, y\rangle : y \in \mathbb{R}_+^m,\ \mathcal{A}^*(y) \succeq \hat{C} \bigr\} && \text{(6.16c)}\\
&\qquad\quad\leq \inf\bigl\{\, \langle b, y\rangle : y \in \mathbb{Z}_+^m,\ \mathcal{A}^*(y) - \hat{S} = \hat{C},\ \hat{S} \in \mathbb{S}_+^{\{0\}\cup[n]},\ \hat{S} \text{ satisfies (6.10)} \bigr\}. && \text{(6.16d)}
\end{aligned}
$$

If there exists either $\hat{X} \in \mathbb{S}_{++}^{\{0\}\cup[n]}$ such that $\mathcal{A}(\hat{X}) \leq b$ or $y \in \mathbb{R}_+^m$ such that $\mathcal{A}^*(y) \succ \hat{C}$, then the middle inequality in (6.16) holds with equality. The chain (6.16) remains true if the constraint $y \in \mathbb{Z}_+^m$ is relaxed to $y \in \mathbb{R}_+^m$ in (6.16d).

Proof. The proof of the chain of the inequalities (6.16) is trivial, except possibly for the middle inequality, which is Weak Duality for SDPs. The statement about the middle inequality holding with equality follows from the Strong Duality Theorem. $\square$

We have seen in the previous section that, when applied to a certain formulation of the Lovász theta number, the optimization problems from (6.16) compute the graph invariants $\alpha(G;w)$, $\vartheta(G;w)$, and $\overline{\chi}(G;w)$. To see why (6.16) "generalizes" (6.1), let us reconsider the diagonal embedding (6.3) of a linear program in the format (6.1b), whose dual SDP is given by (6.4). We proceed as in the proof of Proposition 6.1. Suppose we add the constraint (6.10) to (6.4), so that $\hat{S}$ is of the form $\hat{S} = \sum_{K\in\mathcal{K}}(-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ for some family $\mathcal{K}$ of subsets of $V := [n]$. Then the affine constraints for (6.4) translate to:

$$
\begin{aligned}
|\mathcal{K}| &= \hat{S}_{00} = \eta - \langle b, y\rangle,\\
-\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \hat{S}[V,0] = -u,\\
\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \operatorname{diag}(\hat{S}[V]) \leq 2u + A^{\mathsf{T}}y - c,\\
\sum_{K\in\mathcal{K}} [i\in K][j \in K] &= \hat{S}_{ij} \leq 0 \qquad \forall ij \in \tbinom{V}{2}.
\end{aligned}
$$

The latter two conditions are equivalent to $c \leq u + A^{\mathsf{T}}y$ and $|K| \leq 1$ for all $K \in \mathcal{K}$. Thus, the dual (6.4) with the additional constraint (6.10) may be restated as:

$$
\begin{array}{ll}
\inf & \bar{e}^{\mathsf{T}}u + b^{\mathsf{T}}y\\
 & c \leq u + A^{\mathsf{T}}y,\\
 & y \in \mathbb{R}_+^m,\\
 & u \in \mathbb{Z}_+^n.
\end{array}
\tag{6.17}
$$

Even upon adding the integrality constraint $y \in \mathbb{Z}_+^m$, which appears in (6.16d), every feasible solution for (6.1d) yields a feasible solution for (6.17) with the same objective value, by taking $u := 0$. In this sense, the extended chain (6.16) generalizes (6.1).

In the next sections, we shall repeat the previous procedure for some SDP formulations of MaxCut, vertex cover problem, and others. That is, we assume that dual slack satisfies the constraint (6.10), so that it is determined by a family $\mathcal{K}$ of subsets of V, then we translate the affine constraints of the dual SDP in terms of $\mathcal{K}$, and restate it in an almost purely combinatorial form, as we did in (6.12) and in (6.17).

6.3 Integrality Constraint for the Dual of a MaxCut SDP

Recall that the MaxCut problem is that of, given a graph $G = (V, E)$ and a function $w \in \mathbb{R}^E_+$, find $\max\{\,\langle w, \mathbb{1}_{\delta(S)}\rangle : S \subseteq V,\, S \notin \{\varnothing, V\}\}$, where $\delta(S) \coloneqq \{\,\{i,j\} \in E : |\{i,j\} \cap S| = 1\}$ for each $S \subseteq V$. We set $\delta(i) \coloneqq \delta(\{i\})$ for each $i \in V$. In this section, we shall consider the following SDP formulation for MaxCut:

$$\begin{array}{ll} \max & \langle 0 \oplus \mathcal{L}_G(w), \hat{X}\rangle, \\ & \langle e_0 e_0^{\mathsf{T}}, \hat{X}\rangle = 1, \\ & \langle 2\,\mathrm{Sym}(e_i(e_i - e_0)^{\mathsf{T}}), \hat{X}\rangle = 0 \quad \forall i \in V, \\ & \hat{X}[V] \geq 0, \\ & \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}. \end{array} \tag{6.18}$$

(We refer the reader back to (2.2) for the definition of the Laplacian $\mathcal{L}_G$ of G.) Note that, modulo the nonnegativity constraint $\hat{X}[V] \geq 0$, the SDP (6.18) is obtained from the usual SDP relaxation for MaxCut, namely $\max\{\,\frac{1}{4}\langle 0 \oplus \mathcal{L}_G(w), \hat{Y}\rangle : \hat{Y} \in \mathscr{E}_{\{0\}\cup V}\}$, by using the change of variable $\hat{X} \coloneqq \mathrm{Congr}_{\mathrm{Bool}}(\hat{Y})$; see [52]. The dual of (6.18), written with an explicit slack, is:

$$\begin{array}{ll} \inf & \eta \\ & \eta \in \mathbb{R},\, u \in \mathbb{R}^V,\, Z \in \mathbb{S}^V_{\geq 0}, \\ & \begin{bmatrix} \eta & -u^{\mathsf{T}} \\ -u & \mathrm{Diag}(2u) - Z \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^{\mathsf{T}} \\ 0 & \mathcal{L}_G(w) \end{bmatrix}, \\ & \hat{S} \in \mathbb{S}_+^{\{0\}\cup V}. \end{array} \tag{6.19}$$

Suppose we add the non-convex constraint (6.10) to (6.19), so that the dual slack $\hat{S}$ is required to have the form $\hat{S} = \sum_{K\in\mathcal{K}}(-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ for some family $\mathcal{K}$ of subsets of V. Then the affine constraints of (6.19) translate to

$$\begin{aligned} |\mathcal{K}| &= \hat{S}_{00} = \eta, \\ -\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \hat{S}[V,0] = -u, \\ \sum_{K\in\mathcal{K}} [i \in K] &= \hat{S}_{ii} \leq 2u_i - \langle \mathbb{1}_{\delta(i)}, w\rangle \qquad \forall i \in V, \\ \sum_{K\in\mathcal{K}} [i \in K][j \in K] &= \hat{S}_{ij} \leq [ij \in E]w_{ij} \qquad \forall ij \in \tbinom{V}{2}. \end{aligned}$$

Thus, the problem (6.19) with the additional constraint (6.10) may be restated as:

$$\begin{array}{lll} \min & |\mathcal{K}| & \\ & \mathcal{K} \text{ a family of subsets of } V, & \\ & G[K] \text{ is complete for each } K \in \mathcal{K}, & \\ & \langle \mathbb{1}_{\delta(i)}, w\rangle \leq \sum_{K\in\mathcal{K}}[i \in K] & \forall i \in V, \\ & \sum_{K\in\mathcal{K}}[ij \in E[K]] \leq w_{ij} & \forall ij \in E. \end{array} \tag{6.20}$$

We shall prove that, if $w \in \mathbb{Z}_+^E$, then (6.20) has a unique optimal solution $\mathcal{K}^*$ of a trivial form, namely, the incidence vector of $\mathcal{K}^*$ is precisely $w \oplus 0$. Here, the incidence vector of a family $\mathcal{K}$ of subsets of V is the function that maps each subset of V to its multiplicity in $\mathcal{K}^*$. We shall need the following auxiliary optimization problem:

$$\begin{array}{lll} \min & |\mathcal{K}| & \\ & \mathcal{K} \text{ a family of subsets of } V, & \\ & G[K] \text{ is complete for each } K \in \mathcal{K}, & \\ & \langle \mathbb{1}_{\delta(i)}, w \rangle + d_i \leq \sum_{K \in \mathcal{K}} [i \in K] & \forall i \in V, \\ & \sum_{K \in \mathcal{K}} [ij \in E[K]] \leq w_{ij} & \forall ij \in E, \end{array} \tag{6.21}$$

where $d \in \mathbb{R}^V$.

Lemma 6.4. Let $G = (V, E)$ be a graph, let $w \in \mathbb{Z}_+^E$ and $d \in \mathbb{Z}_+^V$. Let C be a clique of G with $|C| \geq 2$. Set $\bar{w} := w - \mathbb{1}_{E[C]}$ and $\bar{d} := d + (|C| - 2)\mathbb{1}_C$. If $\mathcal{K}$ is a feasible solution for (6.21) with weight functions w and d such that $C \in \mathcal{K}$, then $\mathcal{K} \setminus \{C\}$ is feasible for (6.21) with weight functions $\bar{w}$ and $\bar{d}$, and $\bar{w} \geq 0$. Conversely, if $\bar{\mathcal{K}}$ is a feasible solution for (6.21) with weight functions $\bar{w}$ and $\bar{d}$, then $\bar{\mathcal{K}} \cup \{C\}$ is feasible for (6.21) with weight functions w and d.

Proof. Let $\mathcal{K}$ be feasible for (6.21) with weight functions w and d. Suppose that $C \in \mathcal{K}$. Set $\overline{\mathcal{K}} := \mathcal{K} \setminus \{C\}$. Let $ij \in E$. Then $[ij \in E[C]] + \sum_{K \in \overline{\mathcal{K}}} [ij \in E[K]] = \sum_{K \in \mathcal{K}} [ij \in E[K]] \leq w_{ij}$ whence $\sum_{K \in \overline{\mathcal{K}}} [ij \in E[K]] \leq w_{ij} - [ij \in E[C]] = \bar{w}_{ij}$ and $\bar{w}_{ij} \geq 0$. Next, let $i \in V$. Then

$$\begin{aligned} \langle \mathbb{1}_{\delta(i)}, \bar{w} \rangle + \bar{d}_i + [i \in C] &= \langle \mathbb{1}_{\delta(i)}, w \rangle - [i \in C](|C| - 1) + d_i + [i \in C](|C| - 2) + [i \in C] \\ &= \langle \mathbb{1}_{\delta(i)}, w \rangle + d_i \leq \sum_{K \in \mathcal{K}} [i \in K] = [i \in C] + \sum_{K \in \overline{\mathcal{K}}} [i \in K], \end{aligned} \tag{6.22}$$

whence $\langle \mathbb{1}_{\delta(i)}, \bar{w} \rangle + \bar{d}_i \leq \sum_{K \in \overline{\mathcal{K}}} [i \in K]$. This proves that $\overline{\mathcal{K}}$ is feasible with weights $\bar{w}$ and $\bar{d}$.

Now, let $\overline{\mathcal{K}}$ be feasible for (6.21) with weight functions $\bar{w}$ and $\bar{d}$. Set $\mathcal{K} := \overline{\mathcal{K}} \cup \{C\}$. Let $ij \in E$. Then

$$\sum_{K \in \mathcal{K}} [ij \in E[K]] = [ij \in E[C]] + \sum_{K \in \overline{\mathcal{K}}} [ij \in E[K]] \leq [ij \in E[C]] + \bar{w}_{ij} = w_{ij}.$$

Let $i \in V$. Then

$$\sum_{K \in \mathcal{K}} [i \in K] = [i \in C] + \sum_{K \in \overline{\mathcal{K}}} [i \in K] \geq [i \in C] + \langle \mathbb{1}_{\delta(i)}, \bar{w} \rangle + \bar{d}_i = \langle \mathbb{1}_{\delta(i)}, w \rangle + d_i,$$

where the last equation is derived as in (6.22). Thus, $\mathcal{K}$ is feasible for (6.21) with weight functions w and d. ∎

Lemma 6.5. Let $G = (V, E)$ be a graph. Let $w \in \mathbb{Z}_+^E$. Then, for every $d \in \mathbb{Z}_+^V$, every optimal solution $\mathcal{K}^*$ for (6.21) is such that, for each $i \in V$, the singleton $\{i\}$ occurs in $\mathcal{K}^*$ with multiplicity $\geq d_i$.

