THE THETA NUMBER OF SIMPLICIAL COMPLEXES

CHRISTINE BACHOC, ANNA GUNDERT, AND ALBERTO PASSUELLO

ABSTRACT. We introduce a generalization of the celebrated Lovász theta number of a graph to simplicial complexes of arbitrary dimension. Our generalization takes advantage of real simplicial cohomology theory, in particular combinatorial Laplacians, and provides a semidefinite programming upper bound of the independence number of a simplicial complex. We consider properties of the graph theta number such as the relationship to Hoffman's ratio bound and to the chromatic number and study how they extend to higher dimensions. Like in the case of graphs, the higher dimensional theta number can be extended to a hierarchy of semidefinite programming upper bounds reaching the independence number. We analyse the value of the theta number and of the hierarchy for dense random simplicial complexes.

1. INTRODUCTION

The theta number $\vartheta(G)$ of a graph G was introduced by L. Lovász in his seminal paper [32], in order to provide spectral bounds of the independence number and of the chromatic number of G. In modern terms, $\vartheta(G)$ is the optimal value of a semidefinite program, and as such is computationally easy; in contrast, the independence number $\alpha(G)$ and the chromatic number $\chi(G)$ are difficult to compute. These graph invariants satisfy the following inequalities, where \overline{G} denotes the complement of G:

(1) $\alpha(G) \le \vartheta(G) \le \chi(\overline{G}).$

The inequality $\alpha(G) \leq \vartheta(G)$ was one of the main ingredients in Lovász' proof of the Shannon conjecture on the capacity of the pentagon [32]. More generally, this inequality plays a central role in extremal combinatorics, sometimes in a disguised form: to cite a few, the Delsarte linear programming method in coding theory [8] and recent generalizations of Erdös-Ko-Rado theorems [7, 12, 13] can be interpreted as instances of this inequality. Analogs of the theta number in geometric settings have lead to many advances in packing problems (see [36] and references therein), in particular the very recent solutions to the sphere packing problems in dimensions 8 and 24 [5, 40].

Our aim in this paper is to generalize this graph parameter to higher dimensions, in the framework of *simplicial complexes*. Let us recall that an (abstract) simplicial complex X on a finite set V is a family of subsets of V called *faces* that is closed under taking subsets. We refer to Section 1 for basic definitions and results about simplicial complexes. Graphs fit in this framework, being simplicial complexes of dimension 1. In recent years, considerable work has been devoted to generalizing the classical theory of graphs to this higher-dimensional setting. Much of the efforts have focused on the notion of expansion (see, e.g., [9, 15, 20, 27, 33, 38]), but other natural concepts such as random walks [37], trees [11, 26], planarity [35], girth [10, 34], independence and chromatic numbers [14, 19] have been extended to higher dimensions. Some of these notions were introduced and studied previously in the context of *hypergraphs*. Pure *k*-dimensional simplicial complexes

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are essentially (k + 1)-uniform hypergraphs, but the topological point of view brings the machinery of algebraic topology such as homology theory to the subject.

The familiar graph-theoretic notions of independence number and of chromatic number extend in a natural way to this setting: For a k-dimensional simplicial complex X, an independent set is a set of vertices that does not contain any maximal face of X, and the *independence number* $\alpha(X)$ is the maximal cardinality of an independent set. The *chromatic number*¹ $\chi(X)$ is the least number of colors needed to color the vertices so that no maximal face of X is monochromatic, in other words, it is the smallest number of parts of a partition of the vertices into independent sets.

In order to define the theta number $\vartheta_k(X)$ of a pure k-dimensional simplicial complex X, we will follow an approach that leads in a natural way to the inequality $\alpha(X) \leq \vartheta_k(X)$. The main idea is to associate to an independent set S a certain matrix, and then to design a semidefinite program that captures as many properties of this matrix as possible. The matrix that we associate to an independent set is (up to a multiplicative factor) a submatrix of the *down-Laplacian of the complete complex*. In the case of dimension 1, the down-Laplacian is simply the all-one matrix, and we end up with one of the many formulations of the Lovász theta number.

Our first task will be to compare $\vartheta_k(X)$ to the eigenvalue upper bound of $\alpha(X)$ proved by Golubev in [19]. This upper bound involves for $0 \le i \le k - 1$, the largest eigenvalues μ_i of the *i*-th up-Laplacians of X and the minimal degrees d_i of the *i*-faces of X:

(2)
$$\alpha(X) \le n \left(1 - \frac{(d_0 + 1)(d_1 + 2)\dots(d_{k-2} + k - 1)d_{k-1}}{\mu_0\dots\mu_{k-1}} \right)$$

When every possible (k - 1)-face is contained in at least one k-face, i.e., when X has a *complete* (k - 1)-*skeleton*, this inequality simplifies to

(3)
$$\alpha(X) \le n \left(1 - \frac{d_{k-1}}{\mu_{k-1}} \right)$$

and can thus be seen as a natural generalization of the celebrated *ratio bound* for graphs attributed to Hoffman (see, e.g., [4, Theorem 3.5.2]). In that case, we will show that

$$\vartheta_k(X) \le n \left(1 - \frac{d_{k-1}}{\mu_{k-1}}\right),$$

therefore $\vartheta_k(X)$ provides an upper bound of $\alpha(X)$ that is at least as good as (3). In the case of a non-complete (k-1)-skeleton, Golubev's bound and $\vartheta_k(X)$ turn out to be incomparable, as we will see in examples below.

The theta number of a graph has many very nice properties; some of them, although unfortunately not all of them, can be generalized to higher dimensions. Most of this paper is devoted to determining which of the properties of the graph theta number extend to our notion of the theta number of simplicial complexes.

The relationship to the chromatic number generalizes only partially. Indeed, the inequality $\alpha(X) \leq \vartheta_k(X)$ immediately leads to the inequality $n/\vartheta_k(X) \leq \chi(X)$. However, in the case of graphs, the stronger inequality $\vartheta(\overline{G}) \leq \chi(G)$ holds. We will see that its natural analog in the setting of k-complexes would be that $\vartheta_k(\overline{X}) \leq k\chi(X)$ and that this inequality does not hold in general. Instead, we will introduce an ad hoc notion of chromatic number for simplicial complexes, denoted $\chi_k(X)$, and show that the inequality $\vartheta_k(\overline{X}) \leq \chi_k(X)$ holds. While $\chi(X)$ is defined using vertex colorings, the definition of

¹In the study of hypergraphs, the chromatic number $\chi(X)$ is also known as the *weak chromatic number* while $\chi(X_1)$, the chromatic number of the 1-skeleton, is known as the *strong chromatic number*.

 $\chi_k(X)$ is based on colorings of (k-1)-faces respecting orientations. Moreover, it is tightly related to a notion of *homomorphisms* between pure k-dimensional simplicial complexes that we introduce and that may be of interest by itself.

A very interesting benefit of the theta number of a graph is that it is possible to expand it into *hierarchies* of semidefinite upper bounds of the independence number; Lassere's hierarchy based on polynomial optimization principles is one of the most popular (see [29, 30]). We will see that a similar situation holds in higher dimensions: to a pure kdimensional complex X we will associate a sequence $\hat{\vartheta}_{\ell}(X)$ for $\ell = k, \ldots, \alpha(X)$ such that

$$\alpha(X) = \hat{\vartheta}_{\alpha(X)}(X) \le \dots \le \hat{\vartheta}_{\ell}(X) \le \dots \le \hat{\vartheta}_{k}(X) \le \vartheta_{k}(X).$$

In order to define $\hat{\vartheta}_{\ell}(X)$, we will proceed in two steps: in a first step, we define a natural sequence $\vartheta_{\ell}(X)$ for $\ell = k, k+1, \ldots, \alpha(X)$; in a second step, we modify the definition of $\vartheta_{\ell}(X)$ slightly in such a way that the sequence of its values decreases.

Our last results concern the theta number of random simplicial complexes $X^k(n, p)$ from the model proposed by Linial and Meshulam in [31]. This model is a higher-dimensional analog of the Erdős-Rényi model G(n, p) for random graphs and has gained increasing attention in recent years (see [25] for a survey).

We show that $\vartheta_k(X^k(n,p))$ is of the order of $\sqrt{(n-k)(1-p)/p}$ for probabilities p such that $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$ for some constant c_0 . This result extends the known estimates for the value of the theta number of the random graph G(n,p).

The paper is organized as follows: Sections 2 and 3 recall basic definitions and properties of simplicial complexes and semidefinite programming. Section 4 recalls properties of the theta number of a graph that serve as a guideline for the theta number of a k-dimensional simplicial complex, which is introduced in Section 5. Section 6 computes the theta number of certain basic families of 2-dimensional simplicial complexes. Section 7 discusses chromatic numbers and Section 8 the hierarchy of theta numbers. The final Section 9 contains the analysis of the theta number of random simplicial complexes.

2. SIMPLICIAL COMPLEXES

Let $V = \{v_1, \ldots, v_n\}$ be a finite set. We will use the notation $\binom{V}{k}$ for the set of ksubsets of V. Let us recall that an *(abstract) simplicial complex* X on a vertex set V is a family of subsets of V (called the *faces* of X), such that if $F \in X$, then all subsets of F also belong to X. The *dimension* of a face $F \in X$ is |F| - 1, and we denote by X_i the set of *i*-dimensional faces of X, with the convention $X_{-1} = \{\emptyset\}$. Note that we do not require every element in V to be a 0-face of X, so X_0 can be a proper subset of V. The *i-skeleton* of X is the simplicial complex $X_{-1} \cup X_0 \cup \cdots \cup X_i$.

A simplicial complex X is said to be of dimension $k \ge 0$, if k is the maximal dimension of any of its faces. For example, a graph is a simplicial complex of dimension 1. Going back to the general case, if X is of dimension k, and if moreover all maximal (with respect to inclusion) faces of X are of dimension k, then X is said to be *pure*. Unless explicitly mentioned, we will only consider pure complexes.

A basic example of a pure k-dimensional simplicial complex is the *complete* k-complex K_n^k , whose faces are all the subsets of $[n] = \{1, ..., n\}$ that have at most (k+1) elements.

We note that in order to define a pure simplicial complex of dimension k, it is enough to specify its set of k-dimensional faces. In particular, the *complementary complex* \overline{X} of a pure simplicial complex of dimension k, is again a pure simplicial complex of dimension k, whose k-dimensional faces are those (k + 1)-subsets of V that do not belong to X_k (we adopt the convention that the empty complex, whose set of faces is empty, is pure of dimension k for all $k \ge 0$).

