

# A SEMIDEFINITE PROGRAMMING HIERARCHY FOR PACKING PROBLEMS IN DISCRETE GEOMETRY

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ABSTRACT. Packing problems in discrete geometry can be modeled as finding independent sets in infinite graphs where one is interested in independent sets which are as large as possible. For finite graphs one popular way to compute upper bounds for the maximal size of an independent set is to use Lasserre’s semidefinite programming hierarchy. We generalize this approach to infinite graphs. For this we introduce topological packing graphs as an abstraction for infinite graphs coming from packing problems in discrete geometry. We show that our hierarchy converges to the independence number.

## 1. INTRODUCTION

**1.1. Packing problems in discrete geometry.** Many, often notoriously difficult, problems in discrete geometry can be modeled as packing problems in graphs where the vertex set is an uncountable set having additional geometric structure.

The most famous example is the sphere packing problem in three-dimensional space, the Kepler problem, which was solved by Hales [17] in 1998. Here the vertex set is  $\mathbb{R}^3$  and two points are adjacent whenever their Euclidean distance is in the open interval  $(0, 2)$ .

An *independent set* of an undirected graph  $G = (V, E)$  is a subset of the vertex set which does not span an edge. In the sphere packing case, an independent set corresponds to centers of unit balls which do not intersect in their interior. Now one is trying to find an independent set which covers as much space as possible. What “much” means depends on the situation. When the vertex set  $V$ , the *container*, is compact and when we pack identical shapes we can simply count and we use the *independence number*

$$\alpha(G) = \sup\{|I| : I \subseteq V, I \text{ is independent}\}.$$

If the objects are of different size we provide them with a weight  $w(x)$  and we use the *weighted independence number*

$$\alpha_w(G) = \sup\left\{\sum_{x \in I} w(x) : I \subseteq V, I \text{ is independent}\right\}.$$

In the non-compact sphere packing case one needs to use a density version of the independence number since maximal independent sets have infinite cardinality: The

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(upper) point density of an independent set  $I \subset \mathbb{R}^3$  is

$$\delta(I) = \limsup_{R \rightarrow \infty} \frac{|I \cap [-R, R]^3|}{\text{vol}([-R, R]^3)},$$

where  $[-R, R]^3$  is the cube centered at the origin with side length  $2R$ . This measures the number of centers of unit balls per unit volume. To determine the geometric density of the corresponding sphere packing we multiply  $\delta(I)$  by the volume of the unit ball.

More examples include:

- *Error correcting  $q$ -ary codes:*  $V = \mathbb{F}_q^n$ , where  $\{x, y\} \in E$  if their Hamming distance lies in the open interval  $(0, d)$ . If  $q = 2$  we speak about *binary codes* and if we restrict to all code words having the same Hamming norm we speak about *constant weight codes*.
- *Spherical codes:*  $V = S^{n-1}$ , where  $\{x, y\} \in E$  if their inner product lies in the open interval  $(\cos(\theta), 1)$ .
- *Codes in real projective space:*  $V = \mathbb{RP}^{n-1}$ , where  $\{x, y\} \in E$  if their distance lies in the open interval  $(0, d)$ .
- *Sphere packings:*  $V = \mathbb{R}^n$ , where  $\{x, y\} \in E$  if their Euclidean distance lies in the open interval  $(0, 2)$ .
- *Binary sphere packings:*  $V = \mathbb{R}^n \times \{1, 2\}$  where  $\{(x, i), (y, j)\} \in E$  if the Euclidean distance between  $x$  and  $y$  lies in the open interval  $(0, r_i + r_j)$  and  $w(x, i) = r_i^n \text{vol } B_n$ , where  $B_n$  is the unit ball.
- *Binary spherical cap packings:*  $V = S^{n-1} \times \{1, 2\}$  where  $\{(x, i), (y, j)\} \in E$  if the inner product of  $x$  and  $y$  lies in the open interval  $(\cos(\theta_1 + \theta_2), 1)$  and  $w(x, i)$  is the volume of the spherical cap  $\{z \in S^{n-1} : x \cdot z \geq \cos(\theta_i)\}$ .
- *Packings of congruent copies of a convex body:*  $V = \mathbb{R}^n \times \text{SO}(n)$  where  $\{(x, A), (y, B)\} \in E$  if  $x + AK^\circ \cap y + BK^\circ \neq \emptyset$ , where  $K^\circ$  is the interior of the convex body  $K$ .

Currently, these problems have been solved in only a few special cases. One might expect that they will never be solved in full generality, for all parameters. Finding good lower bounds by constructions and good upper bounds by obstructions are both challenging tasks. Over the last years the best known results were achieved with computer assistance: Algorithms like the adaptive shrinking cell scheme of Torquato and Jiao [36] generate dense packings and give very good lower bounds. The combination of semidefinite programming and harmonic analysis often gives the best known upper bounds for these packing problems. This method originated from work of Hoffman [19], Delsarte [11], and Lovász [28].

**1.2. Lasserre's hierarchy for finite graphs.** Computing the independence number of a finite graph is an NP-hard problem as shown by Karp [21]. Approximating optimal solutions of NP-hard problems in combinatorial optimization with the help of linear and semidefinite optimization is a very wide and active area of research. The most popular semidefinite programming hierarchies for NP-hard combinatorial optimization problems are the Lovász-Schrijver hierarchy [29] (the  $N^+$ -operator) and the hierarchy of Lasserre [24]. Laurent [25] showed that Lasserre's hierarchy is stronger than the Lovász-Schrijver hierarchy.

We now give a formulation of Lasserre’s hierarchy for computing the independence number of a finite graph  $G = (V, E)$ . Here we follow Laurent [25]. The  $t$ -th step of Lasserre’s hierarchy is:

$$\text{las}_t(G) = \max \left\{ \sum_{x \in V} y_{\{x\}} : y \in \mathbb{R}_{\geq 0}^{I_{2t}}, y_\emptyset = 1, M_t(y) \text{ is positive semidefinite} \right\},$$

where  $I_t$  is the set of all independent sets with at most  $t$  elements and where  $M_t(y) \in \mathbb{R}^{I_t \times I_t}$  is the *moment matrix* defined by the vector  $y$ : Its  $(J, J')$ -entry equals

$$(M_t(y))_{J, J'} = \begin{cases} y_{J \cup J'} & \text{if } J \cup J' \in I_{2t}, \\ 0 & \text{otherwise.} \end{cases}$$

The first step in Lasserre’s hierarchy coincides with the  $\vartheta'$ -number, the strengthened version of Lovász  $\vartheta$ -number [28] which is due to Schrijver [33]; for a proof see for instance the book by Schrijver [34, Theorem 67.11]. Furthermore the hierarchy converges to  $\alpha(G)$  after at most  $\alpha(G)$  steps:

$$\vartheta'(G) = \text{las}_1(G) \geq \text{las}_2(G) \geq \dots \geq \text{las}_{\alpha(G)}(G) = \alpha(G).$$

Lasserre [24] showed this convergence in the general setting of hierarchies for 0/1 polynomial optimization problems by using Putinar’s Positivstellensatz [31]. Laurent [25] gave an elementary proof, which we discuss in Section 4.

Many variations are possible to set up a semidefinite programming hierarchy: For instance one can consider only “interesting” principal submatrices to simplify the computation and one can also add more constraints coming from problem specific arguments. In fact, in the definition of  $\text{las}_t(G)$  we used the nonnegativity constraints  $y_S \geq 0$  for  $S \in I_{2t}$ . Even without them, the convergence result holds, and the first step in the hierarchy coincides with the Lovász  $\vartheta$ -number.

A rough classification for all these variations can be given in terms of  $n$ -point bounds. This refers to all variations which make use of variables  $y_S$  with  $|S| \leq n$ . An  $n$ -point bound is capable of using obstructions coming from the local interaction of configurations having at most  $n$  points. For instance the Lovász  $\vartheta$ -number is a 2-point bound and the  $t$ -th step in Lasserre’s hierarchy is a  $2t$ -point bound. The relation between  $n$ -point bounds and Lasserre’s hierarchy was first made explicit by Laurent [26] in the case of bounds for binary codes.

**1.3. Topological packing graphs.** The aim of this paper is to define and analyze a semidefinite programming hierarchy which upper bounds the independence number for infinite graphs arising from packing problems in discrete geometry. For this we consider graphs where vertices which are close are adjacent, and where vertices which are adjacent will stay adjacent after slight perturbations. These two conditions will be essential at many places in this paper. We formalize them by the following definition.

**Definition 1.1.** *A graph whose vertex set is a Hausdorff topological space is called a topological packing graph if each finite clique is contained in an open clique, where a clique is a subset of the vertices where every two vertices are adjacent.*

It clearly suffices to verify the condition for cliques of size one or two.

Of course, every graph is a packing graph when we endow the vertex set with the discrete topology. However, weaker topologies give stronger conditions on the edge

sets. For instance, when the vertex set of a topological packing graph is compact, then the independence number is finite because every single vertex is a clique.