Proof. The proof is by induction on $\bar{e}^\mathsf{T} w$, the case $\bar{e}^\mathsf{T} w = 0$ being trivial. Suppose $w \neq 0$. Let $\mathcal{K}^*$ be an optimal solution for (6.21). If every member of $\mathcal{K}^*$ is a singleton, then the multiplicity of $\{i\}$ in $\mathcal{K}^*$ is the

RHS of the constraint $\langle \mathbb{1}_{\delta(i)}, w\rangle + d_i \leq \sum_{K\in\mathcal{K}^*}[i \in K]$, and we are done, since the LHS is bounded below by d_i. So suppose there exists $C \in \mathcal{K}^*$ such that $|C| \geq 2$. Define $\bar{w} := w - \mathbb{1}_{E[C]}$ and $\bar{d} := d + (|C| - 2)\mathbb{1}_C$. By Lemma 6.4, we find that $\mathcal{K}^* \setminus \{C\}$ is optimal for (6.21) with weight functions $\bar{w} \geq 0$ and $\bar{d}$. Since $\bar{e}^\mathsf{T}\bar{w} < \bar{e}^\mathsf{T}w$, we find by induction that, for each $i \in V$, the singleton $\{i\}$ has multiplicity $\geq \bar{d}_i \geq d_i$ in $\mathcal{K}^* \setminus \{C\}$, and hence in $\mathcal{K}^*$. □

Now we can prove that (6.20) has a unique optimal solution and that it is trivial:

Proposition 6.6. Let $G = (V, E)$ be a graph, and let $w \in \mathbb{Z}_+^E$. Then the optimization problem (6.20) has a unique optimal solution $\mathcal{K}^*$, namely, all members of $\mathcal{K}^*$ are edges of G, and each edge $e \in E$ appears in $\mathcal{K}^*$ with multiplicity w_e.

Proof. Let $\mathcal{K}^*$ be an optimal solution for (6.20). We first show that

$$|K| \leq 2 \qquad \forall K \in \mathcal{K}^*. \tag{6.23}$$

Let $C \in \mathcal{K}^*$ with $|C| \geq 3$. By Lemma 6.4, we know that $\mathcal{K}^* \setminus \{C\}$ is an optimal solution for (6.21) with weight functions $\bar{w} := w - \mathbb{1}_{E[C]}$ and $\bar{d} := d + (|C| - 2)\mathbb{1}_C$, where $d := 0$. By Lemma 6.5, we find that each singleton $\{i\}$ with $i \in C$ has multiplicity $\geq \bar{d}_i \geq |C| - 2$ in $\mathcal{K}^* \setminus \{C\}$, and thus also in $\mathcal{K}^*$. We now modify the feasible solution $\mathcal{K}^*$ as follows. Replace one instance of C and $|C| - 2$ instances of each singleton $\{i\}$ with $i \in C$ with one instance of each member of $E[C]$. This new family $\mathcal{K}'$ is feasible for (6.21) with weight functions w and d, moreover

$$|\mathcal{K}'| = |\mathcal{K}^*| - \big[1 + |C|(|C| - 2)\big] + \binom{|C|}{2} = |\mathcal{K}^*| - \frac{1}{2}\big(|C| - 1\big)\big(|C| - 2\big) < |\mathcal{K}^*|.$$

This proves (6.23).

Now suppose that some edge $ij \in E$ does not occur with multiplicity w_{ij} in $\mathcal{K}^*$. Since the maximum multiplicity that an edge $e \in E$ can have in $\mathcal{K}^*$ is w_e by the edge constraints of (6.20), then the node constraint for i and (6.23) shows that the singleton $\{i\}$ must occur in $\mathcal{K}^*$. Similarly, $\{j\}$ must occur in $\mathcal{K}^*$. By replacing one instance of each of $\{i\}$ and $\{j\}$ in $\mathcal{K}^*$ with ij, we obtain a feasible solution $\mathcal{K}'$ with $|\mathcal{K}'| < |\mathcal{K}^*|$. This proves that each edge ij occurs in $\mathcal{K}^*$ with multiplicity w_{ij}. The result now follows, since clearly no singleton occurs in $\mathcal{K}^*$ by optimality. □

6.4 Integrality Constraints for a Vertex Cover SDP

Recall that the vertex cover problem is that of, given a graph $G = (V, E)$ and a function $w \in \mathbb{R}_+^V$, find $\min\{\langle w, \mathbb{1}_C\rangle : C$ is a vertex cover of $G\}$, where a subset C of V is defined to a *vertex cover* of G if $V \setminus C$ is a stable set of G. An SDP relaxation for this problem is:

$$\begin{aligned} \inf \quad & \langle 0 \oplus \mathrm{Diag}(w), \hat{X}\rangle \\ & \langle e_0 e_0^\mathsf{T}, \hat{X}\rangle = 1, \\ & \langle 2\,\mathrm{Sym}(e_i(e_i - e_0)^\mathsf{T}), \hat{X}\rangle = 0 && \forall i \in V, \\ & \langle 2\,\mathrm{Sym}((e_0 - e_i)(e_0 - e_j)^\mathsf{T}), \hat{X}\rangle = 0 && \forall ij \in E, \\ & \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}. \end{aligned} \tag{6.24}$$

The SDP (6.24) is obtained from the SDP relaxation

$$\begin{aligned} \min\quad & \left\langle \tfrac{1}{4}\textstyle\sum_{i\in V} w_i(e_0+e_i)(e_0+e_i)^\mathsf{T}, \hat{Y}\right\rangle \\ & \operatorname{diag}(\hat{Y}) = 1, \\ & \langle 2\operatorname{Sym}((e_0-e_i)(e_0-e_j)^\mathsf{T}), \hat{Y}\rangle = 0 \quad \forall ij\in E, \\ & \hat{Y}\in \mathbb{S}_+^{\{0\}\cup V} \end{aligned}$$

for the vertex cover problem, studied by Kleinberg and Goemans [77], by using the change of variable $\hat{X} \coloneqq \operatorname{Congr}_{\mathrm{Bool}}(\hat{Y})$. The dual of (6.24), written with an explicit slack, is

$$\begin{aligned} \sup\quad & \eta \\ & \eta\in\mathbb{R},\ u\in\mathbb{R}^V,\ y\in\mathbb{R}^E, \\ & \begin{bmatrix} \eta & -u^\mathsf{T} \\ -u & \operatorname{Diag}(2u)\end{bmatrix} + \sum_{ij\in E} y_{ij}\begin{bmatrix} 2 & -\mathbb{1}_{ij}^\mathsf{T} \\ -\mathbb{1}_{ij} & 2\operatorname{Sym}(e_ie_j^\mathsf{T})\end{bmatrix} + \hat{S} = \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & \operatorname{Diag}(w)\end{bmatrix}, \\ & \hat{S}\in\mathbb{S}_+^{\{0\}\cup V}. \end{aligned} \tag{6.25}$$

Suppose we add the non-convex constraint (6.10) to (6.25), so that the dual slack $\hat{S}$ is required to have the form $\hat{S} = \sum_{K\in\mathcal{K}}(-1\oplus\mathbb{1}_K)(-1\oplus\mathbb{1}_K)^\mathsf{T}$ for some family $\mathcal{K}$ of subsets of V. Then the affine constraints from (6.25) translate to:

$$|\mathcal{K}| = \hat{S}_{00} = -\eta - 2\langle\bar{e}, y\rangle, \tag{6.26a}$$

$$-\sum_{K\in\mathcal{K}}\mathbb{1}_K = \hat{S}[V,0] = u + \sum_{ij\in E} y_{ij}\mathbb{1}_{ij}, \tag{6.26b}$$

$$\sum_{K\in\mathcal{K}}\mathbb{1}_K = \operatorname{diag}(\hat{S}[V]) = w - 2u, \tag{6.26c}$$

$$\sum_{K\in\mathcal{K}}[i\in K][j\in K] = \hat{S}_{ij} = -[ij\in E]y_{ij} \qquad \forall ij\in\tbinom{V}{2}. \tag{6.26d}$$

This implies that $G[K]$ is complete for each $K\in\mathcal{K}$ and $y_e = -\sum_{K\in\mathcal{K}}[e\in E[K]]$ for each $e\in E$. The objective function is

$$\eta = -|\mathcal{K}| + 2\sum_{e\in E}\sum_{K\in\mathcal{K}}[e\in E[K]] = -|\mathcal{K}| + 2\sum_{K\in\mathcal{K}}\tbinom{|K|}{2} = \sum_{K\in\mathcal{K}}\Big(|K|^2 - |K| - 1\Big).$$

From (6.26b) we get

$$u = -\sum_{K\in\mathcal{K}}\mathbb{1}_K + \sum_{K\in\mathcal{K}}(|K|-1)\mathbb{1}_K = \sum_{K\in\mathcal{K}}(|K|-2)\mathbb{1}_K$$

whence (6.26c) becomes $w = \sum_{K\in\mathcal{K}}(2|K|-3)\mathbb{1}_K$. Thus, the problem (6.25) with the additional constraint (6.10) may be restated as

$$\begin{aligned} \max\quad & \textstyle\sum_{K\in\mathcal{K}}\big(|K|^2 - |K| - 1\big) \\ & \mathcal{K} \text{ a family of subsets of } V, \\ & G[K] \text{ is complete for each } K\in\mathcal{K}, \\ & w = \textstyle\sum_{K\in\mathcal{K}}(2|K|-3)\mathbb{1}_K. \end{aligned} \tag{6.27}$$

Note that singleton cliques contribute -1 to the objective function. If $w = \bar{e}$, then the last constraints require $|K| \leq 2$ for each $K \in \mathcal{K}$, so every perfect matching of G is a feasible solution for (6.27).

It is reasonable to argue that we are looking at (6.25) on the wrong scale. The SDP (6.24) is obtained from the SDP (6.5) by applying the map $\mathrm{Congr}_{\mathrm{Flip}}$; see (4.42). Thus, the correct scale to look at dual slacks of the form $\hat{S} = \sum_{K \in \mathcal{K}} (-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ in the dual for (6.5) is to have the dual slacks of (6.25) have the form

$$\sum_{K \in \mathcal{K}} \mathrm{Congr}_{\mathrm{Flip}}^{-*}\big((-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}\big) = \sum_{K \in \mathcal{K}} \big((|K|-1) \oplus -\mathbb{1}_K\big)\big((|K|-1) \oplus -\mathbb{1}_K\big)^{\mathsf{T}}.$$

Then the affine constraints (6.26) translate as follows. We still need each $K \in \mathcal{K}$ to be a clique by (6.26d), and again $y_e = -\sum_{K \in \mathcal{K}} [e \in E[K]]$ for each $e \in E$. The objective function, however, becomes

$$\eta = -\sum_{K \in \mathcal{K}} (|K|-1)^2 + 2 \sum_{K \in \mathcal{K}} \sum_{e \in E} [e \in E[K]] = \sum_{K \in \mathcal{K}} (|K|-1).$$

The LHS of (6.26b) is modified to $-\sum_{K \in \mathcal{K}} (|K|-1)\mathbb{1}_K$, and so it yields $u = 0$. In this setting, the modified dual may be restated as

$$\begin{array}{ll} \max & \sum_{K \in \mathcal{K}} \big(|K|-1\big) \\ & \mathcal{K} \text{ a family of subsets of } V, \\ & G[K] \text{ is complete for each } K \in \mathcal{K}, \\ & w = \sum_{K \in \mathcal{K}} \mathbb{1}_K. \end{array} \tag{6.28}$$

In this new problem, each perfect matching remains feasible, with the same objective value as in (6.27). However, there are much more complex feasible solutions now, such as any partition of V into cliques. This latter example shows that it is not always clear what the "correct" scale is to apply the non-convex constraint (6.10).

6.5 The Lovász-Schrijver Embedding

Lovász and Schrijver [101] introduced a general procedure to generate an SDP relaxation for any binary integer linear program. Their so-called lift-and-project method may be seen as a generalization of the SDP formulation (6.5) for the theta number, and it is guaranteed to yield an exact formulation after a linear number of recursive applications. The method is much more general than our short description for it; see, e.g., [86]. In this section, we will embed a binary integer linear program in the format of (6.1a) into an SDP using the Lovász-Schrijver procedure and specialize it to the formulation of the stable set problem via the polytope $\mathrm{FRAC}(G)$ defined in (5.55). We shall show that every clique covering of G yields a feasible solution for the dual SDP with the additional constraint (6.10).

