# Grothendieck inequalities, nonlocal games and optimization

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## Chapter 5

# The graphical Grothendieck problem with rank constraint

The content of this chapter is based on joint work with Fernando Mário de Oliveira Filho and Frank Vallentin [BOFV10b]

## 5.1 Introduction

In this chapter, we study computational aspects of another optimization problem, the *graphical Grothendieck problem with rank-r constraint*. This problem is based on a graph $G = (V, E)$ with finite vertex set $V$, edge set $E \in \binom{V}{2}$ and a symmetric matrix $A$ whose rows and columns are indexed by $V$. Let us recall that $\mathcal{S}_V^+$ denotes the cone of positive semidefinite matrices whose rows and columns are indexed by $V$. The problem is defined as follows.

**Problem 5.1 (The graphical Grothendieck problem with rank-$r$ constraint).** Takes as input a graph $G = (V, E)$, positive integer $r$ and symmetric matrix $A : V \times V \to \mathbb{R}$.

$$\begin{aligned} \text{maximize} \quad & \textstyle\sum_{\{u,v\}\in E} A(u,v)X(u,v) \\ \text{subject to} \quad & X \in \mathcal{S}_V^+ \\ & X(u,u) = 1 \ \forall u \in V \\ & \operatorname{rank}(X) = r \end{aligned}$$

Like the variant considered in Chapter 4 this problem is almost a semidefinite program. But due to the rank constraint it may not be efficiently solvable or approximable to within arbitrary precision. The case $r = 1$ has MAX CUT (see Section 1.7.2) as a special case, and is therefore NP-hard. To obtain the MAX CUT problem we set the graph $G$ to be the complete bipartite graph $K_{n,n}$ on $2n$ vertices. Take a Laplacian matrix $B$ of some graph on $n$ vertices and set $A = \left[\begin{smallmatrix} 0 & B \\ B^T & 0 \end{smallmatrix}\right]$. An optimal solution for Problem 5.1 then gives a cut of maximal size for the $n$-vertex graph. The problem reduces to the *positive semidefinite Grothendieck problem* treated in Chapter 4 when we replace the above matrix $B$ by an arbitrary positive semidefinite matrix. If we remove the rank constraint (we will denote this by $r = \infty$) then the problem does become a semidefinite program, which can be solved efficiently regardless of the graph $G$.

We can interpret the problem geometrically using the 1-1 correspondence between rank-$r$ positive semidefinite matrices $X : V \times V \to \mathbb{R}$ and matrices of the form $\big(f(u) \cdot f(v)\big)_{u,v \in V}$ where each $f(u)$ is an $r$-dimensional unit vector. The problem thus asks to position $|V|$ vectors on a real $r$-dimensional unit sphere in such a way that a weighted sum of their inner products is maximized. It follows from this that the optimum of Problem 5.1 is given by $\mathrm{SDP}_r(G, A)$ (see Definition 2.3.4) and that the largest possible ratio $\mathrm{SDP}_q(G, A) / \mathrm{SDP}_r(G, A)$ for matrices $A : V \times V \to \mathbb{R}$ is given by $K(q \mapsto r, G)$ (see Definition 2.3.5). In particular, the rank-$r$ Grothendieck constant of the graph $G$, defined by $K(r, G) = K(\infty \mapsto r, G)$, gives the largest possible ratio of the optimum of the natural semidefinite relaxation of Problem 5.1, and its actual optimum.

The case $r = 1$ of Problem 5.1 was studied extensively by the computer science community. The case of bipartite graphs was studied by Alon and Naor [AN06] in the context of computing the cut norm of matrices and finding Szemerédi partitions of graphs. Based on the fact that $K(1, K_{n,n}) \leq K_G$, they gave a polynomial-time $(1/K_G)$-approximation algorithm for computing the cut-norm, thereby kindling a large mass of research related to connections between optimization, semidefinite programming and Grothendieck-like inequalities. Let $K_n$ denote the complete graph on $n$ vertices. For $G = K_n$ Problem 5.1 is known as the *quadratic programming problem with* $\{-1, 1\}$*-constraint*. Independently, Nemirovski, Roos and Terlaky [NRT99], Megretski [Meg01] and Charikar and Wirth [CW04] proved that $K(1, K_n) \leq O(\log n)$. Khot and O'Donnell [KO08] proved that $K(1, K_n) \geq \Omega(\log n)$, showing that in contrast to $K_G$, its graphical versions are not in general constants (see also [AMMN06, ABH$^+$05]). Hardness-of-approximation results for the quadratic programming problem were obtained by Arora et al. [ABH$^+$05]. We refer to Section 2.3.2 for more details on these numbers.

Much less seems to be known about the computational aspects of the more geometric cases of the graphical Grothendieck problem with rank-$r$ constraint, where $r \geq 2$. The main results of this chapter are new upper bounds on the numbers $K(r, G)$ for arbitrary ranks $r$ and graphs $G$ with small chromatic number. These upper bounds are obtained by analyzing an efficient $K(r, G)^{-1}$-approximation algorithm for Problem 5.1, given in Section 5.1.2. At the end of this chapter we derive new upper bounds on $K(r, G)$ for graphs with large chromatic number, by analyzing a straight-forward modification of an efficient approximation algorithm due to Alon, Makarychev, Makarychev, and Naor [AMMN06] (see Section 5.6). Before giving details of the main results we discuss two applications.

### 5.1.1 Applications

We give two interpretations of Problem 5.1, one in ground state energies and one in XOR games. Similar to the problem considered in Chapter 4, the objective function of Problem 5.1 can be interpreted as a kind of energy. Stanley's *n-vector model* [Sta68] describes the interaction of particles in a spin glass with ferromagnetic and antiferromagnetic interactions. Let $G = (V, E)$ be the interaction graph where the vertices represent particles and where edges indicate which particles interact. The potential function $A\colon V \times V \to \mathbb{R}$ is 0 if $u$ and $v$ are not adjacent, positive if there is ferromagnetic interaction between $u$ and $v$, and negative if there is antiferromagnetic interaction. The particles possess a vector-valued spin $f\colon V \to S^{n-1}$. The case $n = 1$ corresponds to the Ising model, the case $n = 2$ to the XY (or classical planar) model, the case $n = 3$ to the Heisenberg model, and the case $n = \infty$ to the Berlin-Kac spherical model. In the absence of an external field, the total energy of the system is given by the *Hamiltonian*

$$-\sum_{\{u,v\}\in E} A(u,v) f(u) \cdot f(v).$$

The *ground state* of this model is a configuration of spins $f\colon V \to S^{n-1}$ which minimizes the total energy. Finding the ground state is the same as solving $\mathrm{SDP}_n(G, A)$. The much-studied Ising model (the case $n = 1$) is a simplification of the spin glass model in which the vectors are two- or three-dimensional (i.e., the XY model and the Heisenberg model) [Sta68, BGJR88, KNS10]. Typically, the interaction graph has small chromatic number. The most common case is when this graph is a finite subgraph of the integer lattice $\mathbb{Z}^n$ where the vertices are the lattice points and where two vertices are connected if their

Euclidean distance is one. These graphs are bipartite since they can be partitioned into even and odd vertices, corresponding to the parity of the sum of the coordinates. We refer to Talagrand's book [Tal03] and the paper Bansal, Bravyi and Terhal [BBT08] for more extensive introductions and mathematical/computational treatments of spin glasses.

The case of bipartite graphs in Problem 5.1 is also of interest to us because it is related to the setting of two-player nonlocal games. Let $L$ and $R$ be disjoint finite sets and let $\mathcal{G} = (\pi, \Sigma)$ be a two-player XOR game given by probability distribution $\pi$ on $L \times R$ and sign matrix $\Sigma : L \times R \to \{-1, 1\}$. The set $L$ contains Alice's questions and the set $R$ Bob's. Let $G = (V, E)$ be the complete bipartite graph on vertex set $V = L \cup R$ where all edges are between the sets $L$ and $R$. Define the matrix $A : L \cap R \to \mathbb{R}$ by setting $A(u, v) = \pi(u, v)\Sigma(u, v)$ if $\{u, v\} \in E$ and $A(u, v) = 0$ otherwise. The optimum of Problem 5.1 is of the form

$$\sum_{\{u,v\} \in E} A(u, v) f(u) \cdot f(v)$$

for some functions $f : V \to S^{r-1}$. Since our graph $G$ is bipartite, we can split the collection of vectors $f(u)$ into two groups corresponding to whether $u \in L$ or $u \in R$. By renaming the vectors $f(u)$ for every $u \in R$ to, say, $g(u)$ we get that the sum above equals

$$\sum_{u \in L} \sum_{v \in R} A(u, v) f(u) \cdot g(v) = \mathbb{E}_{(u,v) \sim \pi} \big[ \Sigma(u, v) f(u) \cdot g(v) \big].$$

By Tsirelson's Theorem (see Section 1.5) we thus have that the optimum above is a *lower bound* on the entangled bias of $\mathcal{G}$ when the players have quantum systems of local dimension $2^{\lceil r/2 \rceil}$, and an *upper bound* on the bias when the local dimensions are $\sqrt{r/2}$.