A *distance graph*  $G = (V, E)$  is a graph where  $(V, d)$  is a metric space, and where there exists  $D \subseteq (0, \infty)$  such that  $x$  and  $y$  are adjacent precisely when  $d(x, y) \in D$ . If  $D$  is open and contains the interval  $(0, \delta)$  for some  $\delta > 0$ , then  $G$  is a topological packing graph. That  $D$  contains an interval starting from 0 implies that vertices which are close are adjacent, and that  $D$  is open implies that adjacent vertices will stay adjacent after slight perturbations. The binary spherical cap packing graph as defined in Section 1.1 is a compact topological packing graph with the usual topology on the vertex set  $S^{n-1} \times \{1, 2\}$ . And although there exists a metric compatible with this topology which gives the graph as a distance graph<sup>1</sup>, it is easier and more natural to work directly with the topological packing graph structure.

Notice that in Definition 1.1 requiring all cliques to be contained in an open clique — which by Zorn’s lemma is equivalent to all maximal cliques being open — would give a strictly stronger condition.<sup>2</sup>

**1.4. Generalization of Lasserre’s hierarchy.** Now we introduce our generalization of Lasserre’s hierarchy for compact topological packing graphs.

Before we go into the technical details we like to comment on the choice of spaces in our generalization: In Lasserre’s hierarchy for finite graphs the optimization variable  $y$  lies in the cone<sup>3</sup>  $\mathbb{R}_{\geq 0}^{I_{2t}}$ . One might try to use the same cone when  $I_{2t}$  is uncountable. But then there are too many variables and it is impossible to express the objective function. At the other extreme one might try to restrict this cone to finitely (or countably) supported vectors. But then we do not know how to develop a duality theory like the one in Section 3. A duality theory is important for concrete computations: Minimization problems can be used to derive upper bounds rigorously. We use a cone of Borel measures where we have “one degree of freedom” for every open set.

In Section 2 we use the topology of  $V$  to equip the set  $I_t$ , consisting of the independent sets which have at most  $t$  elements, with a compact Hausdorff topology. Let  $\mathcal{C}(I_{2t})$  be the set of continuous real-valued functions on  $I_{2t}$ . By the Riesz representation theorem (see e.g. [6, Chapter 2.2]) the topological dual of  $\mathcal{C}(I_{2t})$ , where the topology is defined by the supremum norm, can be identified with the space  $\mathcal{M}(I_{2t})$  of signed Radon measures. A *signed Radon measure* is the difference of two Radon measures, where a *Radon measure*  $\nu$  is a locally finite measure on the Borel algebra satisfying *inner regularity*:  $\nu(B) = \sup\{\nu(C) : C \subseteq B, C \text{ compact}\}$  for each Borel set  $B$ . Nonnegative functions in  $\mathcal{C}(I_{2t})$  form the cone  $\mathcal{C}(I_{2t})_{\geq 0}$ . Its conic dual  $(\mathcal{C}(I_{2t})_{\geq 0})^*$  is the cone of *positive Radon measures*

$$\mathcal{M}(I_{2t})_{\geq 0} = \{\lambda \in \mathcal{M}(I_{2t}) : \lambda(f) \geq 0 \text{ for all } f \in \mathcal{C}(I_{2t})_{\geq 0}\}.$$

<sup>1</sup>Assume  $\theta_1 < \theta_2$  and let  $\epsilon$  be some number strictly between  $(1 - \theta_1/\theta_2)/2$  and 1. Let  $D = (0, 1)$ , and let  $d((x, i), (y, j))$  be given by  $\epsilon\delta_{i \neq j} + (1 - \epsilon\delta_{i \neq j}) \arccos(x \cdot y) (\theta_1 + \theta_2)^{-1}$  when  $x \cdot y < \cos(\theta_i + \theta_j)$  and 1 otherwise.

<sup>2</sup>Consider the graph with vertex set  $[0, 1] \times \mathbb{Z}$  where  $(x, i)$  and  $(y, j)$  are adjacent if  $i = j$  or when  $x$  and  $y$  are both strictly smaller than  $|i - j|^{-1}$  (for  $i \neq j$ ). Here each finite clique is contained in an open clique, but the countable clique  $\{0\} \times \mathbb{Z}$  is not.

<sup>3</sup>In this paper cones are always assumed to be convex.

Denote by  $\mathcal{C}(I_t \times I_t)_{\text{sym}}$  the space of *symmetric kernels*, which are the continuous functions  $K : I_t \times I_t \rightarrow \mathbb{R}$  such that

$$K(J, J') = K(J', J) \text{ for all } J, J' \in I_t.$$

We say that a symmetric kernel  $K$  is *positive semidefinite* if

$$(K(J_i, J_j))_{i,j=1}^m \text{ is positive semidefinite for all } m \in \mathbb{N} \text{ and } J_1, \dots, J_m \in I_t.$$

The positive semidefinite kernels form the cone  $\mathcal{C}(I_t \times I_t)_{\geq 0}$ . The dual of  $\mathcal{C}(I_t \times I_t)_{\text{sym}}$  can be identified with the space of symmetric signed Radon measures  $\mathcal{M}(I_t \times I_t)_{\text{sym}}$ . Here a signed Radon measure  $\mu \in \mathcal{M}(I_t \times I_t)$  is *symmetric* if

$$\mu(E \times E') = \mu(E' \times E) \text{ for all Borel sets } E \text{ and } E'.$$

We say that a measure  $\mu \in \mathcal{M}(I_t \times I_t)_{\text{sym}}$  is *positive definite* if it lies in the dual cone  $\mathcal{M}(I_t \times I_t)_{\geq 0} = (\mathcal{C}(I_t \times I_t)_{\geq 0})^*$ .

Now we are ready to define our generalization:

- The optimization variable is  $\lambda \in \mathcal{M}(I_{2t})_{\geq 0}$ .
- The objective function evaluates  $\lambda$  at  $I_{=t}$ , where in general,

$$I_{=t} = \{S \in I_t : |S| = t\},$$

and so when  $t = 1$  we simply deal with all vertices, as singleton sets. This is similar to the objective function  $\sum_{x \in V} y_{\{x\}}$  in Lasserre's hierarchy for finite graphs.

- The normalization condition reads  $\lambda(\{\emptyset\}) = 1$ .
- For generalizing the moment matrix condition “ $M_t(y)$  is positive semidefinite” we use a dual approach. We define the operator

$$A_t : \mathcal{C}(I_t \times I_t)_{\text{sym}} \rightarrow \mathcal{C}(I_{2t}) \text{ by } A_t K(S) = \sum_{J, J' \in I_t : J \cup J' = S} K(J, J').$$

We have  $\|A_t K\|_{\infty} \leq 2^{2t} \|K\|_{\infty}$ , so  $A_t$  is bounded and hence continuous. Thus there exists the adjoint  $A_t^* : \mathcal{M}(I_{2t}) \rightarrow \mathcal{M}(I_t \times I_t)_{\text{sym}}$  and the moment matrix condition reads  $A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0}$ .

**Definition 1.2.** *The  $t$ -th step of the generalized hierarchy is*

$$\text{las}_t(G) = \sup \left\{ \lambda(I_{=1}) : \lambda \in \mathcal{M}(I_{2t})_{\geq 0}, \lambda(\{\emptyset\}) = 1, A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0} \right\}.$$

Clearly, we have a nonincreasing chain

$$(1) \quad \text{las}_1(G) \geq \text{las}_2(G) \geq \dots \geq \text{las}_{\alpha(G)-1}(G) \geq \text{las}_{\alpha(G)}(G) = \text{las}_{\alpha(G)+1}(G) = \dots,$$

which stabilizes after  $\alpha(G)$  steps, and specializes to the original hierarchy if  $G$  is a finite graph. Each step gives an upper bound for  $\alpha(G)$  because for every independent set  $S$  the measure

$$\lambda = \sum_{R \in I_{2t} : R \subseteq S} \delta_R, \quad \text{where } \delta_R \text{ is the delta measure at } R,$$

is a feasible solution for  $\text{las}_t(G)$  with objective value  $|S|$ . To see this we note that  $\lambda(\{\emptyset\}) = 1$ , and for any  $K \in \mathcal{C}(I_t \times I_t)_{\geq 0}$  we have

$$\begin{aligned} \langle K, A_t^* \lambda \rangle &= \langle A_t K, \lambda \rangle = \sum_{R \in I_{2t}: R \subseteq S} \sum_{J, J' \in I_t: J \cup J' = R} K(J, J') \\ &= \sum_{J, J' \in I_t: J, J' \subseteq S} K(J, J') \geq 0. \end{aligned}$$

In Section 3 we consider the dual program of  $\text{las}_t(G)$ , which is

$$\text{las}_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\geq 0}, A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I_{2t} \setminus \{\emptyset\} \right\},$$

and we show that strong duality holds in every step:

**Theorem 1.3.** *Let  $G$  be a compact topological packing graph. For every  $t \in \mathbb{N}$  we have  $\text{las}_t(G) = \text{las}_t(G)^*$ , and if  $\text{las}_t(G)$  is finite<sup>4</sup>, then the optimum in  $\text{las}_t(G)$  is attained.*

In Section 4 we show that the chain (1) converges to the independence number:

**Theorem 1.4.** *Let  $G$  be a compact topological packing graph. Then,*

$$\text{las}_{\alpha(G)}(G) = \alpha(G).$$

A variation of  $\text{las}_t(G)$  can be used to upper bound the weighted independence number of a weighted compact topological packing graph  $G$  with a continuous weight function  $w: V \rightarrow \mathbb{R}_{\geq 0}$ . We extend  $w$ , with the obvious abuse of notation, to a function  $w: I_{2t} \rightarrow \mathbb{R}_{\geq 0}$  where only singleton sets have positive weight. It turns out, by Lemma 2.2, that also the extension is continuous. Then we replace the objective function  $\lambda(I_{=1})$  by  $\lambda(w)$ .