Let V and E be finite sets. Suppose a polytope $P \subseteq [0,1]^V$ is defined as $P := \{\, x \in \mathbb{R}^V : Ax \leq b\}$, where $A \in \mathbb{R}^{E \times V}$. In fact, in many important cases, every entry of A is an integer, so we shall assume this. Let P_0 be the homogenization

$$P_0 := \mathbb{R}_+(1 \oplus P) = \Big\{\, \hat{x} \in \mathbb{R}^{\{0\} \cup V} : \begin{bmatrix} -b & A \end{bmatrix} \hat{x} \leq 0 \Big\}.$$

Then it is not hard to prove that

$$\{\,x \in \{0,1\}^V : Ax \leq b\} \subseteq \Big\{\operatorname{diag}(\hat{X}[V]) : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\ \hat{X}e_i, \hat{X}(e_0 - e_i) \in P_0\, \forall i \in V,\ \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}\Big\}.$$

Let $w \in \mathbb{R}^V$. Then $\max\{\,\langle w, x\rangle : x \in P \cap \{0,1\}^V\}$ is bounded above by

$$\max\Big\{\,\langle \operatorname{Diag}(0 \oplus w), \hat{X}\rangle : \mathcal{B}_{\{0\}\cup V}(\hat{X}) = 1 \oplus 0,\ \hat{X}e_i, \hat{X}(e_0 - e_i) \in P_0\, \forall i \in V,\ \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}\Big\}. \tag{6.29}$$

The bound is tight if the constraint (6.11) is added to (6.29), since it specializes to $\operatorname{rank}(\hat{X}) = 1$ and ensures that $\hat{X}$ has the form $\hat{X} = (1 \oplus x)(1 \oplus x)^{\mathsf{T}}$ with $x \in \{0,1\}^V$. Set $a_e := A^{\mathsf{T}} e_e$ for each $e \in E$. For a given $i \in V$, the constraint $\hat{X}e_i \in P_0$ is equivalent to $\big\langle \operatorname{Sym}\big((-b_e \oplus a_e)(0 \oplus e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0$ for every $e \in E$, whereas the constraint $\hat{X}(e_0 - e_i) \in P_0$ is equivalent to $\big\langle \operatorname{Sym}\big((-b_e \oplus a_e)(1 \oplus -e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0$ for every $e \in E$. Thus, after scaling some inequalities to ensure that all matrices defining our constraints have integer entries, the problem (6.29) becomes:

$$\begin{array}{lll}
\sup & \langle \operatorname{Diag}(0 \oplus w), \hat{X}\rangle & \\
& \langle \operatorname{Sym}(e_0 e_0^{\mathsf{T}}), \hat{X}\rangle = 1, & \\
& \langle 2\operatorname{Sym}(e_i(e_i - e_0)^{\mathsf{T}}), \hat{X}\rangle = 0 & \forall i \in V, \\
& \big\langle 2\operatorname{Sym}\big((-b_e \oplus a_e)(0 \oplus e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0 & \forall i \in V,\ \forall e \in E, \\
& \big\langle 2\operatorname{Sym}\big((-b_e \oplus a_e)(1 \oplus -e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0 & \forall i \in V,\ \forall e \in E, \\
& \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}. &
\end{array} \tag{6.30}$$

The dual of (6.30) may be written more compactly by using certain matrix variables. Let us associate each constraint of the form $\big\langle \operatorname{Sym}\big((-b_e \oplus a_e)(0 \oplus e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0$ with a dual variable Y_{ie}, where $Y \in \mathbb{R}_+^{V\times E}$. Similarly associate each constraint of the form $\big\langle \operatorname{Sym}\big((-b_e \oplus a_e)(1 \oplus -e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0$ with a dual variable Z_{ie}, where $Z \in \mathbb{R}_+^{V\times E}$. Note that

$$\sum_{i\in V}\sum_{e\in E} Y_{ie} \operatorname{Sym}\big((-b_e \oplus a_e)(0 \oplus e_i)^{\mathsf{T}}\big) = \operatorname{Sym}\left(\begin{bmatrix} 0 & 0^{\mathsf{T}} \\ -Yb & YA \end{bmatrix}\right),$$
$$\sum_{i\in V}\sum_{e\in E} Z_{ie} \operatorname{Sym}\big((-b_e \oplus a_e)(1 \oplus -e_i)^{\mathsf{T}}\big) = \operatorname{Sym}\left(\begin{bmatrix} -\bar{e}^{\mathsf{T}}Zb & \bar{e}^{\mathsf{T}}ZA \\ Zb & -ZA \end{bmatrix}\right).$$

Thus, the dual of (6.30), written with an explicit slack, is

$$\begin{array}{ll}
\inf & \eta \\
& \eta \in \mathbb{R},\ u \in \mathbb{R}^V,\ Y \in \mathbb{R}_+^{V\times E},\ Z \in \mathbb{R}_+^{V\times E}, \\
& \begin{bmatrix} \eta - \bar{e}^{\mathsf{T}}Zb & (-u - (Y-Z)b + A^{\mathsf{T}}Z^{\mathsf{T}}\bar{e})^{\mathsf{T}} \\ -u - (Y-Z)b + A^{\mathsf{T}}Z^{\mathsf{T}}\bar{e} & \operatorname{Diag}(2u) + 2\operatorname{Sym}\big((Y-Z)A\big) \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^{\mathsf{T}} \\ 0 & \operatorname{Diag}(w) \end{bmatrix}, \\
& \hat{S} \in \mathbb{S}_+^{\{0\}\cup V}.
\end{array} \tag{6.31}$$

We are interested in the specialization of (6.31) when $P = \operatorname{FRAC}(G)$. We shall assume that G has no isolated node, so that

$$\operatorname{FRAC}(G) = \{\,x \in \mathbb{R}^V : x \geq 0,\ B_G^{\mathsf{T}}x \leq \bar{e}\}; \tag{6.32}$$

recall that B_G is the $V \times E$ incidence matrix of G. Due to the structure of the system of inequalities defining $\mathrm{FRAC}(G)$ in (6.32), it is convenient to rewrite (6.30) and (6.31) by treating the constraint $x \geq 0$ separately. That is, if $P = \{\, x \in \mathbb{R}^V : x \geq 0,\, Ax \leq b\}$, then the SDP (6.30) may be rewritten as

$$\begin{array}{lll}
\sup & \langle \operatorname{Diag}(0 \oplus w), \hat{X}\rangle & \\
& \langle \operatorname{Sym}(e_0 e_0^{\mathsf{T}}), \hat{X}\rangle = 1, & \\
& \langle 2\operatorname{Sym}(e_i(e_i - e_0)^{\mathsf{T}}), \hat{X}\rangle = 0 & \forall i \in V, \\
& \big\langle 2\operatorname{Sym}\big((-b_e \oplus a_e)(0 \oplus e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0 & \forall i \in V,\ \forall e \in E, \\
& \big\langle 2\operatorname{Sym}\big((-b_e \oplus a_e)(1 \oplus -e_i)^{\mathsf{T}}\big), \hat{X}\big\rangle \leq 0 & \forall i \in V,\ \forall e \in E, \\
& \hat{X}[V] \geq 0, & \\
& \big\langle 2\operatorname{Sym}(e_i(e_j - e_i)^{\mathsf{T}}), \hat{X}\big\rangle \leq 0, & \forall i \in V,\ \forall j \in V, \\
& \hat{X} \in \mathbb{S}_+^{\{0\}\cup V}. &
\end{array} \tag{6.33}$$

The dual of (6.33), written with an explicit slack, is

$$\begin{array}{ll}
\inf & \eta \\
& \eta \in \mathbb{R},\, u \in \mathbb{R}^V,\, Y \in \mathbb{R}_+^{V\times E},\, Z \in \mathbb{R}_+^{V\times E},\, U \in \mathbb{S}_{\geq 0}^V,\, R \in \mathbb{R}_+^{V\times V}, \\
& \begin{bmatrix} \eta - \bar{e}^{\mathsf{T}} Z b & (-u - (Y-Z)b + A^{\mathsf{T}} Z^{\mathsf{T}} \bar{e})^{\mathsf{T}} \\ -u - (Y-Z)b + A^{\mathsf{T}} Z^{\mathsf{T}} \bar{e} & 2\operatorname{Diag}(u - R\bar{e}) + 2\operatorname{Sym}\big(R + (Y-Z)A\big) - U \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^{\mathsf{T}} \\ 0 & \operatorname{Diag}(w) \end{bmatrix}, \\
& \hat{S} \in \mathbb{S}_+^{\{0\}\cup V}.
\end{array} \tag{6.34}$$

We next show that the chain of inequalities (6.16) is at least as tight as (6.1) when applied to the primal SDP (6.33) with $A = B_G^{\mathsf{T}}$:

Proposition 6.7. Let $G = (V, E)$ be a graph, and $w \in \mathbb{Z}_+^V$. Then the optimal value of (6.34), with $A := B_G^{\mathsf{T}}$ and $b := \bar{e}$, and the additional constraint (6.10), is bounded above by $\overline{\chi}(G; w)$.

Proof. We start by rewriting (6.34) with the variables Z and R set to 0:

$$\begin{array}{ll}
\inf & \eta \\
& \eta \in \mathbb{R},\, u \in \mathbb{R}^V,\, Y \in \mathbb{R}_+^{V\times E},\, U \in \mathbb{S}_{\geq 0}^V, \\
& \begin{bmatrix} \eta & (-u - Y\bar{e})^{\mathsf{T}} \\ -u - Y\bar{e} & 2\operatorname{Diag}(u) + 2\operatorname{Sym}\big(Y B_G^{\mathsf{T}}\big) - U \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^{\mathsf{T}} \\ 0 & \operatorname{Diag}(w) \end{bmatrix}, \\
& \hat{S} \in \mathbb{S}_+^{\{0\}\cup V}.
\end{array} \tag{6.35}$$

Suppose we add the non-convex constraint (6.10) to (6.35), so that the dual slack $\hat{S}$ is required to have the form $\hat{S} = \sum_{K\in\mathcal{K}} (-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^{\mathsf{T}}$ for some family $\mathcal{K}$ of subsets of V. Then the affine constraints from (6.35) translate to:

$$\begin{aligned}|\mathcal{K}| &= \hat{S}_{00} = \eta,\\ -\sum_{K\in\mathcal{K}} \mathbb{1}_K &= \hat{S}[V,0] = -u - Y\bar{e}\\ \sum_{K\in\mathcal{K}} [i\in K] &= \hat{S}_{ii} \le 2u_i - w_i + 2e_i^\mathsf{T} Y B_G^\mathsf{T} e_i \qquad \forall i \in V,\\ \sum_{K\in\mathcal{K}} [i\in K][j\in K] &= \hat{S}_{ij} \le e_i^\mathsf{T} Y B_G^\mathsf{T} e_j + e_j^\mathsf{T} Y B_G^\mathsf{T} e_i \qquad \forall ij \in \tbinom{V}{2}.\end{aligned}$$

The latter two constraints may be rewritten as

$$\begin{aligned}w_i + 2e_i^\mathsf{T} Y\big(\mathbb{1}_{\delta(i)} + \mathbb{1}_{E\setminus\delta(i)}\big) &\le \sum_{K\in\mathcal{K}} [i\in K] + 2e_i^\mathsf{T} Y \mathbb{1}_{\delta(i)} \qquad \forall i\in V,\\ \sum_{K\in\mathcal{K}} [i\in K][j\in K] &\le e_i^\mathsf{T} Y \mathbb{1}_{\delta(j)} + e_j^\mathsf{T} Y \mathbb{1}_{\delta(i)} \qquad \forall ij \in \tbinom{V}{2}.\end{aligned}$$

Thus, the modified dual may be restated as

$$\begin{array}{ll}\min & |\mathcal{K}|\\ & \mathcal{K} \text{ a family of subsets of } V,\\ & w_i + 2e_i^\mathsf{T} Y \mathbb{1}_{E\setminus\delta(i)} \le \sum_{K\in\mathcal{K}}[i\in K] \qquad \forall i\in V,\\ & \sum_{K\in\mathcal{K}}[i\in K][j\in K] \le e_i^\mathsf{T} Y\mathbb{1}_{\delta(j)} + e_j^\mathsf{T} Y \mathbb{1}_{\delta(i)} \quad \forall ij\in\tbinom{V}{2}.\end{array} \tag{6.37}$$

Suppose that $\mathcal{K}$ is a clique cover of G with respect to w, i.e., $\mathcal{K}$ is a family of subsets of V such that $\sum_{K\in\mathcal{K}} \mathbb{1}_K = w$. Set

$$Y_{ie} := [e\in\delta(i)] \sum_{K\in\mathcal{K}} [i\in K][e\in E[K]].$$

Then it is easy to check that $(\mathcal{K}, Y)$ is feasible for (6.37). This completes the proof. ☐

6.6 A Burer-like Embedding for Packing Problems

Burer [19] showed that every binary integer linear program $\max\{\langle c, x\rangle : Ax = b,\ x\in\{0,1\}^V\}$ may be formulated exactly as a completely positive program as follows:

$$\begin{array}{ll}\sup & \langle 0\oplus \mathrm{Diag}(c), \hat{X}\rangle\\ & \mathcal{B}_{\{0\}\cup[n]}(\hat{X}) = 1\oplus 0,\\ & \langle 0\oplus \mathrm{Diag}(A^\mathsf{T} e_i), \hat{X}\rangle = b_i \quad \forall i\in[n],\\ & \langle 0\oplus e_i^\mathsf{T} A A^\mathsf{T} e_i, \hat{X}\rangle = b_i^2 \qquad \forall i\in[n],\\ & \hat{X}\in\mathcal{C}^*_{\{0\}\cup V}.\end{array} \tag{6.38}$$

In this section, we consider an SDP relaxation of a slight modification of the embedding (6.38) applied to packing problems.