Let X be a simplicial complex; we assume that every face of X is endowed with an *orientation*, i.e., a local ordering of its vertices. Then, if $F \in X_i$ and $K \in X_{i-1}$, an *oriented incidence number* $[F : K] \in \{0, \pm 1\}$ can be defined. Often, the orientation of the faces is induced by a global ordering of the vertex set V; in that case, if $F = \{x_0, x_1, \ldots, x_i\}$ where $x_0 < x_1 < \cdots < x_i$ with respect to this ordering,

$$[F:K] = \begin{cases} (-1)^j & \text{if } K \subset F \text{ and } F \setminus K = \{x_j\}, \\ 0 & \text{otherwise.} \end{cases}$$

The vector space of functions from X_i to \mathbb{R} is denoted by $\mathcal{C}^i(X; \mathbb{R})$ and its elements are called *i*-dimensional cochains of X with coefficients in \mathbb{R} . The coboundary map δ_i : $\mathcal{C}^i(X; \mathbb{R}) \to \mathcal{C}^{i+1}(X; \mathbb{R})$ is defined for $-1 \leq i < \dim(X)$ by

$$(\delta_i f)(H) = \sum_{F \in X_i} [H : F] f(F).$$

The image of δ_{i-1} is the subspace $B^i(X; \mathbb{R})$ of *i*-dimensional coboundaries, and the kernel of δ_i is the subspace $Z^i(X; \mathbb{R})$ of *i*-dimensional cocycles. Because the coboundary maps satisfy $\delta_i \circ \delta_{i-1} = 0$, we have $B^i(X; \mathbb{R}) \subseteq Z^i(X; \mathbb{R})$. The quotient group

$$H^i(X;\mathbb{R}) := Z^i(X;\mathbb{R})/B^i(X;\mathbb{R}).$$

is then called the *i*-th cohomology group of X with coefficients in \mathbb{R} .

Analogously, we can define the homology groups of a simplicial complex. For this, the spaces $\mathcal{C}^i(X;\mathbb{R})$ are endowed with the standard inner product $\langle f,g\rangle = \sum_{F \in X_i} f(F)g(F)$ and the *boundary map* $\partial_{i+1} = \delta_i^* : \mathcal{C}^{i+1}(X;\mathbb{R}) \to \mathcal{C}^i(X;\mathbb{R})$ is defined as the adjoint of the coboundary map δ_i . We have, for $F \in X_i$,

$$(\partial_{i+1}f)(F) = \sum_{H \in X_{i+1}} [H:F]f(H).$$

The spaces of *boundaries* $B_i(X; \mathbb{R}) := \operatorname{im} \partial_{i+1}$ and of *cycles* $Z_i(X; \mathbb{R}) := \operatorname{ker} \partial_i$ are subspaces of $\mathcal{C}^i(X; \mathbb{R})$ satisfying $B_i(X; \mathbb{R}) \subseteq Z_i(X; \mathbb{R})$ and thus define the *i*-th reduced homology group of X

$$H_i(X;\mathbb{R}) := Z_i(X;\mathbb{R})/B_i(X;\mathbb{R}).$$

Moreover, by duality we have that $Z_i(X; \mathbb{R}) = B^i(X; \mathbb{R})^{\perp}$ and $Z^i(X; \mathbb{R}) = B_i(X; \mathbb{R})^{\perp}$. The following diagram summarizes these linear maps for $0 \le i \le \dim(X) - 1$:

$$\mathcal{C}^{i+1}(X;\mathbb{R}) \xrightarrow[\partial_{i+1}]{\overset{\delta_i}{\longleftrightarrow}} \mathcal{C}^i(X;\mathbb{R}) \xrightarrow[\partial_i]{\overset{\delta_{i-1}}{\longleftrightarrow}} \mathcal{C}^{i-1}(X;\mathbb{R})$$

The *i*-th up-Laplacian L_i^{\uparrow} and *i*-th down-Laplacian L_i^{\downarrow} of X are the following selfadjoint and positive semidefinite operators on $C^i(X; \mathbb{R})$:

$$L_i^{\downarrow} := \delta_{i-1}\partial_i, \quad L_i^{\uparrow} := \partial_{i+1}\delta_i.$$

By definition, $L_i^{\uparrow}L_i^{\downarrow} = L_i^{\downarrow}L_i^{\uparrow} = 0$. Furthermore, it is not hard to see that ker $L_i^{\downarrow} = Z_i(X;\mathbb{R})$, im $L_i^{\downarrow} = B^i(X;\mathbb{R})$, ker $L_i^{\uparrow} = Z^i(X;\mathbb{R})$, and im $L_i^{\uparrow} = B_i(X;\mathbb{R})$. For

$$\mathcal{H}_i(X;\mathbb{R}) := Z_i(X;\mathbb{R}) \cap Z^i(X;\mathbb{R}),$$

we have the *Hodge decomposition* of $\mathcal{C}^i(X;\mathbb{R})$ into pairwise orthogonal subspaces

$$\mathcal{C}^{i}(X;\mathbb{R}) = \mathcal{H}_{i}(X;\mathbb{R}) \oplus B^{i}(X;\mathbb{R}) \oplus B_{i}(X;\mathbb{R}).$$

In particular, $\mathcal{H}_i(X; \mathbb{R}) \simeq H^i(X; \mathbb{R}) \simeq H_i(X; \mathbb{R})$.

The characteristic functions e_F of faces $F \in X_i$ are called *elementary cochains*; they form an orthonormal basis of $C^i(X; \mathbb{R})$. In order to express the matrices of the Laplacian operators in this basis we introduce the following notation: for $F \in X_i$, let deg(F) denote the *degree* of F, i.e., the number of (i + 1)-faces of X that contain F. For $(F, F') \in X_i^2$, such that $|F \cap F'| = i$, let

$$\epsilon_{F,F'} := [F : F \cap F'][F' : F \cap F'].$$

We note that, if $F \cup F' \in X_{i+1}$, we can express $\epsilon_{F,F'}$ also as

$$\epsilon_{F,F'} = -[F \cup F' : F][F \cup F' : F'].$$

For $(F, F') \in X_i^2$, such that $|F \cap F'| \neq i$, we set $\epsilon_{F,F'} = 0$. Then, it is easy to see that

$$(L_i^{\downarrow})_{F,F'} = \begin{cases} i+1 & \text{if } F = F' \\ \epsilon_{F,F'} & \text{otherwise} \end{cases}$$

and

$$(L_i^{\uparrow})_{F,F'} = \begin{cases} \deg(F) & \text{if } F = F' \\ -\epsilon_{F,F'} & \text{if } F \cup F' \in X_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

where we use the same notations for the operators and for their matrices in the basis of elementary cochains.

Example 2.1. In the case of the simplicial complex associated to a graph G = (V, E), defined by $X_{-1} = \{\emptyset\}$, $X_0 = V$ and $X_1 = E$, we find that $L_0^{\downarrow} = J$ is the all-ones matrix and L_0^{\uparrow} is equal to the combinatorial Laplacian L = D - A where D is the diagonal matrix with the degrees of the vertices as diagonal elements and A is the adjacency matrix of the graph.

Example 2.2. For the complete k-complex K_n^k , and for $0 \le i \le k - 1$, it is easy to verify that

$$L_i^{\uparrow} + L_i^{\downarrow} = nI.$$

Together with the property $L_i^{\uparrow}L_i^{\downarrow} = 0$, we obtain that $(L_i^{\uparrow})^2 = nL_i^{\uparrow}$ and that $(L_i^{\downarrow})^2 = nL_i^{\downarrow}$. So *n* is the only non zero eigenvalue of the up and down Laplacians. Computing the traces of these operators gives the multiplicities of this eigenvalue, namely $\binom{n-1}{i}$ for L_i^{\downarrow} and $\binom{n-1}{i+1}$ for L_i^{\uparrow} . So we have

$$\ker(L_i^{\uparrow} - nI) = \operatorname{im}(L_i^{\uparrow}) = B_i, \quad \dim(B_i) = \binom{n-1}{i+1},$$
$$\ker(L_i^{\downarrow} - nI) = \operatorname{im}(L_i^{\downarrow}) = B^i, \quad \dim(B^i) = \binom{n-1}{i},$$

and, as these dimensions add up to $\binom{n}{i+1} = \dim(C^i)$, $\mathcal{H}_i = \{0\}$.

We conclude this section by recalling the definition of the adjacency matrix of a kdimensional simplicial complex X: it is the matrix A such that $L_{k-1}^{\uparrow} = D - A$ where D is the diagonal matrix encoding the degrees of the (k-1)-faces. In other words,

$$A_{F,F'} = \begin{cases} \epsilon_{F,F'} & \text{if } F \cup F' \in X_k \\ 0 & \text{otherwise} \end{cases}$$

We note that in dimension 1 this definition coincides with the usual notion of the adjacency matrix of a graph.

3. Semidefinite programming

In this section, we gather basic facts about semidefinite programs. For further information we refer to standard references such as [2], [3], [39].

Semidefinite programs (SDP for short) are special cases of convex optimization programs that admit efficient algorithms, such as algorithms based on the so-called interior point method. They generalize linear programs and have turned out to be very useful for providing polynomial time approximations of hard problems in many areas, especially in combinatorics (see, e.g., [18] and [1, Chapter 6]).

For a matrix $A \in \mathbb{R}^{n \times n}$ we say that A is positive semidefinite, denoted by $A \succeq 0$, if A is real-valued, symmetric, and if all its eigenvalues are nonnegative. If moreover none of its eigenvalues are equal to zero, A is positive definite $(A \succ 0)$. The set of all positive semidefinite matrices is a cone denoted by $\mathbb{R}^{n \times n}_{\geq 0}$. The space of real symmetric matrices is endowed with the standard inner product $\langle A, B \rangle = \text{trace}(AB)$.

Given $(c_1, \ldots, c_m) \in \mathbb{R}^m$ and symmetric matrices A_0, \ldots, A_m of size *n*, the following optimization problem is a *semidefinite program in primal form*:

$$p^* = \sup\{\langle A_0, Z \rangle : Z \in \mathbb{R}^{n \times n}_{\succ 0}, \langle A_i, Z \rangle = c_i \text{ for all } 1 \le i \le m\}.$$

In other words, this program asks for the supremum of a linear form, where this supremum is taken over the intersection of the cone of positive semidefinite matrices with an affine space.

A feasible solution of this program is a matrix Z that satisfies the required constraints: $Z \in \mathbb{R}_{\geq 0}^{n \times n}$ and $\langle A_i, Z \rangle = c_i$. It is an optimal solution if its objective value $\langle A_0, Z \rangle$ is equal to p^* . If there is no feasible solution, we let $p^* = -\infty$.

The following *dual program* is attached to the primal program:

$$d^* = \inf\{c_1x_1 + \dots + c_mx_m : (x_1, \dots, x_m) \in \mathbb{R}^m, -A_0 + x_1A_1 + \dots + x_mA_m \succeq 0\}$$

The terms 'primal' and 'dual' do not refer to a specific class of programs: Despite their apparent difference, any of these programs can be put in the form of the other, and, as expected, dualizing twice returns the initial program.

The inequality $p^* \leq d^*$, referred to as *weak duality*, always holds, and under some mild conditions even *strong duality*, i.e., $p^* = d^*$, holds. Strong duality is guaranteed if the SDP satisfies the so-called *Slater's conditions*, of which we will use the following version: If an SDP has a strictly feasible primal solution, i.e., if there is a feasible solution Z of the primal program such that $Z \succ 0$, and a strictly feasible dual solution, i.e., there exists (x_1, \ldots, x_m) such that $-A_0 + x_1A_1 + \cdots + x_mA_m \succeq 0$, then strong duality holds and, moreover, there are optimal solutions for both the primal and the dual program.

4. The theta number of a graph

In this section, we introduce the theta number of a graph G = (V, E). Our presentation will serve as a guideline for the generalization to higher dimensional simplicial complexes.