**1.5. Explicit computations in the literature.** Explicit computations of  $n$ -point bounds have been done in a variety of situations. The following table provides a guide to the literature:

Packing problem	2-point bound	3-point bound	4-point bound
Binary codes	Delsarte [11]	Schrijver [35]	Gijswijt, Mittlmann, Schrijver [16]
$q$ -ary codes	Delsarte [11]	Gijswijt, Schrijver, Tanaka [15]	
Constant weight codes	Delsarte [11]	Schrijver [35], Regts [32]	
Spherical codes	Delsarte, Goethals, Seidel [12]	Bachoc, Vallentin [3]	
Codes in $\mathbb{R}P^{n-1}$	Kabatiansky, Levenshtein [20]	Cohn, Woo [10]	
Sphere packings	Cohn, Elkies [9]		
Binary sphere and spherical cap packings	de Laat, Oliveira, Vallentin [23]		
Congruent copies of a convex body	Oliveira, Vallentin [30]		

<sup>4</sup>We show this in Remark 5.4.

For the first three packing problems in this table one can use Lasserre's hierarchy for finite graphs. For the last five packing problems in this table our generalization can be used, where in the last three cases one has to perform a compactification of the vertex set first.

We elaborate on the connection between these  $n$ -point bounds and our hierarchy in Section 5. The convergence of the hierarchy, shows that this approach is in theory capable of solving any given packing problem in discrete geometry. One attractive feature of the hierarchy is that already its first steps give strong upper bounds as one can see from the papers cited in the table above.

## 2. TOPOLOGY ON SETS OF INDEPENDENT SETS

Let  $G = (V, E)$  be a topological packing graph. In this section we introduce a topology on  $I_t$ , the set of independent sets having cardinality at most  $t$ .

We equip the direct product  $V^t$  with the product topology and the image of  $V^t$  under the map

$$q: (v_1, \dots, v_t) \mapsto \{v_1, \dots, v_t\}$$

with the quotient topology. When we add the empty set to the image we obtain the collection  $\text{sub}_t(V)$  of all subsets of  $V$  of cardinality at most  $t$ , which obtains its topology from the disjoint union topology. Compactness of  $\text{sub}_t(V)$  follows immediately from compactness of  $V$ . Handel [18, Proposition 2.7] shows that it is Hausdorff.

Given  $U_1, \dots, U_r \subseteq V$ , define

$$(U_1, \dots, U_r)_t = \{S \in \text{sub}_t(V) : S \subseteq U_1 \cup \dots \cup U_r, S \cap U_i \neq \emptyset \text{ for } 1 \leq i \leq r\}.$$

Handel [18] observes

$$q^{-1}((U_1, \dots, U_r)_t) = \bigcup_{\substack{\tau: \{1, \dots, t\} \rightarrow \{1, \dots, r\} \\ \tau \text{ surjective}}} U_{\tau(1)} \times \dots \times U_{\tau(t)}.$$

This shows that if the sets  $U_i$  are open, then  $(U_1, \dots, U_r)_t$  is open. In fact, if  $\mathcal{B}$  is a base for  $V$ , then

$$\mathcal{B}_t = \{(U_1, \dots, U_r)_t : 1 \leq r \leq t, U_1, \dots, U_r \in \mathcal{B}\}$$

is a base for  $\text{sub}_t(V)$ . Moreover, if  $\{u_1, \dots, u_r\}$  is an element in an open set  $U$  in  $\text{sub}_t(V)$ , then there are open neighborhoods  $U_i$  of  $u_i$  such that the open neighborhood  $(U_1, \dots, U_r)_t$  of  $\{u_1, \dots, u_r\}$  is contained in  $U$ .

We now endow  $I_t$  with a topology as a subset of  $\text{sub}_t(V)$ . Clearly,  $I_{=1}$  is homeomorphic to  $V$ . It is also immediate that  $I_t$  is Hausdorff. Furthermore, it is compact:

**Lemma 2.1.** *Let  $G = (V, E)$  be a compact topological packing graph. Then  $I_t$  is compact for every  $t \in \mathbb{N}$ .*

*Proof.* We will show that  $I_t$  is closed, respectively that its complement  $D_t = \text{sub}_t(V) \setminus I_t$  is open in the compact space  $\text{sub}_t(V)$ . Let  $\{x_1, \dots, x_r\} \in D_t$  be arbitrary. Without loss of generality we may assume that  $x_1$  and  $x_2$  are adjacent. By the topological packing graph condition there exists an open clique  $U \subseteq V$  containing both  $x_1$  and  $x_2$ . Since  $V$  is a Hausdorff space there exist disjoint open sets  $U_1$  and  $U_2$  such that  $x_1 \in U_1 \subseteq U$  and  $x_2 \in U_2 \subseteq U$ . Each set in  $(U_1, U_2, V, \dots, V)_t$  contains at least one edge, so  $(U_1, U_2, V, \dots, V)_t \subseteq D_t$ . The set  $(U_1, U_2, V, \dots, V)_t$  is an open neighborhood of  $\{x_1, \dots, x_r\}$ . Hence,  $D_t$  is open.  $\square$

If the topology on  $V$  comes from a metric, then the topology on  $\text{sub}_t(V)$  is given by the Hausdorff distance, see for example Borsuk and Ulam [7]. This indicates that subsets of nonequal cardinality can be close in the topology on  $\text{sub}_t(V)$ . However, in the following lemma, we use the topological packing graph condition to show that independent sets of different cardinality are in different connected components of  $I_t$ .

**Lemma 2.2.** *Let  $G = (V, E)$  be a topological packing graph. The map  $I_t \rightarrow \mathbb{N}$ ,  $S \mapsto |S|$  is continuous for every  $t \in \mathbb{N}$ . In particular,  $I_{=t}$  is both open and closed.*

*Proof.* Let  $\{S_\alpha\}$  be a net in  $I_t$  converging to  $\{x_1, \dots, x_r\} \in I_t$ , where we assume the  $x_i$  to be pairwise different. By the topological packing graph condition, there exist pairwise disjoint open cliques  $U_i$  such that  $x_i \in U_i$ . The set  $(U_1, \dots, U_r)_t$  is open and contains  $\{x_1, \dots, x_r\}$ . Hence, we eventually have  $S_\alpha \in (U_1, \dots, U_r)_t$ . Then  $|S_\alpha| \geq r$  since the  $U_i$  are pairwise disjoint and  $|S_\alpha| \leq r$  since the  $U_i$  are cliques.  $\square$

### 3. DUALITY THEORY OF THE GENERALIZED HIERARCHY

**3.1. A primal-dual pair.** In this section we derive the dual program of the  $t$ -th step in our hierarchy  $\text{las}_t(G)$ .

We want to have a symmetric situation between primal and dual. We consider the dual pairs  $(\mathcal{C}(I_{2t}), \mathcal{M}(I_{2t}))$  and  $(\mathcal{C}(I_t \times I_t)_{\text{sym}}, \mathcal{M}(I_t \times I_t)_{\text{sym}})$  together with the corresponding nondegenerate bilinear forms

$$\langle f, \lambda \rangle = \lambda(f) = \int f(S) d\lambda(S) \quad \text{and} \quad \langle K, \mu \rangle = \mu(K) = \int K(J, J') d\mu(J, J').$$

We endow the spaces with the weakest topologies compatible with the pairing: the weak topology on the function spaces and the weak\* topology on the measure spaces. From now on we will always use these topologies unless explicitly stated otherwise. Because the cones defined in Section 1.4 are closed, it follows from the bipolar theorem that

$$(\mathcal{M}(I_{2t})_{\geq 0})^* = \mathcal{C}(I_{2t})_{\geq 0} \quad \text{and} \quad (\mathcal{M}(I_t \times I_t)_{\geq 0})^* = \mathcal{C}(I_t \times I_t)_{\geq 0}.$$

Hence, the situation is completely symmetric.

Recall that the operator

$$A_t: \mathcal{C}(I_t \times I_t)_{\text{sym}} \rightarrow \mathcal{C}(I_{2t}), \quad A_t K(S) = \sum_{J, J' \in I_t: J \cup J' = S} K(J, J')$$

is continuous in the norm topologies, so it follows that it is continuous in the weak topologies. In the next subsection we use that its adjoint  $A_t^*$  is injective:

**Lemma 3.1.** *Let  $G = (V, E)$  be a compact topological packing graph. Then the operator  $A_t$  is surjective for every  $t \in \mathbb{N}$ .*

*Proof.* Let  $g$  be a function in  $\mathcal{C}(I_{2t})$ . The continuity of

$$u: I_t \times I_t \rightarrow \text{sub}_{2t}(V), \quad (J, J') \mapsto J \cup J'$$

follows from [18]. Hence

$$h: u^{-1}(I_{2t}) \rightarrow \mathbb{R}, \quad (J, J') \mapsto \frac{g(J \cup J')}{A_t \mathbb{1}(J \cup J')}$$

is continuous where  $\mathbb{1}$  is the kernel which evaluates to 1 everywhere.

