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A RECURSIVE LOVÁSZ THETA NUMBER FOR SIMPLEX-AVOIDING SETS

DAVI CASTRO-SILVA, FERNANDO MÁRIO DE OLIVEIRA FILHO, LUCAS SLOT,
AND FRANK VALLENTIN

(Communicated by Isabella Novik)

Abstract. We recursively extend the Lovász theta number to geometric hypergraphs on the unit sphere and on Euclidean space, obtaining an upper bound for the independence ratio of these hypergraphs. As an application we reprove a result in Euclidean Ramsey theory in the measurable setting, namely that every k -simplex is exponentially Ramsey, and we improve existing bounds for the base of the exponential.

1. Introduction

The Lovász theta number $\vartheta(G)$ of a finite graph G satisfies $\alpha(G) \leq \vartheta(G) \leq \chi(\overline{G})$, where $\alpha(G)$ is the independence number of G and $\chi(\overline{G})$ is the chromatic number of the complement \overline{G} of G , the graph whose edges are the non-edges of G ; the theta number can be computed efficiently using semidefinite programming.

Originally, Lovász [18] introduced ϑ to determine the Shannon capacity of the 5-cycle. The theta number turned out to be a versatile tool in optimization, with applications in combinatorics and geometry. It is related to spectral bounds like Hoffman’s bound, as noted by Lovász in his paper (cf. Bachoc, DeCorte, Oliveira, and Vallentin [2]), and also to Delsarte’s linear programming bound in coding theory, as observed independently by McEliece, Rodemich, and Rumsey [19] and Schrijver [28].

Bachoc, Nebe, Oliveira, and Vallentin [3] extended ϑ to infinite geometric graphs on compact metric spaces. They also showed that this extension leads to the classical linear programming bound for spherical codes of Delsarte, Goethals, and Seidel [9]; the linear programming bound of Cohn and Elkies for the sphere-packing density [6] can also be seen as an appropriate extension of ϑ [17, 21]. These many applications illustrate the power of the Lovász theta number as a unifying concept in optimization; Goemans [15] even remarked that “it seems all paths lead to ϑ !”.

We will show how a recursive variant of ϑ can be used to find upper bounds for the independence ratio of geometric hypergraphs on the sphere and on Euclidean space; this will lead to new bounds for a problem in Euclidean Ramsey theory.

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1.1. Unit sphere. We call a set $\{x_1, \dots, x_k\}$ of $k \geq 2$ points on the $(n - 1)$ -dimensional unit sphere $S^{n-1} = \{x \in \mathbb{R}^n : \|x\| = 1\}$ a (k, t) -simplex if $x_i \cdot x_j = t$ for all $i \neq j$. The convex hull of a (k, t) -simplex has dimension $k - 1$. There is a (k, t) -simplex on S^{n-1} for every $k \leq n$ and $t \in [-1/(k - 1), 1)$.

Fix $n \geq k \geq 2$ and $t \in [-1/(k - 1), 1)$. A set of points on S^{n-1} avoids (k, t) -simplices if no k points in the set form a (k, t) -simplex. We are interested in the parameter

$\alpha(S^{n-1}, k, t) = \sup\{\omega(I) : I \subseteq S^{n-1} \text{ is measurable and avoids } (k, t)\text{-simplices}\}$, where ω is the surface measure on the sphere normalized so the total measure is 1.

This is the independence ratio of the hypergraph whose vertex set is S^{n-1} and whose edges are all (k, t) -simplices.

In §2 we will define the parameter $\vartheta(S^{n-1}, k, t)$ recursively as the optimal value of the problem

$$\begin{aligned} \sup_{f \in C([-1, 1])} \int_{S^{n-1}} \int_{S^{n-1}} f(x \cdot y) d\omega(y) d\omega(x) \\ f(1) = 1, \\ f(t) \leq \vartheta(S^{n-2}, k - 1, t/(1 + t)), \end{aligned}$$

$f \in C([-1, 1])$ is a function of positive type for S^{n-1}

for $k \geq 3$. The base of the recursion is $k = 2$: $\vartheta(S^{n-1}, 2, t)$ is the optimal value of the problem above when “ $f(t) \leq \vartheta(S^{n-2}, k - 1, t/(1 + t))$ ” is replaced by “ $f(t) = 0$ ”.

From Theorem 2.1 it follows that $\vartheta(S^{n-1}, k, t) \geq \alpha(S^{n-1}, k, t)$. Using extremal properties of ultraspherical polynomials, an explicit formula can be computed for this bound, as shown in Theorem 2.2.

1.2. Euclidean space. Transferring these concepts from the compact unit sphere to the non-compact Euclidean space requires a bit of care; this is done in §3.

A unit k -simplex in \mathbb{R}^n is a set $\{x_1, \dots, x_k\}$ of $k \leq n + 1$ points such that $\|x_i - x_j\| = 1$ for all $i \neq j$. As before, the dimension of the convex hull of a unit k -simplex is $k - 1$. A set of points in \mathbb{R}^n avoids unit k -simplices if no k points in the set form a unit k -simplex. We are interested in the parameter

$$\alpha(\mathbb{R}^n, k) = \sup\{\bar{\delta}(I) : I \subseteq \mathbb{R}^n \text{ is measurable and avoids unit } k\text{-simplices}\},$$

where $\bar{\delta}(X)$ is the upper density of $X \subseteq \mathbb{R}^n$, that is,

$$\bar{\delta}(X) = \limsup_{T \rightarrow \infty} \frac{\text{vol}(X \cap [-T, T]^n)}{\text{vol}[-T, T]^n}.$$

Again, this parameter has an interpretation in terms of the independence ratio of a hypergraph on the Euclidean space and again we can bound the independence ratio from above by an appropriately defined parameter $\vartheta(\mathbb{R}^n, k)$. Theorem 3.2 gives an explicit expression for $\vartheta(\mathbb{R}^n, k)$ in terms of Bessel functions and ultraspherical polynomials.

