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NEW UPPER BOUNDS FOR SPHERICAL CODES AND PACKINGS

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Abstract. We improve the previously best known upper bounds on the sizes of θ-spherical codes for every $\theta < \theta^* \approx 62.997^\circ$ at least by a factor of 0.4325, in sufficiently high dimensions. Furthermore, for sphere packing densities in dimensions $n \geq 2000$ we have an improvement at least by a factor of $0.4325 + \frac{51}{n}$. Our method also breaks many non-numerical sphere packing density bounds in small dimensions. Apart from Cohn and Zhao's [CZ14] improvement on the geometric average of Levenshtein's bound [Lev79] over all sufficiently high dimensions by a factor of 0.79, our work is the first improvement for each dimension since the work of Kabatyanskii and Levenshtein [KL78] and its later improvement by Levenshtein [Lev79]. Moreover, we generalize Levenshtein's optimal polynomials and provide explicit formulae for them that may be of independent interest. For $0 < \theta < \theta^*$, we construct a test function for Delsarte's linear programing problem for θ-spherical codes with exponentially improved factor in dimension compared to previous test functions.

1. Introduction

1.1. **Sphere packings.** Packing densities have been studied extensively, for purely mathematical reasons as well as for their connections to coding theory. The work of Conway and Sloane is a comprehensive reference for this subject [CS99]. We proceed by defining the basics of this subject. Consider $\mathbb{R}^n$ equipped with the Euclidean metric $|.|$ and the associated volume vol(.). For each real $r > 0$ and each $x \in \mathbb{R}^n$, we denote by $B_n(x, r)$ the open ball in $\mathbb{R}^n$ centered at x and of radius r. For each discrete set of points $S \subset \mathbb{R}^n$ such that any two distinct points $x, y \in S$ satisfy $|x - y| \geq 2$, we can consider

$$\mathcal{P} := \cup_{x \in S} B_n(x, 1),$$

the union of non-overlapping unit open balls centered at the points of S. This is called a *sphere packing* (S may vary), and we may associate to it the function mapping each real $r > 0$ to

$$\delta_{\mathcal{P}}(r) := \frac{\mathrm{vol}(\mathcal{P} \cap B_n(0, r))}{\mathrm{vol}(B_n(0, r))}.$$

The *packing density* of $\mathcal{P}$ is defined as

$$\delta_{\mathcal{P}} := \limsup_{r\to\infty} \delta_{\mathcal{P}}(r).$$

Clearly, this is a finite number. The *maximal sphere packing density* in $\mathbb{R}^n$ is defined as

$$\delta_n := \sup_{\mathcal{P}\subset\mathbb{R}^n} \delta_{\mathcal{P}},$$

a supremum over all sphere packings $\mathcal{P}$ of $\mathbb{R}^n$ by non-overlapping unit balls.

The linear programming method initiated by Delsarte is a powerful tool for giving upper bounds on sphere packing densities [Del72]. That being said, we only know the optimal sphere packing densities in dimensions 1,2,3,8 and 24 [FT43, Hal05, Via17, CKM$^+$17]. In dimension 1, this is trivial with $\delta_1 = 1$. In dimension 2, the best sphere packing is achieved by the usual hexagonal lattice packing with $\delta_2 = \pi/\sqrt{12}$. A rigorous proof was provided by L. Fejes Tóth in 1943 [FT43]; however, a proof was also given earlier by A.Thue in 1910 [Thu10], but it was considered incomplete by some experts in the field. In dimension 3, this is the subject of the Kepler conjecture, and was resolved in 1998 by T.Hales [Hal05]. As a result of his work, we know that $\delta_3 = \pi/\sqrt{18}$. The other two known cases of optimal sphere packings were famously resolved in dimensions 8 and 24 by M. Viazovska and her collaborators in 2016. Based on some of the ideas of Cohn and Elkies [CE03], M. Viazovska first resolved the dimension 8 case [Via17]. Shortly afterward, she along with Cohn, Kumar, Miller, and Radchenko resolved the case of 24 dimensions [CKM$^+$17]. As a result of her work, we now know that the maximal packing in 8 dimensions is obtained by the E_8-lattice with $\delta_8 = \pi^4/384$. In 24 dimensions, it is achieved by the Leech lattice with $\delta_{24} = \pi^{12}/(12!)$. All these optimal sphere packings come from even unimodular lattices. Very recently, the first author proved an optimal upper bound on the sphere packing density of all but a tiny fraction of even unimodular lattices in high dimensions; see [Sar19, Theorem 1.1].

The best known upper bounds on sphere packing densities in low dimensions are based on the linear programming method developed by Cohn and Elkies [CE03] which itself is inspired by Delsarte's linear programing method. More recently the upper bounds have been improved in low dimensions using the semi-definite linear programing method [dLdOFV14]. However, in high dimensions, the most successful method to date for obtaining asymptotic upper bounds goes back to Kabatyanskii–Levenshtein from 1978 [KL78]. This method is based on first bounding from above the maximal size of spherical codes using Delsarte's linear programming method. We discuss this in the next subsection.

1.2. **Spherical codes.** A notion closely related to sphere packings of Euclidean spaces is that of spherical codes. Given S^{n-1}, the unit sphere in $\mathbb{R}^n$, a *θ-spherical code* is a finite subset $A \subset S^{n-1}$ such that no two distinct $x, y \in A$ are at an angular distance less than θ. For each $0 < \theta \leq \pi$, we define $M(n, \theta)$ to be the largest cardinality of a θ-spherical code $A \subset S^{n-1}$.

Suppose that $p_m^{\alpha,\beta}(t)$ is, up to normalization, the Jacobi polynomial of degree m with parameters (α, β). We denote by $t_{1,m}^{\alpha,\beta}$ its largest root. Levenshtein proved the following inequality using Delsarte's linear programing method. See Section 2 for a summary of results on Jacobi polynomials.

Theorem 1.1 (Levenshtein, Theorem 6.2 of [Lev98]). *If $\cos\theta \leq t_{1,\ell-\varepsilon}^{\alpha+1,\alpha+\varepsilon}$ for some $0 < \theta < \pi/2$, some ℓ, $\varepsilon \in \{0, 1\}$, and $\alpha := \frac{n-3}{2}$, then*

$$M(n, \theta) \leq \binom{\ell + n - 2}{n-1} + \binom{\ell + n - 1 - \varepsilon}{n-1}.$$

This is a less refined version of an upper bound proved by Levenshtein where the right hand side is given by the value of a functional applied to a polynomial depending on θ. We will shortly discuss this functional in the general setting of this paper. This theorem of Levenshtein was preceeded by a weaker theorem of Kabatyanskii–Levenshtein from 1978 [KL78].The bounds on sphere packing densities follow from such bounds on spherical codes via an elementary geometric argument that allows to relate sphere packings in $\mathbb{R}^n$ to spherical codes. Indeed, for any $0 < \theta \leq \pi/2$, Sidelnikov [Sid74] proved that

$$\delta_n \leq \frac{M(n+1,\theta)}{\mu_n(\theta)}, \tag{1}$$

where $\mu_n(\theta) := 1/\sin^n(\theta/2)$. Let $\theta^* := 62.997...^\circ$ be the unique root of the equation $\cos\theta \log(\frac{1+\sin\theta}{1-\sin\theta}) - (1+\cos\theta)\sin\theta = 0$. In [KL78], Kabatyanskii and Levenshtein proved the following bound by using inequality (1) for θ^* and a weaker form of Theorem 1.1 [KL78, (52)] to bound $M(n,\theta^*)$ (it gives the same exponent 0.599 as using Theorem 1.1).

Theorem 1.2 (Kabatyanskii–Levenshtein, 1978)**.** *As $n \to \infty$,*

$$\delta_n \leq 2^{-0.599n(1+o(1))}.$$

Let $0 \leq \theta < \theta' \leq \pi$. We write $\mu_n(\theta,\theta')$ for the *mass* of the cap with radius $\frac{\sin(\theta/2)}{\sin(\theta'/2)}$ on the unit sphere S^{n-1} (with respect to the natural probability measure). The best known bounds on $M(n,\theta)$ for $\theta < \theta^*$ are obtained via a similar elementary argument of Sidelnikov [Sid74] stating that for $0 < \theta < \theta' \leq \pi$

$$M(n,\theta) \leq \frac{M(n+1,\theta')}{\mu_n(\theta,\theta')}. \tag{2}$$

Indeed Barg and Musin [BM07, p.11 (8)], based on the work [AVZ00] of Agrell, Vargy, and Zeger, improved the above inequality and showed that

$$M(n,\theta) \leq \frac{M(n-1,\theta')}{\mu_n(\theta,\theta')}. \tag{3}$$

whenever $\pi > \theta' > 2\arcsin\left(\frac{1}{2\cos(\theta/2)}\right)$. As demonstrated by Kabatyanskii–Levenshtein in [KL78], for large dimensions n and $0 < \theta < \theta^*$ the linear programming upper bound on $M(n,\theta)$ is exponentially weaker than the one obtained from the combination of the linear programming upper bound on $M(n,\theta^*)$ with inequality (2) for $M(n,\theta)$. Cohn and Zhao [CZ14] improved sphere packing density upper bounds by combining the above upper bound of Kabatyanskii–Levenshtein on $M(n,\theta)$ with their analogue of (3) when $\theta \to 0$ [CZ14, Proposition 2.1] stating that for $\pi/3 \leq \theta \leq \pi$,

$$\delta_n \leq \frac{M(n,\theta)}{\mu_n(\theta)}, \tag{4}$$

leading to better bounds than those obtained from (1). Thus, their improvement is a consequence of a geometric argument at the level of comparing sphere packings to spherical codes. Our first result removes the angular restrictions on the Barg and Musin result. In the following, let $s := \cos\theta$, $s' := \cos\theta'$, $r := \sqrt{\frac{s-s'}{1-s'}}$,

$$\gamma_{\theta,\theta'} := 2\arctan\frac{s}{\sqrt{(1-s)(s-s')}} + \arccos(r) - \pi,$$

and

$$R := \cos(\gamma_{\theta,\theta'}).$$

Proposition 1.3. *Let $0 < \theta < \theta' < \pi$. We have*

$$M(n, \theta) \leq \frac{M(n-1, \theta')}{\mu_n(\theta, \theta')}(1 + O(ne^{-nc})), \tag{5}$$

where $c := \frac{1}{2}\log\left(\frac{1-r^2}{1-R^2}\right) > 0$ is independent of n and only depends on θ and θ'.

We prove this Proposition in Section 3. A completely analogous result removes the restriction $\theta \geq \pi/3$ from Cohn and Zhao's result.

Remark 6. Asymptotically as $n \to \infty$, Proposition 1.3 combined with the asymptotic bound on spherical codes due to Kabatyanskii–Levenshtein improves the best bound on $M(n, \theta)$ on (geometric) average by a factor $0.62 \sim (0.79)^2$ for every $\theta < \theta'$ and $\theta' > 2\arcsin\left(\frac{1}{2\cos(\theta/2)}\right)$. This improvement for spherical codes is the square of the improvement of Cohn and Zhao for the sphere packing density.

Our main theorem regarding spherical codes is a linear programming variant of the inequality (5) which we state in the next section. The variant of inequality (5) is improved with an extra factor 0.4325 for each sufficiently large n (rather than averaging over all high dimensions). In the case of sphere packings, we obtain the same asymptotic improvement. Furthermore, we show that for dimensions $n \geq 2000$ we obtain an improvement by a factor of $0.4325 + \frac{51}{n}$. As a consequence, we obtain a constant improvement to all previously known linear programming bounds on spherical codes and sphere packing densities. Our improvement does not lead to an improvement of the exponent 0.599 in Theorem 1.2; this exponent is to this day the best known. That being said, our geometric ideas combined with numerics lead to improvements that are better than the 0.4325 proved above.

1.3. **Constant improvement.** First, we discuss Delsarte's linear programming method, and then we state our main theorem.

Throughout this paper, we work with *probability* measures μ on $[-1, 1]$. μ gives an inner product on the space of real polynomials $\mathbb{R}[t]$, and let $\{p_i\}_{i=0}^{\infty}$ be an orthonormal basis with respect to μ such that the degree of p_i is i and $p_i(1) > 0$ for every i. Note that $p_0 = 1$. Such a basis is uniquely determined by μ. Suppose that the basis elements p_k define positive definite functions on S^{n-1}, namely

$$\sum_{x_i, x_j \in A} h_i h_j p_k\left(\langle x_i, x_j\rangle\right) \geq 0 \tag{7}$$

for any finite subset $A \subset S^{n-1}$ and any real numbers $h_i \in \mathbb{R}$. An example of a probability measure satisfying inequality (7) is

$$d\mu_\alpha := \frac{(1-t^2)^\alpha}{\int_{-1}^{1}(1-t^2)^\alpha dt}dt,$$

where $\alpha \geq \frac{n-3}{2}$ and $2\alpha \in \mathbb{Z}$. Given $s \in [-1, 1]$, consider the space $D(\mu, s)$ of all functions $f(t) = \sum_{i=0}^{\infty} f_i p_i(t)$, $f_i \in \mathbb{R}$, such that

(1) $f_i \geq 0$ and $f_0 > 0$,
(2) $f(t) \leq 0$ for $-1 \leq t \leq s$.

Suppose $0 < \theta < \pi$, and $A = \{x_1, \ldots, x_N\}$ is a θ-spherical code in S^{n-1}. Given a function $f \in D(\mu, \cos\theta)$, we consider

$$\sum_{i,j} f(\langle x_i, x_j\rangle).$$

This may be written in two different ways as

$$Nf(1) + \sum_{i \neq j} f(\langle x_i, x_j \rangle) = f_0 N^2 + \sum_{k=1}^{\infty} f_k \sum_{i,j} p_k(\langle x_i, x_j \rangle).$$

Since $f \in D(\mu, \cos\theta)$ and $\langle x_i, x_j \rangle \leq \cos\theta$ for every $i \neq j$, this gives us the inequality

$$N \leq \frac{f(1)}{f_0}.$$

We define $\mathcal{L}(f) := \frac{f(1)}{f_0}$. In particular, this method leads to the linear programming bound

$$M(n,\theta) \leq \inf_{f \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)} \mathcal{L}(f). \tag{8}$$

Levenshtein proved Theorem 1.1 by introducing a family of even and odd degree polynomials inside $D(d\mu_{\frac{n-3}{2}}, \cos\theta)$ that minimize $\mathcal{L}(f)$ among all polynomials of smaller degrees inside $D(d\mu_{\frac{n-3}{2}}, \cos\theta)$. We call them Levenshtein's polynomials. Let $g_{\theta'} \in D(d\mu_{\frac{n-4}{2}}, \cos\theta')$ be the Levenshtein polynomial associated to angle θ' and dimension $n-1$. As we pointed out, for $\theta < \theta^*$ the best known upper bounds so far are obtained from a combination of variants of inequality (2) or our (5) to linear programming bounds (8) for the angle θ^*, at least in high dimensions. However, it is possible to directly provide a function inside $D(d\mu_{\frac{n-3}{2}}, \cos\theta)$ for $\theta < \theta^*$ that *improves* this bound without relying on inequality (5). We now state one of our main theorems.

Theorem 1.4. *Fix $\theta < \theta^*$. Suppose $0 < \theta < \theta' \leq \pi/2$, where $\cos(\theta') = t_{1,d-\varepsilon}^{\alpha+1,\alpha+\varepsilon}$ for some $\varepsilon \in \{0,1\}$ and $\alpha := \frac{n-4}{2}$. Then there is a function $h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$ such that*

$$\mathcal{L}(h) \leq c_n \frac{\mathcal{L}(g_{\theta'})}{\mu_n(\theta, \theta')},$$

where $c_n \leq 0.4325$ for large enough n independent of θ and θ'.

Corollary 1.5. *Fix $0 < \theta < \theta^*$. There exists a solution to Delsarte's linear programing problem for θ-spherical codes with exponentially improved factor in dimension compared to Levenshtein's optimal polynomials for θ-spherical codes.*

Proof. By [KL78, Theorem 4]

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{L}(g_\theta) = \frac{1+\sin\theta}{2\sin\theta} \log \frac{1+\sin\theta}{2\sin\theta} - \frac{1-\sin\theta}{2\sin\theta} \log \frac{1-\sin\theta}{2\sin\theta}.$$

Let $h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$, which minimizes $\mathcal{L}(h)$. By the first part of Theorem 1.4, we have

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{L}(h) \leq \inf_{\pi/2 \geq \theta' > \theta} \left(\frac{1+\sin\theta'}{2\sin\theta'} \log \frac{1+\sin\theta'}{2\sin\theta'} - \frac{1-\sin\theta'}{2\sin\theta'} \log \frac{1-\sin\theta'}{2\sin\theta'} \right) - \lim_{n\to\infty} \frac{\log \mu_n(\theta, \theta')}{n}.$$

It is easy to show that [KL78, Proof of Theorem 4]

$$\lim_{n\to\infty} \frac{\log \mu_n(\theta, \theta')}{n} = \frac{1}{2} \log \frac{1-\cos\theta}{1-\cos\theta'}.$$

Hence,

$$\lim_{n\to\infty} \frac{1}{n} \log \mathcal{L}(h) \leq \inf_{\pi/2 \geq \theta' > \theta} \Delta(\theta') - \frac{1}{2} \log(1-\cos\theta).$$

where

$$\Delta(\theta') := \frac{1+\sin\theta'}{2\sin\theta'} \log \frac{1+\sin\theta'}{2\sin\theta'} - \frac{1-\sin\theta'}{2\sin\theta'} \log \frac{1-\sin\theta'}{2\sin\theta'} + \frac{1}{2} \log(1-\cos\theta').$$

Note that

$$\frac{d}{d\theta'}\Delta(\theta') = \cos\theta' \log(\frac{1+\sin\theta'}{1-\sin\theta'}) - (1+\cos\theta')\sin\theta'.$$

As we mentioned above, $\theta^* := 62.997...^\circ$ is the unique root of the equation $\frac{d}{d\theta'}\Delta(\theta') = 0$ [KL78, Theorem 4] in the interval $0 < \theta' \leq \pi/2$, which is a unique minimum of $\Delta(\theta')$ for $0 < \theta' \leq \pi/2$. Hence, for $\theta < \theta^*$

$$\lim_{n\to\infty} \frac{1}{n} \left(\log \mathcal{L}(h) - \log \mathcal{L}(g_\theta)\right) \leq \Delta(\theta^*) - \Delta(\theta) < 0.$$

This concludes the proof of our corollary. □

Finding functions $h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$ with smaller value $\mathcal{L}(h)$ than $\mathcal{L}(g_\theta)$ for Levenshtein's polynomials had been suggested by Levenshtein in [Lev98, page 117]. In fact, Boyvalenkov–Danev–Bumova [BDB96] gives necessary and sufficient conditions for constructing extremal *polynomials* that improve Levenshtein's bound. However, their construction does not improve the exponent of Levenshtein's bound as the asymptotic degrees of their polynomials are the same as those of Levenshtein's polynomials.