Let S be an independent set of G, i.e., a subset of V not containing any edges. The set S naturally defines a vector $\mathbf{1}_S \in \mathbb{R}^V$, namely its characteristic vector. We consider the matrix $Y^S := \mathbf{1}_S \mathbf{1}_S^T$, whose entries are given by:

$$Y_{v,v'}^S = \begin{cases} 0 & \text{if } \{v,v'\} \nsubseteq S\\ 1 & \text{otherwise.} \end{cases}$$

The following properties of Y^S motivate the definition of $\vartheta(G)$: Y^S is a positive semidefinite matrix such that $Y_{v,v'}^S = 0$ if $\{v, v'\} \in E$. Furthermore, the cardinality of S can be

recovered in two different ways from Y^S : If I and J stand as usual for the identity matrix and the all-ones matrix, we have $\langle I, Y^S \rangle = |S|$ and $\langle J, Y^S \rangle = |S|^2$. So, if we set

(4)
$$\vartheta(G) = \sup\{\langle J, Y \rangle : Y \in \mathbb{R}^{V \times V}, Y \succeq 0, \langle I, Y \rangle = 1, Y_{v,v'} = 0 \text{ if } \{v, v'\} \in E\}$$

the matrix $|S|^{-1}Y^S$ is feasible for (4) and we get that $|S| \leq \vartheta(G)$.

Because (4) is a semidefinite program, its optimal value $\vartheta(G)$ can be approximated numerically up to arbitrary precision in polynomial time in the size of G. If, instead of a sharp numerical value, one aims for a rougher upper bound of $\vartheta(G)$, the *dual formulation* of (4) is often more convenient:

(5)
$$\vartheta(G) = \inf\{\lambda_{\max}(Z) : Z \in \mathbb{R}^{V \times V}, \ Z = J + T, \ T_{v,v'} = 0 \ \text{if} \ \{v, v'\} \notin E\}.$$

Here, $\lambda_{\max}(Z)$ denotes the largest eigenvalue of Z.

To illustrate this principle we consider a classical example. For any matrix T such that $T_{v,v'} = 0$ for all $\{v, v'\} \notin E$, the dual formulation of $\vartheta(G)$ provides the inequality $\alpha(G) \leq \lambda_{\max}(J+T)$. A possible choice for T is a multiple of the adjacency matrix A of G, say T = tA. The best bound is obtained for t minimizing $\lambda_{\max}(J+tA)$. For d-regular graphs, the matrices J and A commute, so the eigenvalues of J + tA are easy to analyze. The optimal choice of t then leads to the so-called *ratio bound* attributed to Hoffman (see, e.g., [4, Theorem 3.5.2]):

(6)
$$\alpha(G) \le \frac{-|V|\lambda_{\min}(A)}{d - \lambda_{\min}(A)}.$$

5. THE THETA NUMBER OF A SIMPLICIAL COMPLEX

We now move to higher dimensions and define the theta number of a k-dimensional simplicial complex X. As suggested in the introduction, the down-Laplacian L_{k-1}^{\downarrow} of the complete complex K_n^k will play the role of the all-ones matrix J in (4) and (5). Recall that L_{k-1}^{\downarrow} is the matrix indexed by $\binom{V}{k}$ that is defined by:

$$(L_{k-1}^{\downarrow})_{F,F'} = \begin{cases} k & \text{if } F = F' \\ \epsilon_{F,F'} & \text{otherwise} \end{cases}$$

We note that this matrix may not be the down-Laplacian of the complex X. Obviously, this is the case if and only if X has a complete (k - 1)-skeleton, otherwise the down-Laplacian of X is a principal submatrix of L_{k-1}^{\downarrow} . From now on, to avoid confusion, we will denote the matrices associated to X by $L_i^{\downarrow}(X)$, $L_i^{\uparrow}(X)$ and reserve the notations L_i^{\downarrow} , L_i^{\uparrow} for the complete complex.

Let $S \subset V$ be an independent set of X. Following the same strategy as in the case of graphs, we consider the following matrix Y^S , indexed by $\binom{V}{k}$:

(7)
$$(Y^S)_{F,F'} = \begin{cases} 0 & \text{if } F \cup F' \nsubseteq S \\ (L_{k-1}^{\downarrow})_{F,F'} & \text{otherwise.} \end{cases}$$

We have $Y^S = \delta_{\binom{S}{k}} \delta_{\binom{S}{k}}^T$, where as a generalization of the characteristic vector of S, we consider the matrix $\delta_{\binom{S}{k}}$ defined as follows:

$$\left(\delta_{\binom{S}{k}}\right)_{K,F} = \begin{cases} 0 & \text{if } F \nsubseteq S\\ (\delta_S)_{K,F} & \text{otherwise,} \end{cases}$$

where $K \in \binom{V}{k-1}$, $F \in \binom{V}{k}$ and δ is the matrix of the boundary operator δ_{k-2} with respect to the basis of elementary cochains. The properties of Y^S lead to the following definition of $\vartheta_k(X)$:

Definition 5.1. Let X be a pure k-dimensional complex on V, and let L_{k-1}^{\downarrow} be the down Laplacian of the complete complex on V. Let: (8)

$$\begin{split} \vartheta_k(X) &:= \sup \left\{ \langle L_{k-1}^{\downarrow}, Y \rangle \ : \quad Y \in \mathbb{R}^{\binom{V}{k} \times \binom{V}{k}}, \ Y \succeq 0, \ \langle I, Y \rangle = 1, \\ Y_{F,F'} &= 0 \ if \ F \cup F' \in X_k, \\ Y_{F,F'} &= 0 \ if \ |F \cup F'| \ge k+2, \\ \epsilon_{F,F'} Y_{F,F'} &= \epsilon_{F'',F^{\dagger}} Y_{F'',F^{\dagger}} \ if \ F \cup F' = F'' \cup F^{\dagger} \right\} \end{split}$$

Proposition 5.2. We have

$$\alpha(X) \le \vartheta_k(X).$$

Proof. Let S be an independent set with $|S| = \alpha(X)$. As $Y^S = \delta_{\binom{S}{k}} \delta_{\binom{S}{k}}^T$, the matrix Y^S is clearly positive semidefinite. We have

(9)
$$\langle Y^S, I \rangle = k \binom{|S|}{k}$$

and

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$$\langle Y^{S}, L_{k-1}^{\downarrow} \rangle = k^{2} \binom{|S|}{k} + \sum_{\substack{|F \cup F'| = k+1 \\ F \cup F' \subseteq S}} 1$$
$$= k^{2} \binom{|S|}{k} + (k+1)k \binom{|S|}{k+1} = k \binom{|S|}{k} |S|.$$

Moreover, from the fact that S is an independent set, and from the definition of Y^S (7), it is clear that $(Y^S)_{F,F'} = 0$ if $F \cup F' \in X_k$, or if $|F \cup F'| \ge k + 2$.

The conditions $\epsilon_{F,F'}Y_{F,F'} = \epsilon_{F'',F^{\dagger}}Y_{F'',F^{\dagger}}$ if $F \cup F' = F'' \cup F^{\dagger}$ are satisfied by the entries of L_{k-1}^{\downarrow} , so the matrix Y^S inherits this property.

To sum up, we have proved that the matrix $k^{-1} {\binom{|S|}{k}}^{-1} Y^S$ is feasible for $\vartheta_k(X)$. Since its objective value is equal to |S|, we can conclude that $\alpha(X) \leq \vartheta_k(X)$.

Now we consider the dual program of (8), in order to obtain another formulation of $\vartheta_k(X)$, similar to (5).

Proposition 5.3. We have

(11)

$$\vartheta_{k}(X) = \inf \left\{ \lambda_{\max}(Z) : Z = L_{k-1}^{\downarrow} + T, \\
T_{F,F} = 0 \text{ for all } F \in \binom{V}{k} \\
\sum_{F \cup F' = H} \epsilon_{F,F'} T_{F,F'} = 0 \text{ if } H \in \binom{V}{k+1} \setminus X_{k} \right\}$$

Proof. This is just a straightforward rewriting of the dual program. Both programs have the same objective value because Slater's condition holds: $Y = {n \choose k}^{-1}I$ is a strictly feasible solution of (8) and T = 0 gives rise to a strictly feasible solution of (11).

Remark 5.4. Let us make a few obvious observations about $\vartheta_k(X)$. The first one, is that, as expected, $k \leq \vartheta_k(X) \leq n$. Indeed, the lower bound follows by taking $Y = {\binom{n}{k}}^{-1}I$ in (8) while the upper bound follows by taking T = 0 in (11).

The second observation is that $\vartheta_k(X)$ is easy to determine for the empty and the complete k-complexes. Indeed, if X is the empty k-complex, the matrix $Y = k^{-1} {\binom{n}{k}}^{-1} L_{k-1}^{\downarrow}$ is feasible for (8) giving that $\vartheta_k(X) = n$. If X is the complete k-complex, the semidefinite program (8) has only one feasible solution which is $Y = {\binom{n}{k}}^{-1} I$ so $\vartheta_k(X) = k$. We note that, in these trivial cases, the equality $\alpha(X) = \vartheta_k(X)$ holds.

The benefit of the formulation (11) is that any feasible matrix T leads to an upper bound of $\vartheta_k(X)$ and therefore to an upper bound of the independence number of X. Let us illustrate this principle by showing that we can recover the upper bound proved by Golubev

[19] in the case of a k-dimensional simplicial complex X with complete (k-1)-skeleton. We take $T = \gamma(L_{k-1}^{\uparrow}(X) - D_{k-1}(X))$ for some $\gamma \in \mathbb{R}$ that will be chosen later. Clearly T satisfies the conditions required by (11). Then

$$\lambda_{\max}(L_{k-1}^{\downarrow}+T) \leq \lambda_{\max}(L_{k-1}^{\downarrow}+\gamma L_{k-1}^{\uparrow}(X)) + \max_{F \in X_{k-1}}(-\gamma \deg(F)).$$

We assume that X has complete (k-1)-skeleton, so we have $L_{k-1}^{\downarrow} = L_{k-1}^{\downarrow}(X)$ and $L_{k-1}^{\downarrow}L_{k-1}^{\uparrow}(X) = 0$. Let us denote by Λ the set of non zero eigenvalues of $L_{k-1}^{\uparrow}(X)$. Then, the eigenvalues of the matrix $L_{k-1}^{\downarrow} + \gamma L_{k-1}^{\uparrow}(X)$ are: n, associated to the eigenspace B^{k-1} , and $\gamma\lambda$, for $\lambda \in \Lambda$, corresponding to eigenvectors in B_{k-1} . For $\gamma = \frac{n}{\lambda_{\max}(L_{k-1}^{\uparrow}(X))}$, we have $\lambda_{\max}(L_{k-1}^{\downarrow} + \gamma L_{k-1}^{\uparrow}(X)) = n$ and we get:

$$\alpha(X) \le \vartheta_k(X) \le n \bigg(1 - \frac{\deg_{\min}(X)}{\lambda_{\max}(L_{k-1}^{\uparrow}(X))} \bigg).$$

We note that, if X is regular, i.e., if $\deg(F)$ is a constant number for $F \in \binom{V}{k}$, then this upper bound is the exact analog of the ratio bound for graphs (6).

We have just seen that, in the case of a k-complex with complete (k - 1)-skeleton, $\vartheta_k(X)$ is an upper bound of the independence number of X which is as least as good as the bound (2). The case of complexes with noncomplete (k - 1)-skeleton turns out to be more tricky; indeed, in some cases $\vartheta_k(X)$ provides a good bound of $\alpha(X)$, even a sharp one, and beats the bound (2) given by Golubev, while in other cases, Golubev's bound is better. We provide examples illustrating this situation in the next section, where we explicitly work out the computation of $\vartheta_2(X)$ for certain families of 2-dimensional complexes. This will also yield counterexamples for certain properties of the theta number related to the chromatic number that we might expect (see Section 7). It will also be interesting to observe the prominent role plaed by the eigenvalues and eigenspaces of the Laplacian operators in these examples .