1.3. Euclidean Ramsey theory. The central question of Euclidean Ramsey theory is: given a finite configuration P of points in \mathbb{R}^n and an integer $r \geq 1$, does every r -coloring of \mathbb{R}^n contain a monochromatic congruent copy of P ?

The simplest point configurations are unit k -simplices, which are known to have the exponential Ramsey property: the minimum number $\chi(\mathbb{R}^n, k)$ of colors needed to color the points of \mathbb{R}^n in such a way that there are no monochromatic unit k -simplices grows exponentially in n . This was first proved by Frankl and Wilson [14]

for $k = 2$ and by Frankl and Rödl [13] for $k > 2$. Results in this area are usually proved by the linear algebra method; see also Sagdeev [24].

Recently, Naslund [20] used the slice-rank method from the work of Croot, Lev, and Pach [7] and Ellenberg and Gijswijt [11] on the cap-set problem¹ to prove that

$$\chi(\mathbb{R}^n, 3) \geq (1.01466 + o(1))^n.$$

This is the best lower bound known at the moment.

For simplices of higher dimension, Sagdeev [25] used a quantitative version of the Frankl-Rödl theorem to show that

$$\chi(\mathbb{R}^n, k) \geq 1 + \frac{1}{2^{2^{k+3}}} + o(1)^n.$$

Denote by $H(n, k)$ the *unit-distance hypergraph*, namely the k -uniform hypergraph whose vertex set is \mathbb{R}^n and whose edges are all unit k -simplices. The parameter $\chi(\mathbb{R}^n, k)$ is the chromatic number of this hypergraph. A theorem of de Bruijn and Erdős [5] shows² that computing $\chi(\mathbb{R}^n, k)$ is a combinatorial problem: the chromatic number of $H(n, k)$ is the maximum chromatic number of any finite subgraph of $H(n, k)$.

Determining $\chi(\mathbb{R}^n, 2)$ is known as the Nelson-Hadwiger problem. The problem was proposed by Nelson in 1950 (cf. Soifer [29, Chapter 3]), who used the Moser spindle, a 4-chromatic 7-vertex subgraph of $H(2, 2)$, to show that $\chi(\mathbb{R}^2, 2) \geq 4$. Isbell (cf. Soifer, *ibid.*), also in 1950, proved that $\chi(\mathbb{R}^2, 2) \leq 7$ by constructing a coloring of $H(2, 2)$.

The difficulty of finding subgraphs of $H(2, 2)$ with chromatic number higher than 4 led Falconer [12] to define the *measurable chromatic number* $\chi_m(\mathbb{R}^n, 2)$ by requiring the color classes to be Lebesgue-measurable sets; we define $\chi_m(\mathbb{R}^n, k)$ likewise for $k \geq 3$. Of course, $\chi_m(\mathbb{R}^n, k) \geq \chi(\mathbb{R}^n, k)$, but it is not known whether the two numbers differ. Falconer could show that $\chi_m(\mathbb{R}^2, 2) \geq 5$, whereas a proof that $\chi(\mathbb{R}^2, 2) \geq 5$ was only obtained more than three decades later by de Grey [16], who found by computer a 5-chromatic subgraph of $H(2, 2)$ with 1581 vertices.

The restriction to measurable color classes also helps improving asymptotic lower bounds. Frankl and Wilson [14] give a combinatorial proof that

$$\chi(\mathbb{R}^n, 2) \geq (1.2 + o(1))^n.$$

By analyzing a strengthening of the extension of the theta number given by Oliveira and Vallentin [22], Bachoc, Passuello, and Thiery [4] could show that

$$\chi_m(\mathbb{R}^n, 2) \geq (1.268 + o(1))^n.$$

Similarly, the analytical tools developed here can also be used to improve lower bounds for $\chi_m(\mathbb{R}^n, k)$. Since

$$(1) \quad \alpha(\mathbb{R}^n, k)\chi_m(\mathbb{R}^n, k) \geq 1,$$

any upper bound for $\alpha(\mathbb{R}^n, k)$ gives a lower bound for $\chi_m(\mathbb{R}^n, k)$, hence

$$\chi_m(\mathbb{R}^n, k) \geq \frac{1}{\alpha(\mathbb{R}^n, k)}.$$

¹The slice-rank method is only implicit in the original works; the actual notion of slice rank for a tensor was introduced by Tao in a blog post [31].

²De Bruijn and Erdős consider only $k = 2$, but their result can be easily generalized to $k \geq 3$.

In §4 we analyze the upper bounds $\mathcal{G}(S^{n-1}, k, t)$ for simplex-avoiding sets on the sphere and $\mathcal{G}(\mathbb{R}^n, k)$ for simplex-avoiding sets on Euclidean space by using properties of ultraspherical polynomials, obtaining Theorem 1.1.

Theorem 1.1. *If $k \geq 2$, then:*

- (i) *for every $t \in (0, 1)$, there is a constant $c = c(k, t) \in (0, 1)$ such that $\mathcal{G}(S^{n-1}, k, t) \leq (c + o(1))^n$;*
- (ii) *there is a constant $c = c(k) \in (0, 1)$ such that $\mathcal{G}(\mathbb{R}^n, k) \leq (c + o(1))^n$.*

From this theorem we get an exponential lower bound for $\chi_m(\mathbb{R}^n, k)$. Rigorous estimates of the constant c then yield significantly better lower bounds for $\chi_m(\mathbb{R}^n, k)$ than those coming from $\chi(\mathbb{R}^n, k)$.