### 5.1.2 An efficient approximation algorithm for graphs with small chromatic number

In this chapter we prove explicit upper bounds for $K(r, G)$. For the most part, we will focus on the case of small $r$ and graphs with small chromatic number, although our methods for such cases are not restricted to this. The proof of the following theorem gives a randomized polynomial-time approximation algorithm for approximating ground states in the Heisenberg model in the lattice $\mathbb{Z}^3$ with approximation ratio $0.78\ldots = (1.28\ldots)^{-1}$. This result can be regarded as the principal contribution of this chapter.

**5.1.1.** THEOREM. *For $r = 1, \dots, 10$ and in the case of a bipartite or a tripartite graph $G$ the rank-$r$ Grothendieck constant is at most:*

| $r$ | *bipartite* $G$ | *tripartite* $G$ |
|---|---|---|
| 1 | $1.782213\dots$ | $3.264251\dots$ |
| 2 | $1.404909\dots$ | $2.621596\dots$ |
| 3 | $1.280812\dots$ | $2.412700\dots$ |
| 4 | $1.216786\dots$ | $2.309224\dots$ |
| 5 | $1.177179\dots$ | $2.247399\dots$ |
| 6 | $1.150060\dots$ | $2.206258\dots$ |
| 7 | $1.130249\dots$ | $2.176891\dots$ |
| 8 | $1.115110\dots$ | $2.154868\dots$ |
| 9 | $1.103150\dots$ | $2.137736\dots$ |
| 10 | $1.093456\dots$ | $2.124024\dots$ |

Our bound for the original Grothendieck constant $K_G$, which corresponds to the case where $r = 1$ and $G$ is a complete bipartite graph $K_{n,n}$ of any size $n$, is due to Krivine [Kri79]. Our bound for $K(2, K_{n,n})$ coincides with Haagerup's [Haa87] upper bound on $K_G^{\mathbb{C}}$. Though these numbers may be different, it should not be a surprise that the bounds are equal, since we use some of Haagerup's techniques. When the graph $G$ has large chromatic number, then the result of [AMMN06] gives the best known bounds for $K(1, G)$ (see Section 2.3.2). They prove a logarithmic dependence on the chromatic number of the graph whereas the first row in the table has a linear dependence on the chromatic number. We extend the results of [AMMN06] for large chromatic numbers for $r \geq 2$ in Section 5.6.

For the proof of Theorem 5.1.1 we use the framework developed by Krivine and Haagerup for the case of bipartite graphs, explained below. The main new technical tool used in the proof is a matrix version of Grothendieck's Identity given in Lemma 5.2.1. To develop some intuition for the proof we begin by considering the natural strategy for proving upper bounds on $K(r, G)$. Based on the Goemans and Williamson approximation algorithm for MAX CUT and Algorithm 4.1 for Problem 4.1, the natural strategy is to embed a collection of $|V|$-dimensional vectors $\big(f(u)\big)_{u \in V}$ for which the value $\mathrm{SDP}_\infty(G, A)$ is achieved[1] into $S^{r-1}$ using a random projection based on an $r$-by-$|V|$ matrix $Z$ with i.i.d.

[1] Recall that $|V|$-dimensional vectors always suffice since $|V|$ vectors span a space of dimension at most $|V|$.

Gaussian entries. This amounts to defining the random $r$-dimensional unit vectors $g(u) = Zf(u)/\|Zf(u)\|_2$. By linearity of expectation, the expected objective value of this solution for the rank-$r$ case of Problem 5.1 is given by

$$\mathbb{E}\Big[\sum_{\{u,v\}\in E} A(u,v)g(u)\cdot g(v)\Big] = \sum_{\{u,v\}\in E} A(u,v)\mathbb{E}\big[g(u)\cdot g(v)\big].$$

The problem now is lower bound this quantity in terms of the optimum of the problem $\mathrm{SDP}_r(G,A)$. If $r=1$, Grothendieck's Identity gives $\mathbb{E}\big[g(u)\cdot g(v)\big] = (2/\pi)\arcsin\big(f(u)\cdot f(v)\big)$. For larger values of $r$ this expectation is also some nonlinear function of $f(u)\cdot f(v)$. The strategy of Krivine and Haagerup is to "linearize" these functions by using the following new embedding lemma.

**5.1.2.** LEMMA. *Let $G=(V,E)$ be a graph and choose $Z=(Z_{ij})\in\mathbb{R}^{r\times|V|}$ at random so that the entries are i.i.d. $N(0,1)$ random variables. Given $f\colon V\to S^{|V|-1}$, there is a function $g\colon V\to S^{|V|-1}$ such that whenever $u$ and $v$ are adjacent in $G$, then*

$$\mathbb{E}\Big[\frac{Zg(u)}{\|Zg(u)\|_2}\cdot\frac{Zg(v)}{\|Zg(v)\|_2}\Big] = \beta(r,G)f(u)\cdot f(v)$$

*for some constant $\beta(r,G)$ depending only on $r$ and $G$. Moreover, the function $g$ can be found in polynomial time in $|V|$.*

In the statement above we are vague regarding the constant $\beta(r,G)$. We will give the precise statement of the lemma in Section 5.4 (Lemma 5.4.1 there), right now this precise statement is not relevant to our discussion. Now, the strategy of Krivine and Haagerup amounts to analyzing a following four-step procedure that yields a randomized polynomial-time approximation algorithm for Problem 5.1, Algorithm 5.1 shown below.

To analyze this algorithm, we compute the expected value of the feasible solution $h$. By linearity of expectation, we get

$$\begin{aligned}\mathrm{SDP}_r(G,A) &\geq \mathbb{E}\Big[\sum_{\{u,v\}\in E} A(u,v)h(u)\cdot h(v)\Big]\\ &= \sum_{\{u,v\}\in E} A(u,v)\mathbb{E}[h(u)\cdot h(v)]\end{aligned}$$

as before. But now, using Lemma 5.1.2, we get that the above sum equals

$$\beta(r,G)\sum_{\{u,v\}\in E} A(u,v)f(u)\cdot f(v) \;=\; \beta(r,G)\,\mathrm{SDP}_\infty(G,A), \tag{5.1}$$

**Algorithm 5.1** Takes as input graph $G = (V, E)$, positive integer $r$ and symmetric matrix $A : V \times V \to \mathbb{R}$, and returns a feasible solution $h : V \to S^{r-1}$ for $\mathrm{SDP}_r(G, A)$.

(1) Solve the semidefinite relaxation of Problem 5.1, obtaining $f : V \to S^{n-1}$.

(2) Use $f$ to construct $g : V \to S^{|V|-1}$ according to Lemma 5.1.2.

(3) Sample matrix $Z \in \mathbb{R}^{r\times|V|}$ such that the entries $Z_{ij}$ are independently distributed Gaussian random variables with mean 0 and variance 1.

(4) Define $h : V \to S^{r-1}$ by $h(u) = Zg(u)/\|Zg(u)\|_2$ for every $u \in V$.

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and hence $K(r, G) \leq \beta(r, G)^{-1}$. Since $\mathrm{SDP}_\infty(G, A) \geq \mathrm{SDP}_r(G, A)$ it also follows that Algorithm 5.1 is a $\beta(r, G)$-approximation algorithm for Problem 5.1.

The constant $\beta(r, G)$ in Lemma 5.1.2 is defined in terms of the Taylor expansion of the inverse of the function $E_r\colon [-1, 1] \to [-1, 1]$ given by

$$E_r(x \cdot y) = \mathbb{E}\left[\frac{Zx}{\|Zx\|_2} \cdot \frac{Zy}{\|Zy\|_2}\right],$$

where $x, y \in S^\infty$ and $Z = (Z_{ij}) \in \mathbb{R}^{r\times\infty}$ is chosen so that its entries are independently distributed according to the normal distribution with mean 0 and variance 1. In Section 4.2.1 of Chapter 4 we argued that the function $E_r$ is indeed well-defined, which follows because the expectation above is invariant under orthogonal transformations.