We now give a uniform version of our theorem for the Sphere packing problem.

Theorem 1.6. *Suppose that* $1/3 \leq \cos(\theta') < 1/2$*. We have*

$$\delta_{n-1} \leq c_{n-1}(\theta') \frac{\mathcal{L}(g_{\theta'})}{\mu_{n-1}(\theta')},$$

where $c_n(\theta') < 1$ *for every* n*. If, additionally,* $n \geq 2000$ *and* $\cos(\theta') = t_{1,d-\varepsilon}^{\alpha+1,\alpha+\varepsilon}$ *for some* $\varepsilon \in \{0,1\}$*, where* $\alpha = \frac{n-3}{2}$*, we have* $c_n(\theta') \leq 0.515 + \frac{74}{n}$*. Furthermore, for* $n \geq 2000$ *we have* $c_n(\theta^*) \leq 0.4325 + \frac{51}{n}$*.*

Note that by Kabatyanskii–Levenshtein [KL78], the best angle for such a comparison is asymptotically θ^* as comparisons using other angles are exponentially worse. Consequently, this theorem implies that we have an improvement by 0.4325 for sphere packing density upper bounds in high dimensions. Furthermore, note that the constant of improvements $c_n(\theta')$ are non-trivially bounded from above *uniformly* in θ'.

Remark 9. We prove Theorem 1.6 by constructing a test function that satisfies the Cohn–Elkies linear programing conditions. This construction is based on the work of Cohn and Zhao [CZ14] which proves the above theorem for $c_n = 1$. The factor $0.4325 + \frac{51}{n}$ is the constant improvement over the combination of the work of Cohn and Zhao [CZ14] with Levenshtein's optimal polynomials [Lev79]. Furthermore, note that the right hand side corresponds to the dimension $n-1$, and so the dimension of the right hand side does not increase as happens in the case of Sidelnikov's inequality (2).

We begin the proofs of Theorems 1.4 and 1.6 in Section 4 and complete them in Section 5. We start the construction of h in Section 4. In Proposition 4.6, we prove a general version of Theorem 1.4. We construct h for every pair of angles $0 < \theta < \theta^* \leq \theta' < \pi/2$ and any given $g_{\theta'} \in D(d\mu_{\frac{n-4}{2}}, \cos\theta')$ for $c_n = 1$. In particular, Proposition 1.3 and its linear programming version Proposition 4.6 generalize the construction of Cohn and Zhao which works only for $\theta \approx 0$ and $\theta' \geq \pi/3$ [CZ14, Theorem 3.4] to any pair of angles. However, constructing h with $c_n < 1$ is difficult; see Remark 29.

Our novelty is in developing analytic methods for constructing h with $c_n < 1$. Our construction is based on estimating the triple density functions of points in Section 7 and estimating the Jacobi polynomials near their extreme roots in Section 6. It is known that the latter problem is very difficult [Kra07, Conjecture 1]. In Section 6, we overcome this difficulty by using the relation between

n	Rogers	Levenshtein79	K.–L.	Cohn–Zhao	C.–Z.+L79	New bound
12	8.759×10^{-2}	1.065×10^{-1}	1.038×10^{0}	9.666×10^{-1}	3.253×10^{-1}	1.228×10^{-1}
24	2.456×10^{-3}	3.420×10^{-3}	2.930×10^{-2}	2.637×10^{-2}	8.464×10^{-3}	3.194×10^{-3}
36	5.527×10^{-5}	8.109×10^{-5}	5.547×10^{-4}	4.951×10^{-4}	1.610×10^{-4}	6.035×10^{-5}
48	1.128×10^{-6}	1.643×10^{-6}	8.745×10^{-6}	7.649×10^{-6}	2.534×10^{-6}	9.487×10^{-7}
60	2.173×10^{-8}	3.009×10^{-8}	1.223×10^{-7}	1.046×10^{-7}	3.521×10^{-8}	1.317×10^{-8}
72	4.039×10^{-10}	5.135×10^{-10}	1.550×10^{-9}	1.322×10^{-9}	4.496×10^{-10}	1.678×10^{-10}
84	7.315×10^{-12}	8.312×10^{-12}	1.850×10^{-11}	1.574×10^{-11}	5.381×10^{-12}	2.007×10^{-12}
96	1.300×10^{-13}	1.291×10^{-13}	2.111×10^{-13}	1.786×10^{-13}	6.101×10^{-14}	2.273×10^{-14}
108	2.277×10^{-15}	1.937×10^{-15}	2.320×10^{-15}	1.942×10^{-15}	6.662×10^{-16}	2.480×10^{-16}
120	3.940×10^{-17}	2.826×10^{-17}	2.452×10^{-17}	2.051×10^{-17}	7.058×10^{-18}	2.626×10^{-18}

TABLE 1. Upper bounds on maximal sphere packing densities δ_n in $\mathbb{R}^n$. The last column is obtained from Proposition 4.7 by minimizing the right hand side of this proposition as we vary the angle θ between $\pi/3$ and π and maximize $\delta > 0$.

the zeros of Jacobi polynomials; these ideas go back to the work of Stieltjes [Sti87]. More precisely, we use the underlying differential equations satisfied by the Jacobi polynomials and the fact that the roots of the family of Jacobi polynomials are interlacing.

Theorem 1.6 is not optimal. From a numerical perspective, we may use our test functions h to obtain the last column of Table 1, which already gives better improvement in low dimensions than our asymptotic result. We now describe the different columns. The *Rogers* column corresponds to the bounds on sphere packing densities obtained by Rogers [Rog58]. The *Levenshtein79* column corresponds to the bound obtained by Levenshtein in terms of roots of Bessel functions [Lev79]. The *K.–L.* column corresponds to the bound on $M(n, \theta)$ proved by Kabatyanskii and Levenshtein [KL78] combined with Sidelnikov's inequality (2). The *Cohn–Zhao* column corresponds to the column found in the work of Cohn and Zhao [CZ14]; they combined their inequality (4) with the bound on $M(n, \theta)$ proved by Kabatyanskii–Levenshtein. We also include the column *C.–Z.+L79* which corresponds to combining Cohn and Zhao's inequality with improved bounds on $M(n, \theta)$ using Levenshtein's optimal polynomials [Lev79]. The final column corresponds to the bounds on sphere packing densities obtained by our method. Note that our bounds break most of the other bounds also in smaller dimensions. Another advantage is that we provide an explicit function satisfying the Cohn–Elkies linear programming conditions. Our bounds come from this explicit function and only involve explicit integral calculations; in contrast to the numerical method in [CE03], we do not rely on any searching algorithm. Moreover, compared to the Cohn–Elkies linear programming method, in $n = 120$ dimensions, we substantially break the sphere packing density upper bound of 1.164×10^{-17} obtained by forcing eight double roots.

1.4. **Generalizations of Levenshtein's extremal polynomials.** In addition to proving the results mentioned in the previous subsections for $\theta < \theta^*$, we end this paper by providing a new conceptual derivation of Levenshtein's extremal polynomials of both even and odd degrees. This is orthogonal to what was discussed in the previous subsections. Moreover, we derive explicit closed formulae for generalized version of Levenshtein's extremal polynomials in addition to explicit formulae for the value of the functional $\mathcal{L}$ on such extremal functions.

More precisely, we study a problem more general than what has been studied in the literature on optimizing Levenshtein's polynomials. Indeed, we introduce the spaces $\Lambda_{\mu,d,\eta}$, associated to some continuous function η, whose elements satisfy the second condition of the definition of $D(\mu, s)$ trivially. We then find the infimum of the functional $\mathcal{L}$ over $\Lambda_{\mu,d,\eta}$ and show that this infimum is achieved by a function that lies in $\Lambda_{\mu,d,\eta} \cap D(\mu,s)$ under some explicit conditions. We recover Levenshtein's extremal polynomials of odd and even degrees which correspond to $\eta = 1$ and $\eta = 1+t$, respectively.

We now precisely define the spaces $\Lambda_{\mu,d,\eta}$, and state our first theorem regarding the critical functions of the functional $\mathcal{L}$. Suppose that $\eta(t)$ is a continuous non-negative function on $[-1,1]$, where $\int_{-1}^{1}\eta(t)dt > 0$. For example we may take $\eta(t)$ to be a polynomial which is positive on $[-1,1]$, e.g. $\eta(t) = 1+t$. Let $\Lambda_{\mu,d,\eta}$ be the space of all functions $g(t) = (t-s)\eta(t)f(t)^2$, where $f(t)$ is some polynomial of degree at most d and $g_0 > 0$. Let $\{\tilde{p}_i\}$ be the orthonormal basis of polynomials with respect to the measure $\eta(t)\mu$ where $\tilde{p}_i$ has degree i and $\tilde{p}_i(1) > 0$. For example for $\eta(t) = 1$, we have $\tilde{p}_i = p_i$. Let

$$f^{[\mu,d,\eta]}(t) := \sum_{i=0}^{d-1} \frac{\lambda_i^{\mathrm{c}}}{t-s} \det \begin{bmatrix} \tilde{p}_{i+1}(t) & \tilde{p}_{i+1}(s) \\ \tilde{p}_i(t) & \tilde{p}_i(s) \end{bmatrix},$$

where $\lambda_i^{\mathrm{c}} := \frac{1}{\tilde{a}_{i+1}}\left(\frac{\tilde{p}_i(1)}{\tilde{p}_i(s)} - \frac{\tilde{p}_{i+1}(1)}{\tilde{p}_{i+1}(s)}\right)$ ($\tilde{a}_i$ depends on the basis $\{\tilde{p}_n\}$, and is defined in equation (17) in Section 2). Let $g^{[\mu,d,\eta]}(t) := (t-s)\eta(t)f^{[\mu,d,\eta]}(t)^2$, and denote by $d_1(s)$ and $d_2(s)$ the first and second positive integers i such that $\tilde{p}_i(s)\tilde{p}_{i+1}(s) < 0$. Note that we are suppressing s from some of our notations. Next, we state our main theorem.

Theorem 1.7. *$g^{[\mu,d,\eta]}(t)$ (up to a positive scalar multiple) is the unique critical point of $\mathcal{L}$ over $g \in \Lambda_{\mu,d,\eta}$ provided that $g_0^{[\mu,d,\eta]} > 0$. Moreover, $g^{[\mu,d,\eta]}(t)$ (up to a positive scalar multiple) is the unique minimum of $\mathcal{L}$ over $g \in \Lambda_{\mu,d,\eta}$ provided that $d_1(s) \le d < d_2(s)$ and $g_0^{[\mu,d,\eta]} > 0$.*

We prove Theroem 1.7 in Section 8. The argument is based on Lagrange multiplier method and diagonalizing a quadratic from which is the zeroth Fourier coefficients (in the basis p_i) and so we cannot continue to work with the basis p_i because of the presence of $\eta(t)$. This is why we work in the basis $\tilde{p}_i$, an orthonormal basis of $\mathbb{R}[t]$ with respect to the measure $\eta(t)d\mu(t)$. Once we have such a diagonalization, the condition $d_1(s) \le d < d_2(s)$ ensures a signature property which in turn ensures global minimality of the critical function $g^{[\mu,d,\eta]}$ assuming the positivity of the zeroth Fourier coefficient in the expansion in the basis $\{p_i\}$. Note that $\Lambda_{\mu,d,\eta}$ is not a subspace of $D(\mu,s)$; we need to choose μ, d, η (depending on s) appropriately so that $g^{[\mu,d,\eta]}$ is in $D(\mu,s)$. We discuss this in the following subsection.

1.5. **Positivity of Fourier coefficients.** Once we obtain the critical function $g^{[\mu,d,\eta]}$ as above and obtain the strict positivity of the zeroth Fourier coefficient, we need to give conditions under which the other Fourier coefficients are non-negative. As a result, we restrict μ and $\eta(t)$ to have the following positivity properties.

Definition 1.8. We say μ satisfies the *Krein condition* if for every $i,j,k \ge 0$,

$$\int_{-1}^{1} p_i(t)p_j(t)p_k(t)d\mu \ge 0.$$

Note that $d\mu_\alpha$ satisfies the Krein condition; see [KL78, Equation (38)].

Definition 1.9. We say a continuous function η is (μ,s,d)-*positive* if there exists a non-zero $c \in \mathbb{C}$ such that for every $i,j \ge 0$,

$$c\int_{-1}^{1} p_i(t)(t-s)\eta(t)f^{[\mu,d,\eta]}(t)d\mu \ge 0, \tag{10}$$

and

$$c\int_{-1}^{1} p_j(t)f^{[\mu,d,\eta]}(t)d\mu \geq 0. \tag{11}$$

We often use the following expressions for $f^{[\mu,d,\eta]}(t)$ in order to check (μ, s, d)-positivity condition. One may view these formulas as the generalized *Christoffel-Darboux* formula.

Theorem 1.10. *We have*

$$f^{[\mu,d,\eta]}(t) = \frac{\tilde{c}}{(t-1)(t-s)} \det \begin{bmatrix} \tilde{p}_{d+1}(t) & \tilde{p}_{d+1}(s) & \tilde{p}_{d+1}(1) \\ \tilde{p}_{d}(t) & \tilde{p}_{d}(s) & \tilde{p}_{d}(1) \\ \tilde{p}_{d-1}(t) & \tilde{p}_{d-1}(s) & \tilde{p}_{d-1}(1) \end{bmatrix}$$

for some $\tilde{c} \in \mathbb{C}$. Moreover,

$$f^{[\mu,d,\eta]}(t) = \tilde{c}' \sum_{i=0}^{d-1} \tilde{p}_i(t) \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_i(s) & \tilde{p}_i(1) \end{bmatrix}$$

for some $\tilde{c}' \in \mathbb{C}$.

Note that condition (1) for $g^{[\mu,d,\eta]}(t) = (t-s)\eta(t)f^{[\mu,d,\eta]}(t)^2$, is an infinite system of quadratic inequalities in terms of the coefficients of $f^{[\mu,d,\eta]}(t)$, and the quadratic forms depend on the multiplicative structure of the Jacobi polynomials. So, checking condition (1) directly for $g^{[\mu,d,\eta]}$ is very hard. We have the following criteria, though sufficient, is not a necessary condition for (1).

Theorem 1.11. *Suppose that μ satisfies the Krein condition and η is (μ, s, d)-positive. Then*

$$g^{[\mu,d,\eta]} \in D(\mu, s).$$

1.6. **Polynomial η and comparison with other works.** Next, we consider special examples of $g^{[\mu,d,\eta]}(t)$, where η is a polynomial. In particular, we consider $\mu = d\mu_\alpha := (1-t^2)^\alpha dt / \int_{-1}^{1}(1-t^2)^\alpha dt$ with $\alpha > -1$ and $\eta = 1$ or $\eta = 1+t$. These examples are closely related to Levenshtein's extremal polynomials with odd and even degrees respectively; see [Lev98, Lev92, Lev79]. The extremal properties of these polynomials has been studied extensively in the works of Boyvalenkov [Boy95, BDH+19] and also the work of Barg and Nogin [BN08]. Suppose that $\eta(t) \in \mathbb{R}[t]$ is a polynomial with roots $\alpha_1, \ldots, \alpha_h \in \mathbb{C}$. Let

$$b^{[\mu,d,\eta]}(t) := \frac{1}{(t-1)(t-s)\eta(t)} \det \begin{bmatrix} p_{d+h+1}(t) & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \ldots & p_{d+h+1}(\alpha_h) \\ & & \vdots & & & \\ p_d(t) & p_d(s) & p_d(1) & p_d(\alpha_1) & \ldots & p_d(\alpha_h) \\ p_{d-1}(t) & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \ldots & p_{d-1}(\alpha_h) \end{bmatrix}, \tag{12}$$

and

$$r^{[\mu,d,\eta]}(t) := \sum_{i=0}^{d-1} p_i(t) \det \begin{bmatrix} p_{d+h}(s) & p_{d+h}(1) & p_{d+h}(\alpha_1) & \ldots & p_{d+h}(\alpha_h) \\ & & \vdots & & \\ p_d(s) & p_d(1) & p_d(\alpha_1) & \ldots & p_d(\alpha_h) \\ p_i(s) & p_i(1) & p_i(\alpha_1) & \ldots & p_i(\alpha_h) \end{bmatrix}. \tag{13}$$

We prove that $b^{[\mu,d,\eta]}(t)$ and $r^{[\mu,d,\eta]}(t)$ are scalar multiple of each other. In the special case of polynomials we have the following explicit expressions for $f^{[\mu,d,\eta]}(t)$.

Theorem 1.12. *We have $f^{[\mu,d,\eta]}(t) = cb^{[\mu,d,\eta]}(t)$ where $c \in \mathbb{C}$. Moreover, $f^{[\mu,d,\eta]}(t) = c'r^{[\mu,d,\eta]}(t)$, where $c' \in \mathbb{C}$. Note that $\frac{c'}{c} = \prod_{i=d}^{d+h+1} a_i > 0$.*

By using the above explicit formula for $f^{[\mu,d,\eta]}(t)$, we determine the set of d for which η is (μ, s, d)-positive in the following theorem.

Theorem 1.13. *η is (μ, s, d)-positive if and only if there exists a non-zero $\kappa \in \mathbb{C}$ such that for every $0 \le i \le d-1$*

$$\kappa \det \begin{bmatrix} p_{d+h}(s) & p_{d+h}(1) & p_{d+h}(\alpha_1) & \dots & p_{d+h}(\alpha_h) \\ & & \vdots & & \\ p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p_i(s) & p_i(1) & p_i(\alpha_1) & \dots & p_i(\alpha_h) \end{bmatrix} \ge 0, \tag{14}$$

and for every $d-1 \le j \le d+h$

$$\kappa \det \begin{bmatrix} \gamma_{d+h+1,j} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ \gamma_{d,j} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix} \ge 0, \tag{15}$$

where

$$\gamma_{i,j} = \int_{-1}^{1} \frac{(p_i(t) - p_i(1))}{(t-1)} p_j(t) d\mu = \begin{cases} \int_{-1}^{1} \frac{1}{t-1} \det \begin{bmatrix} p_j(1) & p_i(1) \\ p_j(t) & p_i(t) \end{bmatrix} d\mu & \text{for } j < i, \\ 0 & \text{otherwise.} \end{cases}$$

As the value of the functional $\mathcal{L}$, we have the following theorem.