Namely, in the case $k = 3$ we obtain (see §4.1)

$$\alpha(\mathbb{R}^n, 3) \leq (0.95622 + o(1))^n,$$

and so

$$\chi_m(\mathbb{R}^n, 3) \geq (1.04578 + o(1))^n.$$

We also obtain the rougher estimate

$$\alpha(\mathbb{R}^n, k) \leq \left(1 - \frac{1}{9(k-1)^2} + o(1) \right)^n,$$

valid for all $k \geq 3$, which immediately implies

$$\chi_m(\mathbb{R}^n, k) \geq \left(1 + \frac{1}{9(k-1)^2} + o(1) \right)^n.$$

Though our lower bounds for $\chi_m(\mathbb{R}^n, k)$ do not necessarily hold for $\chi(\mathbb{R}^n, k)$, they do imply some structure for general colorings. If a coloring of $H(n, k)$ uses fewer than $1/\alpha(\mathbb{R}^n, k)$ colors, then the closure of one of the color classes is a measurable set with density greater than $\alpha(\mathbb{R}^n, k)$, and so it contains a unit k -simplex. This means that in such a coloring there are monochromatic k -point configurations arbitrarily close to unit k -simplices.

1.4. Notation and preliminaries. We will denote the Euclidean inner product between $x, y \in \mathbb{R}^n$ by $x \cdot y$. The surface measure on the sphere is denoted by ω and is always normalized so the total measure is 1.

We always normalize the Haar measure on a compact group so the total measure is 1. By $O(n)$ we denote the group of $n \times n$ orthogonal matrices. If $X \subseteq S^{n-1}$ is any measurable set and if μ is the Haar measure on $O(n)$, then for every $e \in S^{n-1}$ we have $\mu(\{ T \in O(n) : Te \in X \}) = \omega(X)$.

We will need Lemma 1.2, which will be applied to the sphere and the torus. For a proof, see Lemma 5.5 in DeCorte, Oliveira, and Vallentin [8].

Lemma 1.2. *Let V be a metric space and Γ be a compact group that acts transitively on V ; let ν be a finite Borel measure on V that is positive on open sets. Denote by μ the Haar measure on Γ . If the metric on V and the measure ν are Γ -invariant and if $f \in L^2(V; \nu)$, then the function $K : V \times V \rightarrow \mathbb{R}$ such that*

$$K(x, y) = \int_{\Gamma} f(\sigma x)f(\sigma y) d\mu(\sigma)$$

is continuous.

2. Simplex-avoiding sets on the sphere

We call a continuous kernel $K : S^{n-1} \times S^{n-1} \rightarrow \mathbb{R}$ *positive* if for every finite set

$U \subseteq S^{n-1}$ the matrix $(K(x, y))_{x, y \in U}$ is positive semidefinite. A continuous function $f : [-1, 1] \rightarrow \mathbb{R}$ is of *positive type* for S^{n-1} if the kernel $K \in C(S^{n-1} \times S^{n-1})$ given by $K(x, y) = f(x \cdot y)$ is positive.

Fix $n \geq k \geq 3$ and $t \in [-1/(k - 1), 1)$. For any $\gamma \geq 0$, consider the optimization problem

$$(2) \quad \begin{aligned} & \sup_{S^{n-1}} \int_{S^{n-1}} f(x \cdot y) d\omega(y) d\omega(x) \\ & f(1) = 1, \\ & f(t) \leq \gamma, \\ & f \in C([-1, 1]) \text{ is a function of positive type for } S^{n-1}. \end{aligned}$$

Theorem 2.1. Fix $n \geq k \geq 3$, $t \in [-1/(k - 1), 1)$. If $\gamma \geq \alpha(S^{n-2}, k - 1, t/(1 + t))$, then the optimal value of (2) is an upper bound for $\alpha(S^{n-1}, k, t)$.

Proof. Let $I \subseteq S^{n-1}$ be a measurable set that avoids (k, t) -simplices and assume $\omega(I) > 0$. Consider the kernel $K : S^{n-1} \times S^{n-1} \rightarrow \mathbb{R}$ such that

$$K(x, y) = \int_{O(n)} \chi_I(Tx) \chi_I(Ty) d\mu(T),$$

where χ_I is the characteristic function of I and where μ is the Haar measure on $O(n)$.

By taking $V = S^{n-1}$ and $\Gamma = O(n)$ in Lemma 1.2, we see that K is continuous. By construction, K is also positive and invariant, that is, $K(Tx, Ty) = K(x, y)$ for all $T \in O(n)$ and $x, y \in S^{n-1}$. Such kernels are of the form $K(x, y) = g(x \cdot y)$, where $g \in C([-1, 1])$ is of positive type for S^{n-1} . Note that

$$K(x, x) = \int_{O(n)} \chi_I(Tx) d\mu(T) = \omega(I),$$

so $g(1) = \omega(I) > 0$.

Set $f = g/g(1)$. Immediately we have that f is continuous and of positive type and that $f(1) = 1$; moreover

$$\int_{S^{n-1}} \int_{S^{n-1}} f(x \cdot y) d\omega(y) d\omega(x) = \omega(I).$$

Hence, if we show that $f(t) \leq \gamma$, the theorem will follow.

If $x \in S^{n-1}$ is a point in a (k, t) -simplex, all other points in the simplex are in $U_{x,t} = \{ y \in S^{n-1} : y \cdot x = t \}$. Note that $U_{x,t}$ is an $(n - 2)$ -dimensional sphere with radius $(1 - t^2)^{1/2}$; let ν be the surface measure on $U_{x,t}$ normalized so the total measure is 1.

If $T \in O(n)$ is any orthogonal matrix, then TI avoids (k, t) -simplices. Hence if $x \in TI$, then $TI \cap U_{x,t}$ cannot contain $k - 1$ points with pairwise inner product t , and so $\nu(TI \cap U_{x,t}) \leq \alpha(S^{n-2}, k - 1, t/(1 + t)) \leq \gamma$. Indeed, the natural bijection between $U_{x,t}$ and S^{n-2} maps pairs of points with inner product t to pairs of points with inner product $t/(1+t)$, and so $TI \cap U_{x,t}$ is mapped to a subset of S^{n-2} avoiding $(k - 1, t/(1 + t))$ -simplices.