**Outline of the rest of this chapter.** The Taylor expansion of $E_r$ is computed in Section 5.2. The Taylor expansion of $E_r^{-1}$ is treated in Section 5.3, where we basically follow Haagerup [Haa87]. A precise version of Lemma 5.1.2 is stated and proved in Section 5.4, following Krivine [Kri79]. In Section 5.5 we show that one can refine this analysis and can (strictly) improve the upper bounds on $K(r, G)$ if one takes the size of the vertex set into account. In particular, there we prove upper bounds on $K(q \mapsto r, G)$. In Section 5.6 we show how to generalize the technique of [AMMN06] to deal with graphs with large chromatic numbers and higher values of $r$ and we briefly summarize this chapter in Section 5.7.

## 5.2 A matrix version of Grothendieck's Identity

In this section we prove a generalization of Grothendieck's Identity. This gives the Taylor coefficients of the function $E_r$, which we need to prove Lemma 5.1.2.

**5.2.1.** LEMMA. *For positive integers $r, n$, let $u, v$ be real $n$-dimensional unit vectors and let $Z$ be a random real $r$-by-$n$ matrix with independent $N(0,1)$ entries. Then,*

$$\mathbb{E}\left[\frac{Zu}{\|Zu\|_2} \cdot \frac{Zv}{\|Zv\|_2}\right] = \gamma(r)\,(u \cdot v)\,{}_2F_1\begin{pmatrix} 1/2,\, 1/2 \\ r/2+1 \end{pmatrix} ;\, (u \cdot v)^2 \Bigg),$$

*where*

$$\gamma(r) = \frac{2}{r}\left(\frac{\Gamma\left(\frac{r+1}{2}\right)}{\Gamma\left(\frac{r}{2}\right)}\right)^2$$

*and*

$${}_2F_1\left(\begin{matrix} 1/2,\, 1/2 \\ r/2+1 \end{matrix} ;\, (u \cdot v)^2\right) = \sum_{k=0}^{\infty} \frac{\big(1 \cdot 3 \cdots (2k-1)\big)^2}{\big((r+2)(r+4)\cdots(r+2k)\big)\big(2 \cdot 4 \cdots (2k)\big)}(u \cdot v)^{2k}$$

*is a hypergeometric function (see for example [AAR99]).*

Before proving this lemma, we note a couple of special cases. For the case $r = 1$, we obtain Grothendieck's Identity (Lemma 4.2.4):

$$\begin{aligned}\mathbb{E}[\operatorname{sign}(Zu)\operatorname{sign}(Zv)] &= \frac{2}{\pi}\arcsin(u \cdot v) \\ &= \frac{2}{\pi}\left(u \cdot v + \left(\frac{1}{2}\right)\frac{(u \cdot v)^3}{3} + \left(\frac{1 \cdot 3}{2 \cdot 4}\right)\frac{(u \cdot v)^5}{5} + \cdots\right).\end{aligned}$$

The case $r = 2$ gives a function used by Haagerup [Haa87] to upper bound $K_G^{\mathbb{C}}$:

$$\begin{aligned}\mathbb{E}\left[\frac{Zu}{\|Zu\|_2} \cdot \frac{Zv}{\|Zv\|_2}\right] &= \frac{1}{u \cdot v}\Big(E(u \cdot v) - (1-(u \cdot v)^2)K(u \cdot v)\Big) \\ &= \frac{\pi}{4}\left(u \cdot v + \left(\frac{1}{2}\right)^2\frac{(u \cdot v)^3}{2} + \left(\frac{1 \cdot 3}{2 \cdot 4}\right)^2\frac{(u \cdot v)^5}{3} + \cdots\right),\end{aligned}$$

where $K$ and $E$ are the complete elliptic integrals of the first and second kind (see for example [AAR99]). Note that on page 201 of Haagerup [Haa87] $\pi/2$

should be $\pi/4$. In the previous chapter we computed the first coefficient of the Taylor series of the expectation for every $r$, which turned out to be $\gamma(r)$.

Unfortunately, for $r \geq 2$ we don't have a nice geometric proof as we do for the case $r = 1$. The proof we give here is based on the rotational invariance of the normal distribution and integration with respect to spherical coordinates together with some identities for hypergeometric functions. A similar calculation was done by König and Tomczak-Jaegermann [Kön01]. It would be interesting to find a more geometrical proof of the lemma.[2]

PROOF OF LEMMA 5.2.1: Let $Z_i \in \mathbb{R}^n$ be the $i$-th row of the matrix $Z$, with $i = 1, \ldots r$. We define vectors

$$x = \begin{pmatrix} Z_1 \cdot u \\ Z_2 \cdot u \\ \vdots \\ Z_r \cdot u \end{pmatrix} \qquad \text{and} \qquad y = \begin{pmatrix} Z_1 \cdot v \\ Z_2 \cdot v \\ \vdots \\ Z_r \cdot v \end{pmatrix}$$

so that we have $x \cdot y = (Zu) \cdot (Zv)$. Since the probability distribution of the vectors $Z_i$ is invariant under orthogonal transformations we may assume that $u = (1, 0, \ldots, 0)^T$ and $v = (t, \sqrt{1-t^2}, 0, \ldots, 0)^T$ and so the pair $(x, y) \in \mathbb{R}^r \times \mathbb{R}^r$ is distributed according to the probability density function (see for example [Mui82, Theorem 1.2.9])

$$(2\pi\sqrt{1-t^2})^{-r} \exp\left(-\frac{x \cdot x - 2tx \cdot y + y \cdot y}{2(1-t^2)}\right).$$

Hence,

$$\mathbb{E}\left[\frac{x}{\|x\|_2} \cdot \frac{y}{\|y\|_2}\right] =$$
$$(2\pi\sqrt{1-t^2})^{-r} \int_{\mathbb{R}^r} \int_{\mathbb{R}^r} \frac{x}{\|x\|_2} \cdot \frac{y}{\|y\|_2} \exp\left(-\frac{x \cdot x - 2tx \cdot y + y \cdot y}{2(1-t^2)}\right) dxdy.$$

By using spherical coordinates $x = \alpha\xi$, $y = \beta\eta$, where $\alpha, \beta \in [0, \infty)$ and $\xi, \eta \in S^{r-1}$, and the rotationally invariant (surface area) measure $\tilde{\omega}_r$ on the $r$-dimensional unit sphere, normalized such that $\tilde{\omega}_r(S^{r-1}) = \pi^{r/2}/\Gamma(r/2)$, we rewrite the above integral as

$$\int_0^\infty \int_0^\infty (\alpha\beta)^{r-1} \exp\left(-\frac{\alpha^2 + \beta^2}{2(1-t^2)}\right) \int_{S^{r-1}} \int_{S^{r-1}} \xi \cdot \eta \exp\left(\frac{\alpha\beta t \xi \cdot \eta}{1-t^2}\right)$$
$$d\tilde{\omega}_r(\xi) d\tilde{\omega}_r(\eta) d\alpha d\beta.$$

[2] Oded Regev gave a more intuitive proof based on well-known probabilistic estimates, but we won't give the details of his proof here.