Theorem 1.14. *For $\eta(t) = (t-\alpha_1)\dots(t-\alpha_h)$ real non-negative polynomial with distinct roots $\alpha_i \in \mathbb{C}$,*

$$\mathcal{L}(g^{[\mu,d,\eta]}) = \frac{\omega_0 \det \begin{bmatrix} p'_{d+h+1}(1) & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ & & \vdots & & & \\ p'_d(1) & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p'_{d-1}(1) & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}}{\det \begin{bmatrix} p_{d+h+1}(1) \sum_{l=d-1}^{d+h} \frac{a_{l+1}}{p_l(1) p_{l+1}(1)} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ p_d(1) \sum_{l=d-1}^{d-1} \frac{a_{l+1}}{p_l(1) p_{l+1}(1)} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ 0 & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}}.$$

Our framework subsumes the work of Levenshtein, by recovering his extremal polynomials in both odd and even degrees with $\eta = 1$ and $\eta = 1 + t$.

1.7. **Structure of the paper.** This paper is structured as follows. Section 2 gives a summary of the properties of orthogonal polynomials, especially Jacobi polynomials, that will be used in this paper. Except for Proposition 2.1, there is no claim of originality in this section. In Section 3, we setup some of the notation used in this paper and prove Proposition 1.3. Section 4 concerns the general construction of our test functions that are used in conjunction with the Delsarte and Cohn–Elkies linear programming methods; we prove Propositions 4.6 and 4.7 in this section. In Section 5, we prove our main Theorems 1.4 and 1.6. In this section, we use our estimates on the triple density functions proved in Section 7. We also use our local approximation to Jacobi polynomials proved in Section 6. Sections 8, 9, and 10 concern generalizations of Levenshtein's optimal polynomials and their properties. In the final Section 11, we provide a table of improvement factors.

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2. Orthogonal polynomials

In this section, we record some well-known properties of the Jacobi polynomials (see [Sze39, Chapter IV]) as well as the Christoffel-Dabroux formula that will be used repeatedly in this paper, especially in the later sections. Except possibly for Proposition 2.1, there is no claim of originality.

We denote by $p_n^{\alpha,\beta}(t)$ the Jacobi polynomial of degree n with parameters α and β. These are orthogonal polynomials with respect to the measure $d\mu_{\alpha,\beta} := (1-t)^\alpha(1+t)^\beta dt / \int_{-1}^1 (1-t)^\alpha(1+t)^\beta dt$ on the interval $[-1,1]$. When $\alpha=\beta$, we denote this measure simply as $d\mu_\alpha$. For simplicity, we write $p_n(t)$ for the L^2-normalized Jacobi polynomials $\frac{p_n^{\alpha,\alpha}(t)}{\|p_n^{\alpha,\alpha}\|_2}$. We denote the top coefficient of $p_n(t)$ with k_n. Note that the weight (α,α) is implicit in the notation. The *Christoffel-Darboux* formula states the following (see [Sze39, Theorem 3.2.2]):

$$\frac{1}{(t-s)}\det\begin{bmatrix} p_{n+1}(t) & p_{n+1}(s) \\ p_n(t) & p_n(s)\end{bmatrix} = \frac{k_{n+1}}{k_n}\sum_{j=0}^n p_j(s)p_j(t) = a_{n+1}\sum_{j=0}^n p_j(s)p_j(t), \tag{16}$$

where $a_{n+1} = \frac{k_{n+1}}{k_n} > 0$. In fact, this formula holds more generally for sequences of orthonormal polynomials with respect to some measure on $[-1,1]$. The recursive relation for orthonormal polynomials (see [Sze39, Theorem 3.2.1]) gives

$$p_{n+1}(t) = (a_{n+1}t + b_{n+1})p_n(t) - c_{n+1}p_{n-1}(t), \tag{17}$$

where

$$c_{n+1} = \frac{a_{n+1}}{a_n} = \frac{k_{n+1}k_{n-1}}{k_n^2} > 0, \text{ and } b_{n+1} = 0 \text{ for } \alpha=\beta. \tag{18}$$

We also have; see [KL78, Equation (38)]

$$p_i(t)p_j(t) = \sum_{l=0}^{i+j} a_{i,j}^l p_l(t), \tag{19}$$

where $a_{i,j}^l \geq 0$ when $\alpha \geq \beta$, which means $d\mu_\alpha$ satisfies the Krein condition. The Jacobi polynomials that we use are suitably normalized so that we have the following formulas:

$$p_n^{\alpha,\beta}(1) = \binom{n+\alpha}{n}, \tag{20}$$

$$\omega_n^{\alpha,\beta} := \int_{-1}^1 (p_n^{\alpha,\beta})^2 d\mu_{\alpha,\beta}(t) = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)n!} \text{ for } \alpha,\beta > -1, \tag{21}$$

(22)

$$2n(n+\alpha+\beta)(2n+\alpha+\beta-2)p_n^{\alpha,\beta}(t) = (2n+\alpha+\beta-1)((2n+\alpha+\beta)(2n+\alpha+\beta-2)t+\alpha^2-\beta^2)p_{n-1}^{\alpha,\beta}(t)$$
$$-2(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)p_{n-2}^{\alpha,\beta}(t) \text{ for } n\geq 2,$$

and

$$\frac{d}{dt}p_n^{\alpha,\beta}(t) = \frac{n+\alpha+\beta+1}{2}p_{n-1}^{\alpha+1,\beta+1}(t). \tag{23}$$

Henceforth, we suppress the α from $\omega_n^{\alpha,\alpha}$ and write simply ω_n.

When proving our local approximation result on Levenshtein's optimal polynomials, we will use the fact that the Jacobi polynomial $p_d^{(\alpha,\beta)}(t)$ satisfies the differential equation

$$(1-t^2)x''(t) + (\beta-\alpha-(\alpha+\beta+2)t)x'(t) + d(d+\alpha+\beta+1)x(t) = 0. \tag{24}$$

We also use the following expression for a_n appearing in equation (17) above. This is easily obtained from the other properties above.

$$a_n = \frac{(2n+\alpha+\beta)\sqrt{(2n+\alpha+\beta+1)(2n+\alpha+\beta-1)}}{2\sqrt{n(n+\alpha)(n+\beta)(n+\alpha+\beta)}}. \tag{25}$$

In this paper, we will perform a change of basis of polynomials by changing the measure with respect to which orthogonality is defined. The following proposition will be useful.

Proposition 2.1. *Suppose that $\{p_0, p_1, \dots\}$ is an orthonormal basis for $\mathbb{R}[t]$ with respect to the measure $d\mu$ on $[-1,1]$. For distinct $\alpha_1, \dots, \alpha_k \in \mathbb{C}$, let $d\tilde{\mu}(t) := (t-\alpha_1)\dots(t-\alpha_k)d\mu(t)$ and*

$$\tilde{p}_i(t) := \frac{1}{(t-\alpha_1)\dots(t-\alpha_k)} \det \begin{bmatrix} p_{i+k}(t) & p_{i+k}(\alpha_1) & \dots & p_{i+k}(\alpha_k) \\ p_{i+k-1}(t) & p_{i+k-1}(\alpha_1) & \dots & p_{i+k-1}(\alpha_k) \\ \vdots & \vdots & & \vdots \\ p_i(t) & p_i(\alpha_1) & \dots & p_i(\alpha_k) \end{bmatrix}.$$

Then $\{\tilde{p}_0, \tilde{p}_1, \dots\}$ forms an orthogonal family of polynomials for $d\tilde{\mu}(t)$.

Proof. Suppose that $n > m \geq 0$ are integers. It suffices to show that

$$\int_{-1}^{1} \tilde{p}_m \tilde{p}_n d\tilde{\mu}(t) = 0.$$

We have

$$\int_{-1}^{1} \tilde{p}_m \tilde{p}_n d\tilde{\mu}(t) = \int_{-1}^{1} \tilde{p}_m \det \begin{bmatrix} p_{n+k}(t) & p_{n+k}(\alpha_1) & \dots & p_{n+k}(\alpha_k) \\ p_{n+k-1}(t) & p_{n+k-1}(\alpha_1) & \dots & p_{n+k-1}(\alpha_k) \\ \vdots & \vdots & & \vdots \\ p_n(t) & p_n(\alpha_1) & \dots & p_n(\alpha_k) \end{bmatrix} d\mu(t) = 0,$$

where the last identity follows from the fact that $\tilde{p}_m$ is a polynomial of degree $m < n$ which is orthogonal to any linear combination of $p_n, \dots, p_{n+k}$ with respect to measure $d\mu(t)$. This completes the proof of our proposition. □

3. Geometric improvement

In this section, we give a proof of Proposition 1.3. First, we introduce some notations.

Let $0 < \theta < \theta' < \pi$ be given angles, and let $s := \cos\theta$ and $s' := \cos\theta'$ as before. Throughout, S^{n-1} is the *unit* sphere. Suppose $\boldsymbol{z} \in S^{n-1}$ is a fixed point. Consider the cap $\mathrm{Cap}_{\theta,\theta'}(\boldsymbol{z})$ on S^{n-1} centered at $\boldsymbol{z}$ and of radius $\sqrt{1-r^2}$, where

$$r = \sqrt{\frac{s-s'}{1-s'}}.$$

Consider the tangent hyperplane $T_{\boldsymbol{z}}S^{n-1} := \{\boldsymbol{u} \in \mathbb{R}^n : \langle \boldsymbol{u}, \boldsymbol{z}\rangle = 0\}$ to S^{n-1} at the point $\boldsymbol{z} \in S^{n-1}$. For each $\boldsymbol{x}, \boldsymbol{y} \in S^{n-1}$ of angle at least θ from each other, we may orthogonally project them onto the tangent plane $T_{\boldsymbol{z}}S^{n-1}$ via the map $\Pi_{\boldsymbol{z}} : S^{n-1} \to T_{\boldsymbol{z}}S^{n-1}$. It is easy to see that for every $\boldsymbol{x} \in S^{n-1}$,

$$\Pi_{\boldsymbol{z}}(\boldsymbol{x}) = \boldsymbol{x} - \langle \boldsymbol{x}, \boldsymbol{z}\rangle \boldsymbol{z}.$$

For brevity, we denote $\frac{\Pi_{\boldsymbol{z}}(\boldsymbol{x})}{|\Pi_{\boldsymbol{z}}(\boldsymbol{x})|}$ by $\tilde{\boldsymbol{x}}$ when $\boldsymbol{z}$ is understood. Given $\boldsymbol{x}, \boldsymbol{y} \in S^{n-1}$, we obtain points $\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}$ in the tangent space $T_{\boldsymbol{z}}S^{n-1}$. We will use the following notation.

$$u := \langle \boldsymbol{x}, \boldsymbol{z}\rangle,$$
$$v := \langle \boldsymbol{y}, \boldsymbol{z}\rangle,$$

and

$$t := \langle \boldsymbol{x}, \boldsymbol{y}\rangle.$$

It is easy to see that

$$\langle \tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}\rangle = \frac{t - uv}{\sqrt{(1-u^2)(1-v^2)}}.$$

For $0 < \theta < \theta' < \pi$, we define

$$\gamma_{\theta,\theta'} := 2\arctan\frac{s}{\sqrt{(1-s)(s-s')}} + \arccos(r) - \pi, \tag{26}$$

and

$$R := \cos(\gamma_{\theta,\theta'}).$$

Then $R > r$, and we define the strip

$$\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z}) := \left\{\boldsymbol{x} \in S^{n-1} : \arccos(R) \le \langle \boldsymbol{x}, \boldsymbol{z}\rangle \le \arccos(r)\right\}.$$

By equation (147) and Lemma 42 of [AVZ00], the maximum of

$$\frac{s - uv}{\sqrt{(1-u^2)(1-v^2)}}$$

over this strip occurs when $\boldsymbol{x}, \boldsymbol{y}$ lie on the boundary of the cap $\mathrm{Cap}_{\theta,\theta'}(\boldsymbol{z})$, and so is at most

$$\frac{s - r^2}{1 - r^2} = s'.$$

Consequently, any two points in the strip $\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z})$ that are at least θ apart are projected under $\Pi_{\boldsymbol{z}}$ to points on the tangent plane to $\boldsymbol{z}$ that are at least θ' apart from the point of view of $\boldsymbol{z}$. With this in mind, we are now ready to prove Proposition 1.3. When discussing the measure of strips $\mathrm{Str}_{\theta,\theta'}(x)$, we drop x from the notation and simply write $\mathrm{Str}_{\theta,\theta'}$.

Proof of Proposition 1.3. Suppose $\{x_1, \ldots, x_N\} \subset S^{n-1}$ is a maximal spherical code corresponding to the angle θ. Given $x \in S^{n-1}$, let $m(x)$ be the number of such strips $\mathrm{Str}_{\theta,\theta'}(x_i)$ such that $x \in \mathrm{Str}_{\theta,\theta'}(x_i)$. Note that $x \in \mathrm{Str}_{\theta,\theta'}(x_i)$ if and only if $x_i \in \mathrm{Str}_{\theta,\theta'}(x)$. Therefore, the strip $\mathrm{Str}_{\theta,\theta'}(x)$ contains $m(x)$ points of $\{x_1, \ldots, x_N\}$. From the previous lemma, we know that the projection of these $m(x)$ points onto the tangent plane of S^{n-1} at the points $x \in S^{n-1}$ have pairwise radial angles at least θ'. As a result,

$$m(x) \le M(n-1, \theta'),$$

using which we obtain

$$N \cdot \mu(\mathrm{Str}_{\theta,\theta'}) = \sum_{i=1}^{N} \int_{\mathrm{Str}_{\theta,\theta'}(x_i)} d\mu(x) = \int_{S^{n-1}} m(x)d\mu(x) \le M(n-1,\theta') \int_{S^{n-1}} d\mu(x) = M(n-1,\theta').$$

Hence,

$$M(n,\theta) \le \frac{M(n-1,\theta')}{\mu(\mathrm{Str}_{\theta,\theta'})},$$

as required.

Note that the masses of $\mathrm{Str}_{\theta,\theta'}(x)$ and the cap $\mathrm{Cap}_{\theta,\theta'}$ have the property that

$$\begin{aligned} 1-\frac{\mu(\mathrm{Str}_{\theta,\theta'})}{\mu_n(\theta,\theta')} &= \frac{1}{\mu_n(\theta,\theta')}\int_R^1(1-t^2)^{\frac{n-3}{2}}dt \\ &\leq \frac{(1-R^2)^{\frac{n-3}{2}}}{\mu_n(\theta,\theta')}. \end{aligned}$$

On the other hand, we may also give a lower bound on $\mu_n(\theta,\theta')$ by noting that

$$\begin{aligned} \mu_n(\theta,\theta') &= \frac{1}{\omega_0}\int_r^1(1-t^2)^{\frac{n-3}{2}}dt \\ &\geq \frac{\left(\sqrt{\frac{1+r}{1-r}}\right)^{n-3}}{\omega_0}\int_r^1(1-t)^{n-3}dt \\ &= \frac{\left(\sqrt{\frac{1+r}{1-r}}\right)^{n-3}(1-r)^{n-2}}{(n-2)\omega_0} \\ &\geq \frac{(1-r)(1-r^2)^{\frac{n-3}{2}}}{2(n-2)}. \end{aligned}$$

Here, ω_0 is the volume of the unit sphere S^{n-1}. Combining this inequality with the above, we obtain

$$1\geq\frac{\mu(\mathrm{Str}_{\theta,\theta'})}{\mu_n(\theta,\theta')}\geq 1-\frac{2(n-2)(1-R^2)^{\frac{n-3}{2}}}{(1-r)(1-r^2)^{\frac{n-3}{2}}}=1-\frac{2(n-2)}{(1-r)}e^{-\frac{n-3}{2}\log\left(\frac{1-r^2}{1-R^2}\right)}.$$

Since $R>r$, this lower bound exponentially converges to 1 as $n\to\infty$. □

4. New test functions

In this section, we give linear programming bounds on sizes of spherical codes and sphere packing densities by constructing new test functions using averaging arguments.

4.1. **Spherical codes.** In this subsection, we construct a function inside $D(d\mu_{\frac{n-3}{2}},\cos\theta)$ from a given one inside $D(d\mu_{\frac{n-4}{2}},\cos\theta')$, where $\theta'>\theta$.

Suppose that $g_{\theta'}\in D(d\mu_{\frac{n-4}{2}},\cos\theta')$. Fix $\boldsymbol{z}\in S^{n-1}$. Given $\boldsymbol{x},\boldsymbol{y}\in S^{n-1}$, we define

$$h(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z}):=F(\langle\boldsymbol{x},\boldsymbol{z}\rangle)F(\langle\boldsymbol{y},\boldsymbol{z}\rangle)g_{\theta'}(\langle\tilde{\boldsymbol{x}},\tilde{\boldsymbol{y}}\rangle), \tag{27}$$

where F is an arbitrary integrable real valued function on $[-1,1]$, and $\tilde{\boldsymbol{x}}$ and $\tilde{\boldsymbol{y}}$ are are unit vectors on the tangent space of the sphere at $\boldsymbol{z}$ as defined in the previous section. We also use the notation u,v,t as before. It is easy to see that

$$h(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z}):=F(u)F(v)g_{\theta'}\left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\right).$$

The above types functions in three variables also appear in semi-definite linear programing [BV08]. Indeed this was our main motivation for considering these types of functions.

Lemma 4.1. *$h(\boldsymbol{x},\boldsymbol{y};\boldsymbol{z})$ is a positive definite function in variables $\boldsymbol{x},\boldsymbol{y}$ on S^{n-1}, namely*

$$\sum_{x_i,x_j\in A}a_ia_jh(\boldsymbol{x}_i,\boldsymbol{x}_j;\boldsymbol{z})\geq 0$$

for every finite subset $A \subset S^{n-1}$, and coefficients $a_i \in \mathbb{R}$. Moreover, h is invariant by the diagonal action of $O(n)$, namely

$$h(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{z}) = h(k\boldsymbol{x}, k\boldsymbol{y}; k\boldsymbol{z})$$

for every $k \in O(n)$.

Proof. It follows easily from the definitions. □

Let

$$h(\boldsymbol{x}, \boldsymbol{y}) := \int_{O(n)} h(\boldsymbol{x}, \boldsymbol{y}; k\boldsymbol{z}) d\mu(k), \tag{28}$$

where $d\mu(k)$ is the normalized Haar measure on $O(n)$.

Lemma 4.2. *$h(\boldsymbol{x}, \boldsymbol{y})$ is a positive definite point pair invariant function on S^{n-1}*

Proof. It follows form the previous lemma. □

Since $h(\boldsymbol{x}, \boldsymbol{y})$ is a point pair invariant function, so it only depends on $t = \langle \boldsymbol{x}, \boldsymbol{y} \rangle$. For the rest of this paper, we abuse notation and consider h as a real valued function on $[-1, 1]$, where $h(\boldsymbol{x}, \boldsymbol{y}) = h(t)$.