Therefore, if $x \in S^{n-1}$, then

$$\begin{aligned} g(t) &= \int_{U_{x,t}} K(x, y) \, dv(y) = \int_{U_{x,t}} \int_{O(n)} \chi_I(Tx)\chi_I(Ty) \, d\mu(T)dv(y) \\ &= \int_{O(n)} \chi_I(Tx) \int_{U_{x,t}} \chi_I(Ty) \, dv(y)d\mu(T) \\ &\leq \gamma\omega(I), \end{aligned}$$

whence $f(t) \leq \gamma$, and we are done. □

One obvious choice for γ in Problem (2) is the bound given by the same problem for $(k - 1, t/(1 + t))$ -simplices. The base for the recursion is $k = 2$: then we need an upper bound for the measure of a set of points on the sphere that avoids pairs of points with a fixed inner product. Such a bound was given by Bachoc, Nebe, Oliveira, and Vallentin [3] and looks very similar to (2). They show that, for $n \geq 2$ and $t \in [-1, 1)$, the optimal value of the following optimization problem is an upper bound for $\alpha(S^{n-1}, 2, t)$:

$$\begin{aligned} (3) \quad & \sup_{f: S^{n-1} \rightarrow S^{n-1}} \int_{S^{n-1}} f(x \cdot y) \, d\omega(y)d\omega(x) \\ & f(1) = 1, \\ & f(t) = 0, \\ & f \in C([-1, 1]) \text{ is a function of positive type for } S^{n-1}. \end{aligned}$$

Let $\mathcal{G}(S^{n-1}, 2, t)$ denote the optimal value of the optimization problem above, so $\mathcal{G}(S^{n-1}, 2, t) \geq \alpha(S^{n-1}, 2, t)$. For $k \geq 3$ and $t \in [-1/(k - 1), 1)$, let $\mathcal{G}(S^{n-1}, k, t)$ be the optimal value of Problem (2) when $\gamma = \mathcal{G}(S^{n-2}, k - 1, t/(1 + t))$. It follows that $\mathcal{G}(S^{n-1}, k, t) \geq \alpha(S^{n-1}, k, t)$.

There is a simple analytical expression for $\mathcal{G}(S^{n-1}, k, t)$, as we see now. For $n \geq 2$ and $j \geq 0$, let P_j^α denote the Jacobi polynomial with parameters $\alpha = \beta = (n - 3)/2$ and degree j , normalized so $P_j^\alpha(1) = 1$ (for background on Jacobi polynomials, see the book by Szegő [30]).

In Theorem 6.2 of Bachoc, Nebe, Oliveira, and Vallentin [3] it is shown that for every $t \in [-1, 1)$ there is some $j \geq 0$ such that $P_j^\alpha(t) < 0$. Theorem 8.21.8 in the book by Szegő [30] implies that, for every $t \in (-1, 1)$,

$$(4) \quad \lim_{j \rightarrow \infty} P_j^\alpha(t) = 0.$$

Hence, for every $t \in (-1, 1)$ we can define

$$(5) \quad M_n(t) = \min\{P_j^\alpha(t) : j \geq 0\},$$

and we see that $M_n(t) < 0$. With this we have [3, Theorem 6.2]

$$(6) \quad \mathcal{G}(S^{n-1}, 2, t) = \frac{-M_n(t)}{1 - M_n(t)}.$$

The expression for $\mathcal{G}(S^{n-1}, k, t)$ is very similar.

Theorem 2.2. *If $n \geq k \geq 3$ and if $t \in [-1/(k - 1), 1)$, then*

$$(7) \quad \mathcal{G}(S^{n-1}, k, t) = \frac{\mathcal{G}(S^{n-2}, k - 1, t/(1 + t)) - M_n(t)}{1 - M_n(t)}.$$

The proof requires the following characterization of functions of positive type due to Schoenberg [27]: a function $f: [-1, 1] \rightarrow \mathbb{R}$ is continuous and of positive type for S^{n-1} if and only if there are nonnegative numbers f_0, f_1, \dots such that $\sum_{j=0}^{\infty} f_j < \infty$ and

$$(8) \quad f(t) = \sum_{j=0}^{\infty} f_j P_j^n(t),$$

with uniform convergence in $[-1, 1]$.

Proof of Theorem 2.2. The orthogonality of the Jacobi polynomials P_j^n implies in particular that, if $j \geq 1$, then

$$\int_{S^{n-1}} \int_{S^{n-1}} P_j^n(x \cdot y) d\omega(y) d\omega(x) = 0.$$

Use this and Schoenberg’s characterization of positive type functions to rewrite (2) with $\gamma = \mathcal{G}(S^{n-2}, k - 1, t/(1 + t))$, obtaining the equivalent problem

$$\begin{aligned} \sup & \sum_{j=0}^{\infty} f_j = 1, \\ & \sum_{j=0}^{\infty} f_j P_j^n(t) \leq \mathcal{G}(S^{n-2}, k - 1, t/(1 + t)), \\ & f_j \geq 0 \text{ for all } j \geq 0. \end{aligned}$$

To solve this problem, note that

$$\sum_{j=0}^{\infty} f_j P_j^n(t)$$

is a convex combination of the numbers $P_j^n(t)$. We want to keep this convex combination below $\mathcal{G}(S^{n-2}, k - 1, t/(1 + t))$ while maximizing f_0 . The best way to do so is to concentrate all the weight of the combination on f_0 and f_{j^*} , where j^* is such that $P_{j^*}^n(t)$ is the most negative number appearing in the convex combination, that is, $P_{j^*}^n(t) = M_n(t)$. Now solve the problem using only the variables f_0 and f_{j^*} to get the optimal value as given in the statement of the theorem. \square

The expression for $\mathcal{G}(S^{n-1}, k, 0)$ is particularly simple. Indeed, for $n \geq 2$ it follows from the recurrence relation for the Jacobi polynomials that $M_n(0) = P_n^n(0) = -1/(n - 1)$, whence

$$\mathcal{G}(S^{n-1}, k, 0) = (k - 1)/n.$$

Figure 1 shows the behavior of $\mathcal{G}(S^{n-1}, 3, t)$ for a few values of n as t changes. Plots for $k > 3$ are very similar.