6. THE THETA NUMBER OF CERTAIN FAMILIES OF 2-COMPLEXES

6.1. The complete tripartite 2-complex. To define this complex, we let n = 3m and partition V = [n] into three subsets A, B, C of equal size m. As 2-dimensional faces we select all triangles with exactly one vertex in each of these subsets; as 1-dimensional faces all edges with at most one vertex in each of these subsets. A natural notation for this complex is $K_{m,m,m}^2$. It is clear that $\alpha(K_{m,m,m}^2) = 2m$ because $A \cup B$ is a maximal independent set with 2m vertices. We will show that $\vartheta_2(K_{m,m,m}^2) = 2m$.

With the notations of (2), $d_0 = 2m$, $d_1 = m$, $\mu_0 = 3m$, $\mu_1 = 3m$ and the bound in (2) equals (7m - 1)/3, so this is an example where the theta number beats Golubev's bound.

We will also show that, for the complementary complex $\overline{K_{m,m,m}^2}$, we have $\vartheta_2(\overline{K_{m,m,m}^2}) = 3 = \alpha(\overline{K_{m,m,m}^2})$. This complex has a complete 1-skeleton with $d_1 = 2m - 2$ and $\mu_1 = 3m$, so Golubev's bound (2) equals (m + 2), which is not tight.

Proposition 6.1. We have $\vartheta_2(K^2_{m,m,m}) = 2m$ and $\vartheta_2(\overline{K^2_{m,m,m}}) = 3$.

Proof. To keep notations light we use the generic notation X for $X = K_{m,m,m}^2$ throughout the proof. We will verify that $\vartheta_2(X) = 2m$, by constructing a suitable matrix T feasible for (11). The matrix T will be constructed from the projection matrices associated to certain eigenspaces of $L_1^{\uparrow}(X)$ and $L_1^{\downarrow}(X)$.

We denote by $A \times B$ the set of edges connecting one vertex in A and one vertex in B, and similarly for the other kinds of edges. So, $X_1 = (A \times B) \cup (B \times C) \cup (C \times A)$. We choose the orientations of the triangular faces and of the edges of X following the rule $A \to B \to C \to A$; this way, [G : F] = +1 for all $G \in X_2$ and $F \in X_1$.

It turns out that the up-Laplacian $L_1^{\uparrow}(X)$ has three non zero eigenvalues, 3m, 2m and m, respectively with multiplicity 1, 3(m-1), and $3(m-1)^2$. We will need the projection matrices P_{3m}^{\uparrow} and P_{2m}^{\uparrow} associated to the eigenvalues 3m and 2m.

The all-one vector is clearly an eigenvector of $L_1^{\uparrow}(X)$ for the eigenvalue 3m, so $P_{3m}^{\uparrow} = J_{3m^2}/(3m^2)$. The space $V_A = \{\sum_{a \in A} x_a(\mathbf{1}_{a \times B} + \mathbf{1}_{a \times C}) : \sum_{a \in A} x_a = 0\}$ is easily seen to be an eigenspace of $L_1^{\uparrow}(X)$ for the eigenvalue 2m. Similarly, we have two other (m-1)-dimensional eigenspaces V_B and V_C , and these spaces are pairwise orthogonal. In order to express the projection matrix P_{2m}^{\uparrow} associated to the sum of these spaces, we introduce the following notation: for $(F, F') \in X_1^2$, we denote $F \sim F'$ if F and F' both belong to $A \times B$ (respectively to $B \times C$, $C \times A$). Then,

$$(P_{2m}^{\uparrow})_{F,F'} = \frac{1}{2m^2} \cdot \begin{cases} 2(m-1) & \text{if } F = F' \\ -2 & \text{if } F \sim F' \text{ and } F \cap F' = \emptyset \\ (m-2) & \text{if } F \sim F' \text{ and } F \cap F' \neq \emptyset, F \neq F' \\ -1 & \text{if } F \not\sim F' \text{ and } F \cap F' = \emptyset \\ (m-1) & \text{if } F \not\sim F' \text{ and } F \cap F' \neq \emptyset \end{cases}$$

The down Laplacian $L_1^{\downarrow}(X)$ has two non zero eigenvalues: 3m with multiplicity 2 and 2m with multiplicity 3(m-1). The vector space $\{\gamma \mathbf{1}_{A \times B} + \alpha \mathbf{1}_{B \times C} + \beta \mathbf{1}_{A \times C} : \alpha + \beta + \gamma = 0\}$ is a two-dimensional space of eigenvectors for $L_1^{\downarrow}(X)$ and for the eigenvalue 3m, and the corresponding projection matrix P_{3m}^{\downarrow} is given by:

$$(P_{3m}^{\downarrow})_{F,F'} = \frac{1}{3m^2} \cdot \begin{cases} 2 & \text{if } F \sim F' \\ -1 & \text{otherwise.} \end{cases}$$

So far the matrices that we have defined are indexed by $X_1 = (A \times B) \cup (B \times C) \cup (A \times C)$. We now will consider matrices indexed by the whole set $\binom{V}{2}$, therefore we extend the matrices introduced above by adding zero rows and columns for the indices not belonging to X_1 (we keep the same notation for the enlarged matrices). We are now ready to define the matrix T that will do the job for $\vartheta_2(X)$:

Lemma 6.2. With the previous notations, let

$$T = 2m(P_{3m}^{\uparrow} + P_{2m}^{\uparrow} + P_{3m}^{\downarrow}) - L_1^{\downarrow}(X).$$

This matrix satisfies the following properties:

- (1) $T_{F,F} = 0$ for all $F \in {V \choose 2}$ (2) $T_{F,F'} = 0$ for all F, F' such that $F \cap F' \neq \emptyset$ and $F \cup F' \notin X_2$
- (3) $2m\mathbf{I} L_1^{\downarrow} T \succeq 0.$

Proof. Properties (1) and (2) follow by direct verification. In order to prove (3), we write $L_1^{\downarrow} + T = U + V + W \text{ where } U = 2m(P_{3m}^{\uparrow} + P_{2m}^{\uparrow}), V = 2mP_{3m}^{\downarrow} \text{ and } W = L_1^{\downarrow}(X) - L_1^{\downarrow},$ and make the remark that the product of any two of these matrices is zero. Indeed, for U, Vand for U, W it follows immediately from the property that the product of up and down Laplacians is zero; for V, W, it is due to the fact that the image of P_{3m}^{\downarrow} is an eigenspace for the eigenvalue 3m not only for $L_1^{\downarrow}(X)$ but also for L_1^{\downarrow} . So, we need to prove that $2m\mathbf{I} - U$, $2m\mathbf{I} - V$ and $2m\mathbf{I} - W$ are positive semidefinite. For the first two it is obvious because $2m\mathbf{I} - U = 2m(\mathbf{I} - P_{3m}^{\uparrow} - P_{2m}^{\uparrow})$ and $2m\mathbf{I} - V = 2m(\mathbf{I} - P_{3m}^{\downarrow})$. So now the only missing piece is a proof that $2m\mathbf{I} - (L_1^{\downarrow} - L_1^{\downarrow}(X)) \succeq 0$. For this, we arrange the elements of $\binom{V}{2}$ so that those in $X_1 = (A \times B) \cup (B \times C) \cup (A \times C)$ and we accordingly write

 $(C \times A)$ come before those in $(A \times A) \cup (B \times B) \cup (C \times C)$, and we accordingly write L_1^{\downarrow} by blocks:

$$L_1^{\downarrow} = \begin{pmatrix} L_1^{\downarrow}(X) & M \\ M^T & N \end{pmatrix}.$$

We want to prove that

$$\begin{pmatrix} 2m\mathbf{I} & -M \\ -M^T & 2m\mathbf{I} - N \end{pmatrix} \succeq 0.$$

By the Schur complement lemma, this is equivalent to $2m\mathbf{I} - N - (2m)^{-1}M^TM \succeq 0$. A direct computation shows that $M^T M = 2mN$, so all boils down to $m\mathbf{I} - N \succeq 0$, which is indeed true because N is a block-diagonal matrix with three blocks equal to $L_1^{\downarrow}(K_m^2)$. \Box

Now, we turn our attention to $\overline{K_{m,m,m}^2} = \overline{X}$. In order to prove that $\vartheta_2(\overline{X}) = 3$, we will use the primal formulation (8) and apply a symmetry argument. In the next section we will see a second, simpler, proof, using chromatic numbers, see Example 7.6.

With the previous notations, a feasible matrix Y must be of the form:

$$Y = \begin{pmatrix} Y_1 & 0\\ 0 & \tau \mathbf{I} \end{pmatrix}$$

where Y_1 is supported on the diagonal and on the triangles that belong to X_2 , i.e., the triangles with one vertex in each of A, B, C. It is clear that the automorphism group of X permutes transitively the elements of X_2 and of X_1 , and that, by convexity, (8) has a symmetric solution. So, without loss of generality, we can assume that $Y_1 = \beta L_1^{\uparrow}(X) + \gamma \mathbf{I}$. Restricting the semidefinite program on this set of matrices leads to a linear program in the variables β , γ , τ that can be easily solved and leads to the optimal value 3. We skip the details here.

We note that this approach would not work for $\vartheta_2(X)$ because \overline{X}_2 has two orbits: the triangles that are fully contained in one of the subsets A, B, C and the ones that have two vertices in one of these sets and one vertex in another one.

6.2. The complete bipartite 2-complex. Now n = 2m and V = [n] is partitioned in two subsets A, B, of equal size m. As 2-dimensional faces we select the triangles that meet both sets A and B, thus having two vertices in one of the parts and the third vertex in the other. We denote this complex by $K^2_{m,m}$. It is clear that $\alpha(K^2_{m,m}) = m$ since A is an independent set with m vertices. This complex has a complete 1-skeleton and $d_1 = m$, $\mu_1 = 2m$ so the bound (3) equals m, showing that $\vartheta_2(K_{m,m}^2) = m$ and that the theta number agrees with Golubev's bound.

For the complementary complex $\overline{K_{m,m}^2}$, which is nothing else than the disjoint union of two complete complexes K_m^2 , we have $\alpha(\overline{K_{m,m}^2}) = 4$. Golubev's bound is twice the value corresponding to K_m^2 , thus 4, and it is sharp again. As we will see know, $\vartheta_2(\overline{K_{m,m}^2})$ is much larger:

Proposition 6.3. We have $\vartheta_2(K_{m,m}^2) = m$ and $\vartheta_2(\overline{K_{m,m}^2}) = \frac{8m-4}{m+1}$.