4.1.1. *Computing $\mathcal{L}(h)$.* We now proceed to computing the value of $\mathcal{L}(h)$ in terms of F and $g_{\theta'}$. First, we compute the value of $h(1)$. Let $\|F\|_2^2 := \int_{-1}^1 F(u)^2 d\mu_{\frac{n-3}{2}}(u)$.

Lemma 4.3. *We have*

$$h(1) = g_{\theta'}(1)\|F\|_2^2.$$

Proof. Indeed, by definition, $h(1)$ corresponds to taking $\boldsymbol{x} = \boldsymbol{y}$, from which it follows that $t = 1$, $u = v$ and $\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}} = 1$. Therefore, we obtain

$$h(1) = \int_{-1}^1 F(u)^2 g_{\theta'}(1) d\mu_{\frac{n-3}{2}}(u) = g_{\theta'}(1)\|F\|_2^2.$$

□

Next, we compute the zero Fourier coefficient of h. Let $F_0 = \int_{-1}^1 F(u) d\mu_{\frac{n-3}{2}}(u)$ and $g_{\theta',0} = \int_{-1}^1 g_{\theta'} d\mu_{\frac{n-4}{2}}(u)$.

Lemma 4.4. *We have*

$$h_0 = g_{\theta',0} F_0^2.$$

Proof. Let $O(n-1) \subset O(n)$ be the centralizer of $\boldsymbol{z}$. We identify $O(n)/O(n-1)$ by S^{n-1} via the map $[k_1] := k_1\boldsymbol{z} \in S^{n-1}$. Then we write the Haar measure of $O(n)$ as the product of the Haar measure of $O(n-1)$ and surface area $d\sigma$ of S^{n-1}

$$d\mu(k_1) = d\mu(k_1')d\sigma([k_1]).$$

where $k_1' \in O(n-1)$. By equation (27), (28) and the above, we obtain

$$\begin{aligned} h_0 &= \int_{k_i' \in O(n-1)} \int_{[k_i] \in S^{n-1}} F(\langle k_1'[k_1], \boldsymbol{z} \rangle) F(\langle k_2'[k_2], \boldsymbol{z} \rangle) g_{\theta'} \left(\left\langle k_1'\widetilde{[k_1]}, k_2'\widetilde{[k_2]} \right\rangle \right) d\mu(k_1') d\sigma([k_1]) d\mu(k_2') d\sigma([k_2]) \\ &= \int_{[k_i] \in S^{n-1}} F(\langle [k_1], \boldsymbol{z} \rangle) F(\langle [k_2], \boldsymbol{z} \rangle) d\sigma([k_1]) d\sigma([k_2]) \int_{k_i' \in O(n-1)} g_{\theta'} \left(\left\langle k_1'\widetilde{[k_1]}, k_2'\widetilde{[k_2]} \right\rangle \right) d\mu(k_1') d\mu(k_2'). \end{aligned}$$

We note that

$$\int_{k_i' \in O(n-1)} g_{\theta'} \left(\left\langle k_1'\widetilde{[k_1]}, k_2'\widetilde{[k_2]} \right\rangle \right) d\mu(k_1') d\mu(k_2') = g_{\theta',0},$$

and

$$\int_{[k_i]\in S^{n-1}} F(\langle [k_1], \boldsymbol{z}\rangle)F(\langle [k_2], \boldsymbol{z}\rangle)d\sigma([k_1])d\sigma([k_2]) = \int_{-1}^{1} F(u)F(v)d\mu_{\frac{n-3}{2}}(u)\mu_{\frac{n-3}{2}}(v) = F_0^2.$$

Therefore,

$$h_0 = g_{\theta',0}F_0^2,$$

as required. □

Proposition 4.5. *We have*

$$\mathcal{L}(h) = \mathcal{L}(g_{\theta'})\frac{\|F\|_2^2}{F_0^2}.$$

Proof. This follows immediately from Lemma 4.3 and Lemma 4.4. □

4.1.2. *Criteria for $h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$.* Finally, we give a criterion which implies $h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$. Recall that $0 < \theta < \theta'$, and $0 < r < R < 1$ that we defined in Section 3. Let $s' = \cos(\theta')$ and $s = \cos(\theta)$. Note that $s' < s$, $r = \sqrt{\frac{s-s'}{1-s'}}$, $s' = \frac{s-r^2}{1-r^2}$ and $R = \cos\gamma_{\theta,\theta'}$ as in equation (26). We define

$$\chi(y) := \begin{cases} 1 & \text{for } r < y \le R, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition 4.6. *Suppose that $g_{\theta'} \in D(d\mu_{\frac{n-4}{2}}, \cos\theta')$ is given and h is defined as in (28) for some F. Suppose that $F(x)$ is a positive integrable function giving rise to an h such that $h(t) \le 0$ for every $-1 \le t \le \cos\theta$. Then*

$$h \in D(d\mu_{\frac{n-3}{2}}, \cos\theta),$$

and

$$M(n,\theta) \le \mathcal{L}(h) = \mathcal{L}(g_{\theta'})\frac{\|F\|_2^2}{F_0^2}.$$

In particular, among all positive integrable functions F with compact support inside $[r, R]$, χ minimize the value of $\mathcal{L}(h)$, and for $F = \chi$ we have

$$M(n,\theta) \le \mathcal{L}(h) \le \frac{\mathcal{L}(g_{\theta'})}{\mu_n(\theta,\theta')}(1 + O(ne^{-nc})),$$

where $c = \frac{1}{2}\log\left(\frac{1-r^2}{1-R^2}\right) > 0$.

Proof. The first part follows from the previous lemmas and propositions. Let us specialize to the situation where F is merely assumed to be a positive integrable function with compact support inside $[r, R]$. Let us first show that $h(t) \le 0$ for $t \le s$. We have

$$h(t) := \int_{O(n)} h(\boldsymbol{x}, \boldsymbol{y}; k\boldsymbol{z})d\mu(k),$$

where $h(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{z}) := F(u)F(v)g_{\theta'}\left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\right)$. First, note that $F(u)F(v) \neq 0$ precisely when $\boldsymbol{x}$ and $\boldsymbol{y}$ belong to $\text{Str}_{\theta,\theta'}(\boldsymbol{z})$. By equation (147) and Lemma 42 of [AVZ00], the angular distance between the projected vectors is at least θ', and so

$$\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}} \in [-1, \cos\theta'].$$

Therefore

$$g_{\theta'}\left(\frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}\right) \le 0,$$

when $F(u)F(v) \neq 0$. Since the integrand $h(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ is non-positive when $t \in [-1, \cos\theta]$. Consequently, $h(t) \leq 0$ for $t < s$.

It is easy to see that when $F = \chi$, then

$$\|F\|_2^2 = \mu(\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z}))$$

and

$$F_0 = \mu(\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z})).$$

Therefore, by our estimate in the proof of Proposition 1.3 we have

$$M(n,\theta) \leq \mathcal{L}(h) \leq \frac{\mathcal{L}(g_{\theta'})}{\mu_n(\theta,\theta')}\left(1 + O(ne^{-\frac{n}{2}\log\left(\frac{1-r^2}{1-R^2}\right)})\right).$$

Finally, the optimality follows from the Cauchy–Schwarz inequality. More precisely, since $F(x)$ has compact support inside $[r, R]$, we have

$$\mu(\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z}))\|F\|_2^2 \geq F_0^2.$$

Therefore, $\mathcal{L}(h) = \frac{g_{\theta'}(1)}{g_{\theta',0}}\frac{\|F\|_2^2}{F_0^2} \geq \frac{\mathcal{L}(g_{\theta'})}{\mu(\mathrm{Str}_{\theta,\theta'}(\boldsymbol{z}))}$ with equality only when $F = \chi$. ☐

Remark 29. Proposition 4.6 shows that χ is optimal among all functions F with support $[r, R]$. We used this restriction on the support of F in order to prove that $h(t) \leq 0$ for $t < s$. By continuity, this negativity condition will continue to hold if we expand slightly the support of χ to $[r-\delta, R]$ for some $\delta > 0$. In order to determine explicitly the extent to which we can enlarge the support of χ, we should understand the behaviour of $g_{\theta'}$ at its zero $\cos\theta'$. As Levenshtein's function g_{θ^*} may be written in terms of Jacobi polynomials, this may be understood by understanding the behaviour of Jacobi polynomials at their extreme roots as the dimension and degree grow. We will make this precise in the next section.

4.2. **Sphere packings.** Suppose $0 < \theta \leq \pi$ is a given angle, and suppose $g_\theta \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$. Fixing $\boldsymbol{z} \in \mathbb{R}^n$, for each $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ consider

$$H(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{z}) := F(|\boldsymbol{x} - \boldsymbol{z}|)F(|\boldsymbol{y} - \boldsymbol{z}|)g_\theta\left(\langle\tilde{\boldsymbol{x}}, \tilde{\boldsymbol{y}}\rangle\right),$$

where F is a positive function on $\mathbb{R}$ such that as a radial function it is in $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. The tilde notation denotes normalization to a unit vector from $\boldsymbol{z}$. We may then define $H(\boldsymbol{x}, \boldsymbol{y})$ by averaging over all $\boldsymbol{z} \in \mathbb{R}^n$:

$$H(\boldsymbol{x}, \boldsymbol{y}) := \int_{\mathbb{R}^n} H(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{z})d\boldsymbol{z}.$$

Note that this then makes $H(\boldsymbol{x}, \boldsymbol{y})$ into a point-pair invariant function. As before, we abuse notation and write $H(T)$ instead of $H(\boldsymbol{x}, \boldsymbol{y})$ when $T = |\boldsymbol{x} - \boldsymbol{y}|$. The analogue of Proposition 4.6 is then the following.

Proposition 4.7. *Let $0 < \theta \leq \pi$ and suppose $g_\theta \in D(d\mu_{\frac{n-3}{2}}, \cos\theta)$. Suppose F is as above such that $H(T) \leq 0$ for every $T \geq 1$. Then H is positive definite on $\mathbb{R}^n$ and*

$$\delta_n \leq \frac{\mathrm{vol}(B_1^n)\|F\|_{L^2(\mathbb{R}^n)}^2}{2^n\|F\|_{L^1(\mathbb{R}^n)}^2}\mathcal{L}(g_\theta), \tag{30}$$

where $\mathrm{vol}(B_1^n)$ is the volume of the n-dimensional unit ball. In particular, if $F = \chi_{[0,\overline{r}+\delta]}$, where $\delta \geq 0$ and $\overline{r} + \delta \leq 1$, is such that it gives rise to an H satisfying $H(T) \leq 0$ for every $T \geq 1$, then

$$\delta_n \leq \frac{\mathcal{L}(g_\theta)}{(2(\overline{r}+\delta))^n}. \tag{31}$$

Proof. The proof of this proposition is similar to that of Theorem 3.4 of Cohn–Zhao [CZ14]. The positive-definiteness of H follows as before. We focus our attention on proving inequality (30). Suppose we have a packing of $\mathbb{R}^n$ of density Δ by non-overlapping balls of radius $\frac{1}{2}$. By Theorem 3.1 of Cohn–Elkies [CE03], we have

$$\Delta \leq \frac{\mathrm{vol}(B_1^n)H(0)}{2^n \widehat{H}(0)}.$$

Note that $H(0) = g_\theta(1)\|F\|^2_{L^2(\mathbb{R}^n)}$, and that

$$\widehat{H}(0) = \int_{\mathbb{R}^n} H(|\boldsymbol{z}|)d\boldsymbol{z} = g_{\theta,0}\|F\|^2_{L^1(\mathbb{R}^n)}.$$

As a result, we obtain inequality (30). The rest follows from a simple computation. $\square$

Note that the situation $\delta = 0$ and $\bar{r} = \frac{1}{2\sin(\theta/2)}$ with $\pi/3 \leq \theta \leq \pi$ corresponds to Theorem 3.4 of Cohn–Zhao [CZ14], as checking the negativity condition $H(T) \leq 0$ for $T \geq 1$ follows from Lemma 2.2 therein. The factor of 2^n comes from considering functions where the negativity condition is for $T \geq 1$ instead of $T \geq 2$.

Remark 32. In this paper, we primarily consider characteristic functions; however, it is an interesting open question to determine the optimal such F in order to obtain the best bounds on sphere packing densities through this method.

5. Comparison with previous bounds

In this section, we begin by improving upon the Levenshtein bound on θ-spherical codes. In the second subsection, we improve upon the Cohn–Zhao upper bound on sphere packing densities. Note that the constructions of the functions were provided in the previous Section 4. We complete the proof of our main theorems by providing the necessary functions F for applying Propositions 4.6 and 4.7.

5.1. **Improving spherical codes bound.** Recall Theorem 1.1. In this section, we give a proof of Theorem 1.4].

Proof Theorem 1.4. Recall that $0 < \theta < \theta' \leq \pi/2$. Let $s' = \cos(\theta') = t^{\alpha+1,\alpha+\varepsilon}_{1,d-\varepsilon}$ for some $\varepsilon \in \{0,1\}$ and $\alpha := \frac{n-4}{2}$, and $s = \cos(\theta)$. Note that $s' < s$ and for $r = \sqrt{\frac{s-s'}{1-s'}}$, we have $s' = \frac{s-r^2}{1-r^2}$ and $0 < r < 1$. Let $0 < \delta = O(\frac{1}{n})$ that we specify later, and define the function F for the application of Proposition 4.6 to be

$$F(y) := \chi(y) := \begin{cases} 1 & \text{for } r-\delta < y \leq R, \\ 0 & \text{otherwise.} \end{cases}$$

We cite some results from the work of Levenshtein [Lev98]. By [Lev98, Lemma 5.89]

$$t^{\alpha+1,\alpha+1}_{1,d-1} < t^{\alpha+1,\alpha}_{1,d} < t^{\alpha+1,\alpha+1}_{1,d}.$$

Levenshtein proved Theorem 1.1, by using the following test functions; see [Lev98, Lemma 5.38]

$$g(x) = \begin{cases} \frac{(x+1)^2}{(x-s')}\left(p^{\alpha+1,\alpha+1}_{d-1}(x)\right)^2 & \text{if } s' = t^{\alpha+1,\alpha+1}_{1,d-1}, \\ \frac{(x+1)}{(x-s')}\left(p^{\alpha+1,\alpha}_{d}(x)\right)^2 & \text{if } s' = t^{\alpha+1,\alpha}_{1,d}, \end{cases}$$

where $\alpha := \frac{n-4}{2}$ in our case. Applying Proposition 4.6 with the function F as above and the function g, we obtain the inequality in the statement of the theorem. We now prove the bound on c_n for sufficiently large n.

By Corollary 1.5, we know that if $s' \neq \cos(\theta^*)$ as $n \to \infty$, then $\mathcal{L}(g_{\theta'})/\mu_n(\theta, \theta')$ for large n is exponentially worse than $\mathcal{L}(g_{\theta^*})/\mu_n(\theta, \theta^*)$. Therefore, we assume that $s' = \cos(\theta') = t_{1,d-\varepsilon}^{\alpha+1,\alpha+\varepsilon}$ for some $\varepsilon \in \{0, 1\}$, and that s' is sufficiently close to $\cos\theta^*$. Note that Corollary 1.5 only used the first part of Theorem 1.4 (basically, Proposition 4.6), and so our argument is not circular. Suppose $s' = t_{1,d}^{\alpha+1,\alpha}$. By Proposition 6.1, we have

$$g(x) = (x+1)(x-s')\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^2(1+A(x))^2,$$

where

$$|A(x)| \leq \frac{e^{\sigma(x)}-1}{\sigma(x)} - 1$$

with

$$\sigma(x) := \frac{|x-s'|(ns'+s'+1)}{1-s'^2}.$$

Next, we consider the test functions constructed in the previous section, and check its negativity. By Proposition 7.1, we have

$$\mu(x; s, \chi) = (1+o(1))\, 2\sqrt{2}\left(\delta + \sqrt{\frac{s-x}{1-x}} - r\right)^+ \left(\left(\frac{1-x^2}{x^2}\right)\left(s-r^2\right)^2\right)^{\frac{n-4}{2}} e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)}.$$

We need to find the maximal $\delta > 0$ such that

$$\int_{-1}^{1} g(x)\mu(x; t, \chi)dx \leq 0$$

for every $-1 \leq t \leq s$. We note that it is enough to prove the above inequality for $t = s$. Since for $s' < t < s$,

$$r(t) = \sqrt{\frac{t-s'}{1-s'}} < \sqrt{\frac{s-s'}{1-s'}} - O(1/n) < r - \delta.$$

Let $\delta = O(1/n)$ that we specify later. Note that the integrand is negative for $x < s'$ and positive for $x > s'$. Hence,

$$\begin{aligned} & \operatorname{sign}\left(\int_{-1}^{1} g(x)\mu(x; s, \chi)dx\right) \\ = \; & \operatorname{sign}\left(\left|\int_{s'}^{1} g(x)\mu(x; s, \chi)dx\right| - \left|\int_{-1}^{s'} g(x)\mu(x; s, \chi)dx\right|\right) \end{aligned}$$

Next, we give a lower bound on the absolute value of the integral over $-1 < x < s'$. By our upper bound on $A(x)$, we have

$$|1 + A(x)| \geq \left(2 - \frac{e^{\sigma(x)}-1}{\sigma(x)}\right)^+$$

We note that $2 - \frac{e^\sigma - 1}{\sigma}$ is a concave function with value 1 at $\sigma = 0$ and a root at $\sigma = 1.256431...$. Hence, for $\sigma < 1.25643$, we have

$$|1 + A(x)| \geq \left(2 - \frac{e^{\sigma(x)}-1}{\sigma(x)}\right).$$

Note that $\sigma(x) < 1.25643$ implies

$$|x - s'| \leq \frac{(1.25643)(1-s'^2)}{ns'}.$$

Let

$$\lambda := \frac{(1.25643)(1-s'^2)}{ns'}.$$

Therefore, as $n\to\infty$

(33)

$$2^{-\frac{3}{2}}\left(s-r^2\right)^{-(n-4)}\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^{-2}\left|\int_{-1}^{s'} g(x)\mu(x;s,\chi)dx\right|$$

$$\gtrsim \int_{s'-\lambda}^{s'}(1+x)(s'-x)\left(2-\frac{e^{\sigma(x)}-1}{\sigma(x)}\right)^2\left(\delta+\sqrt{\frac{s-x}{1-x}}-r\right)\left(\frac{1-x^2}{x^2}\right)^{\frac{n-4}{2}}e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)}dx.$$