The set  $I_{2t}$  is closed in  $\text{sub}_{2t}(V)$ , so the preimage  $u^{-1}(I_{2t})$  is closed in  $I_t \times I_t$ . Since  $I_t \times I_t$  is a compact Hausdorff space there exists, by Tietze's extension theorem, a function  $H \in \mathcal{C}(I_t \times I_t)$  such that  $H(J, J') = h(J, J')$  for all  $J, J' \in I_t$ . For each  $S \in I_{2t}$  we then have

$$\begin{aligned} A_t H(S) &= \sum_{J, J' \in I_t: J \cup J' = S} H(J, J') = \sum_{J, J' \in I_t: J \cup J' = S} h(J, J') \\ &= \frac{1}{A_t \mathbb{1}(S)} \sum_{J, J' \in I_t: J \cup J' = S} g(J \cup J') = g(S). \quad \square \end{aligned}$$

Using the theory of duality in conic optimization problems, see for instance Barvinok [5], we derive the dual hierarchy:

$$\text{las}_t(G)^* = \inf \left\{ K(\emptyset, \emptyset) : K \in \mathcal{C}(I_t \times I_t)_{\geq 0}, A_t K(S) \leq -1_{I_{=1}}(S) \text{ for } S \in I_{2t} \setminus \{\emptyset\} \right\},$$

where one should note that by Lemma 2.2 the characteristic function  $1_{I_{=1}}$  is continuous. It follows from weak duality that  $\text{las}_t(G) \leq \text{las}_t(G)^*$ , and hence  $\text{las}_t(G)^*$  upper bounds the independence number. In the following lemma we give a simple direct proof.

**Lemma 3.2.** *Let  $G = (V, E)$  be a compact topological packing graph. Then*

$$\alpha(G) \leq \text{las}_t(G)^*$$

*holds for all  $t \in \mathbb{N}$ .*

*Proof.* Suppose  $K$  is feasible and  $L$  is an independent set. Then

$$\begin{aligned} 0 &\leq \sum_{J, J' \in \text{sub}_t(L)} K(J, J') = \sum_{S \in \text{sub}_{2t}(L)} A_t K(S) \\ &= K(\emptyset, \emptyset) + \sum_{x \in L} A_t K(\{x\}) + \sum_{S \in \text{sub}_{2t}(L) \setminus \text{sub}_1(L)} A_t K(S) \leq K(\emptyset, \emptyset) - |L|. \quad \square \end{aligned}$$

It is immediate that  $\text{las}_t(G)^*$  stabilizes after  $\alpha(G)$  steps and by Lemma 2.2 it follows that the hierarchy is decreasing. These results also follow from strong duality as discussed next.

**3.2. Strong duality; Proof of Theorem 1.3.** In this section we prove Theorem 1.3: We have strong duality between the problems  $\text{las}_t(G)$  and  $\text{las}_t(G)^*$ . We will show the finiteness of  $\text{las}_t(G)^*$  in Remark 5.4.

For proving Theorem 1.3 we make use of a closed cone condition, which for example is explained in Barvinok [5, Chapter IV.7]. For this we have to show that  $\text{las}_t(G)$  has a feasible solution, which we already know from Section 1.4, and that the cone

$$K = \{(A_t^* \xi - \mu, \xi(I_{=1})) : \mu \in \mathcal{M}(I_t \times I_t)_{\geq 0}, \xi \in \mathcal{M}(I_{2t})_{\geq 0}, \xi(\{\emptyset\}) = 0\}$$

is closed in  $\mathcal{M}(I_t \times I_t)_{\text{sym}} \times \mathbb{R}$ . The above cone is the Minkowski difference of

$$K_1 = \{(A_t^* \xi, \xi(I_{=1})) : \xi \in \mathcal{M}(I_{2t})_{\geq 0}, \xi(\{\emptyset\}) = 0\}$$

and

$$K_2 = \{(\mu, 0) : \mu \in \mathcal{M}(I_t \times I_t)_{\geq 0}\}.$$

By a theorem of Klee [22] and Dieudonné [13] the Minkowski difference  $K_1 - K_2$  is closed when the three conditions

- (A)  $K_1 \cap K_2 = \{0\}$ ,
- (B)  $K_1$  and  $K_2$  are closed,
- (C)  $K_1$  is locally compact.

are satisfied. The fact that  $K_2$  is closed follows immediately since  $\mathcal{M}(I_t \times I_t)_{\geq 0}$  is closed. We now verify the other conditions:

**Lemma 3.3.**  $K_1 \cap K_2 = \{0\}$ .

*Proof.* We will show that  $\xi \in \mathcal{M}(I_{2t})_{\geq 0}$  with  $\xi(\{\emptyset\}) = 0$  is the zero measure if  $A_t^* \xi \in \mathcal{M}(I_t \times I_t)_{\geq 0}$ .

Let  $f \in \mathcal{C}(I_t \times I_t)_{\text{sym}}$  be given by

$$f(J, J') = \begin{cases} 1 & \text{if } J = J' = \emptyset, \\ 0 & \text{otherwise.} \end{cases}$$

Then  $A_t^* \xi(\{(\emptyset, \emptyset)\}) = \langle f, A_t^* \xi \rangle = \langle A_t f, \xi \rangle = \xi(\{\emptyset\}) = 0$ .

For  $n \in \mathbb{Z}$  define  $g_n \in \mathcal{C}(I_t)$  by

$$g_n(S) = \begin{cases} |n| & \text{if } S = \emptyset, \\ 1/n & \text{otherwise.} \end{cases}$$

Since  $g_n \otimes g_n \in \mathcal{C}(I_t \times I_t)_{\geq 0}$  and  $A_t^* \xi \in \mathcal{M}(I_t \times I_t)_{\geq 0}$  we have  $A_t^* \xi(g_n \otimes g_n) \geq 0$ . We have that  $A_t^* \xi(g_n \otimes g_n)$  equates to

$$n^2 A_t^* \xi(\{(\emptyset, \emptyset)\}) + \frac{1}{n^2} A_t^* \xi(I_t \setminus \{\emptyset\} \times I_t \setminus \{\emptyset\}) + 2 \text{sign}(n) A_t^* \xi(\{\emptyset\} \times I_t \setminus \{\emptyset\}).$$

The first term is zero, so the sum of the last two terms is nonnegative for each  $n$ . By letting  $n$  tend to plus and minus infinity we see that  $A_t^* \xi(\{\emptyset\} \times I_t \setminus \{\emptyset\}) = 0$ .

Define  $h \in \mathcal{C}(I_t \times I_t)_{\text{sym}}$  by

$$h(J, J') = \begin{cases} 1 & \text{if } J = \emptyset \text{ and } J' = \emptyset, \\ 1/2 & \text{if } J = \emptyset \text{ or } J' = \emptyset, \\ 0 & \text{otherwise.} \end{cases}$$

Since  $\xi$  is a positive measure we have  $\|\xi\| = \xi(I_{2t})$ , but

$$\xi(I_{2t}) = \langle A_t h, \xi \rangle = \langle h, A_t^* \xi \rangle = A_t^* \xi(\{(\emptyset, \emptyset)\}) + A_t^* \xi(\{\emptyset\} \times I_t \setminus \{\emptyset\}) = 0,$$

so  $\xi = 0$ . □

**Remark 3.4.** The set  $I_{2t}$  is a subset of the power set  $2^V$ . A power set is a *monoid* with the associative binary operation  $\cup$  and unit element  $\emptyset$ . Monoids have sufficient structure for defining functions of *positive type*, which in this case are functions  $f: 2^V \rightarrow \mathbb{R}$  for which the matrices  $(f(J_i \cup J_j))_{i,j=1}^m$  are positive semidefinite for all  $m \in \mathbb{N}$  and  $J_1, \dots, J_m \in 2^V$ . This monoid is *commutative* (i.e.,  $J \cup J' = J' \cup J$  for all  $J, J' \in 2^V$ ) and *idempotent* (i.e.,  $J \cup J = J$  for all  $J \in 2^V$ ), so the matrix

$$\begin{pmatrix} f(\emptyset) & f(J) \\ f(J) & f(J) \end{pmatrix} \text{ is positive semidefinite,}$$

and so  $0 \leq f(J) \leq f(\emptyset)$  for all  $J \in 2^V$  [6, p. 119]. In particular, a function of positive type which vanishes at the unit element is identically zero. This resembles the situation in the proof of Lemma 3.3. To see this we show that one can view  $\lambda \in \mathcal{M}(I_{2t})$  with  $A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0}$  as a ‘‘measure of positive type’’. For this we notice that a function  $f: 2^V \rightarrow \mathbb{R}$  is of positive type if and only if

$\sum_{S \in 2^V} f(S) \sum_{J \cup J' = S} g(J)g(J') \geq 0$  for all finitely supported functions  $g: 2^V \rightarrow \mathbb{R}$ . Going from the monoid  $2^V$  to the “truncated monoid”  $I_{2t}$ , and from functions to measures, we have the natural definition that a measure  $\lambda \in \mathcal{M}(I_{2t})$  is of positive type if  $\int A_t(g \otimes g)(S) d\lambda(S) \geq 0$  for all  $g \in \mathcal{C}(I_{2t})$ , which is the case if and only if  $A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0}$ . Moreover, if we define a convolution and an involution on  $\mathcal{C}(I_{2t})$  by  $f * g = A_t(f \otimes g)$  and  $f^* = f$ , respectively, then a measure  $\lambda$  is of positive type if and only if  $\lambda(f^* * f) \geq 0$  for all  $f \in \mathcal{C}(I_{2t})$ . This agrees with the definition of measures of positive type as given for instance in [14, Chapter 6.3] for locally compact groups, where a different algebra is used.