Let V be a finite set. Let $\mathcal{A}$ be a collection of subsets of V and let $w \in \mathbb{Z}_+^V$. Consider the LP

$$\max\{\, w^\mathsf{T} x : x \in \mathbb{R}_+^V,\, \langle x, \mathbb{1}_A \rangle \leq 1 \, \forall A \in \mathcal{A}\}. \tag{6.39}$$

Assume that $\bigcup \mathcal{A} = V$ so that the constraint $x \leq \bar{e}$ is implied. If the constraint $x \in \{0,1\}^V$ is added to (6.39), then one obtains the classical set-packing problem. We shall consider the following SDP relaxation of the formulation (6.38) applied to (6.39):

$$\begin{array}{lll} \sup & \langle 0 \oplus \operatorname{Diag}(w), \hat{X} \rangle & \\ & \langle e_0 e_0^\mathsf{T}, \hat{X} \rangle = 1, & \\ & \langle 2 \operatorname{Sym}(e_i (e_i - e_0)^\mathsf{T}), \hat{X} \rangle = 0 & \forall i \in V, \\ & \langle -1 \oplus \operatorname{Diag}(\mathbb{1}_A), \hat{X} \rangle \leq 0 & \forall A \in \mathcal{A}, \\ & \langle -1 \oplus \mathbb{1}_A \mathbb{1}_A^\mathsf{T}, \hat{X} \rangle \leq 0 & \forall A \in \mathcal{A}, \\ & \hat{X}[V] \geq 0, & \\ & \hat{X} \in \mathbb{S}_+^{\{0\} \cup V}. & \end{array} \tag{6.40}$$

Its dual, written with an explicit slack, is

$$\begin{array}{ll} \inf & \eta \\ & \eta \in \mathbb{R}, u \in \mathbb{R}^V,\, y \in \mathbb{R}_+^{\mathcal{A}}, z \in \mathbb{R}_+^{\mathcal{A}},\, Z \in \mathbb{S}_{\geq 0}^V, \\ & \begin{bmatrix} \eta & -u^\mathsf{T} \\ -u & \operatorname{Diag}(2u) - Z \end{bmatrix} + \displaystyle\sum_{A \in \mathcal{A}} y_A \begin{bmatrix} -1 & 0^\mathsf{T} \\ 0 & \operatorname{Diag}(\mathbb{1}_A) \end{bmatrix} \\ & \qquad\qquad + \displaystyle\sum_{A \in \mathcal{A}} z_A \begin{bmatrix} -1 & 0^\mathsf{T} \\ 0 & \mathbb{1}_A \mathbb{1}_A^\mathsf{T} \end{bmatrix} - \hat{S} = \begin{bmatrix} 0 & 0^\mathsf{T} \\ 0 & \operatorname{Diag}(w) \end{bmatrix}, \\ & \hat{S} \in \mathbb{S}_+^{\{0\} \cup V}. \end{array} \tag{6.41}$$

Suppose we add the non-convex constraint (6.10) to (6.41), so that the dual slack $\hat{S}$ is required to have the form $\hat{S} = \sum_{K \in \mathcal{K}} (-1 \oplus \mathbb{1}_K)(-1 \oplus \mathbb{1}_K)^\mathsf{T}$ for some family $\mathcal{K}$ of subsets of V. Then the affine constraints for (6.41) translate to:

$$\begin{gathered} |\mathcal{K}| = \hat{S}_{00} = \eta - \langle \bar{e}, y \rangle - \langle \bar{e}, z \rangle, \\ -\sum_{K \in \mathcal{K}} \mathbb{1}_K = \hat{S}[V, 0] = -u, \\ \sum_{K \in \mathcal{K}} \mathbb{1}_K = \operatorname{diag}(\hat{S}[V]) \leq 2u - w + \sum_{A \in \mathcal{A}} (y_A + z_A) \mathbb{1}_A, \\ \sum_{K \in \mathcal{K}} [i \in K][j \in K] = \hat{S}_{ij} \leq \sum_{A \in \mathcal{A}} [ij \subseteq A] z_A \qquad \forall ij \in \tbinom{V}{2}. \end{gathered}$$

Thus, the modified dual may be stated as:

$$\begin{array}{ll} \inf & |\mathcal{K}| + \langle \bar{e}, y \rangle + \langle \bar{e}, z \rangle \\ & \mathcal{K} \text{ a family of subsets of } V, \\ & w \leq \sum_{K \in \mathcal{K}} \mathbb{1}_K + \sum_{A \in \mathcal{A}} (y_A + z_A) \mathbb{1}_A, \\ & \sum_{K \in \mathcal{K}} [i \in K][j \in K] \leq \sum_{A \in \mathcal{A}} [ij \subseteq A] z_A \quad \forall ij \in \tbinom{V}{2}, \\ & y \in \mathbb{R}_+^{\mathcal{A}},\, z \in \mathbb{R}_+^{\mathcal{A}}. \end{array} \tag{6.42}$$

Let us apply this formulation for $\mathcal{A} := E$ for a graph $G = (V, E)$ with no isolated node, so that (6.39) corresponds to optimization over $\mathrm{FRAC}(G)$. For a feasible solution $(\mathcal{K}, y, z)$ of (6.42), each $K \in \mathcal{K}$ is a clique in G, and z_e is bounded below by the number of cliques in $\mathcal{K}$ that induce the edge e.

The formulation (6.42) may be roughly interpreted as follows. We want to cover the nodes of G according to the weight function w on V, that is, each node $i \in V$ must be covered at least w_i times. To cover the nodes, there are two options. We may use an edge e of G, corresponding to the variable y_e. The cost to assign weight y_e to the edge e is also y_e. Alternatively, we may want to cover some nodes of G using a clique K. The advantage of using a clique K is that it has unit cost, regardless of its size $|K|$. On the other hand, once we use a clique K in the covering, we need to increase z_e by 1 for each $e \in E[K]$. By doing that, each node $i \in K$ gets its cover increased by $|K|$ units, and the cost of this whole operation is $1 + \binom{|K|}{2}$. To compare the costs and benefits of each of the two options above, consider covering the weight function $w := |C|\mathbb{1}_C$ on a clique C of G. Using only covering by the y variable, an optimal solution is to assign $y_e := \frac{|C|}{|C|-1}$ for each $e \in E[C]$, with a total cost of $\binom{|C|}{2}\frac{|C|}{|C|-1} = \frac{1}{2}|C|^2$. However, if we use the covering with $\mathcal{K} := \{C\}$ and $z := \mathbb{1}_{E[C]}$, the total cost is $1 + \binom{|C|}{2} = \frac{1}{2}|C|^2 - \frac{1}{2}|C| + 1$. For $w := \bar{e}$, however, it is never advantageous to have $\mathcal{K} \neq \varnothing$ in an optimal covering, so that (6.42) reduces to the LP dual of optimization over $\mathrm{FRAC}(G)$.

Next we consider the formulation (6.42) where $\mathcal{A}$ is the set of all cliques of a graph $G = (V, E)$ with no isolated node. We claim that,

$$\text{for every } w \in \mathbb{R}^V_+, \text{ the optimal value of (6.42) is } \overline{\chi^*}(G; w). \tag{6.43}$$

First note that there is a straightforward correspondence between feasible solutions for the LP dual to $\max\{\langle w, x\rangle : \langle x, \mathbb{1}_A\rangle \leq 1\, \forall A \in \mathcal{A}\}$ and feasible solutions for (6.42) with $\mathcal{K} = \varnothing$ and $z = 0$. Now let $(\mathcal{K}, y, z)$ be feasible for (6.42). Define $\bar{y}_A := y_A + z_A + \langle \mathbb{1}_{\mathcal{K}}, e_A\rangle$ for each $A \in \mathcal{A}$; here the component A of the incidence vector $\mathbb{1}_{\mathcal{K}}$ is the multiplicity of A in $\mathcal{K}$. Since each $K \in \mathcal{K}$ is a clique of G, we find that $(\varnothing, \bar{y}, 0)$ is also feasible in (6.42) with the same objective value as $(\mathcal{K}, y, z)$. This concludes the proof of (6.43).

Chapter 7

Future Research Directions

We now summarize some of the main avenues of future research suggested by some of the developments in this thesis.

7.1 Ellipsoidal Representations and Computational Complexity

In Section 3.4, we proved that the problem of computing the ellipsoidal number $\mathcal{E}_p(G; A)$ of a given graph G, with a matrix $A \in \mathbb{S}^d_+$ and for some given $d \in \mathbb{Z}_{++}$, is NP-hard. There, we relied in a fundamental way on the fact that we allow the matrix A to be singular. The optimization problem (3.2) then corresponds not to finding a smallest ellipsoid that contains a unit-distance representation of G, but, rather, it represents the search for a "smallest elliptic cylinder" that contains a unit-distance representation of G. While the latter problem is also interesting (see, for instance, [82]), it is arguably more natural to require A to be nonsingular, so that it defines a standard ellipsoid. We do not know, however, whether the problem of computing $\mathcal{E}_p(G; A)$ remains NP-hard when such a restriction is added, that is, when we require the given matrix A to be positive definite. A natural attempt to adapt our proof of NP-hardness of computing $\mathcal{E}_p(G; A)$ to the latter case leads to some interesting geometric problems and certain issues related to basic questions in Semidefinite Optimization and Computational Complexity, as we discuss next.

Let us try to reduce the NP-hard problem of determining whether a given input graph $G = (V, E)$ has a unit-distance representation in $\mathbb{R}^k$, for a given $k \in \mathbb{Z}_{++}$, to the problem of computing $\mathcal{E}(G; A)$, for a certain positive definite matrix $A \in \mathbb{S}^d_{++}$. Of course, by taking $d \coloneqq k$ and $A \coloneqq I$, then $\mathcal{E}(G; A) < \infty$ if and only if $\dim(G) \leq k$, but let us consider the more interesting question where we take $d \coloneqq n \coloneqq |V|$. Our current proof, where we allow A to be singular, takes $A \coloneqq \operatorname{Diag}(\mathbb{1}_{[n]\setminus[k]}) \in \mathbb{S}^n$, but now we need the cost matrix to be nonsingular. The obvious approach then involves setting the cost matrix to $B \coloneqq \operatorname{Diag}(\varepsilon \mathbb{1}_{[k]} + \mathbb{1}_{[n]\setminus[k]})$ for some $\varepsilon \in \mathbb{R}_{++}$, where ε should be chosen to be "small." Let us try to determine how small ε needs to be. Suppose that G has a unit-distance representation in $\mathbb{R}^k$. Then an optimal solution for the problem (3.1) maps each node $i \in V$ to a point $u_i \in \mathbb{R}^n$ with $\operatorname{supp}(u_i) \subseteq [k]$. Moreover, by sending some node of G to the origin, and assuming that G is connected, we may assume that $\|u_i\|_\infty \leq n$ for each $i \in V$. Thus, $\mathcal{E}(G; B) \leq \varepsilon n$. Next, suppose that G does not have a unit-distance representation in $\mathbb{R}^k$. Then $\mathcal{E}(G; B) \geq \mathcal{E}(G; A) > 0$. Thus, if we choose $\varepsilon > 0$ so that $\mathcal{E}(G; A) > \varepsilon n$, we obtain our desired reduction.

Actually, since our reduction is not supposed to compute $\mathcal{E}(G;A)$, we must choose $\varepsilon > 0$ so that $\varepsilon n < \mu$, where

$$\mu_{n,k} \coloneqq \min_{H} \mathcal{E}(H;A), \tag{7.1}$$

and H ranges over all graphs on at most n nodes such that $\dim(H) > k$. Obviously such a number ε exists, since $\mu_{n,k} > 0$. However, since we want our reduction to be carried out in polynomial time, we need the number $\mu_{n,k}$ to be have *size* polynomial in n. This leads us to the following question:

> given a graph G on n nodes, is there a lower bound on $\mathcal{E}(G;\mathrm{Diag}(\mathbb{1}_{[n]\setminus[k]}))$, where $k \coloneqq \dim(G) - 1$, of size polynomial in n? (7.2)

The existence of the number $\mu_{n,k}$ defined in (7.1) is related to a certain concept of "flattening" an "almost flat" unit-distance representation of a graph. Suppose that $u\colon V \to \mathbb{R}^n$ is a unit-distance representation of a graph $G = (V,E)$ such that $|V| \leq n$ and $|[u_i]_j| \leq \mu_{n,k}$ for every $i \in V$ and $j \in [n] \setminus [k]$. The latter condition may be vaguely described as saying that the representation u is "almost flat:" since we expect $\mu_{n,k}$ to be a small number, in the case $k = 2$, one could describe the representation u as being "almost" contained in the plane. Then, by the definition of u, there exists a unit-distance representation of G in $\mathbb{R}^k$, i.e., the representation u may be "completely flattened," and be made to lie completely in $\mathbb{R}^k$. Note that the previous discussions stems essentially from the attainment of ellipsoidal numbers, proved in Theorem 3.2.