We change the variable $s'-x$ to z and note that

$$\sqrt{\frac{s-x}{1-x}}-r=\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}+O(\lambda^2) \tag{34}$$

$$\frac{1-x^2}{x^2}=\frac{1-s'^2}{s'^2}\left(1+\frac{2z}{s'(1-s'^2)}+O(\lambda^2)\right) \tag{35}$$

for $|x-s'|<\lambda$. Hence, we obtain that as $n\to\infty$ and $|x-s'|<\lambda$,

$$\begin{aligned}
e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)} &= e^{\left(-\frac{2nr\left(\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}\right)}{s-r^2}\right)+O(\lambda)} = e^{\left(\frac{-nz}{s'(1-s')}\right)+O(\lambda)}\\
\left(\frac{1-x^2}{x^2}\right)^{\frac{n-4}{2}} &= \left(\frac{1-s'^2}{s'^2}\right)^{\frac{n-4}{2}}e^{\left(\frac{nz}{s'(1-s'^2)}\right)+O(\lambda)}\\
2-\frac{e^{\sigma(x)}-1}{\sigma(x)} &= \left(2-\frac{e^{\frac{nzs'}{(1-s'^2)}}-1}{\frac{nzs'}{(1-s'^2)}}\right)(1+O(\lambda)).
\end{aligned}$$

for $|x-s'|<\lambda$. We replace the above asymptotic formulas and obtain that as $n\to\infty$, the right hand side of (33) is at least

$$(1+s')\left(\frac{1-s'^2}{s'^2}\right)^{\frac{n-4}{2}}\int_0^\lambda z\left(2-\frac{e^{\frac{nzs'}{(1-s'^2)}}-1}{\frac{nzs'}{(1-s'^2)}}\right)^2\left(\delta+\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}\right)e^{\left(-\frac{nz}{1-s'^2}\right)}dz.$$

Finally, we give an upper bound on the absolute value of the integral over $s'<x<1$. We note that

$$\sqrt{\frac{s-x}{1-x}}-r=\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}+O(\lambda^2).$$

Let $\Lambda := \frac{2(s-s')^{1/2}(1-s')^{3/2}\delta}{(1-s)}$. Hence, we have

$$\left(\delta+\sqrt{\frac{s-x}{1-x}}-r\right)^+=0$$

for $x-s'>\frac{2(s-s')^{1/2}(1-s')^{3/2}\delta}{(1-s)}$. We have

$$|1+A(x)|\le\left(\frac{e^{\sigma(x)}-1}{\sigma(x)}\right).$$

where

$$\sigma(x) = \frac{n|x-s'|s'}{(1-s'^2)}.$$

Therefore,

$$\begin{aligned}
&2^{-\frac{3}{2}}\left(s-r^2\right)^{-(n-4)}\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^{-2}\left|\int_{s'}^1 g(x)\mu(x;s,\chi)dx\right| \\
\lesssim\ & (1+s')\left(\frac{1-s'^2}{s'^2}\right)^{\frac{n-4}{2}}\int_0^\Lambda z\left(\frac{e^{\frac{nzs'}{(1-s'^2)}}-1}{\frac{nzs'}{(1-s'^2)}}\right)^2\left(\delta-\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}\right)e^{\left(\frac{nz}{1-s'^2}\right)}dz.
\end{aligned}$$

We choose δ such that

$$\begin{aligned}
&\int_0^\lambda z\left(2-\frac{e^{\frac{nzs'}{(1-s'^2)}}-1}{\frac{nzs'}{(1-s'^2)}}\right)^2\left(\delta+\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}\right)e^{\left(-\frac{nz}{1-s'^2}\right)}dz \\
&\geq \int_0^\Lambda z\left(\frac{e^{\frac{nzs'}{(1-s'^2)}}-1}{\frac{nzs'}{(1-s'^2)}}\right)^2\left(\delta-\frac{z(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}\right)e^{\left(\frac{nz}{1-s'^2}\right)}dz.
\end{aligned}$$

Since s' converges to $\cos(\theta^*)$ as $n\to\infty$, for large enough n we may replace the numerical value $\cos(1.0995124)$ for s'. Furthermore, write $v := nz$, and divide by δ to obtain

$$\begin{aligned}
&\int_0^{2.196823} v\left(2-\frac{e^{0.571931v}-1}{0.571931v}\right)^2\left(1+\frac{v}{n\Lambda}\right)e^{(-1.259674v)}dv \\
&\geq \int_0^{n\Lambda} v\left(\frac{e^{0.571931v}-1}{0.571931v}\right)^2\left(1-\frac{v}{n\Lambda}\right)e^{(1.259674v)}dv.
\end{aligned}$$

Here, we have also used that $\Lambda = \frac{2\delta(s-s')^{1/2}(1-s')^{3/2}}{(1-s)}$. Also, note that $n\lambda = 2.196823...$ when s' is near $\cos(1.0995124)$. We have the Taylor expansion around $v=0$

$$\begin{aligned}
& v\left(\frac{e^{0.571931v}-1}{0.571931v}\right)^2 e^{(1.259674v)} \\
=\ & v+1.83161v^2+1.70465v^3+1.07403v^4+0.514959v^5+0.200242v^6+0.0657225v^7 \\
+\ & 0.0187113v^8+0.00471321v^9+0.0010662v^{10}+0.000219143v^{11}+0.0000413083v^{12}+Er
\end{aligned}$$

with error $|Er| < 2\times 10^{-5}$ if $n\Lambda < 0.92$, which we assume to be the case. Simplifying, we want to find the maximal $n\Lambda$ such that

$$\begin{aligned}
& 0.195783+\frac{0.140655}{n\Lambda} \geq \int_0^{n\Lambda} v\left(\frac{e^{0.571556v}-1}{0.571556v}\right)^2\left(1-\frac{v}{n\Lambda}\right)e^{(1.259392v)}dv \\
=\ & 3.17756\times 10^{-6}(n\Lambda)^2\Big((n\Lambda)^{11}+5.74715(n\Lambda)^{10}+30.5037(n\Lambda)^9+148.328(n\Lambda)^8+654.286(n\Lambda)^7 \\
+\ & 2585.41(n\Lambda)^6+9002.5(n\Lambda)^5+27010.2(n\Lambda)^4+67600.9(n\Lambda)^3+134116(n\Lambda)^2+192140(n\Lambda)+157353\Big) \\
-\ & \frac{1}{n\Lambda}\left(-0.360653+2.42691e^{1.25967(n\Lambda)}-3.33819e^{1.83161(n\Lambda)}+1.27193e^{2.40354(n\Lambda)}\right)+Er,
\end{aligned}$$

where the error Er again satisfies $|Er| \leq 2 \times 10^{-5}$. A numerical computation gives us that the inequality is satisfied when $n\Lambda \leq 0.915451....$ Therefore, if we choose $\delta = \ell/n$, then we must have

$$\ell \leq 0.915451... \frac{(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}}.$$

In this case, the cap of radius $\sqrt{1-r^2}$ becomes $\sqrt{1-(r-\delta)^2} = \sqrt{1-r^2}\left(1+\frac{\ell r}{n(1-r^2)}\right) + O(1/n^2)$. Note that $r = \sqrt{\frac{s-s'}{1-s'}}$, and so

$$\frac{r}{1-r^2} = \frac{(s-s')^{1/2}(1-s')^{1/2}}{1-s}.$$

We deduce that,

$$\frac{\ell r}{(1-r^2)} \leq 0.915451... \frac{(1-s)}{2(s-s')^{1/2}(1-s')^{3/2}} \cdot \frac{(s-s')^{1/2}(1-s')^{1/2}}{1-s} = \frac{0.457896862...}{1-s'} = 0.83837237...$$

Similarly, one may obtain the same when $s' = t_{1,d-1}^{\alpha+1,\alpha+1}$. Therefore, our improvement to Levenshtein's bound on $M(n,\theta)$ for large n is by a factor of $1/e^{0.83837237...} = 0.432413...$ for any choice of angle $0 < \theta < \theta^*$. As the error is less than 2×10^{-5}, we deduce that we have an improvement by a factor of at most 0.4325 for sufficiently large n. □

5.2. **Comparison with the Cohn–Zhao bound.** In this subsection, we give our improvement to Cohn and Zhao's [CZ14] bound on sphere packings. We are in the situation of wanting to bound from above the maximal density δ_{n-1} introduced in the introduction to this paper. We have $s' = \cos(\theta')$, and $\overline{r} = \frac{1}{\sqrt{2(1-s')}}$. By assumption, $1/3 \leq s' < 1/2$. In this case, we define for each $0 < \delta = \frac{c_1}{n}$ the function F to be used in Proposition 4.7 to be

$$F(y) := \chi(y) := \begin{cases} 1 & \text{for } 0 \leq y \leq \overline{r} + \delta, \\ 0 & \text{otherwise.} \end{cases}$$

Let

$$r_1 := \sqrt{1-(1-x^2)(\overline{r}+\delta)^2} + x(\overline{r}+\delta).$$

Suppose that $|x - s'| \leq \frac{c_2}{n}$ and $\delta = \frac{c_1}{n}$ for some $0 < c_1 < 0.81$, $0 < c_2 < 3.36$. Note that for such a c_1 and $n \geq 2000$, the assumption $s' < 1/2$ implies that $\overline{r} + \delta < 1$. By Proposition 7.2, we have $\mu(x;\chi) = 0$ for $r_1 \geq \overline{r} + \delta$. Otherwise,

$$\mu(x;\chi) = C_n(1+E)(1-x^2)^{\frac{n-4}{2}} \left(\frac{1}{2(1-x)}\right)^{n-3} \sqrt{1+\left(x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}}\right)^2} (\overline{r} + \delta - r_1)$$

for some constant $C_n > 0$ making $\mu(x;\chi)$ a probability measure on $[-1,1]$, and where $|E| < \frac{(4c_2+2c_1+2)^2}{n}$ for $n \geq 2000$. In particular, for such c_1, c_2, we have $|E| < \frac{292}{n}$.

Proof of Theorem 1.6. As in the proof of Theorem 1.4, we consider $g(x)$ chosen for $s' = \cos(\theta')$. Note that Proposition 4.7 applied to the function F above and g Levenshtein's optimal polynomial for angle θ' gives the existence of the inequality in the theorem. We now deal with the more precise version when $n \geq 2000$ and s' is a root of the Jacobi polynomial as before. As in the proof of Theorem 1.4, we let $s' = t_{1,d}^{\alpha+1,\alpha}$ and take g for this s' as before. As before, we begin with the observation that

$$\text{sign}\left(\int_{-1}^{1} g(x)\mu(x;\chi)dx\right) = \text{sign}\left(\left|\int_{s'}^{1} g(x)\mu(x;\chi)dx\right| - \left|\int_{-1}^{s'} g(x)\mu(x;\chi)dx\right|\right).$$

Let us give a lower bound on the absolute value of the negative contribution from $x \le s'$. As before, for $-1 \le x \le s'$, we have

$$|1 + A(x)| \ge \left(2 - \frac{e^{\sigma(x)} - 1}{\sigma(x)}\right),$$

where

$$\sigma(x) = \frac{|x - s'|((n-1)s' + 1)}{(1 - s'^2)}.$$

Note that $\sigma(x) < 1.25643$, ensuring that the right hand side of the bound on $1+A(x)$ is non-negative, implies

$$|x - s'| \le \frac{1.25643(1 - s'^2)}{(n-1)s' + 1}.$$

Let

$$\lambda := \frac{1.25643(1 - s'^2)}{(n-1)s' + 1}.$$

Since $1/3 \le s' < 1/2$ and $n \ge 2000$, this λ is compatible with the restriction $0 < c_2 < 3.36$. From the above considerations, we have

$$\begin{aligned}
& C_n^{-1} 2^{n-3} \frac{dp_d^{(\alpha+1,\alpha)}}{dt} (s')^{-2} \left| \int_{-1}^{s'} g(x)\mu(x;\chi)dx \right| \\
\ge\ & C_n^{-1} 2^{n-3} \frac{dp_d^{(\alpha+1,\alpha)}}{dt} (s')^{-2} \left| \int_{s'-\lambda}^{s'} g(x)\mu(x;\chi)dx \right| \\
\ge\ & (1+E) \int_{s'-\lambda}^{s'} \frac{(1+x)(s'-x)(1+A(x))^2(1-x^2)^{\frac{n-4}{2}}}{(1-x)^{n-3}} \sqrt{1 + \left(x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}}\right)^2} (\overline{r} + \delta - r_1)^+ \, dx \\
\ge\ & \left(1 - \frac{292}{n}\right) \int_{s'-\lambda}^{s'} (s'-x) \left(2 - \frac{e^{\sigma(x)} - 1}{\sigma(x)}\right)^2 \left(\frac{1+x}{1-x}\right)^{\frac{n-2}{2}} \sqrt{1 + \left(x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}}\right)^2} (\overline{r} + \delta - r_1) \, dx.
\end{aligned}$$

Note that if we let $z := s' - x$, then

$$\left(\frac{1+x}{1-x}\right)^{\frac{n-2}{2}} = \left(\frac{1+s'}{1-s'}\right)^{\frac{n-2}{2}} e^{-\frac{(n-2)z}{1-s'^2}} (1 + E')$$

where $|E'| \le \frac{(s'+\lambda)}{n(1-(s'+\lambda)^2)^2} \left(\frac{1.25643(1-s'^2)}{s'}\right)^2 + \frac{0.003}{n} \le \frac{4.74}{n}$ for $|x - s'| \le \lambda$ and $n \ge 2000$. Here, we have also used the assumption that $1/3 \le s' < 1/2$.

Furthermore, using a Taylor expansion around $x = s'$, we obtain

$$\sqrt{1 + \left(x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}}\right)^2} = \sqrt{2}(1 + E''),$$

where $|E''| < \frac{5\sqrt{2}(1.25643)(1-s'^2)}{2ns'} \le \frac{11.85}{n}$ for $|x - s'| \le \lambda$, $n \ge 2000$, and $1/3 \le s' < 1/2$.

We now write the first order Taylor expansion of r_1 in two variables δ and z at $\delta = z = 0$ and obtain

$$\overline{r} + \delta - r_1 = 2\delta + \frac{\overline{r}}{1 - s'} z + O(\delta|z|).$$

When $n \geq 2000$, the error may be numerically bounded in absolute value from above by

$$\frac{2}{n^2}\left(\frac{1.25643(1-s'^2)}{s'}+0.81\right)^2 \leq \frac{34.62}{n^2}.$$

As a result, we obtain

$$\begin{aligned}
&C_n^{-1}2^{n-3-1/2}\left(\frac{1+s'}{1-s'}\right)^{-\frac{n-2}{2}}\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^{-2}\left|\int_{-1}^{s'}g(x)\mu(x;\chi)dx\right| \\
\geq\ & (1-E''')\int_0^\lambda z\left(2-\frac{e^{\frac{((n-1)s'+1)z}{(1-s'^2)}}-1}{\frac{((n-1)s'+1)z}{(1-s'^2)}}\right)^2 e^{\frac{-(n-2)z}{1-s'^2}}(2\delta+\frac{\overline{r}}{1-s'}z-\frac{34.62}{n^2})dz \\
\geq\ & (1-E''')\int_0^\lambda z\left(2-\frac{e^{\frac{((n-1)s'+1)z}{(1-s'^2)}}-1}{\frac{((n-1)s'+1)z}{(1-s'^2)}}\right)^2 e^{\frac{-((n-1)s'+1)z}{s'(1-s'^2)}}(2\delta+\frac{\overline{r}}{1-s'}z-\frac{34.62}{n^2})dz,
\end{aligned}$$

where $0 < E''' < 312/n$. Making the substitution $v = \frac{((n-1)s'+1)z}{(1-s'^2)}$ and dividing by 2δ, we obtain that

$$\begin{aligned}
&C_n^{-1}\left(\frac{((n-1)s'+1)}{(1-s'^2)}\right)\delta^{-1}2^{n-3-3/2}\left(\frac{1+s'}{1-s'}\right)^{-\frac{n-2}{2}}\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^{-2}\left|\int_{-1}^{s'}g(x)\mu(x;\chi)dx\right| \\
\geq\ & (1-E''')\frac{1}{2\delta}\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-\frac{v}{s'}}\left(2\delta+\frac{\overline{r}(1+s')v}{(n-1)s'+1}-\frac{34.62}{n^2}\right)dv \\
\geq\ & \left(1-\frac{312}{n}\right)\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-\frac{v}{s'}}\left(1+\frac{v}{\beta(n,s',c_1)}-\frac{34.62}{2\delta n^2}\right)dv
\end{aligned}$$

where $\beta(n,s',c_1) := \frac{((n-1)s'+1)\Lambda}{1-s'^2}$ with $\Lambda := \frac{2(1-s')\delta}{\overline{r}}$.

On the other hand, the integral from s' to 1 may be bounded from above in a similar way. Indeed, we may show in a similar way that

$$\begin{aligned}
&C_n^{-1}\left(\frac{((n-1)s'+1)}{(1-s'^2)}\right)\delta^{-1}2^{n-3-3/2}\left(\frac{1+s'}{1-s'}\right)^{-\frac{n-2}{2}}\frac{dp_d^{(\alpha+1,\alpha)}}{dt}(s')^{-2}\left|\int_{s'}^{1}g(x)\mu(x;\chi)dx\right| \\
\leq\ & \left(1+\frac{312}{n}\right)\int_0^{\beta(n,s',c_1)} v\left(\frac{e^v-1}{v}\right)^2 e^{\frac{v}{s'}}\left(1-\frac{v}{\beta(n,s',c_1)}+\frac{34.62}{2\delta n^2}\right)dv
\end{aligned}$$

Note that asymptotically, that is, as $n \to \infty$, the negativity condition of Proposition 4.7 is satisfied if

(36)
$$\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-\frac{v}{s'}}\left(1+\frac{v}{\beta(\infty,s',c_1)}\right)dv \geq \int_0^{\beta(\infty,s',c_1)} v\left(\frac{e^v-1}{v}\right)^2 e^{\frac{v}{s'}}\left(1-\frac{v}{\beta(\infty,s',c_1)}\right)dv.$$

Here, $\beta(\infty,s',c_1) := \lim_{n\to\infty}\beta(n,s',c_1) = \frac{2c_1s'}{\overline{r}(1+s')}$. Note that $\beta(\infty,s',c_1)$ is an increasing function of s' in the interval $[0, \sqrt{17}/2-3/2]$. For $1/3 \leq s' < 1/2$, we have $0 < \beta(\infty,s',c_1) \leq \frac{2c_1}{3}$. As a result, for $1/3 \leq s' < 1/2$ inequality (36) is satisfied if

$$\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-3v}\left(1+\frac{3v}{2c_1}\right)dv \geq \int_0^{\frac{2c_1}{3}} v\left(\frac{e^v-1}{v}\right)^2 e^{3v}\left(1-\frac{3v}{2c_1}\right)dv.$$

By a numerics similar to that done for spherical codes, one finds that the maximal such $c_1 < 1$ is 0.66413470.... Therefore, for every $1/3 \le s' < 1/2$ and $n \to \infty$, we have an improvement at least as good as

$$e^{-0.6641347/\bar{r}} = \exp(-0.6641347\sqrt{2(1-s')}).$$

Note that for such s', as $n \to \infty$, this gives us an improvement of at most 0.5148, a universal such improvement factor.