Proof. We let $X = K_{m,m}^2$. To compute $\vartheta_2(\overline{X})$, we again apply the symmetry principle, like in the case of the complement of the tripartite complex. The automorphism group of $K_{m,m}^2$ has two orbits in $X_1 = \binom{V}{2}$: the set X_1^{in} of edges contained in A or in B, having degree m, and the set X_1^{out} of 'crossing' edges, with degree 2(m-1). It acts transitively on the 2-faces. So without loss of generality a feasible matrix Y of the primal formulation of $\vartheta_2(\overline{X})$ can be assumed to be

$$Y = \beta L_1^{\mathsf{T}}(X) + \gamma \mathbf{I}_{\mathsf{out}} + \tau \mathbf{I}_{\mathsf{in}}$$

where \mathbf{I}_{out} and \mathbf{I}_{in} denote the 0-1 diagonal matrices associated to respectively X_1^{out} and X_1^{in} . The expressions of $\langle I, Y \rangle$ and of $\langle L_1^{\downarrow}, Y \rangle$ are linear in the variables β, γ, τ , but the condition that Y is positive semidefinite is slightly more complicated because $L_1^{\uparrow}(X)$ does not commute with \mathbf{I}_{out} and \mathbf{I}_{in} . In fact, this condition leads to quadratic constraints, as it will become clear if we write the matrices by blocks according to $\binom{V}{2} = X_1^{in} \cup X_1^{out}$. It is easy to verify that

$$L_1^{\uparrow}(X) = \begin{pmatrix} m\mathbf{I} & -M\\ -M^T & 2m\mathbf{I} - N \end{pmatrix}, \quad M^T M = mN - 2J$$

and that N has two non zero eigenvalues: 2m, with multiplicity 1 and eigenvector the allone vector, and m, with multiplicity 2(m - 1). Then, by the Schur complement lemma, the condition

$$\beta L_1^{\uparrow}(X) + \gamma \mathbf{I}_{\text{out}} + \tau \mathbf{I}_{\text{in}} = \begin{pmatrix} (m\beta + \tau)\mathbf{I} & -\beta M \\ \beta M^T & (2m\beta + \gamma)\mathbf{I} - \beta N \end{pmatrix} \succeq 0$$

leads to quadratic inequalities. It is a bit technical but not difficult to see that an optimal solution satisfies $\gamma = \tau$, and finally that it is

$$Y = \frac{-1}{m^2(m+1)} L_1^{\uparrow}(X) + \frac{2}{m(m+1)} \mathbf{I},$$

leading to the optimal value $\langle L_1^{\downarrow}, Y \rangle = (8m-4)/(m+1).$

7. CHROMATIC NUMBERS

Let us first review the case of graphs. For a graph G, the *clique number* $\omega(G) = \alpha(\overline{G})$ and the chromatic number $\chi(G)$ are related by the obvious inequality $\alpha(\overline{G}) \leq \chi(G)$, and the theta number $\vartheta(\overline{G})$ lies in between these numbers ([32, Lemma 3, Corollary 3]):

(12)
$$\alpha(\overline{G}) \le \vartheta(\overline{G}) \le \chi(G).$$

Moreover, the inequality $\vartheta(\overline{G}) \leq \chi(G)$ is always at least as strong as the inequality $n/\vartheta(G) \leq \chi(G)$; indeed, we know that $n \leq \vartheta(G)\vartheta(\overline{G})$ from [32, Corollary 2].

Let us consider the situation for pure k-dimensional simplicial complexes. By analogy with graphs, the chromatic number $\chi(X)$ of a complex X, is usually defined to be the least number of colors needed to color the vertices of X such that no k-face is monochromatic.

We remark that for the complete k-complex K_n^k , the color classes of an admissible coloring cannot have more than k elements, and consequently that $\chi(K_n^k) = \lceil n/k \rceil$. So, for all k-dimensional complexes X, we have $\alpha(\overline{X}) \leq k\chi(X)$. Given that we have defined a generalization of the theta number to k-complexes, that satisfies $\alpha(\overline{X}) \leq \vartheta_k(\overline{X})$, it is natural to wonder if the inequality

(13)
$$\vartheta_k(\overline{X}) \le k\chi(X).$$

is also satisfied. Unfortunately, this is not true in general. Indeed, from the results of Section 6, one can see that (13) is satisfied for the complete tripartite complex and for its complement, but fails for the complete bipartite complex $K_{m,m}^2$, for which $\vartheta_2(\overline{K_{m,m}^2}) = (8m-4)/(m+1)$ (Proposition 6.3) while $\chi(K_{m,m}^2) = 2$.

Let us now see if we can modify the definition of the chromatic number of a simplicial complex, so that it fits better with our theta number. To achieve this, we will adapt the concept of graph homomorphisms to simplicial complexes. Indeed, a nice way to understand the notions of chromatic and clique numbers of graphs is through their connection to graph homomorphisms, as we will recall now.

A homomorphism f from a graph G to a graph G' is a mapping from the vertices of G to the vertices of G' that sends an edge of G to an edge of G'. Then, the clique number and the chromatic number have the following interpretations: the clique number $\omega(G)$ is the largest number ℓ such that there is a homomorphism from the complete graph K_{ℓ} to G, and similarly $\chi(G)$ is the smallest number ℓ such that there is a homomorphism from G to K_{ℓ} . Moreover, one can prove that, if there is a homomorphism from G to G', then $\vartheta(\overline{G}) \leq \vartheta(\overline{G'})$. The combination of these properties immediately leads to (12).

In order to follow a similar approach for simplicial complexes, we introduce an ad-hoc notion of homomorphism.

Definition 7.1. Let X and X' be two pure k-dimensional simplicial complexes. A homomorphism f from X to X' is a mapping $f : X_{k-1} \to X'_{k-1}$ with the following property: There exist orientations of X and X' such that for every $H \in X_k$, there is $H' \in X'_k$ such that

(1) $\{f(F) : F \in X_{k-1}, F \subset H\} = \{F' \in X'_{k-1} : F' \subset H'\},\$

(2)
$$[H': f(F)] = [H: F]$$
 for all $F \in X_{k-1}$ with $F \subset H$.

We note that this definition coincides in dimension 1 with the usual notion of a graph homomorphism as one can always find suitable orientations.

Remark 7.2. In this definition, it is important to understand that a homomorphism f may not necessarily be induced by a global mapping f_0 between the vertices, i.e., it may be the case that there is no mapping $f_0 : X_0 \to X'_0$ such that $f(F) = f_0(F)$ for all $F \in X_{k-1}$. As an example consider the 2-dimensional complex X depicted in Figure 1.

Furthermore, condition (2) is not automatically fulfilled. The 2-dimensional complex X depicted in Figure 2 possesses a map $f : X_1 \to (K_3^2)_1$ satisfying condition (1) but there is no homomorphism from X to K_3^2 .

Proposition 7.3. Let X and X' be two pure k-dimensional simplicial complexes, and let f be a homomorphism from X to X'. Then,

(14)
$$\vartheta_k(\overline{X}) \le \vartheta_k(\overline{X'}).$$

Proof. Our strategy will be to start with an optimal solution Y of the primal formulation (8) of $\vartheta_k(\overline{X})$, from which we construct a matrix Y', feasible for $\vartheta_k(\overline{X'})$, and having the same objective value as Y.



FIGURE 1. The homomorphism of X to K_3^2 is not induced by a vertex map.



FIGURE 2. A complex X with no homomorphism to K_3^2

So, let Y be primal optimal for the semidefinite program defining $\vartheta_k(\overline{X})$. We remark that, if $F \notin X_{k-1}$, then, for all $F' \neq F$, $F \cup F' \notin X_k$, and so $Y_{F,F'} = 0$. As a consequence, by the optimality of Y, we have $Y_{F,F} = 0$.

For $(K, K') \in X_{k-1}^2$, we set

$$Y'_{K,K'} = \sum_{\substack{(F,F') \in X^2_{k-1} \\ f(F) = K, \ f(F') = K'}} Y_{F,F'}$$

where the sum is zero if K or K' does not belong to the image of f.

We have trace $(Y') = \sum_{K \in \binom{V}{k}} Y'_{K,K} = \sum_{F \in X_{k-1}} Y_{F,F} = \operatorname{trace}(Y).$

By the property 1) of homomorphisms, if $K \neq K'$ and $K \cup K'$ is not an element of X'_k , and if K = f(F) and K' = f(F'), then $F \cup F'$ cannot belong to X_k , and so $Y_{F,F'} = 0$. So, we have that $Y'_{K,K'} = 0$.

Thanks to property 2), if $K \cup K' \in X'_k$ and $K \cup K' = K'' \cup K^{\dagger}$, the required condition that $\epsilon_{K,K'}Y'_{K,K'} = \epsilon_{K'',K\dagger}Y'_{K'',K\dagger}$ holds. So, we have proved that Y' is primal feasible for $\vartheta_k(\overline{X'})$.

It remains to analyze the objective value $\langle L_{k-1}^{\downarrow}, Y' \rangle.$ We have

$$\langle L_{k-1}^{\downarrow}, Y' \rangle = k \operatorname{trace}(Y') + \sum_{K, K' : K \cup K' \in X'_k} \epsilon_{K, K'} Y'_{K, K'}.$$

$$\sum_{\substack{K,K'\\K\cup K'\in X'_{k}}} \epsilon_{K,K'} Y'_{K,K'} = \sum_{\substack{K,K'\\K\cup K'\in X'_{k}}} \epsilon_{K,K'} \sum_{\substack{(F,F')\in X^{2}_{k-1}\\f(F)=K, f(F')=K'\\F\cup F'\in X_{k}}} Y_{F,F'}$$

where in the last equality we ignore the terms corresponding to $F \cup F' \notin X_k$ because they are equal to zero, and we apply the property 2). It follows that $\langle L_{k-1}^{\downarrow}, Y' \rangle = \langle L_{k-1}^{\downarrow}, Y \rangle$.

Definition 7.4. Let X be a pure k-dimensional simplicial complex. Let $\chi_k(X)$ denote the smallest number ℓ such that there exists a homomorphism from X to the complete k-complex K_{ℓ}^k .

It is not hard to see that $\chi_k(X) \leq \chi(X_1)$ holds for any pure simplicial complex X as a vertex coloring with ℓ colors that is a proper graph coloring for X_1 gives rise to a homomorphism from X to K_{ℓ}^k . The complex X depicted in Figure 1 serves as an example that the three notions of chromatic numbers considered here differ. It has $\chi_2(X) = 3$, $\chi(X) = 2$ and $\chi(X_1) = 4$.

Proposition 7.5. We have

$$\vartheta_k(\overline{X}) \le \chi_k(X).$$

Proof. If there is $f: X \to K_{\ell}^k$ then applying (14) leads to $\vartheta_k(\overline{X}) \leq \vartheta_k(\overline{K_{\ell}^k}) = \ell$ (see Remark 5.4).

Example 7.6. Consider the complex $X = K_{m,m,m}^2$ defined in Section 6. Clearly, $\chi_2(X) = \chi(X_1) = 3$, so we have $3 = \alpha(\overline{X}) \le \vartheta_2(\overline{X}) \le \chi_2(X) = 3$ and hence $\vartheta_2(\overline{X}) = 3$.

A k-dimensional subcomplex C of a pure k-dimensional simplicial complex X is a connected component of X if for every (k-1)-face F of C any k-face of X that contains F is also in C. Note that this condition does not need to hold for lower dimensional simplices, so two distinct connected components can, e.g., share a common vertex. Further observe that the connected components of X correspond to the connected components of the graph that has the k-faces of X as vertices with two vertices forming an edge if the corresponding k-faces intersect in a common (k-1)-face.

As different connected components do not share (k-1)-faces, the inequality $\chi_k(X) \le \chi(X_1)$ can actually be extended to the connected components of X.