Before we consider condition (C) we need some background: A cone is *locally compact* if it is locally compact as a topological space, that is, each point in the cone is contained in a compact neighborhood relative to the cone. A cone is locally compact if the origin has a compact neighborhood relative to the cone: For each point  $x$  in the cone and each neighborhood  $U$  of the origin there is an  $r > 0$  such that  $x \in rU$ . A *convex base*  $B$  of a cone  $K$  is a convex subset of the cone such that every nonzero  $x \in K$  can be written in a unique way as a positive multiple of an element in  $B$ . A cone is *pointed* if it does not contain a line. Now we can state a theorem of Klee and Dieudonné [22, (2.4)]: A nonempty pointed cone in a locally convex vector space is closed and locally compact if and only if it admits a compact convex base.

**Lemma 3.5.**  $K_1$  is closed and locally compact.

*Proof.* Set

$$B = \{\xi \in \mathcal{M}(I_{2t})_{\geq 0} : \langle 1_{I_{2t}}, \xi \rangle = 1, \langle 1_\emptyset, \xi \rangle = 0\}.$$

The maps

$$\mathcal{M}(I_{2t}) \rightarrow \mathbb{R}, \xi \mapsto \langle 1_{I_{2t}}, \xi \rangle \quad \text{and} \quad \mathcal{M}(I_{2t}) \rightarrow \mathbb{R}, \xi \mapsto \langle 1_\emptyset, \xi \rangle$$

are continuous, so the preimage of  $\{1\}$  under the first map and the preimage of  $\{0\}$  under the second map is closed. Hence,  $B$  is closed in the space of probability measures on  $I_{2t}$ , which is compact by the Banach-Alaoglu theorem. So,  $B$  is compact as well.

By Lemma 3.1  $A_t^*$  is injective, so the map  $\xi \mapsto (A_t^* \xi, \xi(I_{-1}))$  is injective and the image of  $B$  under this map is a compact convex base for  $K_1$ . Hence, by Klee, Dieudonné, the cone  $K_1$  is closed and locally compact.  $\square$

**Remark 3.6.** In this remark we show that for infinite graphs the cone  $K_2$  is not locally compact, and hence it is important that only one of the two cones is required to be locally compact in condition (C). If  $V$  is an infinite set, then so is  $I_t$ , which means that  $\mathcal{M}(I_t)$  is an infinite dimensional (Hausdorff) topological vector space which is therefore not locally compact. The Banach-Alaoglu theorem says that the closed ball of radius  $r$  centered about the origin in  $\mathcal{M}(I_t)$  is compact. This means that it cannot be a neighborhood of the origin. Thus, for each  $r > 0$  there exists a net  $\{\lambda_\beta\} \subseteq \mathcal{M}(I_t)$  converging to the origin, such that  $\|\lambda_\beta\| = r$  for all  $\beta$ .

Let  $f \in \mathcal{C}(I_t \times I_t)_{\text{sym}}$  and  $\epsilon > 0$ . The set

$$\text{span}\{cg \otimes g : c \in \mathbb{R}, g \in \mathcal{C}(I_t)\}$$

is a point separating and nowhere vanishing subalgebra of  $\mathcal{C}(I_t \times I_t)_{\text{sym}}$ , so it follows from the Stone-Weierstrass theorem that it is dense in the uniform topology. This

means that there exists a function  $\tilde{f} = \sum_{i=1}^m c_i g_i \otimes g_i$  such that  $\|\tilde{f} - f\|_\infty \leq \epsilon/r^2$ . Then,

$$\begin{aligned} |\lambda_\beta \otimes \lambda_\beta(f)| &\leq |\lambda_\beta \otimes \lambda_\beta(f) - \lambda_\beta \otimes \lambda_\beta(\tilde{f})| + |\lambda_\beta \otimes \lambda_\beta(\tilde{f})| \\ &\leq \|\lambda_\beta \otimes \lambda_\beta\| \|f - \tilde{f}\|_\infty + \sum_{i=1}^m c_i \lambda_\beta(g_i)^2 \rightarrow \epsilon. \end{aligned}$$

So, the net  $\{\lambda_\beta \otimes \lambda_\beta\}$  in  $\mathcal{M}(I_t \times I_t)_{\geq 0}$ , which satisfies  $\|\lambda_\beta \otimes \lambda_\beta\| = r^2$  for each  $\beta$ , converges to the origin. Therefore, none of the closed balls centered about the origin is a neighborhood of the origin in  $\mathcal{M}(I_t \times I_t)_{\geq 0}$ . Since compact sets are bounded, this means that the origin does not have a compact neighborhood in  $\mathcal{M}(I_t \times I_t)_{\geq 0}$ , so this cone is not locally compact and neither is  $K_2$ .

#### 4. CONVERGENCE TO THE INDEPENDENCE NUMBER; PROOF OF THEOREM 1.4

In this section we prove Theorem 1.4: The chain (1) converges to the independence number  $\alpha(G)$ .

Our proof can be seen as an infinite-dimensional version of Laurent's proof of the convergence of the hierarchy for finite graphs  $G = (V, E)$ . In [25] she makes use of the fact that the cone of positive semidefinite moment matrices where rows and columns are indexed by the power set  $2^V$  is a simplicial polyhedral cone; an observation due to Lindström [27] and Wilf [37]. More specifically,

$$(2) \quad \left\{ M \in \mathbb{R}^{2^V \times 2^V} : M \succeq 0, M \text{ is a moment matrix} \right\} = \text{cone}\{\chi_S \chi_S^\top : S \subseteq V\},$$

where a moment matrix  $M$  is a matrix where the entry  $M_{J, J'}$  only depends on the union  $J \cup J'$  and where the vector  $\chi_S \in \mathbb{R}^{2^V}$  is defined componentwise by

$$\chi_S(R) = \begin{cases} 1 & \text{if } R \subseteq S, \\ 0 & \text{otherwise.} \end{cases}$$

The proof of (2) uses the inclusion-exclusion principle. In our proof the following form of the inclusion-exclusion principle will be crucial: Given finite sets  $A$  and  $C$ ,

$$\begin{aligned} \sum_{B: A \subseteq B \subseteq C} (-1)^{|B|} &= (-1)^{|A|} \sum_{B \subseteq C \setminus A} (-1)^{|B|} \\ &= (-1)^{|A|} \sum_{i=0}^{|C \setminus A|} \binom{|C \setminus A|}{i} 1^{|C \setminus A| - i} (-1)^i \\ &= (-1)^{|A|} (1 - 1)^{|C \setminus A|} = \begin{cases} (-1)^{|A|} & \text{if } A = C, \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

When considering infinite graphs we are faced two difficulties: 1. The cone  $\{A_t^* \lambda : \lambda \in \mathcal{M}(I_{2t})\} \cap \mathcal{M}(I_t \times I_t)_{\geq 0}$  is not finitely generated. 2. Also the power set  $2^V$  is too large.

The second problem we solve by considering the set  $I = I_{\alpha(G)}$  instead of  $2^V$ . In fact, already when we defined the hierarchy we used measures on independent sets instead of measures on subsets of the vertices.

The first problem we solve by using weak vector valued integrals (as discussed in for instance [14, Appendix 3]) instead of finite conic combinations: Let  $\tau \in \mathcal{M}(I)$  and  $\nu_S \in \mathcal{M}(I)$  so that  $S \mapsto \nu_S$  is a continuous map from  $I$  to  $\mathcal{M}(I)$  with

$\sup_{S \in I} \|\nu_S\| < \infty$ . Then  $f \mapsto \int \nu_S(f) d\tau(S)$  is a bounded linear map on  $\mathcal{C}(I)$ , and hence defines a unique signed Radon measure  $\nu$  on  $I$  which we denote by  $\nu = \int \nu_S d\tau(S)$ . The point measures

$$\delta_S \quad \text{and} \quad \chi_R = \sum_{Q \subseteq R} \delta_Q$$

which we will use in the next proposition satisfy the above conditions, so we can use them as integrands in vector valued integrals.

Now the proof of Theorem 1.4 will follow immediately from the following proposition.