Returning to the case of general $n \ge 2000$ and $1/3 \le s' < 1/2$, given such an n we need to maximize $c_1 < 0.81$ such that

$$\begin{aligned} &\left(1-\frac{312}{n}\right)\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-\frac{v}{s'}}\left(1+\frac{v}{\beta(n,s',c_1)}-\frac{17.31}{\delta n^2}\right)dv \\ \ge\ &\left(1+\frac{312}{n}\right)\int_0^{\beta(n,s',c_1)} v\left(\frac{e^v-1}{v}\right)^2 e^{\frac{v}{s'}}\left(1-\frac{v}{\beta(n,s',c_1)}+\frac{17.31}{\delta n^2}\right)dv. \end{aligned}$$

Just as in the asymptotic case above, for $1/3 \le s' < 1/2$ and $n \ge 2000$, since

$$\beta(n,s',c_1) \le \frac{2\left(s'+\frac{1-s'}{2000}\right)c_1\sqrt{2(1-s')}}{1+s'} \le 0.667c_1,$$

it suffices to find the largest c_1 such that

$$\begin{aligned} &\left(1-\frac{312}{n}\right)\int_0^{1.25643} v\left(2-\frac{e^v-1}{v}\right)^2 e^{-3v}\left(1+\frac{1.499v}{c_1}-\frac{17.31}{c_1 n}\right)dv \\ \ge\ &\left(1+\frac{312}{n}\right)\int_0^{0.667c_1} v\left(\frac{e^v-1}{v}\right)^2 e^{3v}\left(1-\frac{1.499v}{c_1}+\frac{17.31}{c_1 n}\right)dv. \end{aligned}$$

This is equivalent to

$$\begin{aligned} &\left(1-\frac{312}{n}\right)\left(0.046916643\left(1-\frac{17.31}{c_1 n}\right)+\frac{0.02603702878}{c_1}\right) \\ \ge\ &\left(1+\frac{312}{n}\right)\int_0^{0.667c_1} v\left(\frac{e^v-1}{v}\right)^2 e^{3v}\left(1-\frac{1.499v}{c_1}+\frac{17.31}{c_1 n}\right)dv. \end{aligned}$$

By a numerical calculation with `Sage`, we obtain that the improvement factor for any $1/3 \le s' < 1/2$ and any $n \ge 2000$ is at least as good as

$$0.515 + 74/n.$$

On the other hand, if we fix $s' = s^*$, then the same kind of calculations as above give us an asymptotic improvement constant of 0.4325, the same as in the case of spherical codes. In fact, for $n \ge 2000$, we have an improvement factor at least as good as

$$0.4325 + 51/n$$

over the combination of Cohn–Zhao [CZ14] and Levenshtein's optimal polynomials [Lev79]. In particular, the universal improvement factor $0.515+74/n$ for $1/3 \le s' < 1/2$ and $n \ge 2000$ is not sharp.

The case of $s' = t_{1,d-1}^{\alpha+1,\alpha+1}$ follows in exactly the same way. This completes the proof of our theorem. $\square$

Remark 37. We end this section by saying that our improvements above are based on a *local* understanding of Levenshtein's optimal polynomials, and that there is a loss in our computations. By doing numerics, we may do computations without having to rely on this local understanding. As we will see in Section 11, our numerical calculations lead to even further improvements, even in low dimensions.

6. Local approximation of Jacobi polynomials

As part of our proofs in the previous section, we needed to determine local approximations to Jacobi polynomials $p_d^{(\alpha,\beta)}$ in the neighbourhood of points $s \in (-1,1)$ such that $s \geq t_{1,d}^{\alpha,\beta}$, where $t_{1,d}^{\alpha,\beta}$ denotes the largest root of $p_d^{(\alpha,\beta)}$. This is obtained using the behaviour of the zeros of Jacobi polynomials. Using this, we obtain suitable local approximations of Levenshtein's optimal functions near s.

Proposition 6.1. *Suppose that* $\alpha \geq \beta \geq 0$, $|\alpha-\beta| \leq 1$, $d \geq 0$ *and* $s \in [t_{1,d}^{(\alpha,\beta)}, 1)$. *Then, we have*

$$p_d^{(\alpha,\beta)}(t) = p_d^{(\alpha,\beta)}(s) + (t-s)\frac{dp_d^{(\alpha,\beta)}}{dt}(s)(1+A(t)),$$

where,

$$|A(t)| \leq \frac{e^{\sigma(t)}-1}{\sigma(t)} - 1$$

with

$$\sigma(t) := \frac{|t-s|\,(2\alpha s + 2s + 1)}{1-s^2}.$$

Proof. Consider the Taylor expansion

$$p_d^{(\alpha,\beta)}(t) = \sum_{k=0}^{\infty} \frac{(t-s)^k}{k!}\frac{d^k p_d^{(\alpha,\beta)}}{dt^k}(s)$$

of $p_d^{(\alpha,\beta)}$ centered at s. We prove the proposition by showing that for $s \in [t_{1,d}^{(\alpha,\beta)}, 1)$, the higher degree terms in the Taylor expansion are small in comparison to the linear term. Indeed, suppose $k \geq 1$. Then we have

$$\frac{(d^{k+1}/dt^{k+1})p_d^{(\alpha,\beta)}(s)}{(d^k/dt^k)p_d^{(\alpha,\beta)}(s)} = \frac{(d/dt)p_{d-k}^{(\alpha+k,\beta+k)}(s)}{p_{d-k}^{(\alpha+k,\beta+k)}(s)} = \sum_{i=1}^{d-k}\frac{1}{s-t_{i,d-k}^{\alpha+k,\beta+k}} \leq \sum_{i=1}^{d-1}\frac{1}{s-t_{i,d-1}^{\alpha+1,\beta+1}},$$

where the last inequality follows from the fact that the roots of a Jacobi polynomial interlace with those of its derivative. However, the last quantity is equal to $\frac{(d^2/dt^2)p_d^{(\alpha,\beta)}(s)}{(d/dt)p_d^{(\alpha,\beta)}(s)}$. We proceed to showing that

$$\frac{(d^2/dt^2)p_d^{(\alpha,\beta)}(s)}{(d/dt)p_d^{(\alpha,\beta)}(s)} \leq \frac{2\alpha+2s+1}{1-s^2}. \tag{38}$$

Indeed, we know from the differential equation (24) that

$$(1-s^2)(d^2/dt^2)p_d^{(\alpha,\beta)}(s) + (\beta-\alpha-(\alpha+\beta+2)s)(d/dt)p_d^{(\alpha,\beta)}(s) + d(d+\alpha+\beta+1)p_d^{(\alpha,\beta)}(s) = 0. \tag{39}$$

However, since s is to the right of the largest root of $p_d^{(\alpha,\beta)}$, $p_d^{(\alpha,\beta)}(s) \geq 0$. Therefore,

$$(1-s^2)(d^2/dt^2)p_d^{(\alpha,\beta)}(s) + (\beta-\alpha-(\alpha+\beta+2)s)(d/dt)p_d^{(\alpha,\beta)}(s) \leq 0,$$

from which the inequality (38) follows. As a result, the degree $k+1$ term compares to the linear term as

$$\frac{(d^{k+1}/dt^{k+1})p_d^{(\alpha,\beta)}(s)}{(d/dt)p_d^{(\alpha,\beta)}(s)}\frac{|t-s|^k}{(k+1)!} \quad \leq \quad \frac{|t-s|^k}{(k+1)!}\left(\frac{2(\alpha+1)s+1}{1-s^2}\right)^k$$

Consequently, for every $k \geq 1$,

$$\frac{|t-s|^{k+1}}{(k+1)!}(d^{k+1}/dt^{k+1})p_d^{(\alpha,\beta)}(s) \leq |t-s|(d/dt)p_d^{(\alpha,\beta)}(s)\frac{\left(\frac{|t-s|(2\alpha+2s+1)}{1-s^2}\right)^k}{(k+1)!}$$

As a result, we obtain that

$$p_d^{(\alpha,\beta)}(t) = p_d^{(\alpha,\beta)}(s) + (t-s)\frac{dp_d^{(\alpha,\beta)}}{dt}(s)(1+A(t)),$$

where

$$|A(t)| \le \frac{e^{\sigma(t)}-1}{\sigma(t)} - 1$$

with

$$\sigma(t) = \frac{|t-s|\,(2\alpha s + 2s + 1)}{1-s^2}.$$

□

7. Conditional density functions

In this section, we compute the conditional density functions for spherical codes and sphere packings used previously.

7.1. **Conditional density function for spherical codes.** Let $\boldsymbol{x}, \boldsymbol{y}$ and $\boldsymbol{z}$ be three randomly independently chosen points on S^{n-1} with respect to the Haar measure. Recall the definitions of u, v, t previously introduced as the pairwise inner products of these vectors. The pushforward measure onto (u, v, t) has the following density function

$$\mu(u,v,t) = \det \begin{bmatrix} 1 & t & u \\ t & 1 & v \\ u & v & 1 \end{bmatrix}^{\frac{n-4}{2}}.$$

Let

$$x := \frac{t-uv}{\sqrt{(1-u^2)(1-v^2)}}.$$

Recall that $\theta < \theta'$. Let $s' = \cos(\theta')$ and $s = \cos(\theta)$. Note that $s' < s$ and for $r = \sqrt{\frac{s-s'}{1-s'}}$, we have $s' = \frac{s-r^2}{1-r^2}$ and $0 < r < 1$. Let $0 < \delta = o(\frac{1}{\sqrt{n}})$ that we specify later, and define

$$\chi(y) := \begin{cases} 1 & \text{for } r-\delta < y \le R, \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mu(x; s, \chi)$ be the induced density function on x subjected to the conditions $t = s$, and $r - \delta \le u, v \le R$. We define for *complex* x

$$x^+ = \begin{cases} x & \text{for } x \ge 0, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition 7.1. *Suppose that* $|x - s'| = o(\frac{1}{\sqrt{n}})$. *We have*

$$\mu(x; s, \chi) = (1+o(1))\, 2\sqrt{2}\left(\delta + \sqrt{\frac{s-x}{1-x}} - r\right)^+ \left(\left(\frac{1-x^2}{x^2}\right)\left(s-r^2\right)^2\right)^{\frac{n-4}{2}} e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)}.$$

Proof. We have

$$\mu(x; s, \chi) = \int_{C_x} \chi(u)\chi(v)\mu(u,v,s)dl$$

where the integral is over the curve $C_x \subset \mathbb{R}^2$ that is given by $\frac{s-uv}{\sqrt{(1-u^2)(1-v^2)}} = x$ and dl is the induced Euclidean metric on C_x. We note that

$$\mu(u,v,s) = \left((1-x^2)(1-u^2)(1-v^2)\right)^{\frac{n-4}{2}}.$$

Hence,

$$\begin{aligned}\mu(x;s,\chi) &= \int_{C_x} \chi(u)\chi(v)\mu(u,v,s)dl \\ &= (1-x^2)^{\frac{n-4}{2}} \int_{C_x} \chi(u)\chi(v)\left((1-u^2)(1-v^2)\right)^{\frac{n-4}{2}} dl \\ &= (1-x^2)^{\frac{n-4}{2}} \int_{C_x} \chi(u)\chi(v)\left(\frac{s-uv}{x}\right)^{n-4} dl \\ &= \left(\frac{1-x^2}{x^2}\right)^{\frac{n-4}{2}} \int_{C_x} \chi(u)\chi(v)\left(s-uv\right)^{n-4} dl\end{aligned}$$

Suppose that u and v are in the support of χ. Since $|x-s'| = o(\frac{1}{\sqrt{n}})$, it follows that $u = r+\tilde{u}$ and $v = r+\tilde{v}$, where $\tilde{u}, \tilde{v} = o(\frac{1}{\sqrt{n}})$. We have

$$s - uv = s - r^2 - r(\tilde{u}+\tilde{v}) - \tilde{u}\tilde{v} = (s-r^2)\left(1 - \frac{r(\tilde{u}+\tilde{v})+\tilde{u}\tilde{v}}{s-r^2}\right).$$

Hence,

$$\mu(x;s,\chi) = \left(\left(\frac{1-x^2}{x^2}\right)(s-r^2)^2\right)^{\frac{n-4}{2}} \int_{C_x} \chi(u)\chi(v)\left(1-\frac{r(\tilde{u}+\tilde{v})+\tilde{u}\tilde{v}}{s-r^2}\right)^{n-4} dl.$$

Recall the following inequalities, which follows easily from the Taylor expansion of $\log(1+x)$

$$e^{a-\frac{a^2}{n}} \leq (1+\frac{a}{n})^n \leq e^a$$

for $|a| \leq n/2$. We apply the above inequalities to estimate the integral, and obtain

$$\int_{C_x} \chi(u)\chi(v)\left(1-\frac{r(\tilde{u}+\tilde{v})+\tilde{u}\tilde{v}}{s-r^2}\right)^{n-4} dl = (1+o(1))\int_{C_x} e^{\left(-\frac{nr(\tilde{u}+\tilde{v})}{s-r^2}\right)}\chi(u)\chi(v)dl.$$

We approximate the curve C_x with the following line

$$\tilde{u}+\tilde{v} = 2\left(\sqrt{\frac{s-x}{1-x}} - r\right) + o\left(\frac{1}{n}\right).$$

It follows that

$$\int_{C_x} e^{\left(-\frac{nr(\tilde{u}+\tilde{v})}{s-r^2}\right)}\chi(u)\chi(v)dl = (1+o(1))2\sqrt{2}\left(\delta+\sqrt{\frac{s-x}{1-x}}-r\right)^+ e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)}.$$

Therefore,

$$\mu(x;s,\chi) = (1+o(1))\,2\sqrt{2}\left(\delta+\sqrt{\frac{s-x}{1-x}}-r\right)^+ \left(\left(\frac{1-x^2}{x^2}\right)(s-r^2)^2\right)^{\frac{n-4}{2}} e^{\left(-\frac{2nr\left(\sqrt{\frac{s-x}{1-x}}-r\right)}{s-r^2}\right)}.$$

This completes the proof of our proposition. □

7.2. **Conditional density for sphere packings.** In this section, we describe and estimate the probability density function for sphere packings. Let $s' = \cos(\theta')$ and $\overline{r} = \frac{1}{\sqrt{2(1-s')}}$, where $1/3 \leq s' < 1/2$. Let $0 < \delta = \frac{c_1}{n}$ for some fixed $c_1 > 0$ that we specify later, and define

$$\chi(y) := \begin{cases} 1 & \text{for } 0 \leq y \leq \overline{r}+\delta, \\ 0 & \text{otherwise.}\end{cases}$$

Let $\boldsymbol{x}, \boldsymbol{y}$ be two randomly independently chosen points on $\mathbb{R}^{n-1}$ with respect to the Euclidean measure such that $|\boldsymbol{x}|, |\boldsymbol{y}| \leq \overline{r} + \delta$, where $|.|$ is the Euclidean norm. Let $\alpha := \arccos\langle \boldsymbol{x}, \boldsymbol{y}\rangle$,

$$U := |\boldsymbol{x}|,$$

$$V := |\boldsymbol{y}|,$$

and

$$T := |\boldsymbol{x} - \boldsymbol{y}|.$$

The pushforward measure onto (U, V, α) has the following density

$$\mu(U, V, \alpha) = U^{n-2} V^{n-2} \sin(\alpha)^{n-3} dU dV d\alpha,$$

up to a positive scalar scalar that depends only on n. Similarly, the projection onto (U, V, T) has the following density function up to a positive scalar

$$\mu(U, V, T) = (UVT)\Delta(U, V, T)^{n-4} dU dV dT,$$

where $\Delta(U, V, T)$ is the Euclidean area of the triangle with sides U, V, T. Let

$$x := \cos(\alpha) = \frac{U^2 + V^2 - T^2}{2UV}.$$

Let $\mu(x; \chi)$ be the induced density function on x subjected to the conditions $T = 1$, and $U, V \leq \overline{r} + \delta$. We define for x

$$x^+ = \begin{cases} x & \text{for } x \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Let

$$r_1 := \sqrt{1 - (1 - x^2)(\overline{r} + \delta)^2} + x(\overline{r} + \delta).$$

Proposition 7.2. *Suppose that* $|x - s'| \leq \frac{c_2}{n}$*,* $x < 1/2$ *and* $\delta = \frac{c_1}{n}$ *for some fixed* $0 < c_1 < 1$*,* $0 < c_2 < 2.2$*. We have*

$$\mu(x; \chi) = (1 + E)(1 - x^2)^{\frac{n-4}{2}} \left(\frac{1}{2(1 - x)}\right)^{n-3} \sqrt{1 + \left(x - \frac{(1 - x^2)\overline{r}}{\sqrt{1 - (1 - x^2)\overline{r}^2}}\right)^2} (\overline{r} + \delta - r_1)^+$$

up to a positive scalar multiple making this a probability measure on $[-1, 1]$*, and where* $|E| < \frac{(4c_2 + 2c_1 + 2)^2}{n}$ *for* $n \geq 2000$*.*

Proof. We have

$$\mu(x; \chi) = \int_{C_x} \chi(U)\chi(V)\mu(U, V, 1) dl,$$

where the integral is over the curve $C_x \subset \mathbb{R}^2$ that is given by $\frac{U^2 + V^2 - 1}{2UV} = x$ and dl is the induced Euclidean metric on C_x. We note that

$$\mu(U, V, 1) = UV \left((1 - x^2)U^2V^2\right)^{\frac{n-4}{2}}.$$

Hence,

$$\mu(x; \chi) = (1 - x^2)^{\frac{n-4}{2}} \int_{C_x} \chi(U)\chi(V) \, (UV)^{n-3} \, dl.$$

Suppose that U and V are in the support of χ. Let $U = \overline{r} + \tilde{U}$ and $V = \overline{r} + \tilde{V}$, then $\tilde{U}, \tilde{V} \leq \frac{c_1}{n}$. We have

$$\tilde{U} + \tilde{V} = \frac{1}{2\overline{r}(1 - x)} - \overline{r} + O(1/n^2) = \frac{(x - s')}{2\overline{r}(1 - x)^2} + O(1/n^2).$$

Since $|x - s'| \leq \frac{c_2}{n}$, and $0.5 < 2\overline{r}(1-x)^2$, it follows that $-\frac{c_1+2c_2}{n} < \tilde{U}, \tilde{V} \leq \frac{c_1}{n}$ for $n \geq 2000$. Hence,

$$\tilde{U} + \tilde{V} = \frac{1}{2\overline{r}(1-x)} - \overline{r} + E_1.$$

where

$$|E_1| = \left| \frac{1}{2\overline{r}(1-x)} \left(2x\tilde{U}\tilde{V} - \tilde{U}^2 - \tilde{V}^2 \right) \right| \leq 3\frac{(c_1+2c_2)^2}{n^2}.$$