Proposition 7.7. Let C be the collection of connected components of X. Then

$$\chi_k(X) \le \max_{C \in \mathcal{C}} \chi(C_1).$$

It is well-known that a *d*-regular graph *G* has a bipartite connected component if and only if the largest eigenvalue of the Laplacian is 2*d*. In [23] Horak and Jost present a combinatorial criterion that can be considered as a higher-dimensional analog of this: They show that for a *d*-regular *k*-complex *X* the largest eigenvalue of the Laplacian $L_{k-1}^{\uparrow}(X)$ is (k+1)d if and only if there is a connected component *C* of *X* and an orientation of the *k*-faces of *X* such that [H : F] = [H' : F] for all $F \in C_{k-1}, F \subset H, H'$. Note that for a connected graph the existence of such an orientation is equivalent to bipartiteness.

But

If a k-dimensional simplicial complex X has chromatic number $\chi_k(X) = k + 1$, this guarantees the existence of such an orientation. Hence, we have the following observation.

Proposition 7.8. Let X be a d-regular k-dimensional simplicial complex. If $\chi_k(X) = k + 1$, then the maximal eigenvalue of the up-Laplacian L_{k-1}^{\uparrow} is (k+1)d.

We remark that these results extend to arbitrary complexes for a normalized version of the Laplacian that we do not study here.

8. A HIERARCHY OF SEMIDEFINITE RELAXATIONS FOR THE INDEPENDENCE NUMBER OF A k-SIMPLICIAL COMPLEX

In this section, X is again a pure k-dimensional simplicial complex. We consider a straightforward generalization of $\vartheta_k(X)$ that leads to higher order theta numbers $\vartheta_\ell(X)$ for $\ell > k$. We will see that all these numbers provide upper bounds of $\alpha(X)$, until $\ell = \alpha(X)$, where $\vartheta_{\alpha(X)} = \alpha(X)$. Finally, we will modify this sequence of theta numbers in order to get a decreasing sequence.

It will be convenient to denote by Ind_i the set of independent sets of dimension *i*. We make the remark that $\operatorname{Ind} := \operatorname{Ind}_{-1} \cup \cdots \cup \operatorname{Ind}_{\alpha(X)-1}$ is a simplicial complex, the *independence complex* of X, and that it has complete (k-1)-skeleton, i.e., $\operatorname{Ind}_{k-1} = \binom{V}{k}$. For $\ell > k$, the matrices involved in the program defining $\vartheta_\ell(X)$ are indexed by $\operatorname{Ind}_{\ell-1}$. We define, for $k \leq \ell \leq \alpha(X)$:

(15)

$$\vartheta_{\ell}(X) = \sup \left\{ \langle L_{\ell-1}^{\downarrow}(\mathrm{Ind}), Y \rangle : Y \in \mathbb{R}^{\mathrm{Ind}_{\ell-1} \times \mathrm{Ind}_{\ell-1}}, Y \succeq 0, \langle I, Y \rangle = 1, \\ Y_{F,F'} = 0 \text{ if } F \cup F' \in \binom{V}{\ell+1} \setminus \mathrm{Ind}_{\ell}, \\ Y_{F,F'} = 0 \text{ if } |F \cup F'| \ge \ell + 2, \\ \epsilon_{F,F'}Y_{F,F'} = \epsilon_{F'',F^{\dagger}}Y_{F'',F^{\dagger}} \text{ if } F \cup F' = F'' \cup F^{\dagger} \right\}$$

and its dual formulation:

(16)
$$\vartheta_{\ell}(X) = \inf \left\{ \lambda_{\max}(Z) : Z = L_{\ell-1}^{\downarrow}(\operatorname{Ind}) + T, \\ T_{F,F} = 0 \text{ for all } F \in \operatorname{Ind}_{\ell-1}, \\ \sum_{F \sqcup F' = H} \epsilon_{F,F'} T_{F,F'} = 0 \text{ if } H \in \operatorname{Ind}_{\ell} \right\}$$

The above definition matches for $\ell = k$ with that of $\vartheta_k(X)$. Both primal and dual programs are strictly feasible: $Y = I/\langle I, I \rangle$ and respectively T = 0 give rise to strictly feasible solutions. We note that, if $\ell = \alpha(X)$, the feasible matrices of the primal program are diagonal matrices and hence $\vartheta_\ell(X) = \ell = \alpha(X)$. We have

Proposition 8.1.

$$\alpha(X) \le \vartheta_{\ell}(X).$$

Proof. The same proof as the one of Proposition 5.2 works. For an independent set S such that $|S| \ge \ell$, we define $Y^S \in \mathbb{R}^{\operatorname{Ind}_{\ell-1} \times \operatorname{Ind}_{\ell-1}}$ by

$$(Y^S)_{F,F'} = \begin{cases} 0 & \text{if } F \cup F' \notin S \\ (L_{\ell-1}^{\downarrow}(\operatorname{Ind}))_{F,F'} & \text{otherwise.} \end{cases}$$

It is then easy to verify, as every subset of an independent set S is also an independent set, that $\ell^{-1} {\binom{|S|}{\ell}}^{-1} Y^S$ is feasible for the primal program (15) and that its objective value is equal to |S|.

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However, it is not clear that the sequence $(\vartheta_{\ell}(X))_{k \leq \ell \leq \alpha(X)}$ is decreasing, because the constraints on the ℓ -sets involved in $\vartheta_{\ell-1}(X)$ do not occur explicitly in $\vartheta_{\ell}(X)$. We now define a variant of $\vartheta_{\ell}(X)$ that provides a decreasing sequence of upper bounds of $\alpha(X)$.

To start with, we note that, if a matrix Y is feasible for (15), then the value of $\epsilon_{F,F'}Y_{F,F'}$ for (F, F') such that $|F \cup F'| = \ell + 1$ only depends on $F \cup F'$. So, we can associate to Y a function $y \in \mathbb{R}^{\text{Ind}_{\ell}}$ such that $\epsilon_{F,F'}Y_{F,F'} = y(H)$ if $H = F \cup F'$. If we extend y to $\text{Ind}_{\ell-1}$ by $y(F) := Y_{F,F}$, we see that y encodes every nonzero entry of Y. Said differently, we have a one to one correspondence between $\mathbb{R}^{\text{Ind}_{\ell-1} \cup \text{Ind}_{\ell}}$ and the set

$$\mathcal{Y}_{\ell-1} = \left\{ Y \in \mathbb{R}^{\mathrm{Ind}_{\ell-1} \times \mathrm{Ind}_{\ell-1}} : \begin{array}{l} Y_{F,F'} = 0 \text{ if } F \cup F' \in \binom{V}{\ell+1} \setminus \mathrm{Ind}_{\ell}, \\ Y_{F,F'} = 0 \text{ if } |F \cup F'| \ge \ell+2, \\ \epsilon_{F,F'}Y_{F,F'} = \epsilon_{H,H'}Y_{H,H'} \text{ if } F \cup F' = H \cup H' \end{array} \right\}$$

We record for later use that, if $y \in \mathbb{R}^{\mathrm{Ind}_{\ell-1} \cup \mathrm{Ind}_{\ell}}$ corresponds to $Y \in \mathcal{Y}$ as above, then

(17)
$$\langle I, Y \rangle = \sum_{F \in \operatorname{Ind}_{\ell-1}} y(F)$$

and

(18)
$$\langle L_{\ell-1}^{\downarrow}(\mathrm{Ind}), Y \rangle = \ell \sum_{F \in \mathrm{Ind}_{\ell-1}} y(F) + \ell(\ell+1) \sum_{H \in \mathrm{Ind}_{\ell}} y(H).$$

Now, we introduce, for $\ell \geq 2$, a map $\tau_{\ell-1} : \mathcal{Y}_{\ell-1} \to \mathcal{Y}_{\ell-2}$. It will be more convenient to define $\tau_{\ell-1}$ on the corresponding functions $y \in \mathbb{R}^{\mathrm{Ind}_{\ell-1} \cup \mathrm{Ind}_{\ell}}$, in the following way: let

$$\begin{aligned} \tau_{\ell-1} : & \mathbb{R}^{\mathrm{Ind}_{\ell-1} \cup \mathrm{Ind}_{\ell}} & \to & \mathbb{R}^{\mathrm{Ind}_{\ell-2} \cup \mathrm{Ind}_{\ell-1}} \\ & y & \mapsto & \tau_{\ell-1}(y) = z \end{aligned}$$

where

$$\begin{cases} z(K) = \frac{1}{\ell} \sum_{F \in \operatorname{Ind}_{\ell-1} : K \subset F} y(F) & \text{if } K \in \operatorname{Ind}_{\ell-2} \\ z(F) = \frac{1}{\ell(\ell-1)} y(F) + \frac{1}{\ell-1} \sum_{H \in \operatorname{Ind}_{\ell} : F \subset H} y(H) & \text{if } F \in \operatorname{Ind}_{\ell-1} \end{cases}$$

We are now in the position to define our strengthening of $\vartheta_{\ell}(X)$: Let

(19)

$$\hat{\vartheta}_{\ell}(X) = \sup \left\{ \langle L_{\ell-1}^{\downarrow}(\operatorname{Ind}), Y \rangle : Y \in \mathbb{R}^{\operatorname{Ind}_{\ell-1} \times \operatorname{Ind}_{\ell-1}}, Y \succeq 0, \langle I, Y \rangle = 1, \\
\tau_{i} \circ \tau_{i+1} \circ \cdots \circ \tau_{\ell-1}(Y) \succeq 0 \text{ for all } i = 1, \dots, \ell-1, \\
Y_{F,F'} = 0 \text{ if } F \cup F' \in \binom{V}{\ell+1} \setminus \operatorname{Ind}_{\ell}, \\
Y_{F,F'} = 0 \text{ if } |F \cup F'| \ge \ell+2, \\
\epsilon_{F,F'}Y_{F,F'} = \epsilon_{F'',F^{\dagger}}Y_{F'',F^{\dagger}} \text{ if } F \cup F' = F'' \cup F^{\dagger} \right\}.$$

Theorem 8.2. The numbers $\hat{\vartheta}_{\ell}(X)$, $k \leq \ell \leq \alpha(X)$, satisfy:

(1)
$$\vartheta_{\ell}(X) \leq \vartheta_{\ell}(X)$$

(2) $\alpha(X) = \hat{\vartheta}_{\alpha(X)}(X) \leq \hat{\vartheta}_{\alpha(X)-1}(X) \leq \cdots \leq \hat{\vartheta}_{k}(X).$

Proof. That $\hat{\vartheta}_{\ell}(X) \leq \vartheta_{\ell}(X)$ is clear since we have only added constraints on Y in the definition of $\hat{\vartheta}_{\ell}(X)$.

Let S be an independent set, with $|S| \ge \ell$. Let, like in the proof of Proposition 8.1, $Y_{\ell-1}^S \in \mathbb{R}^{\mathrm{Ind}_{\ell-1} \times \mathrm{Ind}_{\ell-1}}$ be defined by:

(20)
$$(Y_{\ell-1}^S)_{F,F'} = \begin{cases} 0 \text{ if } F \cup F' \nsubseteq S\\ (L_{\ell-1}^{\downarrow}(\operatorname{Ind}))_{F,F'} \text{ otherwise.} \end{cases}$$

The element $y_{\ell-1}^S \in \mathbb{R}^{\operatorname{Ind}_{\ell-1} \cup \operatorname{Ind}_{\ell}}$ corresponding to $Y_{\ell-1}^S$ is given by: $y_{\ell-1}^S(F) = \ell$ if $F \subset S$, $y_{\ell-1}^S(H) = 1$ if $H \subset S$, and otherwise $y_{\ell-1}^S$ takes the value 0. We will need the following lemma:

Lemma 8.3. We have

$$\tau_{\ell-1}(y_{\ell-1}^S) = \frac{|S| - \ell + 1}{\ell - 1} y_{\ell-2}^S$$

for $y_{\ell-1}^S$ as defined in (20).