If $r = 1$, we get for the inner double integral

$$\int_{S^0}\int_{S^0} \xi\cdot\eta \exp\left(\frac{\alpha\beta t\xi\cdot\eta}{1-t^2}\right) d\tilde{\omega}_r(\xi)d\tilde{\omega}_r(\eta)$$
$$= 4\sinh\left(\frac{\alpha\beta t}{1-t^2}\right)$$
$$= 4\frac{\alpha\beta t}{1-t^2}{}_0F_1\left(\begin{matrix} \text{---} \\ 3/2 \end{matrix};\left(\frac{\alpha\beta t}{2(1-t^2)}\right)^2\right).$$

Now we consider the case when $r \geq 2$. Since the inner double integral over the spheres only depends on the inner product $p = \xi\cdot\eta$, it can be rewritten as

$$\tilde{\omega}_{r-1}(S^{r-2})\tilde{\omega}_r(S^{r-1})\int_{-1}^{1} p\exp\left(\frac{\alpha\beta tp}{1-t^2}\right)(1-p^2)^{(r-3)/2}\,dp.$$

Integration by parts yields

$$\int_{-1}^{1} p(1-p^2)^{(r-3)/2}\exp\left(\frac{\alpha\beta tp}{1-t^2}\right)\,dp$$
$$= \frac{\alpha\beta t}{(r-1)(1-t^2)}\int_{-1}^{1}(1-p^2)^{(r-1)/2}\exp\left(\frac{\alpha\beta tp}{1-t^2}\right)dp.$$

The last integral can be rewritten using the modified Bessel function of the first kind (see for example [AAR99, p. 235, Exercise 9])

$$\int_{-1}^{1}(1-p^2)^{(r-1)/2}\exp\left(\frac{\alpha\beta tp}{1-t^2}\right)\,dp$$
$$= \Gamma((r+1)/2)\sqrt{\pi}\left(\frac{2(1-t^2)}{\alpha\beta t}\right)^{r/2} I_{r/2}\left(\frac{\alpha\beta t}{1-t^2}\right).$$

One can write $I_{r/2}$ as a hypergeometric function [AAR99, Eq. (4.12.2)]

$$I_{r/2}(x) = (x/2)^{r/2}\sum_{k=0}^{\infty}\frac{(x/2)^{2k}}{k!\Gamma(r/2+k+1)} = \frac{(x/2)^{r/2}}{\Gamma((r+2)/2)}{}_0F_1\left(\begin{matrix} \text{---} \\ (r+2)/2 \end{matrix};\left(\frac{x}{2}\right)^2\right).$$

Putting things together, we get

$$\tilde{\omega}_{r-1}(S^{r-2})\tilde{\omega}_r(S^{r-1})\int_{-1}^{1} p\exp\left(\frac{\alpha\beta tp}{1-t^2}\right)(1-p^2)^{(r-3)/2}\,dp$$
$$= \frac{4\pi^r}{\Gamma(r/2)^2 r}\frac{\alpha\beta t}{1-t^2}{}_0F_1\left(\begin{matrix} \text{---} \\ (r+2)/2 \end{matrix};\left(\frac{\alpha\beta t}{2(1-t^2)}\right)^2\right).$$

Notice that the last formula also holds for $r = 1$. So we can continue without case distinction.

Now we evaluate the outer double integral

$$\int_0^\infty \int_0^\infty (\alpha\beta)^r \exp\left(-\frac{\alpha^2+\beta^2}{2(1-t^2)}\right) {}_0F_1\left(\frac{\text{---}}{(r+2)/2}; \left(\frac{\alpha\beta t}{2(1-t^2)}\right)^2\right) d\alpha d\beta.$$

Here the inner integral equals

$$\int_0^\infty \alpha^r \exp\left(-\frac{\alpha^2}{2(1-t^2)}\right) {}_0F_1\left(\frac{\text{---}}{(r+2)/2}; \left(\frac{\alpha\beta t}{2(1-t^2)}\right)^2\right) d\alpha,$$

and doing the substitution $\zeta = \alpha^2/(2(1-t^2))$ gives

$$2^{(r-1)/2}(1-t^2)^{(r+1)/2} \int_0^\infty \zeta^{(r-1)/2} \exp(-\zeta)\, {}_0F_1\left(\frac{\text{---}}{(r+2)/2}; \frac{\zeta(\beta t)^2}{2(1-t^2)}\right) d\zeta,$$

which, by the Bateman Manuscript Project [EMOT54, p. 337 Eq. (11)], equals

$$2^{(r-1)/2}(1-t^2)^{(r+1)/2}\Gamma((r+1)/2)\, {}_1F_1\left(\frac{(r+1)/2}{(r+2)/2}; \frac{(\beta t)^2}{2(1-t^2)}\right).$$

Now we treat the remaining outer integral in a similar way, using [EMOT54, p. 219 Eq. (17)], and get that

$$\begin{aligned}\int_0^\infty \beta^r \exp\left(-\frac{\beta^2}{2(1-t^2)}\right) {}_1F_1\left(\frac{(r+1)/2}{(r+2)/2}; \frac{(\beta t)^2}{2(1-t^2)}\right) d\beta \\ = 2^{(r-1)/2}(1-t^2)^{(r+1)/2}\Gamma((r+1)/2)\, {}_2F_1\left(\frac{(r+1)/2, (r+1)/2}{(r+2)/2}; t^2\right).\end{aligned}$$

By applying Euler's transformation (see for example [AAR99, Eq. (2.2.7)])

$${}_2F_1\left(\frac{(r+1)/2, (r+1)/2}{(r+2)/2}; t^2\right) = (1-t^2)^{-r/2}\, {}_2F_1\left(\frac{1/2, 1/2}{(r+2)/2}; t^2\right)$$

and after collecting the remaining factors we arrive at the result. □

## 5.3 Convergence radius

To construct the new vectors in the step (2) of Algorithm 5.1 that are used to linearize the expectation, we will make use of the Taylor series expansion of the inverse of $E_r$. Locally around zero we can expand the function $E_r^{-1}$ as

$$E_r^{-1}(t) = \sum_{k=0}^{\infty} b_{2k+1} t^{2k+1},$$

for some coefficients $b_{2k+1}$, but in the proof of Lemma 5.1.2 it will be essential that this expansion be valid for all $t \in [-1, 1]$.

In the case $r = 1$ we have $E_1^{-1}(t) = \sin(\pi t/2)$ and here the convergence radius is even infinity. The case $r = 2$ was treated by Haagerup and it requires quite some technical work which we sketch very briefly now. He shows that $|b_k| \leq C/k^2$ for some constant $C$, independent of $k$, using tools from complex analysis. Using Cauchy's integral formula and after doing some simplifications [Haa87, p. 208] one can express $b_k$ for any choice of $\alpha > 1$ as

$$b_k = \frac{2}{\pi k} \int_1^{\alpha} \Im(E_2(z)^{-k})\, dz + \frac{2}{\pi k} \Im\left( \int_{C'_\alpha} E_2(z)^{-k}\, dz \right),$$

where $C'_\alpha$ is the quarter circle $\{ \alpha e^{i\theta} : \theta \in [0, \pi/2] \}$.

For an appropriate choice of $\alpha$ the first integral is in absolute value bounded above by $C/k$ and the second integral is in absolute value exponentially small in $k$. We refer to the original paper for the details. One key point in the arguments is the following integral representation of $E_2$ giving an analytic continuation of $E_2$ on the complex plane slit along the half line $(1, \infty)$:

$$E_2(z) = \int_0^{\pi/2} \sin\theta \arcsin(z \sin\theta)\, d\theta.$$

Here, the term $\arcsin(z \sin\theta)$ gives the main contribution in the estimates.

Now we derive a similar representation of $E_r$ and using it in Haagerup's analysis with obvious changes shows that also for $r > 2$ we have $b_k \leq C/k^2$ for some constant $C$, independent of $k$.

**5.3.1.** LEMMA. *For $r \geq 2$ we have*

$$E_r(z) = \frac{2(r-1)\Gamma((r+1)/2)}{\Gamma(1/2)\Gamma(r/2)} \int_0^{\pi/2} \cos^{r-2}\theta \sin\theta \arcsin(z \sin\theta)\, d\theta.$$

PROOF: Using Euler's integral representation of the hypergeometric function (see for example [AAR99, Theorem 2.2.1]) we can rewrite $E_r$ as

$$E_r(z) = \frac{\Gamma((r+1)/2)}{\Gamma(1/2)\Gamma(r/2)} \int_0^1 \frac{(1-t)^{(r-1)/2} z}{\sqrt{t(1-z^2 t)}}\, dt,$$

which is valid in the complex plane slit along the half line $(1, \infty)$. Using the substitution $t = \sin^2\theta$ we get

$$E_r(z) = 2\frac{\Gamma((r+1)/2)}{\Gamma(1/2)\Gamma(r/2)} \int_0^{\pi/2} \frac{\cos^r\theta z}{\sqrt{1 - z^2\sin^2\theta}}\, d\theta.$$

Now integration by parts and the identity

$$\frac{d}{d\theta}\arcsin(z\sin\theta) = \frac{z\cos\theta}{\sqrt{1-z^2\sin^2\theta}}$$

gives the result. □

## 5.4 Constructing new vectors

In this section, we prove Lemma 5.1.2, of which Lemma 5.4.1 below is the detailed version. Roughly speaking, we define the function $g : V \to S^{|V|-1}$ such that the inner product $g(u) \cdot g(v)$, for adjacent vertices $u$ and $v$, inverts the function $E_r$ and leaves a linear function of $f(u) \cdot f(v)$. For this, we use the Taylor expansion of the inverse of $E_r$ and build on a construction of Krivine [Kri79], who proved the lemma for the case of bipartite graphs.