We have

$$UV = \overline{r}^2 + \overline{r}(\tilde{U}+\tilde{V}) + \tilde{U}\tilde{V} = \overline{r}^2 \left(1 + \frac{\tilde{U}+\tilde{V}}{\overline{r}} \right) + \tilde{U}\tilde{V} = \frac{1}{2(1-x)} + E_2,$$

where $|E_2| < 4\frac{(c_1+2c_2)^2}{n^2}$. Hence,

$$\mu(x;\chi) = (1-x^2)^{\frac{n-4}{2}} \left(\frac{1}{2(1-x)} \right)^{n-3} \int_{C_x} \left(1 + \frac{E_2}{2(1-x)} \right)^{n-3} \chi(U)\chi(V)dl.$$

Note that

$$\left(1 + \frac{E_2}{2(1-x)} \right)^{n-3} = 1 + E_2',$$

where $E_2' \leq 4\frac{(c_1+2c_2)^2}{n}$ for $n \geq 2000$. Hence,

$$\int_{C_x} \left(1 + \frac{E_2}{2(1-x)} \right)^{n-3} \chi(U)\chi(V)dl = (1+\bar{E}_2) \int_{C_x} \chi(U)\chi(V)dl,$$

where $\bar{E}_2 \leq 4\frac{(c_1+2c_2)^2}{n}$. We parametrize the curve C_x with V to obtain

$$U(V) = \sqrt{1-(1-x^2)V^2} + xV.$$

We have

$$\frac{dU}{dV} = x - \frac{(1-x^2)V}{\sqrt{1-(1-x^2)V^2}} = x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}} + E_3,$$

where

$$|E_3| = \left| (V-\overline{r}) \frac{(1-x^2)}{(1-(1-x^2)V_1^2)^{3/2}} \right|$$

for some $V_1 \in (\overline{r} - \frac{c_1+2c_2}{n}, \overline{r} + \frac{c_1}{n})$, which implies $\left| \frac{(1-x^2)}{(1-(1-x^2)V_1^2)^{3/2}} \right| < 6$. Hence,

$$|E_3| \leq 6 \left(\frac{c_1+2c_2}{n} \right).$$

Hence,

$$\begin{aligned}
\int_{C_x} \chi(U)\chi(V)dl &=^{+} \int_{r_1}^{\overline{r}+\delta} \sqrt{1 + \left(\frac{dU}{dV} \right)^2} dV \\
&= \sqrt{1 + \left(x - \frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}} \right)^2} \left(\overline{r} + \delta - r_1 \right)^{+} (1+\bar{E}_3)
\end{aligned}$$

where

$$r_1 := \sqrt{1-(1-x^2)(\overline{r}+\delta)^2} + x(\overline{r}+\delta),$$

and

$$|E_3| \leq 6 \left(\frac{c_1+2c_2}{n} \right).$$

The first equality $=^+$ above means equal to 0 if $\overline{r}+\delta<r_1$. Therefore,

$$\mu(x;\chi)=(1+E)(1-x^2)^{\frac{n-4}{2}}\left(\frac{1}{2(1-x)}\right)^{n-3}\sqrt{1+\left(x-\frac{(1-x^2)\overline{r}}{\sqrt{1-(1-x^2)\overline{r}^2}}\right)^2}\,(\overline{r}+\delta-r_1)^+$$

up to a positive scalar multiple, where $|E|<\frac{(4c_2+2c_1+2)^2}{n}$ for $n\geq 2000$. This completes the proof of our Proposition. □

8. The critical function

In this section, we give a proof of Theorems 1.7 and 1.10. Consider the function

$$g(t;s,\boldsymbol{\lambda}):=(t-s)\eta(t)\left(\sum_{i=0}^{d-1}\frac{\lambda_i}{(t-s)}\det\begin{bmatrix}\tilde{p}_{i+1}(t) & \tilde{p}_{i+1}(s)\\ \tilde{p}_i(t) & \tilde{p}_i(s)\end{bmatrix}\right)^2.$$

We write $g(t;s,\boldsymbol{\lambda})=\sum_{i=0}^{2d+h-1}g_i(s,\boldsymbol{\lambda})p_i(t)$.

8.1. **Computing $g_0(s,\boldsymbol{\lambda})$.** We show that $g_0(s,\boldsymbol{\lambda})$ as a quadratic form in $\boldsymbol{\lambda}$ has a diagonal form.

Proposition 8.1. *We have*

$$g_0(s,\boldsymbol{\lambda})=-\sum_{j=0}^{d-1}\tilde{a}_{j+1}\tilde{p}_j(s)\tilde{p}_{j+1}(s)\lambda_j^2.$$

As a result for every $0\leq i\leq m-1$, we have

$$\frac{\partial g_0}{\partial\lambda_i}=-2\tilde{a}_{i+1}\lambda_i\tilde{p}_i(s)\tilde{p}_{i+1}(s).$$

Proof. We have

$$\begin{aligned}
g_0(s,\boldsymbol{\lambda})&=\int_{-1}^1 g(t;s,\boldsymbol{\lambda})d\mu_\alpha(t)\\
&=\int_{-1}^1\sum_{j=0}^{d-1}\left(\sum_{l=j}^{d-1}\tilde{a}_{l+1}\lambda_l\right)\tilde{p}_j(t)\tilde{p}_j(s)\\
&\times\left(\lambda_{d-1}\tilde{p}_{d-1}(s)\tilde{p}_d(t)+\sum_{i=0}^{d-1}(-\lambda_i\tilde{p}_{i+1}(s)+\lambda_{i-1}\tilde{p}_{i-1}(s))\tilde{p}_i(t)\right)\eta(t)d\mu_\alpha(t)\\
&=\sum_{j=0}^{d-1}\left(\sum_{l=j}^{d-1}\tilde{a}_{l+1}\lambda_l\right)\tilde{p}_j(s)(-\lambda_j\tilde{p}_{j+1}(s)+\lambda_{j-1}\tilde{p}_{j-1}(s))\\
&=\sum_{j=0}^{d-1}\lambda_j\tilde{p}_j(s)\tilde{p}_{j+1}(s)\left(\sum_{l=j+1}^{d-1}\tilde{a}_{l+1}\lambda_l-\sum_{l=j}^{m-1}\tilde{a}_{l+1}\lambda_l\right)\\
&=-\sum_{j=0}^{d-1}\tilde{a}_{j+1}\tilde{p}_j(s)\tilde{p}_{j+1}(s)\lambda_j^2.
\end{aligned}$$

Hence, we also have

$$\frac{\partial g_0}{\partial\lambda_i}=-2\tilde{a}_{i+1}\lambda_i\tilde{p}_i(s)\tilde{p}_{i+1}(s).$$

This completes the proof of our proposition. □

8.2. **Lagrange multiplier.** Let

$$R(s,\boldsymbol{\lambda}) := \frac{g(1;s,\boldsymbol{\lambda})}{g_0(s,\boldsymbol{\lambda})}.$$

Note that for fixed s, $R(s,\boldsymbol{\lambda})$ is invariant under multiplying $\boldsymbol{\lambda}$ with a scalar. So, for fixed s, we may consider $R(s,\boldsymbol{\lambda})$ as a function on the projective space $\mathbb{P}^{d-1}(\mathbb{R})$. We define

$$\boldsymbol{\lambda}^c := (\lambda_0^c,\ldots,\lambda_{d-1}^c), \tag{40}$$

where

$$\lambda_i^c = \frac{1}{\tilde{a}_{i+1}}\left(\frac{\tilde{p}_i(1)}{\tilde{p}_i(s)} - \frac{\tilde{p}_{i+1}(1)}{\tilde{p}_{i+1}(s)}\right).$$

We prove Theorem 1.7 in the following.

Proof of Theorem 1.7. We apply a version of the Lagrange multiplier method and show that $\boldsymbol{\lambda}^c$ (up to scalar) is the unique critical point of $R(s,\boldsymbol{\lambda})$ subjected to $g_0>0$. Since $R(s,\boldsymbol{\lambda})$ is a function on the projective space, without loss of generality we may assume $g_0(s,\boldsymbol{\lambda})=1$. So, minimizing $R(s,\boldsymbol{\lambda})$ subjected to $g_0>0$ is equivalent to finding the minimum of

$$g(1;s,\boldsymbol{\lambda}) = \frac{1}{1-s}\left(\sum_{i=0}^{d-1}\lambda_i \det\begin{bmatrix}\tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s)\\ \tilde{p}_i(1) & \tilde{p}_i(s)\end{bmatrix}\right)^2$$

on the quadric $g_0(s,\boldsymbol{\lambda})=1$. First, we show that $(\lambda_0^c,\ldots,\lambda_{d-1}^c)$ is a critical point for the restriction of R on $g_0(s,\boldsymbol{\lambda})=1$. We have

$$\nabla R = \frac{1}{g_0}\nabla g(1;s,\boldsymbol{\lambda}) - \frac{g(1;s,\boldsymbol{\lambda})}{g_0^2}\nabla g_0.$$

Therefore, $\boldsymbol{\lambda}$ is a critical point for the restriction of R on $g_0(s,\boldsymbol{\lambda})=1$ if and only if $\nabla g(1;s,\boldsymbol{\lambda})$ is parallel to ∇g_0. In other words, it is enough to show that $\nabla g(1;s,\boldsymbol{\lambda})=\nabla g_0$ as points in the projective space $\mathbb{P}^{d-1}(\mathbb{R})$. In what follows we consider vectors as elements of $\mathbb{P}^{d-1}(\mathbb{R})$, so we ignore the scalars.

$$\begin{aligned}\nabla g(1;s,\boldsymbol{\lambda}) &= \left(\frac{\partial g(1;.)}{\partial \lambda_i}\right)_{0\le i\le d-1}\\ &= \frac{\left(\sum_{i=0}^{d-1}\lambda_i\det\begin{bmatrix}\tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s)\\ \tilde{p}_i(1) & \tilde{p}_i(s)\end{bmatrix}\right)}{1-s}\left(\det\begin{bmatrix}\tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s)\\ \tilde{p}_i(1) & \tilde{p}_i(s)\end{bmatrix}\right)_{0\le i\le d-1}\\ &= \left(\det\begin{bmatrix}\tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s)\\ \tilde{p}_i(1) & \tilde{p}_i(s)\end{bmatrix}\right)_{0\le i\le d-1} \in \mathbb{P}^{d-1}(\mathbb{R}).\end{aligned}$$

By Proposition 8.1, we have

$$\nabla g_0(s,\boldsymbol{\lambda}) = (\tilde{a}_{i+1}\lambda_i\tilde{p}_i(s)\tilde{p}_{i+1}(s))_{0\le i\le d-1}\in\mathbb{P}^{d-1}(\mathbb{R}).$$

If $\boldsymbol{\lambda}=(\lambda_i)_{0\le i\le d-1}$ is a critical point then

$$(\lambda_i)_{0\le i\le d-1} = \left(\frac{1}{\tilde{a}_{i+1}}\left(\tilde{p}_i(1)/\tilde{p}_i(s) - \tilde{p}_{i+1}(1)/\tilde{p}_{i+1}(s)\right)\right)_{0\le i\le d-1} = \boldsymbol{\lambda}^c \in \mathbb{P}^{d-1}(\mathbb{R}).$$

This implies that $\boldsymbol{\lambda}^c\in\mathbb{P}^{d-1}(\mathbb{R})$ is the unique critical point for R subjected to $g_0>0$.

If we additionally have $d_1(s)\le d<d_2(s)$, then the quadratic form $g_0(s,\boldsymbol{\lambda})$ has signature $(1,d-1)$. Therefore the set

$$C := \{\boldsymbol{\lambda} : g_0(s,\boldsymbol{\lambda})\ge 1\}$$

is a convex set. Furthermore, note that

$$\begin{aligned}
&\sum_{i=0}^{d-1} \lambda_i^c \det \begin{bmatrix} \tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s) \\ \tilde{p}_i(1) & \tilde{p}_i(s) \end{bmatrix} \\
= \quad & -\sum_{i=0}^{d-1} \tilde{a}_{i+1}\tilde{p}_i(s)\tilde{p}_{i+1}(s)(\lambda_i^c)^2 = g_0^{[\mu,d,\eta]} > 0,
\end{aligned}$$

where the final equality follows from Proposition 8.1. Therefore, the tangent hyperplane of the quadric $g_0(s, \boldsymbol{\lambda}) = 1$ at $\boldsymbol{\lambda}^c$ separates the origin and the quadric. Hence, it follows that $\boldsymbol{\lambda}^c$ is the unique global minimum of R. This concludes the proof of Theorem 1.7. □

We now prove Theorem 1.10 providing us with a clean expression for $f^{[\mu,d,\eta]}$.

Proof of Theorem 1.10. Recall that

$$f^{[\mu,d,\eta]}(t) := \sum_{i=0}^{d-1} \frac{\lambda_i^{\mathrm{c}}}{t-s} \det \begin{bmatrix} \tilde{p}_{i+1}(t) & \tilde{p}_{i+1}(s) \\ \tilde{p}_i(t) & \tilde{p}_i(s) \end{bmatrix}.$$

We have for every $i \leq d-1$,

$$\begin{aligned}
&\int_{-1}^{1} f^{[\mu,d,\eta]}(t)\tilde{p}_i(t)(t-s)\eta(t)d\mu \\
= \quad & -\lambda_i^{\mathrm{c}}\tilde{p}_{i+1}(s) + \lambda_{i-1}^{\mathrm{c}}\tilde{p}_{i-1}(s) \\
= \quad & \frac{1}{\tilde{a}_{i+1}}\left(\tilde{p}_{i+1}(1) - \frac{\tilde{p}_i(1)\tilde{p}_{i+1}(s)}{\tilde{p}_i(s)}\right) + \frac{1}{\tilde{a}_i}\left(\tilde{p}_{i-1}(1) - \frac{\tilde{p}_i(1)\tilde{p}_{i-1}(s)}{\tilde{p}_i(s)}\right) \\
= \quad & \frac{1}{\tilde{p}_i(s)}\left(\frac{1}{\tilde{a}_{i+1}}\det\begin{bmatrix} \tilde{p}_{i+1}(1) & \tilde{p}_{i+1}(s) \\ \tilde{p}_i(1) & \tilde{p}_i(s) \end{bmatrix} - \frac{1}{\tilde{a}_i}\det\begin{bmatrix} \tilde{p}_i(1) & \tilde{p}_i(s) \\ \tilde{p}_{i-1}(1) & \tilde{p}_{i-1}(s) \end{bmatrix}\right) \\
= \quad & \frac{(1-s)}{\tilde{p}_i(s)}\left(\sum_{j=0}^{i}\tilde{p}_j(1)\tilde{p}_j(s) - \sum_{j=0}^{i-1}\tilde{p}_j(1)\tilde{p}_j(s)\right) = (1-s)\tilde{p}_i(1).
\end{aligned}$$

This implies that

$$\int_{-1}^{1} f^{[\mu,d,\eta]}(t)q(t)(t-1)(t-s)\eta(t)d\mu = 0, \tag{41}$$

where $q(t)$ is any polynomial of degree at most $d-2$. Note that $f^{[\mu,d,\eta]}(t)$ is uniquely determined (up to a constant) by being a polynomial of degree $d-1$ that satisfies equation (41). It is easy to check that

$$\frac{1}{(t-1)(t-s)} \det \begin{bmatrix} \tilde{p}_{d+1}(t) & \tilde{p}_{d+1}(s) & \tilde{p}_{d+1}(1) \\ \tilde{p}_d(t) & \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_{d-1}(t) & \tilde{p}_{d-1}(s) & \tilde{p}_{d-1}(1) \end{bmatrix},$$

is of degree $d-1$ and satisfies equation (41). Therefore,

$$f^{[\mu,d,\eta]}(t) = \frac{c}{(t-1)(t-s)} \det \begin{bmatrix} \tilde{p}_{d+1}(t) & \tilde{p}_{d+1}(s) & \tilde{p}_{d+1}(1) \\ \tilde{p}_d(t) & \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_{d-1}(t) & \tilde{p}_{d-1}(s) & \tilde{p}_{d-1}(1) \end{bmatrix},$$

where $c \in \mathbb{C}$. Similarly, we show that

$$\sum_{i=0}^{d-1} \tilde{p}_i(t) \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_i(s) & \tilde{p}_i(1) \end{bmatrix}$$

satisfies equation (41). It is enough to check it for every

$$q_l(t) = \frac{1}{(t-1)(t-s)} \det \begin{bmatrix} \tilde{p}_{l+1}(t) & \tilde{p}_{l+1}(s) & \tilde{p}_{l+1}(1) \\ \tilde{p}_l(t) & \tilde{p}_l(s) & \tilde{p}_l(1) \\ \tilde{p}_{l-1}(t) & \tilde{p}_{l-1}(s) & \tilde{p}_{l-1}(1) \end{bmatrix},$$

where $l < d$. We have

$$\begin{aligned} &\int_{-1}^{1} \left(\sum_{i=0}^{d-1} \tilde{p}_i(t) \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_i(s) & \tilde{p}_i(1) \end{bmatrix} \right) \det \begin{bmatrix} \tilde{p}_{l+1}(t) & \tilde{p}_{l+1}(s) & \tilde{p}_{l+1}(1) \\ \tilde{p}_l(t) & \tilde{p}_l(s) & \tilde{p}_l(1) \\ \tilde{p}_{l-1}(t) & \tilde{p}_{l-1}(s) & \tilde{p}_{l-1}(1) \end{bmatrix} \eta(t) d\mu \\ = \; &\det \begin{bmatrix} \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_{l+1}(s) & \tilde{p}_{l+1}(1) \end{bmatrix} & \tilde{p}_{l+1}(s) & \tilde{p}_{l+1}(1) \\ \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_l(s) & \tilde{p}_l(1) \end{bmatrix} & \tilde{p}_l(s) & \tilde{p}_l(1) \\ \det \begin{bmatrix} \tilde{p}_d(s) & \tilde{p}_d(1) \\ \tilde{p}_{l-1}(s) & \tilde{p}_{l-1}(1) \end{bmatrix} & \tilde{p}_{l-1}(s) & \tilde{p}_{l-1}(1) \end{bmatrix} = 0, \end{aligned}$$

where that last identity follows from the fact that the first column is a linear combination of the other two columns. This concludes the proof of our theorem. □

Proof of Theroem 1.12. Our method is based on the proof of Theroem 1.10. It is enough to show that $b^{[\mu,d,\eta]}(t)$ and $r^{[\mu,d,\eta]}(t)$ are of degree $d-1$ and satisfies equation (41). It is clear that they are of degree $d-1$ and $b^{[\mu,d,\eta]}(t)$ satisfy equation (41). Similarly, it is enough to show that $r^{[\mu,d,\eta]}(t)$ satisfies equation (41) for every

$$q_i(t) := \frac{1}{(t-\alpha_1)\dots(t-\alpha_h)} \det \begin{bmatrix} p_{i+k}(t) & p_{i+k}(\alpha_1) & \dots & p_{i+k}(\alpha_h) \\ p_{i+k-1}(t) & p_{i+k-1}(\alpha_1) & \dots & p_{i+k-1}(\alpha_h) \\ \vdots & \vdots & & \vdots \\ p_i(t) & p_i(\alpha_1) & \dots & p_i(\alpha_h) \end{bmatrix},$$

where $i < d-1$. This follows from a similar argument as in the proof of Theorem 1.10. □

We end this section with a computation of the $\gamma_{i.j}$.