Proof. Let $z := \tau_{\ell-1}(y_{\ell-1}^S)$. Let $K \in \text{Ind}_{\ell-2}$. Every subset of S is independent so the number of $F \in \text{Ind}_{\ell-1}$ such that $K \subset F \subset S$ is $|S| - \ell + 1$. So,

$$z(K) = \frac{1}{\ell} \sum_{F \in \text{Ind}_{\ell-1} : K \subset F} y_{\ell-1}^S(F) = |S| - \ell + 1.$$

Now let $F \in \text{Ind}_{\ell-1}$. It is clear that, if F is not contained in S, z(F) = 0. If $F \subset S$,

$$z(F) = \frac{1}{\ell(\ell-1)}\ell + \frac{1}{\ell-1}\sum_{\substack{H \in \text{Ind}_{\ell}: F \subset H \subset S}} 1$$
$$= \frac{1}{\ell-1} + \frac{1}{\ell-1}(|S|-\ell) = \frac{|S|-\ell+1}{\ell-1}.$$

Lemma 8.3 shows that $\tau_{\ell}(Y_{\ell-1}^S)$ is positive semidefinite, and so, iteratively, that $\tau_i \circ \tau_{i+1} \circ \cdots \circ \tau_{\ell-1}(Y_{\ell-1}^S)$ is positive semidefinite for every $i \leq \ell-1$. We conclude that $Y_{\ell-1}^S$ (after a suitable rescaling) is feasible for $\hat{\vartheta}_{\ell}(X)$, and consequently that $\alpha(X) \leq \hat{\vartheta}_{\ell}(X)$. We have already remarked that $\vartheta_{\alpha(X)} = \alpha(X)$ so also $\hat{\vartheta}_{\alpha(X)} = \alpha(X)$.

It remains to prove that the sequence of $\hat{\vartheta}_{\ell}$ is decreasing. For this, we start from an optimal solution Y of $\hat{\vartheta}_{\ell}$, and we show that $Z := \tau_{\ell-1}(Y)$ is feasible for $\hat{\vartheta}_{\ell-1}$ and that $\langle L_{\ell-1}^{\downarrow}(\mathrm{Ind}), Y \rangle = \langle L_{\ell-2}^{\downarrow}(\mathrm{Ind}), Z \rangle$.

It is clear that $Z \in \mathcal{Y}_{\ell-2}$ and that Z is positive semidefinite, as well as $\tau_i \circ \tau_{i+1} \circ \cdots \circ \tau_{\ell-2}(Z) \succeq 0$ for all $i \leq \ell - 2$. That $\langle I, Z \rangle = 1$ follows easily from (17) and from the definition of $\tau_{\ell-1}$. It remains to take care of the objective value. Applying (18),

$$\langle L_{\ell-2}^{\downarrow}(\mathrm{Ind}), Z \rangle = (\ell-1) \sum_{K \in \mathrm{Ind}_{\ell-2}} z(K) + \ell(\ell-1) \sum_{F \in \mathrm{Ind}_{\ell-1}} z(F)$$

= $(\ell-1) \sum_{K} \frac{1}{\ell} \sum_{F: K \subset F} y(F) + (\ell-1)\ell \sum_{F} \left(\frac{1}{\ell(\ell-1)} y(F) + \frac{1}{\ell-1} \sum_{H: F \subset H} y(H) \right)$

where in the sums we restrict to elements in Ind. Taking account of the fact that every subset of an independent set is also an independent set, we obtain

$$\langle L_{\ell-2}^{\downarrow}(\mathrm{Ind}), Z \rangle = \ell \sum_{F \in \mathrm{Ind}_{\ell-1}} y(F) + \ell(\ell+1) \sum_{H \in \mathrm{Ind}_{\ell}} y(H) = \langle L_{\ell-1}^{\downarrow}(\mathrm{Ind}), Y \rangle.$$

9. THETA NUMBERS OF RANDOM COMPLEXES

A random model $X^k(n, p)$ for simplicial complexes of arbitrary fixed dimension k was introduced by Linial and Meshulam [31] as a higher dimensional analog of the Erdös-Rényi model G(n, p) for random graphs. It has vertex set $[n] = \{1, \ldots, n\}$, complete (k-1)-skeleton, and each element of $\binom{[n]}{k+1}$ is added as a k-dimensional face of $X^k(n, p)$ independently with probability p. Here p = p(n) is a function of n, and we let q := 1 - p. In this section we analyze the theta number of $X^k(n, p)$ for 'dense' complexes, i.e., for pin the range $[c_0 \log(n)/n, 1 - c_0 \log(n)/n]$.

The study of the theta number of random graphs G(n, p) was initiated by Juhász in [24] who proved that, in the case of constant probability $p, \vartheta(G(n, p)) = \Theta(\sqrt{nq/p})$ holds with probability tending to 1. In subsequent works, the range of probabilities for which Juhász' result holds was extended, until in [6], Coja-Oghlan was able to cover $c_0/n \le p \le 1-c_0/n$ for some sufficiently large constant c_0 .

We will restrict ourselves to the range $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$ because we will need the following estimates:

Theorem 9.1 ([16, 22]). Let A denote the adjacency matrix of G(n, p). For every c > 0 there exists $c_0 > 0, c' > 0, c'' > 0$ such that, if $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$,

(21)
$$\lambda_{\max}(pJ-A) \le c'\sqrt{pq(n-1)}$$

and

(22)
$$|\lambda_{\min}(A)| \le c'' \sqrt{pq(n-1)}.$$

with probability at least equal to $1 - n^{-c}$.

With the above, it is rather straightforward to obtain:

Theorem 9.2. For every c > 0 there exists $c_0 > 0, c_1 > 0, c_2 > 0$ such that, if $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$,

(23)
$$c_1\sqrt{(n-1)q/p} \le \vartheta(G(n,p)) \le c_2\sqrt{(n-1)q/p}$$

with probability at least equal to $1 - n^{-c}$.

Indeed, following the method of Juhász, the upper bound is obtained via the dual formulation for the theta number (5) and the matrix Z = J - A/p, where A is the adjacency matrix of G(n, p), while the lower bound follows from the choice $Y = Y'/\langle I, Y' \rangle$ in the primal formulation (4), where $Y = \overline{A} - \lambda_{\min}(\overline{A})I$, \overline{A} being the adjacency matrix of the complementary graph of G(n, p).

9.1. The theta number of $X^k(n, p)$. We will establish the following similar result for random simplicial complexes $X^k(n, p)$:

Theorem 9.3. For every $k \ge 1$ and c > 0, there exists $c_0 > 0, c_1 > 0, c_2 > 0$ such that, if $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$,

$$c_1\sqrt{(n-k)q/p} \le \vartheta_k(X^k(n,p)) \le c_2\sqrt{(n-k)q/p}.$$

with probability at least equal to $1 - n^{-c}$.

For comparison, the independence number of $X^k(n, p)$ is of the order $(\log(n^k p)/p)^{1/k}$ (see [28]). In the range $c_0 \log(n)/n \le p \le 1 - c_0 \log(n)/n$, the eigenvalues of the adjacency matrix of $X^k(n, p)$ have been studied in [21]. We will closely follow the methods developed in [21], in particular the role played by the so-called *links* of X, an idea going back to the work of Garland [17]. By definition, for a k-dimensional simplicial complex X and a (k - 2)-face K of X, the link $lk_X(K)$ is the graph with vertices $\{v \in V : K \cup \{v\} \in X_{k-1}\}$, and edges $\{\{v, w\} : K \cup \{v, w\} \in X_k\}$. In view of the proof of Theorem 9.3, we will first establish a relationship between the theta number of a simplicial complex and that of its links.

Proposition 9.4. Let X be a k-dimensional simplicial complex with complete (k - 1)-skeleton. Then

(24)
$$\vartheta_k(X) \le k \max_{K \in X_{k-2}} \vartheta(\operatorname{lk}_X(K)).$$

Proof. Let $K \in X_{k-2}$. For a matrix $Y \in \mathbb{R}^{\binom{V}{k} \times \binom{V}{k}}$, we introduce its *localization at* K denoted Y_K and defined by:

$$(Y_K)_{F,F'} = \begin{cases} Y_{F,F'} & \text{if } K \subset F \cap F \\ 0 & \text{otherwise.} \end{cases}$$

Let $\rho_K \in \mathbb{R}^{\binom{V}{k} \times \binom{V}{k}}$ denote the diagonal matrix with [F : K] as diagonal entries. Then we observe that

(25)
$$L_{k-1}^{\downarrow} = \sum_{K \in X_{k-2}} \rho_K J_K \rho_K.$$

and that, if $Y_{F,F'} = 0$ for all (F, F') such that $|F \cup F'| \ge k + 2$,

(26)
$$Y = \sum_{K \in X_{k-2}} Y_K - (k-1) \operatorname{diag}(Y).$$

Now let Y be an optimal solution of (8). Taking account of (25) and (26),

$$\begin{split} \vartheta_k(X) &= \langle L_{k-1}^{\downarrow}, Y \rangle = \langle \sum_K \rho_K J_K \rho_K, \sum_K Y_K \rangle - (k-1) \langle L_{k-1}^{\downarrow}, \operatorname{diag}(Y) \rangle \\ &= \sum_{K,K'} \langle \rho_K J_K \rho_K, Y_{K'} \rangle - k(k-1). \end{split}$$

If $K \neq K'$, we have

$$\langle \rho_K J_K \rho_K, Y_{K'} \rangle = \begin{cases} Y_{F,F} & \text{if } K \cup K' = F \\ 0 & \text{otherwise} \end{cases}$$

so, since $\operatorname{trace}(Y) = 1$,

$$\vartheta_k(X) = \sum_K \langle \rho_K J_K \rho_K, Y_K \rangle = \sum_K \langle J_K, \rho_K Y_K \rho_K \rangle.$$

Now, the crucial observation is that the matrix $\rho_K Y_K \rho_K$ gives rise to a feasible matrix of the semidefinite program (4) defining the theta number of $lk_X(K)$. Indeed, let Z_K be the matrix indexed by $V \setminus K$ and defined by $(Z_K)_{v,w} = (\rho_K Y_K \rho_K)_{K \cup \{v\}, K \cup \{w\}}$. This matrix inherits some properties of Y: The matrix Z_K is positive semidefinite, the entries of Z_K associated to edges of $lk_X(K)$ are equal to 0. With obvious notations, we have $\langle J_K, \rho_K Y_K \rho_K \rangle = \langle J, Z_K \rangle$ and $\langle I, Z_K \rangle = \langle I, Y_K \rangle$ so we obtain

$$\vartheta_k(X) \leq \sum_K \langle I, Y_K \rangle \vartheta(\mathrm{lk}_X(K)).$$

We have $\sum_{K} \langle I, Y_K \rangle = k \langle I, Y \rangle = k$ so the announced inequality follows immediately.