The problem of determining lower bounds as requested in (7.2) seems hard to address. Even applying the basic tools of Semidefinite Optimization may be insufficient: unlike the case of linear programs, there exist some quite simple SDPs for which no feasible solution has size polynomially bounded by the size of the input: consider, e.g., the feasible region

$$\left\{ x \in \mathbb{R}^k : \begin{bmatrix} 1 & 2 \\ 2 & x_1 \end{bmatrix} \succeq 0,\ \begin{bmatrix} 1 & x_i \\ x_i & x_{i+1} \end{bmatrix} \succeq 0\ \forall i \in [k-1] \right\}.$$

Of course, there are other very basic issues regarding complexity theory about SDPs using the Turing machine model, such as SDPs for which there is no rational optimal solution.

The question (7.2) remains difficult even as we restrict our attention to the polynomially solvable problem of determining whether a given graph G is such that $\dim(G) = 1$. Obviously these are precisely the bipartite graphs. Thus, question (7.2) essentially reduces to that of providing a polynomial-size lower bound for $\mathcal{E}(C_n;\mathrm{Diag}(\mathbb{1}_{[n]\setminus[1]}))$ for any odd cycle C_n. Yet, we do not know of any such bounds.

7.2 Boundary Structure of Combinatorial Spectrahedra

In Chapter 4, we made progress on the boundary structure of some important "combinatorial spectrahedra," i.e., spectrahedra arising from problems in Combinatorial Optimization. We improved Laurent and Poljak's characterization of the vertices of the elliptope [87, 88] to the lifted theta body of an arbitrary graph. In the latter setting, the vertices of the spectrahedron under scrutiny remains precisely the exact solutions to the combinatorial problem for which the spectrahedron provides a relaxation. An important open problem is to determine whether this phenomenon also occurs for other combinatorial spectrahedra.

As we pointed out in Section 4.5, we currently do not know whether the simple spectrahedron $\mathrm{BQ}'_{\{0\}\cup V} \cap \mathrm{BQ}''_{\{0\}\cup V}$ has only rank-one vertices, and similarly for the spectrahedron described in (4.51). We noted that the former set is a relaxation of the lifting (4.18) of the boolean quadric polytope, whereas the constraints of the latter arise from the Lovász-Schrijver lift-and-project operator discussed in Section 6.5. We do not know either whether the spectrahedron obtained by applying the Lovász-Schrijver procedure to $\mathrm{FRAC}(G)$ has only rank-one vertices.

A more open-ended fundamental research direction is the development of other aspects of the boundary structure of combinatorial spectrahedra to a comparable extent to that of polyhedral combinatorics. As mentioned in Chapter 4, everything that is known from polyhedral combinatorics may in principle be proved using SDP Strong Duality. Still, the union of known results relating combinatorial and geometric structures in combinatorial spectrahedra, as illustrated in the introduction of the aforementioned chapter, is rather meager when compared to Schrijver's monumental book [132, 133, 134] on a classical subset of polyhedral combinatorics.

An essential difficulty, stemming from the potential non-linearity of spectrahedra, is that it is not clear what satisfactory descriptions of the boundary should look like. More specifically, what would be a useful compact representation of a smooth, nonlinear portion of the boundary of a combinatorial spectrahedron? Here, 'usefulness' should be measured in terms of strong correspondences with natural combinatorial structures of the associated problems. Knuth [78, Sec. 37] poses, for instance, the following problem: "Describe $\mathrm{TH}(C_5)$ geometrically." It is not clear what a solution should look like. A potential answer could be a closed-form formula for the function $\vartheta(C_5;\cdot)$ in terms of familiar functions. Another answer could be a finite system of polynomial inequalities defining $\mathrm{TH}(C_5)$. However, whereas a small system of linear inequalities makes it quite easy to compute the support function of the corresponding polyhedron (one could even run the simplex method by hand), this is harder to argue for a system of polynomial inequalities. The application of Algebraic Geometry tools to SDPs, however, has gained a lot of attention recently [16], which may lead to more satisfactory answers. Note that it is easy to obtain a finite system of polynomial inequalities describing a spectrahedron, e.g., using the principal minors criterion. However, $\mathrm{TH}(C_5)$ is only known to be the projection of the spectrahedron $\widehat{\mathrm{TH}}(C_5)$.

Beside the issue about compact representation of smooth portions of the boundary of a spectrahedron, it seems desirable to encode the adjacency structure of these portions, in some kind of structure analogous to the face lattice of a polytope. It is not clear what this structure should look like either.

7.3 Exactness and Interpretation of Dual SDPs

In Chapter 6, we discussed a non-convex constraint that may be regarded as an analogue of the standard integrality constraints in integer linear programs. This non-convex constraint sometimes reduces to the usual rank-one constraint, but when applied to the dual SDP, it yields reasonable "combinatorial duals" both for the standard diagonal embedding of LPs into SDPs, and for a certain formulation of the Lovász theta function, where it yields the weighted clique covering problem.

Some very natural questions arise from this viewpoint of SDPs with the additional non-convex constraint. Namely, is there a sufficiently well-behaved analogue of the notion of *total dual integrality* for SDPs? Even without the non-convex constraint in the dual, one might pose questions about the SDPs analogues of perfect and ideal matrices. Some progress in this direction was obtained in [125].

In some sections from Chapter 6, we focused some effort in trying to get "good interpretations" of the modified dual SDP, i.e., the dual SDP with the additional non-convex constraint (6.10). In Section 6.1, we interpreted the modified dual as precisely the clique covering problem. In Section 6.3, while we did not describe the modified dual problem exactly, we understood it well enough that we could prove a complete description of the optimal solution (Proposition 6.6). Our understanding of the combinatorial nature of the modified dual is considerably worse in Sections 6.4, 6.5, and 6.6. This is in contrast to the situation in combinatorial optimization, where the dual LP with additional integrality constraints, corresponding to (6.1d), usually yield easy-to-interpret, natural combinatorial problems.

Even without adding the non-convex constraint (6.10), dual SDPs are harder to interpret than dual LPs. For several classical combinatorial optimization problems, the dual of the LP relaxation of a natural integer programming formulation seems interesting in its own right, that is, regardless of the fact that it appears as the dual of another problem. This is the case, for instance, for the dual LPs described in the paragraph following the chain (6.1). One of these dual LPs defines the fractional chromatic number of a graph $G = (V, E)$, which may be described as

$$\chi^*(G) = \min\Big\{ \langle \bar{e}, y \rangle : \sum_{K \in \mathcal{K}} y_K \mathbb{1}_K = \bar{e} \Big\};$$

here, $\mathcal{K}$ denotes the set of all cliques of G. Even though the coefficients y_K are allowed to take on real values, the graph invariant χ^* is very natural combinatorially and it is deeply connected to graph homomorphisms into Kneser graphs; see, e.g., [62, Proposition 4.26].

The situation seems to be rather different in the context of SDPs. This was already hinted at in Chapter 6, and slightly more explicitly in Section 2.2, where dual SDP (2.4) for the hypersphere number was interpreted as a purely geometric optimization problem, that is, without an explicit positive semidefinite constraint. For that, however, we used the projective transformation underlying (2.22) in the proof of Theorem 2.4. The reason is that it is not easy to interpret the dual SDP (2.4) directly using its own coordinate system. This may be done, however, using some concepts from rigidity theory, as was already done in, e.g., [144, 55, 53]. We shall show some of the elementary concepts in what follows.

Let $G = (V, E)$ be a graph and let $u \colon V \to \mathbb{R}^d$ for some $d \in \mathbb{Z}_{++}$. A function $\sigma \colon E \to \mathbb{R}$ is a *stress function for u* (describing a *stress coefficient* for each edge) if

$$\sum_{j \in N(i)} \sigma_{ij}\big(u_j - u_i\big) = 0 \qquad \forall i \in V. \tag{7.3}$$

(Here, $N(i)$ denotes the set of neighbors of node i.) This condition, for a fixed $i \in V$, can be interpreted as follows. For an edge $ij \in E$ with $\sigma_{ij} > 0$, we regard the edge ij as a rubber band pulling node i towards node j. If $\sigma_{ij} < 0$, then the edge ij can be thought of as a strut pushing nodes i and j apart. An edge $ij \in E$ with $\sigma_{ij} = 0$ is effectively non-existing. Then each of the terms of the sum in (7.3) can be seen as the force acting on node i arising from the physical structure associated with the corresponding edge. In this context, condition (7.3) means that the physical structure is in equilibrium.

The above interpretation shows why stress functions show up naturally in graph rigidity and tensegrity theory. A related concept is that of an "energy function" (see, e.g., [97, ch. 4] and [30]). Fix a function $\sigma \colon E \to \mathbb{R}$. We can associate to each map $u \colon V \to \mathbb{R}^d$ the energy of u as

$$\mathscr{E}_\sigma(u) \coloneqq \sum_{ij \in E} \sigma_{ij} \|u_j - u_i\|^2.$$

An interpretation of this energy is given as follows. Suppose $\sigma_e > 0$ for every $e \in E$. Then, as above, we can interpret each edge as a rubber band pulling its ends closer together, and the term $\sigma_{ij}\|u_j - u_i\|^2$ can be seen as the contribution of edge ij to the total potential energy $\mathscr{E}_\sigma(u)$ of the system.

In [92], the following problem is considered, in connection with Tutte's barycentric representations [151]: for a certain subset $S \subseteq V$ of nodes, fix a position $u_0 \colon S \to \mathbb{R}^d$, and find an extension $u \colon V \to \mathbb{R}^d$ of u_0 that minimizes the energy $\mathscr{E}_\sigma(u)$, where $\sigma \colon E \to \mathbb{R}_{++}$ is fixed. This corresponds to nailing down the nodes of S into their prescribed positions, then taking each edge e as a rubber band with "constant of elasticity" given by σ_e, and letting the system vibrate until it reaches equilibrium. Thus, an optimal solution u of the above optimization problem corresponds to a configuration in static equilibrium. Optimality conditions then show that σ is "almost" a stress function for u, namely, (7.3) holds for all $i \in V \setminus S$.

The situation is a bit more complicated when we allow some entries of σ to be negative. Indeed, if $\sigma_{ij} < 0$, then we should interpret the edge ij as a strut pushing its ends further apart, but then the contribution $\sigma_{ij}\|u_j - u_i\|^2$ of edge ij to the total potential energy $\mathscr{E}_\sigma(u)$ of the system is negative. This might seem counterintuitive, but given the fact that edge ij is constantly pushing its ends apart, it somewhat makes sense. The most important property that we must preserve for the above ideas to carry through is that the energy function $\mathscr{E}_\sigma$ must have a minimum.

Let us briefly investigate for which functions $\sigma \colon E \to \mathbb{R}$ the energy function $\mathscr{E}_\sigma$ has a minimum. Given $u \colon V \to \mathbb{R}^d$, define a $[d] \times V$ matrix U^T by setting $U^\mathsf{T} e_i := u_i$ for every $i \in V$. Let D be an arbitrary orientation of G, i.e., D is any digraph whose underlying graph is G, and let B_D denote the node-arc incidence matrix of D. Then

$$\begin{aligned}\mathscr{E}_\sigma(u) &= \sum_{k=1}^{d} \sum_{ij \in E} \bigl([u_j]_k - [u_i]_k\bigr)\sigma_{ij}\bigl([u_j]_k - [u_i]_k\bigr)\\ &= \sum_{k=1}^{d} e_k^\mathsf{T} U^\mathsf{T} B_D \operatorname{Diag}(\sigma) B_D^\mathsf{T} U e_k = \operatorname{Tr}\bigl(U^\mathsf{T} \mathcal{L}_G(\sigma) U\bigr),\end{aligned}$$

where we used the factorization

$$\mathcal{L}_G(z) = B_D \operatorname{Diag}(z) B_D^\mathsf{T} \qquad \forall z \in \mathbb{R}^E \tag{7.4}$$

of the Laplacian $\mathcal{L}_G$ of G.

Now it is easy to see that

$$\mathscr{E}_\sigma \text{ has a minimum if and only if } \mathcal{L}_G(\sigma) \succeq 0. \tag{7.5}$$

Indeed, suppose $\mathcal{L}_G(\sigma) \succeq 0$. Then $\mathscr{E}_\sigma(u) \geq 0$ for every $u \colon V \to \mathbb{R}^d$, so $u = 0$ is a minimum of $\mathscr{E}_\sigma$. Now suppose $h^\mathsf{T}\mathcal{L}_G(\sigma)h < 0$ for some $h \in \mathbb{R}^V$. Set $U^\mathsf{T} := e_1 h^\mathsf{T}$, and define $u \colon V \to \mathbb{R}^d$ accordingly. Then $\mathscr{E}_\sigma(u) = (h^\mathsf{T}\mathcal{L}_G(\sigma)h)\operatorname{Tr}\bigl(e_1 e_1^\mathsf{T}\bigr) < 0$, so $\mathscr{E}_\sigma(\lambda u) \to -\infty$ as $\lambda \to \infty$.