3. Simplex-avoiding sets in Euclidean space

An optimization problem similar to (2) provides an upper bound for $\alpha(\mathbb{R}^n, k)$. To introduce it, we need some definitions and facts from harmonic analysis on \mathbb{R}^n ; for background, see e.g. the book by Reed and Simon [23].

A continuous function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is of *positive type* if for every finite set $U \subseteq \mathbb{R}^n$ the matrix $f(x - y)_{x,y \in U}$ is positive semidefinite. Such a function f has a well-defined *mean value*

$$M(f) = \lim_{T \rightarrow \infty} \frac{1}{\text{vol}[-T, T]^n} \int_{[-T, T]^n} f(x) dx.$$

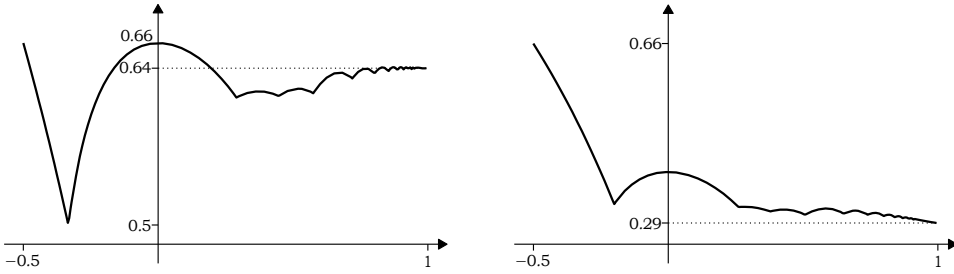


Figure 1. Plots of $g(S^{n-1}, 3, t)$ for $t \in [-0.5, 1]$ and $n = 3$ (left) and 5 (right)

We say that a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is *radial* if $f(x)$ depends only on $\|x\|$. In this case we denote by $f(t)$ the common value of f for vectors of norm t .

Fix $n \geq 2$ and $k \geq 3$ such that $k \leq n + 1$. For every $\gamma \geq 0$, consider the optimization problem

$$(9) \quad \begin{aligned} &\sup M(f) \\ &f(0) = 1, \\ &f(1) \leq \gamma, \\ &f: \mathbb{R}^n \rightarrow \mathbb{R} \text{ is continuous, radial, and of positive type.} \end{aligned}$$

We have the analogue of Theorem 2.1:

Theorem 3.1. Fix $n \geq 2$ and $k \geq 3$ such that $k \leq n + 1$. If $\gamma \geq a(S^{n-1}, k-1, 1/2)$, then the optimal value of (9) is an upper bound for $a(\mathbb{R}^n, k)$.

We need a few facts about periodic sets and functions. A set $X \subseteq \mathbb{R}^n$ is *periodic* if it is invariant under some lattice Λ , that is, if $X + v = X$ for all $v \in \Lambda$. Similarly, a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is *periodic* if there is a lattice Λ such that $f(x + v) = f(x)$ for all $v \in \Lambda$. We say that Λ is a *periodicity lattice* of X or f . A periodic function f with periodicity lattice Λ can be seen as a function on the torus \mathbb{R}^n/Λ ; its mean value is

$$\frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n/\Lambda} f(x) dx.$$

Proof of Theorem 3.1. Let $I \subseteq \mathbb{R}^n$ be a measurable set of positive upper density avoiding unit k -simplices. The first step is to see that we can assume that I is periodic. Indeed, fix $R > 1/2$. Erase a border of width $1/2$ around $I \cap [-R, R]^n$ and paste the resulting set periodically in such a way that there is an empty gap of width 1 between any two pasted copies. The resulting periodic set still avoids unit k -simplices and is measurable. Its upper density is

$$\frac{\text{vol}(I \cap [-R + 1/2, R - 1/2]^n)}{\text{vol}[-R, R]^n};$$

by taking R large enough, we can make this density as close as we want to the upper density of I .

Assume then that I is periodic, so its characteristic function χ_I is also periodic; let Λ be a periodicity lattice of I . Set

$$g(x) = \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n/\Lambda} \chi_I(y) \chi_I(x + y) dy.$$

Lemma 1.2 with $V = \Gamma = \mathbb{R}^n/\Lambda$ applied to χ_I implies that g is continuous. Direct verification yields that g is of positive type, $g(\mathbf{o}) = \bar{\delta}(I)$, and $M(g) = \bar{\delta}(I)^2$.

Now set

$$f(x) = \bar{\delta}(I)^{-1} \int_{\mathbf{O}(n)} g(Tx) \, d\mu(T),$$

where μ is the Haar measure on $\mathbf{O}(n)$. The function f is continuous, radial, and of positive type. Moreover, $f(\mathbf{o}) = 1$ and $M(f) = \bar{\delta}(I)$. If we show that $f(\mathbf{1}) \leq \gamma$, then f is a feasible solution of (9) with $M(f) = \bar{\delta}(I)$, and so the theorem will follow.