Proof of Theorem 9.3. For the upper bound, we apply Proposition 9.4. The link $lk_X(K)$ of a (k-2)-face K in a random complex $X = X^k(n, p)$ is an Erdös-Renyi random graph on $V \setminus K$ with the same probability p. We can thus apply Theorem (9.2) and a union bound to obtain the result. We note that, since the number of such faces is of the order of n^{k-1} , for the probability of the bad event to be, say, less than n^{-c} we need to apply Theorem (9.2) for the larger value c + k - 1 instead of c, explaining the need for an arbitrary large power of n in the convergence speed of probabilities.

In order to find a lower bound of $\vartheta_k(X)$, we consider the matrix $Y = \overline{A} - \lambda_{\min}(\overline{A})I$ where \overline{A} denotes the adjacency matrix of the complementary k-complex \overline{X} . The feasibility conditions of (8) are fulfilled by Y except for the normalization condition $\langle I, Y \rangle = 1$. We have $\langle I, Y \rangle = -\binom{n}{k} \lambda_{\min}(\overline{A})$. Moreover, $\langle L_{k-1}^{\downarrow}, Y \rangle = k(k+1) |\overline{X}_k| - k\binom{n}{k} \lambda_{\min}(\overline{A})$, so

$$\vartheta_k(X) \ge k \bigg(1 + \frac{(k+1)|\overline{X}_k|}{-\binom{n}{k}\lambda_{\min}(\overline{A})} \bigg)$$

The number $|\overline{X}_k|$ of k-faces of $\overline{X} = X^k(n,q)$ is a random variable binomially distributed in $[\binom{n}{k+1}]$ with probability q. Hence, by a straightforward application of a Chernoff bound, for every c > 0, $|\overline{X}_k|$ is at least of the order $\binom{n}{k+1}q$ with probability at least $1 - n^{-c}$. It remains to upper bound $|\lambda_{\min}(\overline{A})|$. For this, we apply the localization procedure that we have already encountered in the proof of Proposition 9.4:

$$\overline{A} = \sum_{K \in X_{k-2}} \overline{A}_K$$

Then, for every $x = (x_F)_{F \in \binom{V}{k}}$, if x_K denotes the vector obtained from x by setting to 0 the coordinates of x associated to faces F not containing K,

$$\langle \overline{A}x, x \rangle = \sum_{K} \langle \overline{A}_{K}x, x \rangle = \sum_{K} \langle \overline{A}_{K}x_{K}, x_{K} \rangle.$$

The matrix \overline{A}_K has the same spectrum as $\rho_K \overline{A}_K \rho_K$. The latter is identical to the adjacency matrix $A_{\text{lk}_{\overline{X}}(K)}$ of the graph $\text{lk}_{\overline{X}}(K)$ on the entries indexed by $\{F = K \cup \{v\}, v \in V \setminus K\}$, and zero elsewhere. So, its non-zero spectrum is that of $A_{\text{lk}_{\overline{Y}}(K)}$ and hence:

$$\langle \overline{A}x, x \rangle \ge \sum_{K} \lambda_{\min}(A_{\operatorname{lk}_{\overline{X}}(K)}) \langle x_K, x_K \rangle.$$

The links $lk_{\overline{X}}(K)$ are random graphs G(n-k+1,q) so, applying (22) and a union bound, we find that, with probability at least equal to $1 - n^{-c}$, for a large enough constant c'',

$$\langle \overline{A}x, x \rangle \ge -c'' \sqrt{pq(n-k)} \sum_{K} \langle x_K, x_K \rangle = -c'' k \sqrt{pq(n-k)} \langle x, x \rangle.$$

We have obtained the desired upper bound $|\lambda_{\min}(\overline{A})| \leq c''' \sqrt{pq(n-k)}$. Putting everything together, we obtain the announced lower bound for $\vartheta_k(X)$.

9.2. The hierarchy of theta numbers of G(n, p). In this last subsection, we restrict ourselves to the case of random graphs G(n, p) and analyze the hierarchy of theta numbers $\vartheta_{\ell}(G(n, p))$ for constant values of ℓ . The restriction to random graphs, i.e., random complexes of dimension 1, is purely for simplicity. The assumption of constant ℓ , however, is essential. Analyzing the complete hierarchy $\hat{\vartheta}_{\ell}(X)$ of a random complex X for non-constant ℓ appears to be a difficult task. It would be interesting to know for which values of ℓ the theta number $\vartheta_{\ell}(G(n, p))$ is close to the independence number. Unfortunately, such questions seem to be out of the reach of the methods we apply here.

Theorem 9.5. For every $\ell \ge 1$ and c > 0, there exists $c_0 > 0, c_1 > 0, c_2 > 0$ such that, if $q^{\ell} \ge c_0 \log(n)/n$ and $pq^{\ell-1} \ge c_0 \log(n)/n$,

$$c_1 \sqrt{nq^{\ell}/p} \le \vartheta_{\ell}(G(n,p)) \le c_2 \sqrt{nq^{\ell}/p}.$$

with probability at least equal to $1 - n^{-c}$.

Proof. We will sometimes use the expression with high probability for an inequality that holds with probability at least $1 - n^{-c}$ for all c > 0, with appropriate constants depending on c.

For an upper bound of $\vartheta_{\ell}(G(n, p))$, we apply

$$\vartheta_{\ell}(G) \leq \ell \max_{K \in \binom{V}{\ell-1}} \vartheta(\operatorname{lk}_{G}(K)).$$

Here, $\operatorname{lk}_G(K)$ is the graph on $V_K := \{v \in V : \{v, k\} \notin E(G(n, p)) \text{ for all } k \in K\}$ with edges $\{v, w\}$ if $K \cup \{v, w\} \in {V \choose \ell+1} \setminus \operatorname{Ind}_{\ell}$. If K is independent, this condition simply means that $\{v, w\}$ is an edge of G, so $\operatorname{lk}_G(K)$ is the graph $G[V_K]$ induced by Gon V_K . If G = G(n, p), the number of vertices $n_K = |V_K|$ is itself a random variable. Since $|K| = \ell - 1$, n_K follows a binomial distribution with parameters $(n - \ell + 1)$ and $q^{\ell-1}$. For n_K to be concentrated around its expected value $q^{\ell-1}(n - \ell + 1)$ we need $q^{\ell-1} \ge c_0 \log(n)/n$ for some $c_0 > 0$.

Assuming $n_K \leq cq^{\ell-1}n$ for some c > 0, we have

$$\vartheta(G[V_K]) \le \vartheta(G(cq^{\ell-1}n, p))$$

because $G[V_K]$ can be viewed as an induced subgraph of $G(cq^{\ell-1}n, p)$. We would like to apply Theorem 9.2. It requires p and q to be greater that $c'_0 \log(q^{\ell-1}n)/(q^{\ell-1}n)$ and holds with probability at least $1 - (q^{\ell-1}n)^c$. All this will be fine if we assume:

$$pq^{\ell-1} \ge c_1 \log(n)/n \text{ and } q^{\ell} \ge c_1 \log(n)/n$$

for a sufficiently large c_1 . With a union bound we obtain with high probability:

$$\vartheta_\ell(G) \le c \sqrt{nq^\ell/p}$$

For the lower bound, we consider the matrix $Y = A - \lambda_{\min}(A)I$ where A is the adjacency matrix of the ℓ -skeleton of Ind and we apply (15). We obtain

$$\vartheta_{\ell}(X) \geq \frac{\langle L_{\ell-1}^{\downarrow}(\mathrm{Ind}), Y \rangle}{\langle I, Y \rangle} = \ell \Big(1 + \frac{(\ell+1)|\operatorname{Ind}_{\ell}|}{-\lambda_{\min}(A)|\operatorname{Ind}_{\ell-1}|} \Big)$$

In order to estimate $|\lambda_{\min}(A)|$ we use $A = \sum_{K \in \operatorname{Ind}_{\ell-2}} A_K$ and remark that A_K has the same non-zero eigenvalues as the adjacency matrix of the graph $\operatorname{lk}_{\operatorname{Ind}}(K)$, itself being the graph $\overline{G}[V_K]$ induced by \overline{G} on V_K . We have

$$\begin{split} \langle Ax, x \rangle &= \sum_{K \in \operatorname{Ind}_{\ell-2}} \langle A_K x, x \rangle = \sum_{K \in \operatorname{Ind}_{\ell-2}} \langle A_K x_K, x_K \rangle \\ &\geq \sum_{K \in \operatorname{Ind}_{\ell-2}} \lambda_{\min}(A_K) \langle x_K, x_K \rangle \\ &\geq \min_{K \in \operatorname{Ind}_{\ell-2}} \lambda_{\min}(A_K) \sum_{K \in \operatorname{Ind}_{\ell-2}} \langle x_K, x_K \rangle \\ &\geq \min_{K \in \operatorname{Ind}_{\ell-2}} \lambda_{\min}(A_K) \ell \langle x, x \rangle, \end{split}$$

so

$$-\lambda_{\min}(A) = |\lambda_{\min}(A)| \le \ell \cdot \max_{K} |\lambda_{\min}(\overline{G}[V_K])|.$$

Like for the upper bound we have with high probability $n_K \leq cq^{\ell-1}n$ for some c > 0 and thus

$$|\lambda_{\min}(\overline{G}[V_K])| \le |\lambda_{\min}(G(cq^{\ell-1}n,q))| \le c'\sqrt{pq^{\ell}n}$$

for some c' > 0, under the same conditions on p and q.

It remains to deal with the ratio $|\operatorname{Ind}_{\ell}|/|\operatorname{Ind}_{\ell-1}|$. For this we will argue that Ind is almost regular. To be more precise we apply double counting to the set

$$D = \{ (A, B) \in \operatorname{Ind}_{\ell-1} \times \operatorname{Ind}_{\ell} : A \subset B \}.$$

The number of ℓ -subsets of B is $\ell + 1$ so $|D| = (\ell + 1) |\operatorname{Ind}_{\ell}|$. For a given A, the number X_A of B containing A follows a binomial distribution with parameters $n - \ell$ and q^{ℓ} , with expected value $q^{\ell}(n - \ell)$. With high probability (requires $q^{\ell} \ge c \log(n)/n$) X_A is larger that $c'q^{\ell}(n - \ell)$ and so

$$\frac{|\operatorname{Ind}_{\ell}|}{|\operatorname{Ind}_{\ell-1}|} \ge \frac{c'q^{\ell}(n-\ell)}{\ell+1}.$$

Putting everything together and applying another union bound we obtain

$$\vartheta_\ell(G) \ge c\sqrt{nq^\ell/p}.$$

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INSTITUT DE MATHÉMATIQUES DE BORDEAUX, UMR 5251, UNIVERSITÉ DE BORDEAUX, 351 COURS DE LA LIBÉRATION, 33400 TALENCE, FRANCE.

E-mail address: christine.bachoc@u-bordeaux.fr

MATHEMATISCHES INSTITUT, UNIVERSITÄT ZU KÖLN, WEYERTAL 86-90, 50931 KÖLN, GERMANY. *E-mail address*: anna.gundert@uni-koeln.de

Institut de Mathématiques de Bordeaux, UMR 5251, Université de Bordeaux, 351 Cours de la Libération, 33400 Talence, France.

E-mail address: alberto.passuello@u-bordeaux.fr