The previous concepts may be used to interpret the dual SDP (2.4). In fact, we will first look at the following augmented SDP for hypersphere number:

$$t(G) = \min\Bigl\{\, t : \mathcal{L}_H^*(\hat{X}) - t\mathbb{1}_{\delta_H(0)} = \mathbb{1}_{E(G)},\, X \in \mathbb{S}_+^{\{0\}\cup V},\, t \in \mathbb{R} \Bigr\} \tag{7.6}$$

where H denotes the cosum of G and the graph $K_{\{0\}}$; see Subsection 2.3.1 for the definition of cosum. Note that (7.6) really models $t(G)$, and the only difference between this formulation of $t(G)$ and the one given by (2.3) is that here we do not insist that the hypersphere is centered at the origin. Thus, (7.6) has an optimal solution. Moreover, since $\bar{X} \oplus \bar{t} = \frac{1}{2}(I \oplus 1)$ is a Slater point of (7.6) and the dual SDP

$$\max\Big\{ \langle \mathbb{1}_{E(G)}, r\rangle : r \in \mathbb{R}^{E(H)},\, \mathcal{L}_H(r) \preceq 0,\, \langle -\mathbb{1}_{\delta_H(0)}, r\rangle = 1 \Big\} \tag{7.7}$$

is feasible, it follows from SDP Strong Duality that there is no duality gap, and the dual has an optimal solution. It should be easy to interpret (7.7) from our previous discussion of energy functions, by using the change of variables $\sigma = -r$. Among all vectors $\sigma\colon E(H) \to \mathbb{R}$ giving rise to an energy function $\mathscr{E}_\sigma$ that has a minimum, normalized so that $\langle \mathbb{1}_{\delta_H(0)}, \sigma\rangle = 1$, choose one that minimizes $\langle \mathbb{1}_{E(G)}, \sigma\rangle$.

Let $X \oplus t$ be an optimal solution for (7.6) and let r be an optimal solution for (7.7). Set $\sigma := -r$, write $X = UU^\mathsf{T}$ for some $[d] \times V(H)$ matrix U^T, and put $u_i := U^\mathsf{T} e_i$ for every $i \in V(H)$. By complementarity, we have $0 = \langle \mathcal{L}_H(\sigma), UU^\mathsf{T}\rangle = U^\mathsf{T}\mathcal{L}_H(\sigma)U$, whence $U^\mathsf{T}\mathcal{L}_H(\sigma) = 0$. The latter equation is easily seen to be equivalent to the fact that σ is a stress function for u.

It is easy to see how the augmented formulations (7.6) and (7.7) relate to the SDPs (2.3) and (2.4) studied in Chapter 2. Namely, by writing $r = -y \oplus z$, with $y \in \mathbb{R}^{V(G)}$ and $z \in \mathbb{R}^{E(G)}$, using the natural correspondence between $V(G)$ and $\delta_H(0)$, we have

$$\mathcal{L}_H(r) = \begin{bmatrix} -\langle \bar{e}, y\rangle & y^\mathsf{T} \\ y & -\operatorname{Diag}(y) + \mathcal{L}_G(z) \end{bmatrix}.$$

Thus, the rigidity interpretations using energy functions translate directly to the SDP (2.4). As before, the parameters $y \oplus z$ which give rise to energy functions that have a minimum are precisely the ones for which $-\operatorname{Diag}(y) + \mathcal{L}_G(z) \preceq 0$. Thus, (2.4) can be seen as the search for the "best" such parameters, normalized so that $\langle \bar{e}, y\rangle = 1$. Moreover, any optimal solution $y \oplus z$ for (2.4) also yields a stress function for any optimal hypersphere representation of G, where we assume an extra node, corresponding to the single node of $K_{\{0\}}$, has been placed at the origin.

The rigidity interpretation of (2.4) may be extended by regarding the constraint $\langle \bar{e}, y\rangle = 1$ as an instance of a general constraint of the form $y \oplus z \in P$ for some polyhedron P. The interpretation thus carries over to the duals of the SDPs arising as the LHS of (2.50), and in particular to the dual SDPs for the variants t' and t^+ of the hypersphere number, defined in (2.60) and (2.63), respectively. In these cases, nonnegativity or nonpositivity constraints on the dual variables require some edges rubber bands and others to be struts. In all these cases, the automorphism group of the dual SDP acts transitively on the dual variables in y, and its action on the edge variables is either transitive or, for the variant t^+, it has only two orbits.

One way to write the MaxCut SDP used by Goemans and Williamson [52] on a graph G and with weights given by $w \in \mathbb{R}^E_+$ is

$$\max\big\{ \langle \tfrac{1}{4}\mathcal{L}_G(w), X\rangle : \operatorname{diag}(X) = \bar{e},\, X \in \mathbb{S}^V_+ \big\},$$

and its dual is

$$\min\big\{ \langle \bar{e}, y\rangle : y \in \mathbb{R}^V,\, \operatorname{Diag}(y) \succeq \tfrac{1}{4}\mathcal{L}_G(w) \big\}.$$

This dual SDP also admits the rigidity interpretation where we require the variable $y \oplus z$ to lie in the polyhedron $\mathbb{R}^V \oplus \{w\}$.

It would be desirable to find deeper connections between concepts from tensegrity theory, geometric representations such as hypersphere and orthonormal representations, the Lovász theta function and the MaxCut SDP, via SDP Duality. It is possible that, with an improved understanding of the dual SDPs for some problems on graphs, more results of a polyhedral combinatorics flavor may be obtained in the context of SDPs, and potentially for SDPs whose duals do not arise directly from graphs as well.

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Appendices

Appendix A

Proofs for the Sake of Completeness

A.1 Ellipsoidal Numbers of Triangles

Our goal in this section is to provide a formula for the ellipsoidal number of K_3, i.e., to prove that the upper bound (3.48) from Proposition 3.13 is tight for $n = 2$. We shall reuse the notation set in the beginning of Chapter 3.

The proof is long but rather pedestrian. It boils down to calculus applied to a formula for the radius of the smallest circle enclosing a given triangle in the plane. The latter formula depends on which edge of the triangle is longest. This dependence creates a complication, since it does not seem to play well with the "smooth" functions we want to deal with to apply calculus.

To overcome this complication, we use a parametrization of the feasible region $\mathcal{U}_2(K_3)$ of $\mathcal{E}(K_3; \cdot)$ for which we always know which edge of our triangle is longest. In fact, we use the symmetries of the plane to restrict ourselves to a subset of the full feasible region of $\mathcal{E}(K_3; \cdot)$, which we show is enough.

The rest is just a long computation.

A.1.1 A Parametrization with a Known Longest Edge

Let us set the notation for the remainder of the section. The parametrization of $\mathcal{U}_2(K_3)$ that we will work with is

$$\mathcal{U} := \left\{ R(\theta)U_0^{\mathsf{T}} + s\bar{e}^{\mathsf{T}} : \theta \in [0, \pi/3],\, s \in \mathbb{R}^2 \right\}, \tag{A.1}$$

where

$$R(\theta) := \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}, \qquad \forall \theta \in \mathbb{R}, \tag{A.2}$$

$$U_0^{\mathsf{T}} := \frac{1}{2} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & \sqrt{3} \end{bmatrix}. \tag{A.3}$$

Pay special attention to the range of θ in the definition of $\mathcal{U}$. We shall show in Theorem A.3 below that we may restrict our attention to $\mathcal{U}$ when computing $\mathcal{E}(K_3;\cdot)$. For now, we content ourselves with identifying the longest edge in a certain triangle arising from the parametrization given by $\mathcal{U}$.

When reading the intermediate results in this section, the reader should keep in mind that our goal is to compute $\mathcal{E}(K_3;\operatorname{Diag}(a,1))$ where $a \in (0,1)$.

Proposition A.1. Let $a \in (0,1)$ and $A \coloneqq \operatorname{Diag}(a,1)$. Let $U^{\mathsf{T}} \in \mathcal{U}$ and set $P^{\mathsf{T}} \coloneqq A^{1/2}U^{\mathsf{T}}$ and $p_i \coloneqq P^{\mathsf{T}} e_i$ for $i \in [3]$. Then the longest edge of the triangle with vertex set $\{p_1, p_2, p_3\}$ is $[p_2, p_3]$, i.e.,

$$\|p_3 - p_2\|_2 \geq \|p_2 - p_1\|_2 \qquad \text{and} \qquad \|p_3 - p_2\|_2 \geq \|p_3 - p_1\|_2.$$

Proof. Let $\theta \in [0, \pi/3]$ and $s \in \mathbb{R}^2$ such that $U^{\mathsf{T}} = R(\theta)U_0^{\mathsf{T}} + s\bar{e}^{\mathsf{T}}$. We have

$$P^{\mathsf{T}} = \frac{1}{2}\begin{bmatrix} a^{1/2}\cos\theta & -a^{1/2}\cos\theta & -\sqrt{3a}\sin\theta \\ \sin\theta & -\sin\theta & \sqrt{3}\cos\theta \end{bmatrix} + A^{1/2}s\bar{e}^{\mathsf{T}}. \tag{A.4}$$

Thus,

$$p_2 - p_1 = \begin{bmatrix} -a^{1/2}\cos\theta \\ -\sin\theta \end{bmatrix}, \tag{A.5a}$$

$$p_3 - p_1 = \frac{1}{2}\begin{bmatrix} -a^{1/2}(\sqrt{3}\sin\theta + \cos\theta) \\ \sqrt{3}\cos\theta - \sin\theta \end{bmatrix}, \tag{A.5b}$$

$$p_3 - p_2 = \frac{1}{2}\begin{bmatrix} -a^{1/2}(\sqrt{3}\sin\theta - \cos\theta) \\ \sqrt{3}\cos\theta + \sin\theta \end{bmatrix}, \tag{A.5c}$$

whence

$$\|p_2 - p_1\|_2^2 = a\cos^2\theta + \sin^2\theta, \tag{A.6a}$$

$$4\|p_3 - p_1\|_2^2 = (3a+1)\sin^2\theta - 2\sqrt{3}(1-a)\sin\theta\cos\theta + (3+a)\cos^2\theta, \tag{A.6b}$$

$$4\|p_3 - p_2\|_2^2 = (3a+1)\sin^2\theta + 2\sqrt{3}(1-a)\sin\theta\cos\theta + (3+a)\cos^2\theta. \tag{A.6c}$$

Thus, $\theta \in [0,\pi/3] \subseteq [0,\pi/2]$ implies that $\|p_3 - p_2\|_2^2 - \|p_3 - p_1\|_2^2 = \frac{\sqrt{3}}{2}(1-a)\sin(2\theta) \geq 0$.

Next note that

$$\begin{aligned} 4\big(\|p_3 - p_2\|_2^2 - \|p_2 - p_1\|_2^2\big) &= (3a-3)\sin^2\theta + 2\sqrt{3}(1-a)\sin\theta\cos\theta + (3-3a)\cos^2\theta \\ &= 3(1-a)\cos(2\theta) + \sqrt{3}(1-a)\sin(2\theta) \\ &= 2\sqrt{3}(1-a)\sin(2\theta + \pi/3) \geq 0, \end{aligned}$$

where the last inequality holds since $\theta \in [0,\pi/3]$ implies $2\theta + \pi/3 \in [0,\pi]$. □

A.1.2 The Parametrization Contains an Optimal Representation

We need to describe some symmetries of the plane that allow us to focus on the parametrization given by $\mathcal{U}$ instead of the full feasible region $\mathcal{U}_2(K_3)$. Recall that, for a permutation $\sigma \in \operatorname{Sym}_V$ of a finite set V, the linear map $P_\sigma \colon \mathbb{R}^V \to \mathbb{R}^V$ is the linear extension of the map $e_i \mapsto e_{\sigma(i)}$. We shall use the standard cycle notation for permutations.

Lemma A.2. Let $x_0 \in \{\pm 1\}^2$, $\theta_0 \in \mathbb{R}$, $s_0 \in \mathbb{R}^2$, and $\sigma_0 \in \mathrm{Sym}_3$. Set $\theta_1 \coloneqq \theta_0 - \pi/3$. Then there exist $x_1 \in \{\pm 1\}^2$, $s_1 \in \mathbb{R}^2$, and $\sigma_1 \in \mathrm{Sym}_3$ such that

$$\mathrm{Diag}(x_0)R(\theta_0)U_0^\top P_{\sigma_0} + s_0\bar{e}^\top = \mathrm{Diag}(x_1)R(\theta_1)U_0^\top P_{\sigma_1} + s_1\bar{e}^\top. \tag{A.7}$$

Proof. Set

$$D \coloneqq \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Using the fact that the sine function is odd and the cosine function is even, it is easy to check that, for every $\theta \in \mathbb{R}$, we have

$$R(-\theta)U_0^\top = -DR(\theta)U_0^\top P_{(12)}, \tag{A.8a}$$

$$R(\theta)D = DR(-\theta), \tag{A.8b}$$

$$R(\tfrac{\pi}{3})U_0^\top = DU_0^\top P_{(23)} + s_2\bar{e}^\top \tag{A.8c}$$

where $s_2 \coloneqq (-1, \sqrt{3})^\top/4$.