To see that $f(\mathbf{1}) \leq \gamma$, note that if x is a point of a unit k -simplex in \mathbb{R}^n , then all the other points in the simplex lie on the unit sphere $x + S^{n-1}$ centered at x . Hence if $x \in I$, then $I \cap (x + S^{n-1})$ is a measurable subset of $x + S^{n-1}$ that avoids $(k - 1, 1/2)$ -simplices, and so the measure of $I \cap (x + S^{n-1})$ as a subset of the unit sphere is at most $\alpha(S^{n-1}, k - 1, 1/2)$. Hence if $\zeta \in \mathbb{R}^n$ is any unit vector, then

$$\begin{aligned} f(\mathbf{1}) &= \bar{\delta}(I)^{-1} \int_{\mathbf{O}(n)} g(T\zeta) \, d\mu(T) \\ &= \bar{\delta}(I)^{-1} \int_{\mathbf{O}(n)} \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n/\Lambda} \chi_I(x) \chi_I(T\zeta + x) \, dx \, d\mu(T) \\ &= \bar{\delta}(I)^{-1} \frac{1}{\text{vol}(\mathbb{R}^n/\Lambda)} \int_{\mathbb{R}^n/\Lambda} \chi_I(x) \int_{\mathbf{O}(n)} \chi_I(T\zeta + x) \, d\mu(T) \, dx \\ &\leq \alpha(S^{n-1}, k - 1, 1/2) \leq \gamma, \end{aligned}$$

as we wanted. □

Denote by $\mathcal{G}(\mathbb{R}^n, k)$ the optimal value of (9) when setting $\gamma = \mathcal{G}(S^{n-1}, k - 1, 1/2)$. Then $\mathcal{G}(\mathbb{R}^n, k) \geq \alpha(\mathbb{R}^n, k)$.

An expression akin to the one for $\mathcal{G}(S^{n-1}, k, t)$ can be derived for $\mathcal{G}(\mathbb{R}^n, k)$. For $n \geq 2$, let

$$\Omega_n(\mathbf{o}) = 1 \quad \text{and} \quad \Omega_n(u) = \Gamma(n/2)(2/u)^{(n-2)/2} J_{(n-2)/2}(u) \quad \text{for } u > \mathbf{o},$$

where J_α is the Bessel function of the first kind with parameter α . Let m_n be the global minimum of Ω_n , which is a negative number (cf. Oliveira and Vallentin [22]). Theorem 3.2 is the analogue of Theorem 2.2.

Theorem 3.2. *For $n \geq 2$ we have*

$$\mathcal{G}(\mathbb{R}^n, k) = \frac{\mathcal{G}(S^{n-1}, k - 1, 1/2) - m_n}{1 - m_n}.$$

The proof uses again a theorem of Schoenberg [26], that this time characterizes radial and continuous functions of positive type on \mathbb{R}^n : these are the functions $f: \mathbb{R}^n \rightarrow \mathbb{R}$ such that

$$(10) \quad f(x) = \int_0^\infty \Omega_n(z \setminus x \setminus) \, d\nu(z)$$

for some finite Borel measure ν .

Proof. If f is given as in (10), then $M(f) = \nu(\{\mathbf{o}\})$ (see e.g. §6.2 in DeCorte, Oliveira, and Vallentin [8]). Using Schoenberg's theorem, we can rewrite (9) (with

Table 1. The bound $\mathcal{G}(\mathbb{R}^n, k)$ for $n = 2, \dots, 10$ and $k = 3, \dots, 11$, with values of n on each row and of k on each column

n / k	3	4	5	6	7	8	9	10	11
2	0.64355	—	—	—	—	—	—	—	—
3	0.42849	0.69138	—	—	—	—	—	—	—
4	0.29346	0.49798	0.73225	—	—	—	—	—	—
5	0.20374	0.36768	0.55035	0.76580	—	—	—	—	—
6	0.15225	0.28471	0.42777	0.60262	0.79563	—	—	—	—
7	0.11866	0.22740	0.34071	0.48493	0.64681	0.81972	—	—	—
8	0.09339	0.18405	0.27471	0.39559	0.53374	0.68268	0.83882	—	—
9	0.07387	0.15030	0.22864	0.33042	0.44903	0.57816	0.71431	0.85537	—
10	0.05846	0.12340	0.19194	0.27851	0.38158	0.49496	0.61521	0.74026	0.86882

$\gamma = \mathcal{G}(S^{n-1}, k - 1, 1/2)$ equivalently as:

$$\begin{aligned} & \sup v(\{0\}) \\ & v([0, \infty)) = 1, \\ & \int_0^\infty \Omega_n(z) dv(z) \leq \mathcal{G}(S^{n-1}, k - 1, 1/2), \\ & v \text{ is a Borel measure.} \end{aligned}$$

We are now in the same situation as in the proof of Theorem 2.2. If z^* is such that $m_n = \Omega_n(z^*)$, then the optimal v is supported at 0 and z^* . Solving the resulting system yields the theorem. \square

Table 1 contains some values for $\mathcal{G}(\mathbb{R}^n, k)$.

4. Exponential density decay

In this section we analyze the asymptotic behavior of $\mathcal{G}(S^{n-1}, k, t)$ and $\mathcal{G}(\mathbb{R}^n, k)$ as functions of n , proving Theorem 1.1.

The main step in our analysis is to understand the asymptotic behavior of

$$M_n(t) = \min\{P_j^n(t) : j \geq 0\},$$

as defined in (5). For $t \in [-1, 0)$ we have $M_n(t) \leq P_0^n(t) = t$, and so $M_n(t)$ does not approach 0 . We have seen in §2 that $M_n(0) = -1/(n - 1)$, so for $t = 0$ we have that $M_n(t)$ approaches 0 linearly fast as n grows. Things get interesting when $t \in (0, 1)$: then $M_n(t)$ approaches 0 exponentially fast as n grows.