**Proposition 4.1.** *Let  $G$  be a compact topological packing graph and suppose  $\lambda$  is feasible for  $\text{las}_{\alpha(G)}(G)$ . Then there exists a unique probability measure*

$$\sigma \in \mathcal{P}(I) = \{\lambda \in \mathcal{M}(I)_{\geq 0} : \|\lambda\| = 1\}$$

such that

$$\lambda = \int \chi_R d\sigma(R).$$

*Proof. Existence:* We have

$$\lambda = \int \delta_S d\lambda(S) = \int \sum_{R \subseteq S} (-1)^{|S \setminus R|} \chi_R d\lambda(S),$$

because by the inclusion-exclusion principle

$$\sum_{R \subseteq S} (-1)^{|S \setminus R|} \chi_R = \sum_{R \subseteq S} (-1)^{|S \setminus R|} \sum_{Q \subseteq R} \delta_Q = \sum_{Q \subseteq S} \delta_Q \sum_{R: Q \subseteq R \subseteq S} (-1)^{|S \setminus R|} = \delta_S.$$

The image of  $f \in \mathcal{C}(I)$  under the linear map

$$\mathcal{C}(I) \rightarrow \mathbb{R}, \quad f \mapsto \int \sum_{R \subseteq S} (-1)^{|S \setminus R|} f(R) d\lambda(S)$$

has norm at most  $2^{\alpha(G)} \|\lambda\| \|f\|_{\infty}$ , so the above linear functional is bounded and hence defines a signed Radon measure  $\sigma$  on  $I$ . Then

$$\int \chi_R(f) d\sigma(R) = \int \sum_{R \subseteq S} (-1)^{|S \setminus R|} \chi_R(f) d\lambda(S) = \lambda(f),$$

for each  $f \in \mathcal{C}(I)$ , so  $\lambda = \int \chi_R d\sigma(R)$ .

*Uniqueness:* If  $\sigma' \in \mathcal{M}(I_{2t})$  is another measure such that  $\lambda = \int \chi_R d\sigma'(R)$ , then  $\int \chi_R d(\sigma - \sigma')(R) = 0$ . Evaluating the above measure at a Borel set  $L \subseteq I_{=t}$  with  $t = \alpha(G)$  gives

$$0 = \int \chi_R(L) d(\sigma - \sigma')(R) = (\sigma - \sigma')(L),$$

so  $\sigma|_{I_{=t}} = \sigma'|_{I_{=t}}$ . Repeating this argument for  $t = \alpha(G) - 1, \dots, 1, 0$  shows  $\sigma = \sigma'$ , which shows that  $\sigma$  is unique.

*Positivity:* Let  $g \in \mathcal{C}(I)_{\geq 0}$  be arbitrary and define  $f \in \mathcal{C}(I)$  by

$$f(Q) = \sum_{P \subseteq Q} (-1)^{|Q \setminus P|} \sqrt{g(P)},$$

so that

$$\begin{aligned} \sum_{Q \subseteq R} f(Q) &= \sum_{Q \subseteq R} \sum_{P \subseteq Q} (-1)^{|Q \setminus P|} \sqrt{g(P)} \\ &= \sum_{P \subseteq R} (-1)^{|P|} \sqrt{g(P)} \sum_{Q: P \subseteq Q \subseteq R} (-1)^{|Q|} = \sqrt{g(R)}. \end{aligned}$$

We have

$$0 \leq \langle f \otimes f, A_{\alpha(G)}^* \lambda \rangle = \langle A_{\alpha(G)} f \otimes f, \lambda \rangle,$$

and since  $\lambda = \int \chi_R d\sigma(R)$ , the right hand side above is equal to

$$\int \sum_{Q \subseteq R} A_{\alpha(G)}(f \otimes f)(Q) d\sigma(R).$$

Since we are in the final step of the hierarchy, we have that  $A_{\alpha(G)}(f \otimes f)(Q)$  can be written as  $\sum_{J \cup J' = Q} f(J)f(J')$ , so the above equals

$$\int \sum_{Q \subseteq R} \sum_{J \cup J' = Q} f(J)f(J') d\sigma(R) = \int \left( \sum_{Q \subseteq R} f(Q) \right)^2 d\sigma(R) = \int g(R) d\sigma(R),$$

which shows that  $\sigma$  is a positive measure.

*Normalization:*  $\sigma$  is a probability measure, because

$$1 = \lambda(\{\emptyset\}) = \int \chi_S(\{\emptyset\}) d\sigma(S) = \|\sigma\|. \quad \square$$

**Proposition 4.2.** *Let  $G$  be a compact topological packing graph. Then the extreme points of the feasible region of  $\text{las}_{\alpha(G)}(G)$  are precisely the measures  $\chi_R$  with  $R \in I$ .*

*Proof.* If  $\sigma \in \mathcal{P}(I)$  and  $\lambda = \int \chi_R d\sigma(R)$ , then

$$\lambda(\{\emptyset\}) = \int \chi_R(\{\emptyset\}) d\sigma(R) = 1,$$

and for each  $K \in \mathcal{C}(I \times I)_{\geq 0}$  we have

$$\langle K, A_{\alpha(G)}^* \lambda \rangle = \int \chi_R(A_{\alpha(G)} K) d\sigma(R) = \int \sum_{J, J' \subseteq R} K(J, J') d\sigma(R) \geq 0,$$

so  $\lambda$  is feasible for  $\text{las}_{\alpha(G)}(G)$ . So we have the surjective linear map

$$L: \mathcal{P}(I) \rightarrow \mathcal{F}, \quad \sigma \mapsto \int \chi_R d\sigma(R),$$

where  $\mathcal{F}$  denotes the feasible set of  $\text{las}_{\alpha(G)}(G)$ . By Proposition 4.1 the map  $L$  is also injective. This means that

$$\text{ex}(\mathcal{F}) = \text{ex}(L(\mathcal{P}(I))) = L(\text{ex}(\mathcal{P}(I)))$$

and since  $\text{ex}(\mathcal{P}(I)) = \{\delta_S : S \in I\}$  (see for instance Barvinok [5, Proposition 8.4]), the right hand side above is equal to  $L(\{\delta_S : S \in I\}) = \{\chi_R : R \in I\}$ .  $\square$

**Proof of Theorem 1.4.** Let  $\lambda$  be feasible for  $\text{las}_{\alpha(G)}(G)$ . By Proposition 4.1 there exists a probability measure  $\sigma$  on  $I$  such that  $\lambda = \int \chi_S d\sigma(S)$ . Substituting this integral for  $\lambda$  in the definition of  $\text{las}_{\alpha(G)}(G)$  gives

$$\text{las}_{\alpha(G)}(G) \leq \max \left\{ \int \underbrace{\chi_R(I_{=1})}_{|R|} d\sigma(R) : \sigma \in \mathcal{P}(I) \right\} = \alpha(G),$$

and since we already know that  $\text{las}_{\alpha(G)}(G) \geq \alpha(G)$ , this completes the proof.  $\square$

## 5. TWO AND THREE-POINT BOUNDS

**5.1. Two-point bounds.** The Lovász  $\vartheta$ -number is a two-point bound originally defined for finite graphs. Bachoc, Nebe, Oliveira, and Vallentin [4] generalized this to the spherical code graph, and they showed that it is equivalent to the linear programming bound of Delsarte, Goethals, and Seidel [12]. The following generalization of the  $\vartheta'$ -number for compact topological packing graphs  $G$  is natural:

$$\vartheta'(G)^* = \inf \left\{ a : a \in \mathbb{R}, F \in \mathcal{C}(V \times V)_{\geq 0}, \right. \\ \left. \begin{aligned} F(x, x) &\leq a - 1 \text{ for } x \in V, \\ F(x, y) &\leq -1 \text{ for } \{x, y\} \in I_{=2} \end{aligned} \right\}.$$

**Lemma 5.1.** *Let  $G$  be a compact topological packing graph. Then  $\vartheta'(G)^*$  has a feasible solution.*

For finite graphs one can show  $\vartheta'(G)^*$  admits a feasible solution by selecting a matrix  $F$  with  $F(x, y) = -1$  for  $\{x, y\} \in I_{=2}$  and the diagonal of  $F$  large enough so as to make it diagonally dominant and hence positive semidefinite. For infinite graphs it is not clear how to adapt this argument, so we use a different approach.

*Proof of Lemma 5.1.* By the topological packing graph condition there is for each  $x \in V$  an open clique  $C_x$  containing  $x$ . Since  $V$  is a compact Hausdorff space, it is a normal space, so there exists an open neighborhood  $U_x$  of  $x$  such that its closure does not intersect  $V \setminus C_x$ . By compactness there exists an  $S \subseteq V$  such that  $\{U_x : x \in S\}$  is a finite open cover of  $V$ . By Urysohn's lemma there is a function  $f_x \in \mathcal{C}(V)$  such that

$$f_x(y) \begin{cases} = |S| & \text{if } y \in U_x, \\ \in [-1, |S|] & \text{if } y \in C_x \setminus U_x, \\ = -1 & \text{if } y \in V \setminus C_x. \end{cases}$$

Define

$$F \in \mathcal{C}(V \times V)_{\geq 0} \text{ by } F = \sum_{x \in S} f_x \otimes f_x, \text{ and } a = |S|^3 + 1.$$

Then,

$$F(y, y) = \sum_{x \in S} f_x(y)^2 \leq |S|^3 = a - 1 \text{ for all } y \in V.$$

Moreover, if  $\{y, y'\} \in I_{=2}$ , then at most one of  $y$  and  $y'$  lies in  $C_x$  for every given  $x \in S$ . So,  $f_x(y)f_x(y') = -|S|$  if either  $y$  or  $y'$  lies in  $U_x$  and  $f_x(y)f_x(y') \leq 1$  if neither  $y$  nor  $y'$  lies in  $U_x$ . Hence,  $F(y, y') \leq -1$  for all  $\{y, y'\} \in I_{=2}$ , and it follows that  $(a, F)$  is feasible for  $\vartheta'(G)^*$ .  $\square$

Now we show that the first step of our hierarchy equals the  $\vartheta'$ -number for compact topological packing graphs, as it is known for finite graphs.