For the nonbipartite case we use the theta number, which is a graph parameter introduced by Lovász [Lov79]. Let $G = (V, E)$ be a graph. The *theta number* of the complement of $G$, denoted by $\vartheta(\overline{G})$, introduced in Section 1.7.3. We restate it here for convenience. It is the optimal value of the following semidefinite program:

$$\begin{aligned} \vartheta(\overline{G}) = \min\Big\{ \lambda :\ & Z \in \mathcal{S}_V^+, \\ & Z(u,u) = \lambda - 1 \ \text{ for } u \in V, \\ & Z(u,v) = -1 \ \text{ for } \{u,v\} \in E \Big\}. \end{aligned} \tag{5.2}$$

**5.4.1.** LEMMA. *Let $G = (V, E)$ be a graph with at least one edge. Given $f : V \to S^{|V|-1}$, there exists $g : V \to S^{|V|-1}$ such that for all $\{u, v\} \in E$, we have*

$$E_r\big(g(u) \cdot g(v)\big) = \beta(r, G) f(u) \cdot f(v),$$

*where the constant $\beta(r, G)$ is defined by the unique positive solution of the equation*

$$\sum_{k=0}^{\infty} |b_{2k+1}| \beta(r, G)^{2k+1} = \frac{1}{\vartheta(\overline{G}) - 1},$$

*where the coefficients $b_{2k+1}$ come from the expansion*

$$E_r^{-1}(t) = \sum_{k=0}^{\infty} b_{2k+1} t^{2k+1}.$$

With this lemma we can now prove Theorem 5.1.1.

PROOF OF THEOREM 5.1.1: We combine Lemma 5.4.1 with the analysis of Algorithm 5.1. To compute the table in the theorem, we use the formula

$$b_k = \frac{1}{k! a_1^k} \left[ \frac{d^{k-1}}{dt^{k-1}} \left( 1 + \frac{a_2}{a_1} t + \cdots + \frac{a_k}{a_1} t^{k-1} \right)^{-k} \right]_{t=0}, \tag{5.3}$$

where $a_i$ are the Taylor coefficients of $E_r$ (see for example Morse and Feshbach [MF53, (4.5.13)]). □

PROOF OF LEMMA 5.4.1: We construct the vectors $g(u) \in S^{|V|-1}$ by constructing vectors $R(u)$ in an infinite-dimensional Hilbert space $\mathcal{H}$ whose inner product matrix coincides with the one of the $g(u)$. We construct the vectors $R(u)$ from two pairs of vector-valued functions, *inner functions* $S, T : \mathbb{R}^{|V|} \to \mathcal{H}$, and *outer functions* $s, t : V \to \mathbb{R}^{2|V|}$. The inner functions serve to invert the function $E_r$ and the outer functions serve to control the pairwise inner products for adjacent vertices $u$ and $v$. We proceed in three steps.

In the first step, we construct the inner functions. Set $H = \mathbb{R}^{|V|}$ and

$$\mathcal{H} = \bigoplus_{k=0}^{\infty} H^{\otimes(2k+1)}.$$

For a unit vector $x \in H$, define the vectors $S(x)$, $T(x) \in \mathcal{H}$ given componentwise by

$$S(x)_k = \sqrt{|b_{2k+1}| \beta(r, G)^{2k+1}} x^{\otimes(2k+1)}$$

and

$$T(x)_k = \operatorname{sign}(b_{2k+1}) \sqrt{|b_{2k+1}| \beta(r, G)^{2k+1}} x^{\otimes(2k+1)}.$$

Then for vectors $x, y \in S^{|V|-1}$ we have

$$S(x) \cdot T(y) = E_r^{-1}(\beta(r, G) x \cdot y)$$

and moreover by the definition of $\beta(r, G)$ given in the lemma,

$$S(x) \cdot S(x) = T(x) \cdot T(x) = \sum_{k=0}^{\infty} |b_{2k+1}| \beta(r, G)^{2k+1} = \frac{1}{\vartheta(\overline{G}) - 1}.$$

Notice that here it is essential that the Taylor expansion of $E_r^{-1}$ has a convergence radius of at least one.

In the second step, we define the outer functions. Let $\lambda = \vartheta(\overline{G})$, and $Z$ be an optimal solution for (5.2). We have $\lambda \geq 2$ since $G$ has at least one edge. Set

$$A = \frac{(\lambda-1)(J+Z)}{2\lambda} \qquad \text{and} \qquad B = \frac{(\lambda-1)J - Z}{2\lambda},$$

where $J$ is the all-ones matrix, and consider the matrix

$$U = \begin{pmatrix} A & B \\ B & A \end{pmatrix}.$$

By applying a Hadamard transformation

$$\frac{1}{\sqrt{2}}\begin{pmatrix} I & I \\ I & -I \end{pmatrix} U \frac{1}{\sqrt{2}}\begin{pmatrix} I & I \\ I & -I \end{pmatrix} = \begin{pmatrix} A+B & 0 \\ 0 & A-B \end{pmatrix}$$

we see that $U$ is positive semidefinite, since both $A+B$ and $A-B$ are positive semidefinite. We define the functions $s\colon V \to \mathbb{R}^{2|V|}$ and $t\colon V \to \mathbb{R}^{2|V|}$ so that $U$ is the Gram matrix of the vectors $\big(s(u)\big)_{u\in V}$ and $\big(t(v)\big)_{v\in V}$ with inner products

$$s(u)\cdot s(v) = t(u)\cdot t(v) = A(u,v) \qquad \text{and} \qquad s(u)\cdot t(v) = B(u,v).$$

It follows that the functions $s$ and $t$ have the following properties:

1. $s(u)\cdot t(u) = 0$ for every $u \in V$,
2. $s(u)\cdot s(u) = t(u)\cdot t(u) = (\vartheta(\overline{G}) - 1)/2$ for every $u \in V$,
3. $s(u)\cdot s(v) = t(u)\cdot t(v) = 0$ whenever $\{u,v\} \in E$,
4. $s(u)\cdot t(v) = s(v)\cdot t(u) = 1/2$ whenever $\{u,v\} \in E$.

In the third step, we combine the two pairs of functions $S, T$ and $s, t$ to define

$$R(u) = s(u) \otimes S(f(u)) + t(u) \otimes T(f(u)).$$

Then, for adjacent vertices $u, v \in V$ we have

$$R(u)\cdot R(v) = E_r^{-1}(\beta(r,G) f(u)\cdot f(v)),$$

and moreover the $R(u)$ are unit vectors. Finally, we use the Gram decomposition of $(R(u)\cdot R(v)) \in \mathcal{S}_V^{+}$ to define the function $g : V \to S^{|V|-1}$. □

We conclude this section with a few remarks on the lemma and its proof:

1. The last sentence of the above proof of Lemma 5.4.1 states that there is a positive semidefinite matrix $Y \in \mathcal{S}_V^+$ which satisfies $Y(u,u) = 1$ and

$$Y(u,v) = E_r^{-1}(\beta(r,G)) f(u) \cdot f(v)$$

for every edge $\{u,v\}$ of $G$. As this matrix only has to satisfy linear constraints, it can be found in polynomial time in $|V|$ using a semidefinite program. Hence, the function $g : V \to S^{|V|-1}$ of the lemma, defined by the Gram decomposition of $Y$, can be found in polynomial time.

2. Krivine proved the statement of the lemma in the case $r = 1$ and for bipartite graphs $G$. Then, $\vartheta(\overline{G}) = 2$ holds. In this case one has various simplifications: One only needs the first step of the proof. Also, $\beta(1,G)$ can be computed analytically. We have $E_1^{-1}(t) = \sin(\pi/2t)$ and

$$\sum_{k=0}^{\infty} \left| (-1)^{2k+1} \frac{(\pi/2)^{2k+1}}{(2k+1)!} \right| t^{2k+1} = \sinh(\pi/2t).$$

Hence, $\beta(1,G) = 2 \operatorname{arcsinh}(1)/\pi = 2\ln(1+\sqrt{2})/\pi$.

3. In the second step one can also work with any feasible solution of the semidefinite program (5.2). For instance one can replace $\vartheta(\overline{G})$ in the lemma by the chromatic number $\chi(G)$ albeit getting a potentially weaker bound.