Theorem 4.1. *For every $t \in (0, 1)$ there is $c \in (0, 1)$ such that $|M_n(t)| \leq (c + o(1))^n$.*

We will need Lemma 4.2 showing that, for every $t \in (0, 1)$, if $j = \Omega(n)$, then $|P_j^n(t)|$ decays exponentially in n . Theorem 4.1 will follow from an application of this lemma after we show that the minimum in (5) is attained for some $j^* = \Omega(n)$. The statement of the lemma is quite precise since we later want to do a more detailed analysis of the base of the exponential. The proof is a refinement of the analysis carried out by Schoenberg [27].

Lemma 4.2. *If for $\theta \in (0, \pi)$ and $\delta \in (0, \pi/2)$ we write*

$$C = (\cos^2 \theta + \sin^2 \theta \sin^2 \delta)^{1/2},$$

then $|P_j^n(\cos \theta)| \leq \pi n^{1/2} \cos^{n-3} \delta + C^j$ for all $n \geq 3$.

Proof. An integral representation for the ultraspherical polynomials due to Gegenbauer (take $\lambda = (n - 2)/2$ in Theorem 6.7.4 from Andrews, Askey, and Roy [1]) gives us the formula

$$P_j^n(\cos \theta) = R(n)^{-1} \int_0^\pi F(\varphi)^j \sin^{n-3} \varphi \, d\varphi,$$

where

$$F(\varphi) = \cos \theta + i \sin \theta \cos \varphi \quad \text{and} \quad R(n) = \int_0^\pi \sin^{n-3} \varphi \, d\varphi.$$

Note that $|F(\varphi)|^2 = \cos^2 \theta + \sin^2 \theta \cos^2 \varphi$ and that $|F(\varphi)| \leq 1$. Split the integration domain into the intervals $[0, \pi/2 - \delta]$, $[\pi/2 - \delta, \pi/2 + \delta]$, and $[\pi/2 + \delta, \pi]$ to obtain

$$\begin{aligned} |P_j^n(\cos \theta)| &\leq R(n)^{-1} \int_0^\pi |F(\varphi)|^j \sin^{n-3} \varphi \, d\varphi \\ &\leq 2R(n)^{-1} \int_0^{\pi/2-\delta} \sin^{n-3} \varphi \, d\varphi + R(n)^{-1} \int_{\pi/2-\delta}^{\pi/2+\delta} |F(\varphi)|^j \sin^{n-3} \varphi \, d\varphi. \end{aligned}$$

For the first term above, note that

$$R(n) = \frac{\pi^{1/2} \Gamma(n/2 - 1)}{\Gamma((n - 1)/2)}.$$

Use Gautschi's inequality (alternatively, take $x = (n - 2)/2$ and $a = 1/2$ in (7) of Wendel [32]) to get

$$R(n)^{-1} \leq \pi^{-1/2} ((n - 2)/2)^{1/2} < n^{1/2}.$$

Now

$$\begin{aligned} 2R(n)^{-1} \int_0^{\pi/2-\delta} \sin^{n-3} \varphi \, d\varphi &\leq 2n^{1/2} \int_0^{\pi/2-\delta} \sin^{n-3}(\pi/2 - \delta) \, d\varphi \\ &= 2n^{1/2}(\pi/2 - \delta) \cos^{n-3} \delta \\ &\leq \pi n^{1/2} \cos^{n-3} \delta. \end{aligned}$$

For the second term we get directly

$$R(n)^{-1} \int_{\pi/2-\delta}^{\pi/2+\delta} |F(\varphi)|^j \sin^{n-3} \varphi \, d\varphi \leq R(n)^{-1} \int_{\pi/2-\delta}^{\pi/2+\delta} C^j \sin^{n-3} \varphi \, d\varphi \leq Cj,$$

and we are done. □

We can now prove the theorem.

Proof of Theorem 4.1. Our strategy is to find a lower bound on the largest j_0 such that $P_j^n(t) \geq 0$ for all $j \leq j_0$. Then we know that $M_n(t)$ is attained by some $j \geq j_0$, and we can use Lemma 4.2 to estimate $|M_n(t)|$.

Recall [30, Theorem 3.3.2] that the zeros of P_j^n are all in $[-1, 1]$ and that the rightmost zero of P_{j+1}^n is to the right of the rightmost zero of P_j^n . Let C_j^λ denote the ultraspherical (or Gegenbauer) polynomial with parameter λ and degree j , so

$$(11) \quad P_j^n(t) = \frac{C_j^{(n-2)/2}(t)}{C_j^{(n-2)/2}(1)}.$$

Let x_j be the largest zero of C_j^λ . Elbert and Laforgia [10, p. 94] show that, for $\lambda \geq 0$,

$$x_j^2 < \frac{j^2 + 2\lambda j}{(j + \lambda)^2}.$$

If for a given j we have that

$$(12) \quad \frac{j^2 + 2\lambda j}{(j + \lambda)^2} \leq t^2,$$

then we know that the rightmost zero of C_j^λ is to the left of t , and so $C_j^\lambda(t) \geq 0$.

The left-hand side in (12) is increasing in j ; let us estimate the largest j for which (12) holds. We want

$$j^2 + 2\lambda j - t^2(j + \lambda)^2 \leq 0.$$

The left-hand side above is quadratic in j and, since $t^2 < 1$, the coefficient of j^2 is positive. So all we have to do is to compute the largest root of the left-hand side, which is $2a(t)\lambda$, where $a(t) = ((1 - t^2)^{-1/2} - 1)/2$. Hence for $j \leq 2a(t)\lambda$ we have $C_j^\lambda(t) \geq 0$. From (11) we see that $P_j^n(t) \geq 0$ if

$$j \leq a(t)n - 2a(t).$$

Now plug the right-hand side above into the upper bound of Lemma 4.2 to get

$$\begin{aligned} |M_n(t)| &\leq (\pi n^{1/2} \cos^{-3} \delta) \cos^n \delta + C^{a(t)n-2a(t)} \\ &= O(n^{1/2})(\cos \delta)^n + O(1)(C^{a(t)})^n, \end{aligned}$$

with C as defined in Lemma 4.2 with $\cos \theta = t$. Since $a(t) > 0$, for any choice of $\delta \in (0, \pi/2)$ we have that $b = \max\{\cos \delta, C^{a(t)}\} \in (0, 1)$. Hence if c is any number such that $b < c < 1$, then $\lim_{n \rightarrow \infty} O(n^{1/2})b^n/c^n = 0$, and the theorem follows. \square