**Theorem 5.2.** *Let  $G$  be a compact topological packing graph. Then*

$$\text{las}_1(G)^* = \vartheta'(G)^*.$$

We prove this theorem by Lemma 5.3 and Lemma 5.6. We first show the easy inequality.

**Lemma 5.3.**  $\text{las}_1(G)^* \leq \vartheta'(G)^*$ .

*Proof.* Assume  $(a, F)$  is feasible for  $\vartheta'(G)^*$  and define  $K \in \mathcal{C}(I_1 \times I_1)_{\text{sym}}$  by

$$\begin{aligned} K(\emptyset, \emptyset) &= a, \\ K(\emptyset, \{x\}) &= K(\{x\}, \emptyset) = -1 \text{ for } x \in V, \\ K(\{x\}, \{y\}) &= (F(x, y) + 1)/a \text{ for } x, y \in V. \end{aligned}$$

To show that  $K$  is positive semidefinite we show that the matrix  $(K(J_i, J_j))_{i,j=1}^m$  is positive semidefinite for all  $m \in \mathbb{N}$  and  $J_1, \dots, J_m \in I_1$  pairwise different. If none of the  $J_i$ 's is empty, then it follows directly. Otherwise we may assume that there are  $x_2, \dots, x_m \in V$  such that  $J_1 = \emptyset$  and  $J_i = \{x_i\}$  for  $i = 2, \dots, m$ . We have

$$\left( K(J_i, J_j) - K(J_i, J_1)K(J_1, J_1)^{-1}K(J_1, J_j) \right)_{i,j=2}^m = a^{-1}(F(x_i, x_j))_{i,j=2}^m,$$

so by the Schur complement  $(K(J_i, J_j))_{i,j=1}^m$  is positive semidefinite.

For  $x \in V$  we have

$$A_1 K(\{x\}) = K(\{x\}, \{x\}) + K(\{x\}, \emptyset) + K(\emptyset, \{x\}) = (F(x, x) + 1)/a - 2 \leq -1,$$

and for  $\{x, y\} \in I_{-2}$  we have

$$\begin{aligned} A_1 K(\{x, y\}) &= K(\{x\}, \{y\}) + K(\{y\}, \{x\}) \\ &= (F(x, y) + 1)/a + (F(y, x) + 1)/a \leq 0. \end{aligned}$$

So  $K$  is feasible for  $\text{las}_t(G)^*$  and since  $K(\emptyset, \emptyset) = a$  we have  $\text{las}_t(G)^* \leq \vartheta'(G)^*$ .  $\square$

**Remark 5.4.** From this lemma we can see that for each  $t \in \mathbb{N}$  the optimization problem  $\text{las}_t(G)^*$  has a feasible solution and so by strong duality the maximum in  $\text{las}_t(G)$  is attained: By Lemma 5.1,  $\vartheta'(G)^*$  has a feasible solution, hence by the lemma above  $\text{las}_1(G)^*$  also has one. Then this can be extended trivially to a feasible solution for every  $\text{las}_t(G)^*$ .

To prove the other inequality we will use the following generalization of the Schur complement.

**Lemma 5.5.** *Let  $X$  be a compact Hausdorff space and let  $x_1, \dots, x_n \in X$  be elements such that the singletons  $\{x_i\}$  are open. Suppose  $\mu \in \mathcal{M}(X \times X)_{\text{sym}}$  is such that the matrix  $A = (\mu(\{(x_i, x_j)\}))_{i,j=1}^n$  is positive definite. Denote by  $\mathcal{F} \subseteq \mathcal{C}(X)$  the set of functions which are zero on  $\{x_1, \dots, x_n\}$  and for  $g \in \mathcal{F}$  define the vector  $v_g \in \mathbb{R}^n$  by  $(v_g)_i = \mu(1_{\{x_i\}} \otimes g)$ . Then  $\mu$  is positive definite if and only if*

$$\mu(g \otimes g) - v_g^\top A^{-1} v_g \geq 0 \quad \text{for all } g \in \mathcal{F}.$$

*Proof.* Mercer's theorem says that a kernel  $K \in \mathcal{C}(X \times X)_{\text{sym}}$  is positive semidefinite if and only if there exist sequences  $(f_i)_i$  and  $(\lambda_i)_i$  in  $\mathcal{C}(X)$  and  $\mathbb{R}_{\geq 0}$  such that  $K(x, y) = \sum_{i=1}^{\infty} \lambda_i f_i \otimes f_i(x, y)$ , where convergence is uniform and absolute. It follows that  $\mu \in \mathcal{M}(X \times X)_{\geq 0}$  if and only if  $\mu(f \otimes f) \geq 0$  for all  $f \in \mathcal{C}(X)$ . Now we use the technique as described in for instance the book by Boyd and Vandenberghe [8, Appendix A.5.5] and note that the measure  $\mu$  is positive definite if and only if the function  $p: \mathbb{R}^n \times \mathcal{F} \rightarrow \mathbb{R}$  given by

$$\begin{aligned} p(r, g) &= \mu((r_1 1_{\{x_1\}} + \cdots + r_n 1_{\{x_n\}} + g) \otimes (r_1 1_{\{x_1\}} + \cdots + r_n 1_{\{x_n\}} + g)) \\ &= \mu(g \otimes g) + r^T A r + 2r^T v_g \end{aligned}$$

is nonnegative on its domain. We have  $\nabla_r p(r, g) = 2Ar + 2v_g$ , so for fixed  $g$ , the minimum of  $p$  is attained for  $r = -A^{-1}v_g$ . Hence  $p$  is nonnegative on its domain if and only if  $\mu(g \otimes g) - v_g^T A^{-1}v_g \geq 0$  for all  $g \in \mathcal{F}$ .  $\square$

**Lemma 5.6.**  $\text{las}_1(G)^* \geq \vartheta'(G)^*$ .

*Proof.* We will use the duals of  $\vartheta'(G)^*$  and  $\text{las}_1(G)^*$ . We derive the dual  $\vartheta'(G)$  of  $\vartheta'(G)^*$  similarly to Section 3.1. We have

$$\vartheta'(G) = \sup \left\{ \eta(I_2 \setminus \{\emptyset\}) : \eta \in \mathcal{M}(I_2 \setminus \{\emptyset\})_{\geq 0}, \eta(I_{=1}) = 1, T^* \eta \in \mathcal{M}(I_{=1} \times I_{=1})_{\geq 0} \right\},$$

where  $T: \mathcal{C}(I_{=1} \times I_{=1}) \rightarrow \mathcal{C}(I_2 \setminus \{\emptyset\})$  is the operator defined by

$$TF(S) = \begin{cases} F(\{x\}, \{x\}) & \text{if } S = \{x\}, \\ \frac{1}{2}(F(\{x\}, \{y\}) + F(\{y\}, \{x\})) & \text{if } S = \{x, y\}. \end{cases}$$

Now we prove strong duality:  $\vartheta'(G) = \vartheta'(G)^*$  and the optimum in  $\vartheta'(G)$  is attained. Following the approach from Section 3.2 we first observe that every probability measure on  $I_{=1}$  is feasible for  $\vartheta'(G)$ . To complete the proof we show that

$$K = \{(T^* \eta - \nu, \eta(I_2 \setminus \{\emptyset\})) : \nu \in \mathcal{M}(I_{=1} \times I_{=1})_{\geq 0}, \eta \in \mathcal{M}(I_2 \setminus \{\emptyset\})_{\geq 0}, \eta(I_{=1}) = 0\}$$

is closed in  $\mathcal{M}(I_{=1} \times I_{=1})_{\text{sym}} \times \mathbb{R}$ . We decompose  $K$  as the Minkowski difference of

$$K_1 = \{(T^* \eta, \eta(I_2 \setminus \{\emptyset\})) : \eta \in \mathcal{M}(I_2 \setminus \{\emptyset\})_{\geq 0}, \eta(I_{=1}) = 0\}$$

and

$$K_2 = \{(\nu, 0) : \nu \in \mathcal{M}(I_{=1} \times I_{=1})_{\geq 0}\}.$$

It is immediate that  $K_1 \cap K_2 = \{0\}$  and again using the approach from Section 3.2 we see that  $K_1$  and  $K_2$  are closed and that  $K_1$  is locally compact.