4. Alon, Makarychev, Makarychev, and Naor [AMMN06] also provide an upper bound for $K(1,G)$ using the theta number of the complement of $G$. They show that

$$K(1,G) \leq O(\log \vartheta(\overline{G}))$$

which is much better than our result in the case of large $\vartheta(\overline{G})$. However, our bound is favourable when $\vartheta(\overline{G})$ is small. In particular, we obtain

$$K(1,G) \leq \frac{2}{\pi \arcsin^{-1}\left(\vartheta(\overline{G}) - 1\right)}.$$

## 5.5 A refined, dimension-dependent analysis

So far we only bounded $K(\infty \mapsto r, G)$. One can perform a refined, dimension-dependent analysis by bounding $K(q \mapsto r, G)$ when $q \geq r$. This is of interest because for instance $\mathrm{SDP}_\infty(G, A) = \mathrm{SDP}_{|V|}(G, A)$. In this section we prove an upper bound for $K(q \mapsto r, G)$ that depends on $q$ and $r$. For fixed $r$, this upper bound will approach 1 as $q$ approaches $r$. Krivine [Kri79] gave such a refined analysis for bipartite graphs. We show that our upper bound on $K(q \mapsto r, G)$ is *strictly* smaller than our upper bound for $K(q + 1 \mapsto r, G)$.

**5.5.1.** LEMMA. *Let $G = (V, E)$ be a graph with at least one edge. Given $f\colon V \to S^{q-1}$, there is a function $g\colon V \to S^{|V|-1}$ such that whenever $u$ and $v$ are adjacent, then*

$$E_r(g(u) \cdot g(v)) = \beta(q \mapsto r, G) f(u) \cdot f(v),$$

*where $0 < \beta(q \mapsto r, G) \leq 1$ is such that $\beta(q \mapsto r, G) > \beta(q + 1 \mapsto r, G)$ and $\beta(q \mapsto r, G) > \beta(r, G)$ for all $q \geq 2$.*

Together with the analysis of Algorithm 5.1, this lemma implies the following bounds on $K(q \mapsto r, G)$.

**5.5.2.** THEOREM. *Let $G = (V, E)$ be a graph with at least one edge and let $q \geq r \geq 1$ be integers. Then $K(q \mapsto r, G) \leq \beta(q \mapsto r, G)^{-1}$.*

PROOF: Combine Lemma 5.5.1 with Algorithm 5.1. □

The proof of the lemma uses a few more basic facts from harmonic analysis, which we now summarize. Let $\overline{P}_k^n$ denote the renormalized version of the Gegenbauer polynomial $P_k^n$ (introduced in Section 4.3) such that $\overline{P}_k^n(1) = 1$. Let us recall the the Gegenbauer polynomials form a completely orthonormal basis for $L^2([-1, 1])$ for the inner product

$$(f, g)_n = \int_{-1}^{1} f(t)g(t)(1 - t^2)^{(n-3)/2}.$$

A polynomial in $\mathbb{R}[x_1, \ldots, x_n]$ is *harmonic* if it is homogeneous and vanishes under the Laplace operator $\Delta = \partial^2/\partial x_1^2 + \cdots + \partial^2/\partial x_n^2$. When restricted to $S^{n-1}$, harmonic polynomials are usually referred to as *spherical harmonics*. We endow the space of measurable functions on $S^{n-1}$ with the inner product

$$(f, g) = \int_{S^{n-1}} f(x)g(x)d\omega_n(x).$$

Spherical harmonics are related to Gegenbauer polynomials by the *addition formula* (see for example [AAR99, Theorem 9.6.3]): Let $H_k$ be the space of degree-$k$

spherical harmonics on $n$ variables. Any orthonormal basis of $H_k$ can be scaled to give a basis $e_{k,1}, \ldots, e_{k,d_k}$ of $H_k$ such that for every $x, y \in S^{n-1}$, we have

$$\overline{P}_k^n(x \cdot y) = \sum_{i=1}^{d_k} e_{k,i}(x) e_{k,i}(y).$$

With this we have all that we need to prove the lemma. We only consider the bipartite case in the proof in order to simplify the notation and to make the argument more transparent. One can handle the nonbipartite case exactly in the same way as in the proof of Lemma 5.4.1.

PROOF OF LEMMA 5.5.1: As before, we construct the function $g : V \to S^{|V|-1}$ from functions $S$ and $T$ that satisfy $S(x) \cdot T(y) = E_r^{-1}(\beta x \cdot y)$ for some real number $\beta$. Consider the expansion

$$E_r^{-1}(\beta t) = \sum_{k=0}^{\infty} c_k^q(\beta) \overline{P}_k^q(t).$$

**7.** CLAIM. *The function $h_q : [0,1] \to \mathbb{R}$ given by*

$$h_q(\beta) = \sum_{k=1}^{\infty} |c_k^q(\beta)|$$

*is continuous on its domain.*

Before proving the claim, we show how it is used to prove Lemma 5.5.1. Let $\beta(q \mapsto r, G)$ be the largest number $\beta \in [0,1]$ such that $h_q(\beta) = 1$. The fact that such a $\beta$ exists follows by the Intermediate Value Theorem, from the fact that $h_q(0) = 0$, $h_q(1) \geq E_r^{-1}(1) = 1$ and continuity of $h_q$.

Consider the Hilbert space

$$\mathcal{H} = \bigoplus_{k=0}^{\infty} \mathbb{R}^{d_k},$$

where $d_k$ is the dimension of $H_k$, the space of harmonic polynomials of degree $k$ on $q$ variables. For a vector $x \in S^{q-1}$, consider the vectors $S(x)$ and $T(x) \in \mathcal{H}$ given componentwise by

$$\begin{aligned} S(x)_k &= \sqrt{|c_k^q(\beta(q \mapsto r, G))|}\big(e_{k,1}(x), \ldots, e_{k,d_k}(x)\big) \\ T(x)_k &= \operatorname{sign}\big(c_k^q(\beta(q \mapsto r, G))\big)\sqrt{|c_k^q(\beta(q \mapsto r, G))|}\big(e_{k,1}(x), \ldots, e_{k,d_k}(x)\big). \end{aligned}$$

By the addition formula, we have

$$S\big(f(u)\big) \cdot T\big(f(v)\big) = E_r^{-1}\big(\beta(q \mapsto r, G) f(u) \cdot f(v)\big).$$

Moreover, from our normalization of the Gegenbauer polynomials $\overline{P}_k^q$ and the addition formula, it follows that we have

$$\|S\big(f(u)\big)\|_2^2 = \|T\big(f(v)\big)\|_2^2 = h_q\big(\beta(q \mapsto r, G)\big) = 1.$$

The desired function $g : V \to S^{|V|-1}$ can be obtained from the $2|V|$-by-$2|V|$ Gram matrix of the vectors $S\big(f(u)\big)$ and $T\big(f(v)\big)$.

Next, we show that for every $q \geq 2$, we have

$$\beta(q \mapsto r, G) > \beta(q+1 \mapsto r, G).$$

We prove this by showing that $h_q\big(\beta(q+1 \mapsto r, G)\big) < 1$, which is sufficient since, by definition, $\beta(q \mapsto r, G)$ is the largest $\beta \in [0,1]$ such that $h_q(\beta) = 1$. Recall that

$$h_q(\beta) \quad = \quad \sum_{k=0}^{\infty} |c_k^q(\beta)|,$$

where the functions $c_k^q$ came from the expansion

$$E_r^{-1}(\beta t) = \sum_{k=0}^{\infty} c_k^q(\beta) \overline{P}_k^q(t).$$

Using the expansion of $E_r^{-1}(\beta t)$ in terms of the polynomials $\overline{P}_1^{q+1}, \overline{P}_2^{q+1}, \ldots,$ we can thus write

$$c_k^q(\beta) = \frac{1}{\|\overline{P}_k^q\|_q^2}\big(E_r^{-1}(\beta t), \overline{P}_k^q\big)_q = \frac{1}{\|\overline{P}_k^q\|_q^2} \sum_{\ell=0}^{\infty} c_\ell^{q+1}(\beta)(\overline{P}_\ell^{q+1}, \overline{P}_k^q)_q.$$

The function $E_r^{-1}$ is not of positive type because the coefficient $b_3$ of its Taylor expansion is always negative (this can easily be checked using Eq. (5.3)). It follows that some of the $c_k^{q+1}(\beta)$ are negative. Hence,

$$h_q(\beta) = \sum_{k=0}^{\infty} |c_k^q(\beta)| <$$

$$\frac{1}{\|\overline{P}_k^q\|_q^2} \sum_{k,\ell=0}^{\infty} |c_\ell^{q+1}(\beta)| (\overline{P}_\ell^{q+1}, \overline{P}_k^q)_q =$$

$$\sum_{\ell=0}^{\infty} |c_\ell^{q+1}(\beta)| \left( \frac{1}{\|\overline{P}_k^q\|_q^2} \sum_{k=1}^{\infty} (\overline{P}_\ell^{q+1}, \overline{P}_k^q)_q \right).$$

It follows from the fact that the polynomials $\overline{P}_1^q, \overline{P}_2^q, \ldots$ form a complete orthogonal basis for $L^2([-1,1])$ with respect to the inner product $(\cdot,\cdot)_q$ and our choice of normalization $\overline{P}_k^{q+1}(1) = \overline{P}_k^q(1) = 1$ that the expression between brackets equals 1. This establishes that for any $\beta \in (0,1)$, we have $h_q(\beta) < h_{q+1}(\beta)$.