Now using (A.8), we find that

$$\begin{aligned} \mathrm{Diag}(x_0)R(\theta_0)U_0^\top P_{\sigma_0} + s_0\bar{e}^\top &= \mathrm{Diag}(x_0)R(\theta_1)R(\tfrac{\pi}{3})U_0^\top P_{\sigma_0} + s_0\bar{e}^\top \\ &= \mathrm{Diag}(x_0)R(\theta_1)\big(DU_0^\top P_{(23)} + s_2\bar{e}^\top\big)P_{\sigma_0} + s_0\bar{e}^\top \\ &= \mathrm{Diag}(x_0)DR(-\theta_1)U_0^\top P_{(23)}P_{\sigma_0} + s_3\bar{e}^\top P_{\sigma_0} + s_0\bar{e}^\top \\ &= \mathrm{Diag}(-x_0)R(\theta_1)U_0^\top P_{(12)}P_{(23)}P_{\sigma_0} + s_1\bar{e}^\top \end{aligned}$$

where $s_3 \coloneqq \mathrm{Diag}(x_0)R(\theta_1)s_2$ and $s_1 \coloneqq s_3 + s_0$. This completes the proof of (A.7). ☐

Now we may finally state precisely what we mean when we say that it is enough to restrict our attention to the subset $\mathcal{U}$ of the full feasible region $\mathcal{U}_2(K_3)$:

Theorem A.3. Let $A \in \mathbb{S}^2_+$ be diagonal. Then

$$\mathcal{E}(K_3; A) = \inf\big\{ \|\mathrm{diag}(UAU^\top)\|_\infty : U^\top \in \mathcal{U}\big\}. \tag{A.9}$$

Proof. Define

$$\mathcal{U}' \coloneqq \Big\{ \mathrm{Diag}(x)U^\top P_\sigma : x \in \{\pm 1\}^2,\, U^\top \in \mathcal{U},\, \sigma \in \mathrm{Sym}_3 \Big\}.$$

Let us show that

$$\mathcal{U}_2(K_3) = \mathcal{U}'. \tag{A.10}$$

We first show '$\supseteq$' in (A.10). Note that

$$\mathcal{U} \subseteq \mathcal{U}_2(K_3) \tag{A.11}$$

since $U_0 \in \mathcal{U}_2(K_3)$ and $\mathcal{U}_2(K_3)$ is closed under orthogonal transformations and shifts. Since $\mathcal{U}_2(K_3)$ is also closed under permutation of columns, it follows that $\mathcal{U}' \subseteq \mathcal{U}_2(K_3)$. For the reverse inclusion, let $U^\top \in \mathcal{U}_2(K_3)$. Then there exists $Q \in \mathbb{O}^2$ and $s_0 \in \mathbb{R}^2$ such that $U^\top = QU_0^\top + s_0\bar{e}^\top$. Thus, for some

$x_0 \in \{\pm 1\}^2$, we know that U^T is of the form $U^\mathsf{T} = \mathrm{Diag}(x_0) R(\theta_0) U_0^\mathsf{T} + s_0 \bar{e}^\mathsf{T}$, where $0 \le \theta_0 < 2\pi$. Let $k \in \mathbb{Z}_+$ be minimal such that $0 \le \theta_0 - k\pi/3 < \pi/3$. Then, by Lemma A.2, we find that

$$U^\mathsf{T} = \mathrm{Diag}(x_0) R(\theta_0) U_0^\mathsf{T} I + s_0 \bar{e}^\mathsf{T} = \mathrm{Diag}(x_k) R(\theta - k\pi/3) U_0^\mathsf{T} P_k + s_k \bar{e}^\mathsf{T}.$$

This proves (A.10).

Now we will show that

$$\inf\Big\{ \|\mathrm{diag}(UAU^\mathsf{T})\|_\infty : U^\mathsf{T} \in \mathcal{U}\Big\} = \inf\Big\{ \|\mathrm{diag}(UAU^\mathsf{T})\|_\infty : U^\mathsf{T} \in \mathcal{U}'\Big\}. \tag{A.12}$$

The inequality '$\le$' follows from (A.11) and (A.10). For the reverse inequality, let $x \in \{\pm 1\}^d$, $U^\mathsf{T} \in \mathcal{U}$ and $\sigma \in \mathrm{Sym}_3$. Since diagonal matrices commute, the objective value of $\mathrm{Diag}(x) U^\mathsf{T} P_\sigma$ in the RHS of (A.12) is

$$\begin{aligned}
\max\Big\{ \|A^{1/2}\,\mathrm{Diag}(x) U^\mathsf{T} P_\sigma e_i\|_2^2 : i \in [n]\Big\} &= \max\Big\{ \|\mathrm{Diag}(x) A^{1/2} U^\mathsf{T} e_i\|_2^2 : i \in [n]\Big\} \\
&= \max\Big\{ \|A^{1/2} U^\mathsf{T} e_i\|_2^2 : i \in [n]\Big\},
\end{aligned}$$

which is the objective value of $U^\mathsf{T} \in \mathcal{U}$ in the LHS of (A.12). This proves (A.12).

Since $\mathcal{E}(K_3; A) = \inf\{ \|\mathrm{diag}(UAU^\mathsf{T})\|_\infty : U^\mathsf{T} \in \mathcal{U}_2(K_3)\}$ by definition, the theorem follows from (A.12) and (A.10). □

A.1.3 Reduction to Smallest Enclosing Circle

Now we show that we may formulate $\mathcal{E}(K_3; \cdot)$ as a smallest enclosing circle problem.

Proposition A.4. Let $A \in \mathbb{S}^2_{++}$ be diagonal. Then

$$\mathcal{E}(K_3; A) = \inf_{\theta \in [0, \frac{\pi}{3}]} \inf\Big\{ t : \|A^{1/2} R(\theta) U_0^\mathsf{T} e_i - c\|_2^2 \le t,\ \forall i \in [3],\ c \in \mathbb{R}^2,\ t \in \mathbb{R}\Big\}. \tag{A.13}$$

Proof. By Theorem A.3, we have

$$\begin{aligned}
\mathcal{E}(K_3; A) &= \inf\Big\{ t : \|A^{1/2} U^\mathsf{T} e_i\|_2^2 \le t,\ \forall i \in [3],\ U^\mathsf{T} \in \mathcal{U}\Big\} \\
&= \inf\Big\{ t : \|A^{1/2} R(\theta) U_0^\mathsf{T} e_i + A^{1/2} s \bar{e}^\mathsf{T} e_i\|_2^2 \le t,\ \forall i \in [3],\ \theta \in [0, \tfrac{\pi}{3}],\ s \in \mathbb{R}^2\Big\} \\
&= \inf\Big\{ t : \|A^{1/2} R(\theta) U_0^\mathsf{T} e_i - c\|_2^2 \le t,\ \forall i \in [3],\ \theta \in [0, \tfrac{\pi}{3}],\ c \in \mathbb{R}^2\Big\}.
\end{aligned}$$

This completes the proof of (A.13). □

Thus, given $\theta \in [0, \pi/3]$, the optimal value of t in the inner minimization problem of (A.13) is obtained by finding the smallest enclosing circle containing the triangle whose vertices are the columns of the matrix

$$P^\mathsf{T} = A^{1/2} R(\theta) U_0^\mathsf{T}. \tag{A.14}$$

Next we provide an analytic solution for an arbitrary smallest enclosing circle problem.

Proposition A.5 (Smallest Enclosing Circle)**.** Let $p_1, p_2, p_3 \in \mathbb{R}^2$ be affinely independent. Let $c^* \oplus t^* \in \mathbb{R}^2 \oplus \mathbb{R}$ be an optimal solution for

$$\min\{\, t : \|p_i - c\|_2^2 \le t,\, \forall i \in [3],\, c \in \mathbb{R}^2,\, t \in \mathbb{R}\}. \tag{A.15}$$

Suppose that the triangle with vertex set $\{p_1, p_2, p_3\}$ has $[p_2, p_3]$ as its longest edge, i.e., $\|p_3 - p_2\|_2 \ge \|p_2 - p_1\|_2$ and $\|p_3 - p_2\|_2 \ge \|p_3 - p_1\|_2$. If

$$\langle p_1, p_2 + p_3 - p_1\rangle \ge \langle p_2, p_3\rangle, \tag{A.16}$$

then

$$t^* = \frac{\|p_3 - p_2\|_2^2}{4}. \tag{A.17}$$

Otherwise,

$$t^* = \frac{\|p_3 - p_2\|_2^2}{4}\left[1 + \left(\frac{\langle p_1, p_2 + p_3 - p_1\rangle - \langle p_2, p_3\rangle}{\langle d, p_2 - p_1\rangle}\right)^2\right], \tag{A.18}$$

where

$$d \coloneqq \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} (p_3 - p_2). \tag{A.19}$$

Proof. First note that (A.15) indeed has an optimal solution, as it may be equivalently formulated as the unconstrained minimization over $c \in \mathbb{R}^2$ of the continuous and coercive function $\max\{\, \|p_i - c\|_2^2 : i \in [3]\}$.

It is also clear that, at an optimal solution, there are at least two active constraints, say the ones corresponding to points $p_i, p_j \in \{p_1, p_2, p_3\}$. So c^* lies at the perpendicular bisector of $[p_i, p_j]$. If the constraint of the other point is not active and c^* is not the midpoint of $[p_i, p_j]$, then a perturbation argument shows that c^* is not optimal. Thus, either all three constraints are tight, or c^* is the midpoint of an edge. In either case, c^* lies at the perpendicular bisector of $[p_2, p_3]$, the longest edge. So c^* is of the form

$$c^* = c_\lambda \coloneqq m + \lambda d, \qquad \lambda \in \mathbb{R} \tag{A.20}$$

where $m \coloneqq \frac{1}{2}(p_2 + p_3)$. Moreover, $t^* = \|p_2 - c^*\|_2^2$. Hence,

$$t^* = \inf\{\, \|p_2 - c_\lambda\|_2^2 : \|p_1 - c_\lambda\|_2^2 \le \|p_2 - c_\lambda\|_2^2,\, \lambda \in \mathbb{R}\}. \tag{A.21}$$

Since $p_2 - m \perp d$, the objective function in (A.21) is:

$$\|p_2 - c_\lambda\|_2^2 = \|p_2 - m - \lambda d\|_2^2 = \|p_2 - m\|_2^2 + \lambda^2\|d\|_2^2 = \|p_3 - p_2\|_2^2\big(\tfrac{1}{4} + \lambda^2\big).$$

The feasibility condition in (A.21) is:

$$\begin{aligned} \|p_1 - c_\lambda\|_2^2 \le \|p_2 - c_\lambda\|_2^2 &\iff \|p_1\|_2^2 - 2\langle p_1, c_\lambda\rangle + \|c_\lambda\|_2^2 \le \|p_2\|_2^2 - 2\langle p_2, c_\lambda\rangle + \|c_\lambda\|_2^2 \\ &\iff \|p_1\|_2^2 - \langle p_1, p_2 + p_3\rangle - 2\lambda\langle p_1, d\rangle \le \|p_2\|_2^2 - \langle p_2, p_2 + p_3\rangle - 2\lambda\langle p_2, d\rangle \\ &\iff \|p_1\|_2^2 - \langle p_1, p_2 + p_3\rangle + \langle p_2, p_3\rangle \le 2\lambda\langle p_1 - p_2, d\rangle. \end{aligned}$$

Hence, (A.21) may be rewritten as

$$t^* = \inf\left\{ \|p_3 - p_2\|_2^2\Big(\frac{1}{4} + \lambda^2\Big) : \|p_1\|_2^2 - \langle p_1, p_2 + p_3\rangle + \langle p_2, p_3\rangle \le 2\lambda\langle p_1 - p_2, d\rangle,\ \lambda \in \mathbb{R}\right\}. \tag{A.22}$$

Note further that $\langle p_1 - p_2, d\rangle \neq 0$. For if $p_1 - p_2$ were orthogonal to d, then $p_1 - p_2$ would be parallel to $p_3 - p_2$, which is orthogonal to d by construction, so that p_1, p_2, p_3 would be affinely dependent.

Thus, (A.16) holds if and only if $\lambda = 0$ is feasible in (A.22), in which case t^* is given by (A.17). Otherwise, the optimal value is

$$\|p_3 - p_2\|_2^2\left[\frac{1}{4} + \Big(\frac{\|p_1\|_2^2 - \langle p_1, p_2 + p_3\rangle + \langle p_2, p_3\rangle}{2\langle d, p_1 - p_2\rangle}\Big)^2\right],$$

which is equal to (A.18). □

Define the functions $f_0, f_1 \colon [0, \frac{\pi}{3}] \to \mathbb{R}$ by

$$\begin{aligned} f_1(\theta) &:= \frac{(1+a) + (1-a)\sin(2\theta + \frac{\pi}{6})}{8}, \\ f_0(\theta) &:= f_1(\theta)\left(1 + \frac{(\frac{1}{2}(1-a)[2\sin(2\theta + \frac{\pi}{6}) + 1] - 1)^2}{3a}\right). \end{aligned} \tag{A.23}$$

Let us apply Proposition A.5 to the triangle given by (A.13). We shall have occasion to apply Proposition A.1 that identified the longest edge of the triangle.