Now we show the inequality  $\vartheta'(G) \leq \text{las}_1(G)$ . Let  $\eta$  be an optimal solution for  $\vartheta'(G)$  and define  $\lambda \in \mathcal{M}(I_2)$  by  $\lambda(\{\emptyset\}) = 1$  and

$$\lambda(L) = \begin{cases} \vartheta'(G)\eta(L) & \text{if } L \text{ is a Borel set in } I_{=1}, \\ \frac{1}{2}\vartheta'(G)\eta(L) & \text{if } L \text{ is a Borel set in } I_{=2}. \end{cases}$$

Then

$$\lambda(I_{=1}) = \vartheta'(G)\eta(I_{=1}) = \vartheta'(G).$$

To complete the proof we have to show  $A_1^* \lambda \in \mathcal{M}(I_1 \times I_1)_{\geq 0}$ . We apply our generalized Schur complement: Let  $g \in \mathcal{C}(I_1)$  be a function with  $g(\emptyset) = 0$ . We have

$$A_1^* \lambda(g \otimes g) = \vartheta'(G) T^* \eta(g \otimes g).$$

The symmetric bilinear form  $(h, g) \mapsto T^*\eta(h \otimes g)$  is positive semidefinite because  $T^*\eta \in \mathcal{M}(I_{=1} \times I_{=1})_{\geq 0}$ , so we can apply the Cauchy-Schwarz inequality and optimality of  $\eta$  to obtain

$$\vartheta'(G)T^*\eta(g \otimes g) \geq \frac{\vartheta'(G)}{T^*\eta(1_{I_{=1}} \otimes 1_{I_{=1}})}(T^*\eta(1_{I_{=1}} \otimes g))^2 = (T^*\eta(1_{I_{=1}} \otimes g))^2.$$

In the remainder of this proof we show

$$T^*\eta(1_{I_{=1}} \otimes g) = \vartheta'(G)\eta(g).$$

Since

$$\vartheta'(G)\eta(g) = \lambda(g) = A_1^*\lambda(1_\emptyset \otimes g)$$

the proof is then complete by using the generalized Schur complement, Lemma 5.5.

Inspired by Schrijver [34, Theorem 67.10] we use Lagrange multipliers. First observe that

$$T(1_{I_{=1}} \otimes 1_{I_{=1}}) = 1_{I_2 \setminus \{\emptyset\}} \quad \text{and} \quad T^*\eta(1_{I_{=1}} \otimes 1_{I_{=1}}) = \eta(I_2 \setminus \{\emptyset\}).$$

For  $u \in \mathbb{R}^2$  define  $g_u \in \mathcal{C}(I_{=1})$  by  $g_u = u_1g + u_2(1_{I_{=1}} - g)$ . For each  $u \in \mathbb{R}^2$  with  $\eta(g_u^2) = 1$ , the measure  $\tilde{\eta}$  defined by  $d\tilde{\eta}(S) = T(g_u \otimes g_u)(S)d\eta(S)$  is feasible for  $\vartheta'(G)$ . So, if we consider the problem of maximizing  $T^*\eta(g_u \otimes g_u)$  over all  $u \in \mathbb{R}^2$  for which  $\eta(g_u^2) = 1$ , then optimality of  $\eta$  implies that an optimal solution is attained for  $u = 1$ .

It follows that there exists a Lagrange multiplier  $c \in \mathbb{R}$  such that

$$\left. \frac{\partial}{\partial u_i} \right|_{u=(1,1)} T^*\eta(g_u \otimes g_u) = c \left. \frac{\partial}{\partial u_i} \right|_{u=(1,1)} \eta(g_u^2) \quad \text{for } i = 1, 2.$$

Since

$$T^*\eta(g_u \otimes g_u) = u^\top \begin{pmatrix} T^*\eta(g \otimes g) & T^*\eta(g \otimes (1_{I_{=1}} - g)) \\ T^*\eta(g \otimes (1_{I_{=1}} - g)) & T^*\eta((1_{I_{=1}} - g) \otimes (1_{I_{=1}} - g)) \end{pmatrix} u$$

and

$$\eta(g_u^2) = u^\top \begin{pmatrix} \eta(g^2) & \eta(g(1_{I_{=1}} - g)) \\ \eta(g(1_{I_{=1}} - g)) & \eta((1_{I_{=1}} - g)^2) \end{pmatrix} u$$

we have

$$T^*\eta(g \otimes 1_{I_{=1}}) = c\eta(g) \quad \text{and} \quad T^*\eta((1_{I_{=1}} - g) \otimes 1_{I_{=1}}) = c\eta(1_{I_{=1}} - g).$$

By summing the last two equations we see that  $c = \vartheta'(G)$ , hence we have the desired equality  $T^*\eta(g \otimes 1_{I_{=1}}) = \vartheta'(G)\eta(g)$ .  $\square$

**5.2. Three-point bounds.** In this section we modify the  $2t$ -point bound  $\text{las}_t(G)$  to obtain a  $2t+1$ -point bound for sufficiently symmetric graphs  $G$ . For the spherical code graph this gives an easy derivation of a variation of the three-point bound given by Bachoc and Vallentin in [3].

Let  $G = (V, E)$  be a compact topological packing graph. We are interested in two groups related to  $G$ . The group of graph automorphisms of  $G$  and the group of homeomorphisms of the topological space  $V$ . When we endow the latter group with the compact-open topology, it is a topological group with a continuous action on  $V$ ; see Arens [1]. In the special case when  $G$  is a distance graph, as defined in Section 1.3, the former group is contained in the latter. We say that  $G$  is *homogeneous* if there exists a compact subgroup of the group of homeomorphisms which consists only of graph automorphisms and is such that the action of  $\Gamma$  on  $V$  is transitive.

Fix a point  $e \in V$ . By  $G^e$  we denote the induced subgraph of  $G$  with vertex set

$$V^e = \{x \in V : x \neq e \text{ and } \{e, x\} \notin E\}.$$

It follows that  $G^e$  is also a compact topological packing graph. We have  $\alpha(G) \geq 1 + \alpha(G^e)$ , and if  $G$  is homogeneous, then  $\alpha(G) = 1 + \alpha(G^e)$ : If  $S$  is an independent set of  $G$ , then there exists a graph automorphism  $\gamma$  with  $e \in \gamma S$ , and  $(\gamma S) \setminus \{e\} \subseteq V^e$  is an independent set for  $\alpha(G^e)$ . So, for computing an upper bound on the independence number of  $G$  we can also compute  $1 + \text{las}_t(G^e)$ . This yields a bound which is at least as good as  $\text{las}_t(G)$ :

**Lemma 5.7.** *Suppose  $G$  is a compact topological packing graph. Then*

$$1 + \text{las}_t(G^e) \leq \text{las}_t(G).$$

*Proof.* We denote the sets of independent sets of  $G^e$  by  $I_t^e$  and  $I_{=t}^e$ . Suppose  $\lambda^e$  is feasible for  $\text{las}_t(G^e)$ . Let  $\lambda = \delta_e + \lambda^e$ . We have  $\lambda \geq 0$  and  $\lambda(\{\emptyset\}) = 1$ . Moreover, since  $A_t^* \lambda = \delta_e \otimes \delta_e + A_t^* \lambda^e$  and  $A_t^* \lambda^e \in \mathcal{M}(I_t^e \times I_t^e)_{\geq 0} \subseteq \mathcal{M}(I_t \times I_t)_{\geq 0}$  we have  $A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0}$ . So  $\lambda$  is feasible for  $\text{las}_t(G)$ . We have  $1 + \lambda^e(I_{=1}^e) = \lambda(I_{=1})$  which completes the proof.  $\square$

In the handbook chapter [2, Theorem 9.15] Bachoc, Gijswijt, Schrijver, and Vallentin gave a simplified, but computationally slightly less powerful, variation of the three-point bound given by Bachoc and Vallentin [3] for spherical codes. In both cases the bounds are formulated using the representation theory coming from the action of the orthogonal group on the unit sphere  $S^{n-1}$ . The variation admits a generalization to compact topological packing graphs which we can formulate as

$$1 + \inf \left\{ \begin{array}{l} F(e, e) : F \in \mathcal{C}(V^e \cup \{e\} \times V^e \cup \{e\})_{\geq 0}, \\ F(x, x) + F(e, x) + F(x, e) \leq -1 \text{ for } \{e, x\} \in I_{=2}, \\ F(x, y) \leq 0 \text{ for } \{e, x, y\} \in I_{=3} \end{array} \right\}.$$

**Proposition 5.8.** *Suppose  $G$  is a compact topological packing graph. Then the optimal value of the optimization problem above equals  $1 + \text{las}_1(G^e)^*$ .*

*Proof.* Given  $F \in \mathcal{C}(V^e \cup \{e\} \times V^e \cup \{e\})_{\text{sym}}$  we define  $K \in \mathcal{C}(I_1 \times I_1)_{\text{sym}}$  by

$$\begin{aligned} K(\emptyset, \emptyset) &= F(e, e), \\ K(\emptyset, \{x\}) &= K(\{x\}, \emptyset) = F(e, x) \text{ for } \{e, x\} \in I_{=2}, \\ K(\{x\}, \{y\}) &= F(x, y) \text{ for } \{e, x, y\} \in I_{=3}. \end{aligned}$$

The above construction gives a bijection from the feasible region of the above optimization problem onto the feasible region of  $\text{las}_1(G^e)$ , and since it preserves objective values this completes the proof.  $\square$

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