What is left to do, is to prove the claim.

PROOF OF CLAIM 7: We begin by showing that for any $\beta \in [0,1]$, the series

$$\sum_{k=0}^{\infty} |c_k^q(\beta)| \tag{5.4}$$

converges. For this, we use the comparison test. Consider the Taylor expansion of the function $E_r^{-1}$, given by

$$E_r^{-1}(t) = \sum_{k=0}^{\infty} b_k t^k,$$

and recall that the series $\sum_{k=0}^{\infty} |b_k|$ converges. Hence, by Schoenberg's Theorem (Theorem 4.2.3), the function

$$\overline{E}_r^{-1}(t) = \sum_{k=0}^{\infty} |b_k| t^k$$

is of positive type for $S^\infty$. In particular, this function is of positive type for $S^{q-1}$, and can therefore, by Theorem 4.3.1, be expanded in terms of the Gegenbauer polynomials as $\sum_{k=0}^{\infty} \bar{c}_k^q \overline{P}_k^q(t)$, for some $\bar{c}_0^q, \bar{c}_1^q, \cdots \geq 0$ such that $\sum_{k=0}^{\infty} \bar{c}_k^q$ converges.

By orthogonality of the Gegenbauer polynomials with respect to the inner product $(\cdot,\cdot)_q$, we have

$$\bar{c}_k^q = \frac{1}{\|\overline{P}_k^q\|_q^2} (\overline{E}_r^{-1}, \overline{P}_k^q)_q = \frac{1}{\|\overline{P}_k^q\|_q^2} \sum_{\ell=0}^{\infty} |b_\ell| (t^\ell, \overline{P}_k^q)_q \tag{5.5}$$

$$c_k^q(\beta) = \frac{1}{\|\overline{P}_k^q\|_q^2} (E_r^{-1}(\beta t), \overline{P}_k^q)_q = \frac{1}{\|\overline{P}_k^q\|_q^2} \sum_{\ell=0}^{\infty} b_\ell \beta^\ell (t^\ell, \overline{P}_k^q)_q. \tag{5.6}$$

Since for every $\ell$, the function $t \mapsto t^\ell$ is of positive type for $S^{q-1}$ (since it is of positive type for every dimension), we have $(t^\ell, \overline{P}_k^q)_q \geq 0$. Comparing Eq.'s (5.5) and (5.6), we see that for every $k$ and any $\beta \in [0,1]$, we have $|c_k^q(\beta)| \leq \bar{c}_k$. The fact that the series (5.4) converges now follows from the fact that $\sum_{k=0}^{\infty} \bar{c}_k$ converges.

The above discussion also establishes that for every every $k$, the function $c_k^q$ is continuous in $\beta$ on the interval $[0, 1]$, from which it follows that $\beta \mapsto |c_k^q(\beta)|$ is continuous there as well. The fact that the function $h_q$ is continuous now follows because, by convergence of (5.4), it can be approximated arbitrarily well by a finite sum of continuous functions. ♦

This completes the proof. □

## 5.6 Bounds for graphs with large chromatic number

For graphs with large chromatic number, our bounds on $K(r, G)$ proved above can be improved using the techniques of [AMMN06], which rely on so-called Gaussian Hilbert spaces (see also [JL01, AN06, KNS10]). In this section, we show how their bounds on $K(1, G)$ can be generalized to higher values of $r$.

**5.6.1.** THEOREM. *Given graph $G = (V, E)$ and positive integer $1 \le r \le \log \vartheta(\overline{G})$, we have*

$$K(r, G) \le \Theta\left(\frac{\log \vartheta(\overline{G})}{r}\right).$$

PROOF: It suffices to show that for any matrix $A : V \times V \to \mathbb{R}$, we have

$$\mathrm{SDP}_r(G, A) \ge \Omega\left(\frac{r}{\log \vartheta(\overline{G})}\right) \mathrm{SDP}_\infty(G, A).$$

Fix a matrix $A : V \times V \to \mathbb{R}$. Let $f : V \to S^{|V|-1}$ be optimal for the semidefinite relaxation of Problem 5.1 given the matrix $A$, so that

$$\sum_{\{u,v\} \in E} A(u, v) f(u) \cdot f(v) = \mathrm{SDP}_\infty(G, A).$$

Let $\widetilde{Z} : V \times V \to \mathbb{R}$ be an optimal solution for the Lovász-theta SDP. Let $J$ be the $2|V|$-by-$2|V|$ all-ones matrix and $I$ the 2-by-2 identity matrix. Since the matrix $(I \otimes \widetilde{Z} + J)/\lambda$ is positive semidefinite, we obtain from its Gram decomposition functions $s, t : V \to \mathbb{R}^{2|V|}$ that satisfy

1. $s(u) \cdot s(u) = t(u) \cdot t(u) = 1$ for all $u \in V$.

2. $s(u) \cdot t(u) = 1/\vartheta(\overline{G})$ for all $u, v \in V$.

3. $s(u) \cdot s(v) = t(u) \cdot t(v) = 0$ for all $\{u, v\} \in E$.

Let $\mathcal{H}$ be the Hilbert space of *vector-valued* functions $h : \mathbb{R}^{r\times|V|} \to \mathbb{R}^r$ such that for a random $r$-by-$|V|$ matrix $Z$ whose entries are i.i.d. $N(0, 1/r)$ distributed random variables, the inner product on $\mathcal{H}$ is defined by

$$(g, h) = \mathbb{E}_Z[g(Z) \cdot h(Z)].$$

We emphasize that elements of $\mathcal{H}$ map matrices to $r$-dimensional vectors.

Let $R \geq 2$ be some number to be set later. Define for every $u \in V$ the function $g_u \in \mathcal{H}$ by

$$g_u(Z) = \begin{cases} \frac{Zf(u)}{R} & \text{if } \|Zf(u)\|_2 \leq R \\ \frac{Zf(u)}{\|Zf(u)\|_2} & \text{otherwise,} \end{cases}$$

for $R$ satisfying the assumptions in the theorem. Notice that for every matrix $Z \in \mathbb{R}^{r\times|V|}$, the vector $g_u(Z) \in \mathbb{R}^r$ has Euclidean norm at most 1. It follows by linearity of expectation that

$$\mathrm{SDP}_r(G, A) \geq \mathbb{E}_Z\Bigg[\sum_{\{u,v\}\in E} A(u,v)\, g_u(Z) \cdot g_v(Z)\Bigg] = \sum_{\{u,v\}\in E} A(u,v)(g_u, g_v).$$

We proceed by lower bounding the right-hand side of the above inequality.

Based on the definition of $g_u$ we define two functions $h_u^0, h_u^1 \in \mathcal{H}$ by

$$h_u^0(Z) = \frac{Zf(u)}{R} + g_u(Z) \qquad \text{and} \qquad h_u^1(Z) = \frac{Zf(u)}{R} - g_u(Z).$$

Next, we define a function in the space $\mathbb{R}^{2|V|} \otimes \mathcal{H}$ by combining the vectors $s(u), t(v) \in \mathbb{R}^{2|V|}$ and $h_u^0, h_u^1 \in \mathcal{H}$. We endow this space with the natural inner product: For $x \otimes g, y \otimes h \in \mathbb{R}^{2|V|} \otimes \mathcal{H}$, define $\langle x \otimes g, y \otimes h\rangle = (x \cdot y)\,(g, h)$, and extend this inner product linearly so that it is defined for all of $\mathbb{R}^{2|V|} \otimes \mathcal{H}$. For every $u \in V$, define the function $H_u \in \mathbb{R}^{2|V|} \otimes \mathcal{H}$ by

$$H_u = \frac{1}{4}s(u) \otimes h_u^0 + 2\vartheta(\overline{G})\, t(u) \otimes h_u^1.$$

We expand the inner products $(g_u, g_v)$ in terms of $f(u) \cdot f(v)$ and $\langle H_u, H_v\rangle$.