Proposition A.6. Let $\theta \in [0, \pi/3]$ and $a \in (0, 1)$. Set $A := \left[\begin{smallmatrix} a & 0 \\ 0 & 1 \end{smallmatrix}\right]$ and define P^T as in (A.14). Let $c^* \oplus t^* \in \mathbb{R}^2 \oplus \mathbb{R}$ be an optimal solution for (A.15) applied to p_1, p_2, p_3, where $p_i := P^\mathsf{T} e_i$ for $i \in [3]$. If

$$2\sin(2\theta + \tfrac{\pi}{6}) \le \frac{1+a}{1-a}, \tag{A.24}$$

then $t^* = f_0(\theta)$. Otherwise, $t^* = f_1(\theta)$. Moreover, if (A.24) holds with equality, then $f_0(\theta) = f_1(\theta)$.

Proof. We apply Proposition A.5 together with Proposition A.1. Let $x := \langle p_1, p_2 + p_3 - p_1\rangle - \langle p_2, p_3\rangle$. We may use the same calculations for $p_2 - p_1$, $p_3 - p_1$, and $p_3 - p_2$ from (A.5). Using the fact that $p_1 = -p_2$, we find that

$$\begin{aligned} 2x &= 2\langle p_1, p_3 - 2p_1\rangle + 2\langle p_1, p_3\rangle = 4\langle p_1, p_3 - p_1\rangle \\ &= -a\cos^2\theta - \sin^2\theta + \sin\theta\cos\theta(\sqrt{3} - \sqrt{3}a) \\ &= (1-a)\sqrt{3}\sin\theta\cos\theta - a\cos^2\theta + \cos^2\theta - 1 \\ &= (1-a)\big[\sqrt{3}\sin\theta\cos\theta + \cos^2\theta\big] - 1 \\ &= (1-a)\Big[\tfrac{\sqrt{3}}{2}\sin(2\theta) + \tfrac{1}{2}(\cos(2\theta) + 1)\Big] - 1 \\ &= (1-a)\Big[\sin(2\theta + \tfrac{\pi}{6}) + \tfrac{1}{2}\Big] - 1 \\ &= \tfrac{1}{2}(1-a)\Big[2\sin(2\theta + \tfrac{\pi}{6}) + 1\Big] - 1. \end{aligned} \tag{A.25}$$

Hence, $x \geq 0$ is equivalent to $2\sin(2\theta+\frac{\pi}{6}) \geq \frac{1+a}{1-a}$. Thus, if (A.24) does not hold, then by Proposition A.5 and (A.6), we have

$$\begin{aligned}
16t^* &= 4\|p_3 - p_2\|_2^2 = (1+a) + 2a\sin^2\theta + 2\cos^2\theta + 2\sqrt{3}(1-a)\sin\theta\cos\theta \\
&= (1+a) + 2a(1-\cos^2\theta) + 2\cos^2\theta + 2\sqrt{3}(1-a)\sin\theta\cos\theta \\
&= (1+3a) + 2(1-a)\tfrac{1}{2}(\cos(2\theta)+1) + \sqrt{3}(1-a)\sin(2\theta) \\
&= 2(1+a) + 2(1-a)\Big(\tfrac{1}{2}\cos(2\theta) + \tfrac{\sqrt{3}}{2}\sin(2\theta)\Big) \\
&= 2\big[(1+a) + (1-a)\sin(2\theta+\tfrac{\pi}{6})\big] = 16f_1(\theta).
\end{aligned} \tag{A.26}$$

So suppose that (A.24) holds. Define d as in (A.19), i.e.,

$$d := \frac{1}{2}\begin{bmatrix} -\sqrt{3}\cos\theta - \sin\theta \\ -a^{1/2}(\sqrt{3}\sin\theta - \cos\theta) \end{bmatrix}.$$

Then by Proposition A.5 and equations (A.25) and (A.26), we have

$$t^* = \frac{\|p_3 - p_2\|_2^2}{4}\left(1 + \frac{x^2}{3a/4}\right) = f_1(\theta)\left(1 + \frac{\left(\frac{1}{2}(1-a)[2\sin(2\theta+\frac{\pi}{6})+1]-1\right)^2}{3a}\right) = f_0(\theta). \tag{A.27}$$

Finally, note that $f_0(\theta) = f_1(\theta)$ if $x = 0$, i.e., if (A.24) holds with equality. □

A.1.4 Calculus Application

Let us first compute a normalized version of $\mathcal{E}(K_3;\cdot)$:

Theorem A.7. Let $a \in (0,1)$. Set

$$A := \begin{bmatrix} a & 0 \\ 0 & 1 \end{bmatrix}.$$

Then

$$\mathcal{E}(K_3;A) = \frac{(a+3)^2}{48}. \tag{A.28}$$

Proof. By Propositions A.4 and A.6, we have

$$\mathcal{E}(K_3;A) = \inf\{\, f(\theta) : \theta \in [0,\tfrac{\pi}{3}]\},$$

where

$$f(\theta) := \begin{cases} f_0(\theta) & \text{if } 2\sin(2\theta+\frac{\pi}{6}) \leq \frac{1+a}{1-a}, \\ f_1(\theta) & \text{otherwise.} \end{cases}$$

We first show that

$$\mathcal{E}(K_3;A) = \inf\{\, f_0(\theta) : \theta \in [0,\tfrac{\pi}{3}]\} \tag{A.29}$$

Let $x \coloneqq \frac{1+a}{1-a}$ and note that $x > 1$. Let us solve the inequality $2\sin(2\theta + \frac{\pi}{6}) > x$ for $\theta \in [0, \frac{\pi}{3}]$. Then $\alpha \coloneqq 2\theta + \frac{\pi}{6} \in [\frac{\pi}{6}, \frac{5\pi}{6}]$, so either the inequality $2\sin(\alpha) > x$ has no solution, in which case (A.29) follows trivially, or its solution set for α is $(\frac{\pi}{2}-\varphi, \frac{\pi}{2}+\varphi)$ for some $\varphi \in [0, \frac{\pi}{3}]$. Hence, $\alpha = 2\theta+\frac{\pi}{6} \in (\frac{\pi}{2}-\varphi, \frac{\pi}{2}+\varphi) \iff 2\theta \in (\frac{\pi}{3} - \varphi, \frac{\pi}{3} + \varphi) \iff \theta \in (\frac{\pi}{6} - \frac{\varphi}{2}, \frac{\pi}{6} + \frac{\varphi}{2}) \eqqcolon (\theta_0, \theta_1)$, so that $\theta_0, \theta_1 \in [0, \frac{\pi}{3}]$. In this case, we have

$$f(\theta) = \begin{cases} f_1(\theta) & \text{if } \theta \in (\theta_0, \theta_1), \\ f_0(\theta) & \text{otherwise.} \end{cases}$$

Now $16f_1'(\theta) = 4(1-a)\cos(2\theta+\frac{\pi}{6})$ and $16f_1''(\theta) = -8(1-a)\sin(2\theta+\frac{\pi}{6})$. Thus, if $\theta \in (\theta_0, \theta_1)$, then $\sin(2\theta+\frac{\pi}{6}) > 0$ and hence $f_1''(\theta) < 0$. So the function f_1 is concave on (θ_0, θ_1), and so $\inf\{\, f_1(\theta) : \theta \in (\theta_0, \theta_1)\} = \min\{f_1(\theta_0), f(\theta_1)\}$. However, at either θ_0 or θ_1, the functions f_1 and f_0 coincide by Proposition A.6, and it is clear that $f_1(\theta) \leq f_0(\theta)$. These facts put together complete the proof of (A.29).

To compute (A.29), it suffices to compute $f_0(\theta)$ at the stationary points of f_0 in $(0, \frac{\pi}{3})$ and the endpoints of the interval $[0, \frac{\pi}{3}]$. It is easy to check that $16af_0'(\theta) = (1-a)^3(4\sin^2(2\theta + \frac{\pi}{6}) - 1)\cos(2\theta + \frac{\pi}{6})$. Thus, the stationary points of f_0 in $[0, \frac{\pi}{3}]$ are $\{0, \frac{\pi}{6}, \frac{\pi}{3}\}$. We have

$$f_0(0) = f_0(\tfrac{\pi}{3}) = \frac{(3+a)^2}{48}, \qquad f_0(\tfrac{\pi}{6}) = \frac{(3a+1)^2}{48a}.$$

The inequality $f_0(0) \leq f_0(\frac{\pi}{6})$ is equivalent to $(1-a)^3 \geq 0$. Thus, $\mathcal{E}(K_3; A) = f_0(0)$. $\square$

Now we can finally prove the general formula for $\mathcal{E}(K_3; \cdot)$:

Theorem A.8. Let $0 < a < b$. Then

$$\mathcal{E}(K_3; \operatorname{Diag}(a, b)) = \frac{(a+3b)^2}{48b}. \tag{A.30}$$

Proof. Define $a' \coloneqq a/b$. Then by Theorem A.7 we have

$$\mathcal{E}(K_3; \operatorname{Diag}(a, b)) = b\mathcal{E}(K_3; \operatorname{Diag}(a', 1)) = b\frac{(a'+3)^2}{48} = \frac{(a+3b)^2}{48b}.$$

$\square$

A.2 Some Folklore Results

The next result establishes a well-known identity involving the optimal values of two conic optimization problems related by a projective transformation. We provide a proof for the sake of completeness.

Lemma A.9. Let $\mathbb{K} \subseteq \mathbb{E}$ be a pointed closed convex cone with nonempty interior. Let $c \in \mathbb{K}^* \setminus \{0\}$ and $c' \in \operatorname{int}(\mathbb{K}^*)$. Let $\mathcal{A} \colon \mathbb{E} \to \mathbb{Y}^*$ be a linear transformation. Define the optimization problems

$$\beta \coloneqq \sup\big\{\, \langle c, x\rangle : \mathcal{A}(x) = 0,\ \langle c', x\rangle = 1,\ x \in \mathbb{K} \big\}, \tag{A.31}$$

$$\beta' \coloneqq \inf\big\{\, \langle c', y\rangle : \mathcal{A}(y) = 0,\ \langle c, y\rangle = 1,\ y \in \mathbb{K} \big\} \tag{A.32}$$

and suppose both are feasible. Then β and β' are both positive and attained, and $\beta\beta' = 1$.

Proof. If y is feasible for (A.32), then $y/\langle c', y\rangle$ is feasible for (A.31) with positive objective value, whence $\beta > 0$. Moreover, β is attained by continuity and compactness. Let x^* be an optimal solution for (A.31). Then $y^* := x^*/\langle c, x^*\rangle$ is feasible for (A.32) with objective value $1/\beta$. If y is a feasible solution for (A.32), then $y/\langle c', y\rangle$ is feasible for (A.31), so $\beta \geq 1/\langle c', y\rangle$. Thus, $\langle c', y\rangle \geq 1/\beta = \langle c', y^*\rangle$, so y^* is an optimal solution for (A.32) and $\beta\beta' = 1$. □

Theorem A.10. Let $A \in \mathbb{S}^n$. Consider the optimization problem

$$\max\{\, x^\mathsf{T} A x : x \in \mathbb{R}^n,\ \|x\| = 1\}. \tag{A.33}$$

Then every local optimal solution of (A.33) is also a global optimal solution.

Proof. Let x_0 be a local optimal solution of (A.33). Let $x_1 \in \mathbb{R}^n$ such that $\|x_1\| = 1$ and $Ax_1 = \lambda x_1$, where $\lambda := \lambda_{\max}(A)$. Assume that the set $\{x_0, x_1\}$ is linearly independent; otherwise we are done. For each $t \in \mathbb{R}$, define

$$x_t := \frac{x_0 + t x_1}{\|x_0 + t x_1\|}$$

and

$$f(t) := x_t^\mathsf{T} A x_t.$$

Then

$$f(t) = \frac{x_0^\mathsf{T} A x_0 + 2t\lambda x_0^\mathsf{T} x_1 + t^2\lambda}{1 + 2t x_0^\mathsf{T} x_1 + t^2},$$

so

$$f'(0) = 2x_0^\mathsf{T} x_1 \frac{\lambda - x_0^\mathsf{T} A x_0}{\left(1 + 2t x_0^\mathsf{T} x_1 + t^2\right)^2}.$$

Thus, either $x_0^\mathsf{T} A x_0 = \lambda$, in which case we are done, or we must have $x_0^\mathsf{T} x_1 = 0$. Assume the latter. Since

$$f(t) = \frac{x_0^\mathsf{T} A x_0 + t^2\lambda}{1 + t^2},$$

we find that

$$f''(0) = 2(\lambda - x_0^\mathsf{T} A x_0).$$

From the fact that x_0 is a local optimal solution for (A.33), we find that $\lambda \leq x_0^\mathsf{T} A x_0$, whence equality must hold. □