We now get exponential decay for $\mathcal{G}(S^{n-1}, k, t)$ for any $k \geq 3$ and $t \in (0, 1)$. Indeed, consider the recurrence $F_0 = t$ and $F_i = F_{i-1}/(1 + F_{i-1})$ for $i \geq 1$, whose solution is $F_i = t/(1 + it)$. Using Theorem 4.1 to develop our analytic solution (7), we get

$$(13) \quad \mathcal{G}(S^{n-1}, k, t) \sim \sum_{i=0}^{k-2} |M_{n-i}(F_i)| = \sum_{i=0}^{k-2} |M_{n-i}(t/(1 + it))|,$$

where $a_n \sim b_n$ means that $\lim_{n \rightarrow \infty} a_n/b_n = 1$. Since $t/(1 + it) > 0$ for all i , each term decays exponentially fast, and so we get exponential decay for the sum.

We also get exponential decay for $\mathcal{G}(R^n, k)$ for any $k \geq 3$. Indeed, from Theorem 3.2 we have that

$$(14) \quad \mathcal{G}(R^n, k) \sim |m_n| + \sum_{i=0}^{k-3} |M_{n-i}(1/(2 + i))|.$$

From Theorem 4.1 we know that every term in the summation above decays exponentially fast. Bachoc, Nebe, Oliveira, and Vallentin [3] give an asymptotic bound for $|m_n|$ that shows that it also decays exponentially in n , namely

$$|m_n| \leq (2/e + o(1))^{n/2} = (0.8577\dots + o(1))^n.$$

This finishes the proof of Theorem 1.1.

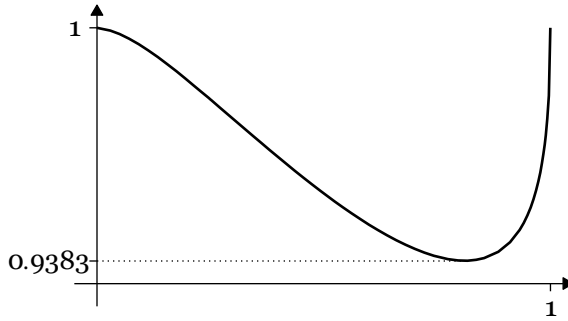


Figure 2. The best constant c obtained in our proof of Theorem 4.1 for each value of $t \in (0, 1)$.

4.1. Explicit bounds. We now compute explicit constants $c(k, t)$ and $c(k)$ which can serve as bases for the exponentials in Theorem 1.1, in particular obtaining the bounds advertised in §1.3.

The constant c given in Theorem 4.1 depends on t . Following the proof, we can find the best constant for every $t \in (0, 1)$ by finding $\delta \in (0, \pi/2)$ such that $\cos \delta = C^{a(t)}$, that is, by solving the equation

$$(15) \quad \cos^4 \delta = (t^2 + (1 - t^2) \sin^2 \delta)^{(1-t^2)^{-1/2}-1}$$

and taking $c = \cos \delta > 0$.

For any given $t \in (0, 1)$ it is easy to solve (15) numerically. For $t = 1/2$ we get $\cos \delta = 0.95621 \dots$ as a solution, and so $|M_n(1/2)| \leq (0.95622 + o(1))^n$, leading to the the bound

$$\mathcal{G}(\mathbb{R}^n, 3) \sim |M_n(1/2)| \leq (0.95622 + o(1))^n.$$

Figure 2 shows a plot of the best constant c for every $t \in (0, 1)$.

With a little extra work, it is possible to show that, for all $k \geq 2$,

$$(16) \quad |M_n(1/k)| \leq \left(1 - \frac{1}{9k^2} + o(1) \right)^n,$$

whence

$$\mathcal{G}(\mathbb{R}^n, k) \sim |M_{n-k+3}(1/(k-1))| \leq \left(1 - \frac{1}{9(k-1)^2} + o(1) \right)^n$$

for all $k \geq 3$.

Direct verification shows that (16) holds for $k = 2$, so let us assume $k \geq 3$. Writing c for the (unique) positive solution $\cos \delta$ of (15) and taking $\theta \in (0, \pi/2)$ such that $\cos \theta = t$, we can rewrite (15) in the more convenient form

$$(17) \quad c^{4 \sin \theta / (1 - \sin \theta)} = 1 - c^2 \sin^2 \theta.$$

Now say $c = 1 - x$ and use Bernoulli's inequality $(1 + z)^r \geq 1 + rz$ to get

$$(1 - x)^{4 \sin \theta / (1 - \sin \theta)} \geq 1 - \frac{4 \sin \theta}{1 - \sin \theta} x \quad \text{and}$$

$$1 - (1 - x)^2 \sin^2 \theta \leq 1 - (1 - 2x) \sin^2 \theta.$$

Equating the left-hand sides of both inequalities above and solving for x , we get

$$c = 1 - x \leq 1 - \frac{\sin \theta(1 - \sin \theta)}{4 + 2 \sin \theta(1 - \sin \theta)}.$$

In particular, when $\cos \theta = 1/k$ we get

$$\begin{aligned} |M_n(1/k)| &\leq 1 - \frac{1}{4k^2(1 + \sqrt{\frac{1}{k^2(k^2 - 1)}}) + 2} + o(1)^n \\ &\leq 1 - \frac{1}{9k^2} + o(1)^n \end{aligned}$$

for all $k \geq 3$.

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