**8.** CLAIM. *For every $\{u, v\} \in E$ we have*

$$(g_u, g_v) \quad = \quad \frac{1}{R^2} f(u) \cdot f(v) - \langle H_u, H_v\rangle.$$

PROOF: Simply expanding the inner product $\langle H_u, H_v \rangle$ gives

$$\begin{aligned}\langle H_u, H_v \rangle &= \frac{s(u)\cdot s(v)}{16}(h_u^0, h_v^0) \;+\; 4\vartheta(\overline{G})^2\big(t(u)\cdot t(v)\big)\,(h_u^1, h_v^1) + \\ &\quad \frac{\vartheta(\overline{G})}{2}\Big[\big(s(u)\cdot t(v)\big)\,(h_u^0, h_v^1) \;+\; \big(t(u)\cdot s(v)\big)\,(h_u^1, h_v^0)\Big].\end{aligned}$$

It follows from property 3 of $s$ and $t$ that the above terms involving $s(u)\cdot s(v)$ and $t(u)\cdot t(v)$ vanish. By property 2, the remaining terms reduce to

$$\begin{aligned}\frac{1}{2}\Big((h_u^0, h_v^1) + (h_u^1, h_u^0)\Big) &= \frac{1}{2}\mathbb{E}_Z\left[\left(\frac{Zf(u)}{R} + g_u(Z)\right)\cdot\left(\frac{Zf(v)}{R} - g_v(Z)\right)\right] + \\ &\quad \frac{1}{2}\mathbb{E}_Z\left[\left(\frac{Zf(u)}{R} - g_u(Z)\right)\cdot\left(\frac{Zf(v)}{R} + g_v(Z)\right)\right].\end{aligned}$$

Expanding the first expectation gives

$$\frac{1}{R^2}\mathbb{E}_Z[f(u)^T Z^T Z f(v)] - (g_u, g_v) - \mathbb{E}_Z\left[\frac{Zf(u)}{R}\cdot g_v(Z)\right] + \mathbb{E}_Z\left[g_u(Z)\cdot\frac{Zf(v)}{R}\right]$$

and expanding the second gives

$$\frac{1}{R^2}\mathbb{E}_Z[f(u)^T Z^T Z f(v)] - (g_u, g_v) + \mathbb{E}_Z\left[\frac{Zf(u)}{R}\cdot g_v(Z)\right] - \mathbb{E}_Z\left[g_u(Z)\cdot\frac{Zf(v)}{R}\right].$$

Adding these two gives that the last two terms cancel. Since $\mathbb{E}_Z[Z^T Z] = I$, what remains equals

$$\frac{1}{R^2}f(u)\cdot f(v) - (g_u, g_v),$$

which proves the claim. ♦

From the above claim it follows that

$$\begin{aligned}\sum_{\{u,v\}\in E} A(u,v)(g_u, g_v) &= \frac{1}{R^2}\mathrm{SDP}_\infty(G,A) - \sum_{\{u,v\}\in E} A(u,v)\langle H_u, H_v\rangle \\ &\geq \left(\frac{1}{R^2} - \max_{u\in V}\|H_u\|_2^2\right)\mathrm{SDP}_\infty(G,A),\end{aligned}$$

where $\|H_u\|_2^2 = \langle H_u, H_u\rangle$.

By the triangle inequality, we have for every $u \in V$,

$$\|H_u\|_2^2 \leq \frac{1}{R^2}\left(\frac{1}{2} + 2\vartheta(\overline{G})R\,\mathbb{E}_Z\left[\left\|\frac{Zf(u)}{R} - g_u(Z)\right\|_2^2\right]\right)^2.$$

By the definition of $g_u$, the vectors $Zf(u)$ and $g_u$ are parallel. Moreover, they are equal if $\|Zf(u)\|_2 \leq R$. Since $f(u)$ is a unit vector, the $r$ entries of the random vector $Zf(u)$ are i.i.d. $N(0, 1/r)$ random variables. Hence,

$$\begin{aligned}
\mathbb{E}_Z \left[ \left\| \frac{Zf(u)}{R} - g_u(Z) \right\|_2^2 \right] &= \int_{\mathbb{R}^r} \mathbf{1}[\|x\| \geq R] \Big( \frac{\|x\|}{R} - 1 \Big) \Big( \frac{r}{2\pi} \Big)^{r/2} e^{-r\|x\|^2/2} dx \\
&= \int_R^\infty \int_{S^{r-1}} \rho^{r-1} \Big( \frac{\rho}{R} - 1 \Big) \Big( \frac{r}{2\pi} \Big)^{r/2} e^{-r\rho^2/2} d\rho d\tilde{\omega}_r(\xi) \\
&\leq \frac{r^{r/2}}{R\Gamma\big(\frac{r}{2}\big)} \int_R^\infty \rho^r e^{-r\rho^2/2} d\rho,
\end{aligned}$$

where $\tilde{\omega}_r$ is the unique rotationally invariant measure on $S^{r-1}$, normalized such that $\tilde{\omega}_r(S^{r-1}) = r^{r/2}/\Gamma(r/2)$. Using a substitution of variables, we get

$$\int_R^\infty \rho^r e^{-r\rho^2/2} d\rho = \frac{1}{2} \Big( \frac{2}{r} \Big)^{(r+1)/2} \Gamma\Big( \frac{r+1}{2}, \frac{rR^2}{2} \Big),$$

where $\Gamma(a, x)$ is the lower incomplete Gamma function [AAR99, Eq. (4.4.5)].

Collecting the terms from above then gives the bound

$$\mathrm{SDP}_r(G, A) \geq \frac{1}{R^2} \left( 1 - \left( \frac{1}{2} + \vartheta(\overline{G}) \frac{2^{(r+1)/2}}{\sqrt{r}\Gamma\big(\frac{r}{2}\big)} \Gamma\Big( \frac{r+1}{2}, \frac{rR^2}{2} \Big) \right)^2 \right) \mathrm{SDP}_\infty(G, A). \tag{5.7}$$

The bound in the theorem follows by setting $R$ as small as possible such that the above factor between brackets is some positive constant.

By Stirling's formula, we have that for some constant $C_1 > 0$, the inequality $\Gamma(x) \geq C_1 e^{-x} x^{x-1/2}$ holds (see for example [AS64, Eq. (6.1.37)]). Hence, for some constants $c, C > 0$, we have

$$\frac{2^{(r+1)/2}}{\sqrt{r}\Gamma\big(\frac{r}{2}\big)} \leq C \left( \frac{c}{r} \right)^{r/2} \tag{5.8}$$

The power series of the incomplete gamma function (see for example [AS64, Eq. (6.5.32)]) gives that if $a \leq x$, for some constant $C_2 > 0$, the inequality $\Gamma(a, x) \leq C_2 x^a e^{-x}$ holds. As $R \geq 2$, for some constants $d, D > 0$, we have

$$\Gamma\left( \frac{r+1}{2}, \frac{rR^2}{2} \right) \leq D\sqrt{r} \left( \frac{r}{d^{R^2}} \right)^{r/2}. \tag{5.9}$$

Putting together estimates (5.8) and (5.9) gives

$$\vartheta(\overline{G}) \frac{2^{(r+1)/2}}{\sqrt{r}\Gamma\big(\frac{r}{2}\big)} \Gamma\left( \frac{r+1}{2}, \frac{rR^2}{2} \right) \;\leq\; CD\sqrt{r}\vartheta(\overline{G}) \left( \frac{c}{d^{R^2}} \right)^{r/2}.$$

Since $r \leq \log \vartheta(\overline{G})$ there is some constant $C'$ such that for $R^2 = C'\big(\log \vartheta(\overline{G})\big)/r$, the above value is less than $1/4$. It follows that for this value of $R$, Inequality (5.7) is nontrivial and we get the result. □

## 5.7 Summary

In this chapter, we proved the first upper bounds depending on $r$ on the rank-$r$ graphical Grothendieck constants $K(r, G)$ for $r > 1$, giving a $1/K(r, G)$-approximation algorithm for the graphical Grothendieck problem with rank-$r$ constraint based on its natural semidefinite relaxation. In particular, we obtained the best known approximation results for approximating the ground state energy for the Heisenberg model when the interaction graph has small chromatic number.