Lemma 8.2.

$$\gamma_{i,j} = \begin{cases} p_i(1)p_j(1) \sum_{l=j}^{i-1} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & \textit{for } j < i, \\ 0 & \textit{otherwise.} \end{cases}$$

Proof. We will prove this using the Christoffel-Darboux formula (16). Indeed, we may rewrite

$$\begin{aligned} \gamma_{i,j} &= p_i(1) \int_{-1}^{1} \frac{\frac{p_i(t)}{p_i(1)} - 1}{t-1} p_j(t) d\mu \\ &= p_i(1) \sum_{l=0}^{i-1} \int_{-1}^{1} \frac{\frac{p_{l+1}(t)}{p_{l+1}(1)} - \frac{p_l(t)}{p_l(1)}}{t-1} p_j(t) d\mu \\ &= p_i(1) \sum_{l=j}^{i-1} \int_{-1}^{1} \frac{\frac{p_{l+1}(t)}{p_{l+1}(1)} - \frac{p_l(t)}{p_l(1)}}{t-1} p_j(t) d\mu. \end{aligned}$$

Using the Christoffel-Darboux formula (16), we may write

$$\frac{\frac{p_{l+1}(t)}{p_{l+1}(1)} - \frac{p_l(t)}{p_l(1)}}{t-1} = \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} \sum_{k=0}^{l} p_k(1)p_k(t).$$

Substituting this into the above, we obtain

$$\gamma_{i,j} \quad = \quad p_i(1)\sum_{l=j}^{i-1}\sum_{k=0}^{l}\int_{-1}^{1}\frac{a_{l+1}p_k(1)}{p_l(1)p_{l+1}(1)}p_k(t)p_j(t)d\mu = p_i(1)p_j(1)\sum_{l=j}^{i-1}\frac{a_{l+1}}{p_l(1)p_{l+1}(1)}.$$

□

9. Critical value of functional

In this section, we give a proof of Theorem 1.14. We now take our function $g^{[\mu,d,\eta]}$ for general polynomials η. By Theorem 1.12, *up to a nonzero constant*, $f^{[\mu,d,\eta]}$ has the equivalent expressions $b^{[\mu,d,\eta]}(t) = \left(\prod_{i=d}^{d+h+1} a_i\right) r^{[\mu,d,\eta]}$, where $b^{[\mu,d,\eta]}$ and $r^{[\mu,d,\eta]}$ are defined in equations (12) and (13), respectively. Consider the function

$$h^{[\mu,d,\eta]}(t) := (t-s)\eta(t)b^{[\mu,d,\eta]}(t)^2.$$

$h^{[\mu,d,\eta]}$ is, up to a constant multiple, equal to $g^{[\mu,d,\eta]}$, and so $\mathcal{L}(g^{[\mu,d,\eta]}) = \mathcal{L}(h^{[\mu,d,\eta]})$. We now compute the value of the functional $\mathcal{L}$ at $h^{[\mu,d,\eta]}$. First, let us compute $h_0^{[\mu,d,\eta]}$.

Lemma 9.1.

$$h_0^{[\mu,d,\eta]} = b^{[\mu,d,\eta]}(1)\det\begin{bmatrix} p_{d+h+1}(1)\sum_{l=d-1}^{d+h}\frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ p_d(1)\sum_{l=d-1}^{d-1}\frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ 0 & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}.$$

Proof. By definition,

$$h_0^{[\mu,d,\eta]} = \int_{-1}^{1} h^{[\mu,d,\eta]}(t)d\mu(t).$$

Let $c' := \prod_{i=d}^{d+h+1} a_i$. Using the explicit expression for $h^{[\mu,d,\eta]}$, we obtain

$$\begin{aligned} & h_0^{[\mu,d,\eta]} \\ = \;& c'\int_{-1}^{1}(t-s)\eta(t)b^{[\mu,d,\eta]}(t)r^{[\mu,d,\eta]}(t)d\mu \\ = \;& c'\int_{-1}^{1}\left(\frac{1}{t-1}\det\begin{bmatrix} p_{d+h+1}(t) & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ & & \vdots & & & \\ p_d(t) & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p_{d-1}(t) & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}\right) r^{[\mu,d,\eta]}(t)d\mu(t) \\ = \;& c'\int_{-1}^{1}\left(\sum_{j=0}^{d+h}\det\begin{bmatrix} \gamma_{d+h+1,j} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ \gamma_{d,j} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix} p_j(t)\right) r^{[\mu,d,\eta]}(t)d\mu(t). \end{aligned}$$

Note that Lemma 8.2 gives us that for $j < d$,

$$\det \begin{bmatrix} \gamma_{d+h+1,j} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ \gamma_{d,j} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}$$

$$= p_j(1) \det \begin{bmatrix} p_{d+h+1}(1) \sum_{l=j}^{d+h} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ p_d(1) \sum_{l=j}^{d-1} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p_{d-1}(1) \sum_{l=j}^{d-2} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}$$

$$= p_j(1) \det \begin{bmatrix} p_{d+h+1}(1) \sum_{l=d-1}^{d+h} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ p_d(1) \sum_{l=d-1}^{d-1} \frac{a_{l+1}}{p_l(1)p_{l+1}(1)} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ 0 & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix},$$

where the last equality follows from subtracting a multiple of the third colum from the first column. Denote by A the determinant expression in the final line. A is independent of j. Using this and the computation above for $h_0^{[\mu,d,\eta]}$, we obtain

$$\begin{aligned} h_0^{[\mu,d,\eta]} &= c' A \int_{-1}^{1} \left(\sum_{j=0}^{d+h} p_j(1) p_j(t) \right) r^{[\mu,d,\eta]}(t) d\mu \\ &= c' A r^{[\mu,d,\eta]}(1) = A b^{[\mu,d,\eta]}(1). \end{aligned}$$

The conclusion follows. □

Combining the previous results, we obtain Theorem 1.14.

10. Positivity of Fourier coefficients

Proof of Theorem 1.13. By definition 1.9 and Theorem 1.12, the inequalities (11) and (15) are equivalent. Next, we show that the inequalities (10) and the inequalities (14) are equivalent. For $j > d + h$, p_j is orthogonal to any polynomial of degree at most $d + h$, hence

$$\int_{-1}^{1} p_j(t)(t-s)\eta(t) c f^{[\mu,d,\eta]}(t) d\mu = 0.$$

This implies inequalities (10) for $j > d + h$. Suppose that $d - 1 \le j \le d + h$. By the definition of $\gamma_{i,j}$.

$$\det \begin{bmatrix} \gamma_{d+h+1,j} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ \gamma_{d,j} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix}$$

and

$$\int_{-1}^{1} \frac{1}{(t-1)} \det \begin{bmatrix} p_{d+h+1}(t) & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ & & \vdots & & & \\ p_d(t) & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p_{d-1}(t) & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix} p_j(t) d\mu$$

are equal. This implies that the inequalities (10) and the inequalities (14) are equivalent for $d-1 \le j \le d+h$. Note that for $j < i$, we have

$$\gamma_{i,j} = \int_{-1}^{1} \frac{1}{t-1} \det \begin{bmatrix} p_j(1) & p_i(1) \\ p_j(t) & p_i(t) \end{bmatrix} d\mu$$

Hence, for $j < d$

$$\det \begin{bmatrix} \gamma_{d+h+1,j} & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ \vdots & \vdots & & & & \\ \gamma_{d,j} & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix} = p_j(1)D$$

where,

$$(42)\quad D := \int_{-1}^{1} \frac{1}{(t-1)} \det \begin{bmatrix} p_{d+h+1}(t) & p_{d+h+1}(s) & p_{d+h+1}(1) & p_{d+h+1}(\alpha_1) & \dots & p_{d+h+1}(\alpha_h) \\ & & \vdots & & & \\ p_d(t) & p_d(s) & p_d(1) & p_d(\alpha_1) & \dots & p_d(\alpha_h) \\ p_{d-1}(t) & p_{d-1}(s) & p_{d-1}(1) & p_{d-1}(\alpha_1) & \dots & p_{d-1}(\alpha_h) \end{bmatrix} d\mu.$$

Inequality (10) for $j = d-1$ and the positivity of $p_{d-1}(1)$, implies that $\kappa D > 0$. Therefore, the inequalities (10) for $j < d-1$ follow from $j = d-1$. This completes the proof of our theorem. ☐

Corollary 10.1. *If the measure μ satisfies the Krein condition and s is such that $p_d(s) < 0$ and $\frac{p_d(s)}{p_d(1)} - \frac{p_i(s)}{p_i(1)} \le 0$ for $0 \le i \le d$, then $\eta(t) := 1$ is (μ, s, d)-positive.*

Proof. Since $\frac{p_d(s)}{p_d(1)} - \frac{p_i(s)}{p_i(1)} \le 0$ for $0 \le i \le d$, $\det \begin{bmatrix} p_d(s) & p_d(1) \\ p_i(s) & p_i(1) \end{bmatrix} \le 0$ for every $0 \le i \le d-1$ and for $j = d$

$$\det \begin{bmatrix} \gamma_{d+1,j} & p_{d+1}(s) & p_{d+1}(1) \\ \gamma_{d,j} & p_d(s) & p_d(1) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) \end{bmatrix} \le 0.$$

Since $p_d(s) < 0$, it is easy to check that $D < 0$ which is defined in (42). This implies

$$\det \begin{bmatrix} \gamma_{d+1,j} & p_{d+1}(s) & p_{d+1}(1) \\ \gamma_{d,j} & p_d(s) & p_d(1) \\ \gamma_{d-1,j} & p_{d-1}(s) & p_{d-1}(1) \end{bmatrix} \le 0.$$

for every $0 \le j \le d-1$. By Theorem 1.13, $\eta(t) := 1$ is (μ, s, d)-positive. ☐

Remark 43. In particular, $d\mu_{\alpha,\beta}$ satisfies the Krein condition whenever $\alpha \ge \beta$, and so Corollary 10.1 is true for the corresponding Jacobi polynomials. This recovers the extremal polynomials of Levenshtein of odd degree.

Corollary 10.2. *For $\eta = 1 + t$ and $\mu = d\mu_\alpha$, if d is such that $\tilde{p}_d(s) < 0$ and $\frac{\tilde{p}_j(s)}{\tilde{p}_j(1)} - \frac{\tilde{p}_{j+1}(s)}{\tilde{p}_{j+1}(1)} \ge 0$ for every $0 \le j \le d-1$, then η is $(d\mu_\alpha, s, d)$-positive.*

Proof. By Theorem 1.13 it is enoguh to verify inequalities (14) and (15) for some $\kappa \in \mathbb{C}$. First, we check inequality (15). The inequality (15) is equivalent to

$$\int_{-1}^{1} p_i(t)(t-s)(1+t) f^{[\mu,d,\eta]}(t) d\mu_\alpha \ge 0.$$

Let $\tilde{p}_i$ be L^2-normalized versions of the Jacobi polynomials $p_i^{\alpha,\alpha+1}$ which satisfy

$$(44)\qquad p_n^{\alpha,\alpha+1}(t) = \frac{(n+1)}{(n+\alpha+1)(1+t)} p_{n+1}^{\alpha,\alpha}(t) + \frac{p_n^{\alpha,\alpha}(t)}{1+t}.$$

Note that the coefficients on the right hand side of the above are positive. Hence, it is enough to show that $(t-s)f^{[d\mu_\alpha,d,1+t]}(t)$ has non-negative coefficients when expanded in the basis $\tilde{p}_i$. As in the proof of Corollary 10.1, this is true since $\tilde{p}_d(s)<0$ and $\frac{\tilde{p}_d(s)}{\tilde{p}_d(1)}-\frac{\tilde{p}_{d-1}(s)}{\tilde{p}_{d-1}(1)}\leq 0$.

For the inequality (14), it suffices to show that

$$\begin{bmatrix} p_{d+1}(s) & p_{d+1}(1) & p_{d+1}(-1) \\ p_d(s) & p_d(1) & p_d(-1) \\ p_j(s) & p_j(1) & p_j(-1) \end{bmatrix}$$

have the same sign as j varies. Since, $p_j(-t)=(-1)^j p_j(t)$, we are reduced to showing that the determinants

$$\det\begin{bmatrix} 1 & 1 & 1 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ (-1)^j & (-1)^d & (-1)^{d+1} \end{bmatrix}$$

have the same sign as j varies. We split this verification into two cases based on the parity of d. If d is even, this determinant is

$$\det\begin{bmatrix} 1 & 1 & 1 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ (-1)^j & 1 & -1 \end{bmatrix}.$$

For j even, this reduces to

$$\det\begin{bmatrix} 1 & 1 & 1 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ 1 & 1 & -1 \end{bmatrix}=\det\begin{bmatrix} 0 & 0 & 2 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ 1 & 1 & -1 \end{bmatrix}=2\left(\frac{p_j(s)}{p_j(1)}-\frac{p_d(s)}{p_d(1)}\right).$$

For odd j (and d even), we have

$$\det\begin{bmatrix} 1 & 1 & 1 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ -1 & 1 & -1 \end{bmatrix}=\det\begin{bmatrix} 0 & 2 & 0 \\ \frac{p_j(s)}{p_j(1)} & \frac{p_d(s)}{p_d(1)} & \frac{p_{d+1}(s)}{p_{d+1}(1)} \\ -1 & 1 & -1 \end{bmatrix}=2\left(\frac{p_j(s)}{p_j(1)}-\frac{p_{d+1}(s)}{p_{d+1}(1)}\right).$$

If d is chosen so that these two quantities are non-negative, then we have the $(d\mu_\alpha,s,d)$-positivity of $1+t$. In the case of Levenshtein, d is the chosen to be the first index at which $\frac{\tilde{p}_j(s)}{\tilde{p}_j(1)}-\frac{\tilde{p}_{j+1}(s)}{\tilde{p}_{j+1}(1)}$ changes sign from positive to negative. This quantity is, after multiplication by $1+s$, equal to

$$\frac{p_j(s)}{p_j(1)}-\frac{p_{j+2}(s)}{p_{j+2}(1)}.$$

The equality follows from relation (44). This implies that for d even, the determinants above are non-negative for every $0\leq j\leq d-1$. Similarly, we can settle the case when d is odd. □

Therefore, the positivity conditions we impose subsume those of Levenshtein.

11. Numerics

In this section, we give a list of improvement factors to maximal sphere packing densities when using the linear programming method. The table consists of our factors of improvement to the right hand side of the inequality (4)

$$\delta_n\leq \sin^n(\theta/2)M(n,\theta)$$

of Cohn and Zhao as θ varies between 61° and 90° and when when $M(n, \theta)$ is bounded using Levenshtein's optimal polynomials [Lev79]. For each given n and θ, the factor of improvement is, by Proposition 4.7,

$$\left(1 + \frac{\delta}{r(\theta)}\right)^{-n},$$

where $\delta > 0$ is maximally chosen so that the negativity condition in the Cohn–Elkies linear programming method holds for the function H constructed in this paper in Section 4 with $\overline{r} = r(\theta) := \frac{1}{\sqrt{2(1-\cos\theta)}}$, $F = \chi_{[0,r(\theta)+\delta]}$, and such that $\overline{r}+\delta \le 1$. In Theorem 1.6, we restricted to the case where $\cos\theta'$ were roots of Jacobi polynomials for the simplicity of computations in Section 5. When doing numerics, however, in order to find the maximal δ, no such restriction is necessary; the following table neither needs nor imposes such a restriction. As all quantities but δ are easily computable or given, Table 2 may be used to compute the value of the appropriate δ. Though we do not include dimensions higher than 130, our preliminary numerics suggest that our 0.4325 in Theorem 1.6 may be improved.

n	61°	62°	63°	64°	65°	66°	67°	68°	69°	70°	71°	72°	73°	74°	75°	76°	77°	78°	79°	80°	81°	82°	83°	84°	85°	86°	87°	88°	89°	90°
4	.942	.889	.839	.793	.750	.711	.674	.640	.608	.578	.550	.524	.500	.477	.456	.436	.417	.399	.392	.396	.400	.405	.409	.413	.416	.418	.420	.420	.420	.419
5	.928	.863	.803	.748	.698	.653	.611	.572	.537	.504	.474	.446	.420	.400	.374	.371	.377	.382	.387	.392	.396	.401	.404	.408	.410	.412	.412	.412	.411	.408
6	.915	.838	.768	.706	.650	.599	.553	.512	.474	.439	.408	.385	.389	.393	.397	.368	.374	.379	.384	.389	.393	.398	.401	.404	.406	.407	.407	.406	.404	.401
7	.901	.813	.735	.666	.605	.550	.501	.457	.418	.395	.373	.378	.383	.388	.391	.395	.371	.377	.382	.387	.391	.395	.398	.401	.403	.404	.403	.402	.400	.396
8	.888	.789	.704	.629	.563	.505	.454	.409	.394	.394	.393	.373	.378	.383	.387	.391	.369	.374	.380	.385	.389	.393	.396	.399	.400	.401	.401	.399	.396	.392
9	.874	.766	.673	.593	.524	.464	.411	.389	.391	.392	.392	.391	.373	.378	.383	.387	.391	.372	.378	.383	.387	.391	.394	.397	.398	.399	.398	.397	.394	.389
10	.862	.744	.644	.560	.488	.426	.382	.386	.389	.390	.391	.391	.389	.374	.379	.384	.388	.371	.376	.381	.385	.389	.393	.395	.397	.397	.397	.395	.391	.387
11	.849	.722	.617	.528	.454	.391	.378	.382	.386	.388	.390	.390	.389	.370	.376	.380	.385	.369	.374	.379	.384	.388	.391	.394	.395	.396	.395	.393	.390	.385
12	.836	.701	.590	.498	.422	.384	.387	.379	.383	.386	.388	.389	.389	.387	.372	.377	.382	.386	.373	.378	.383	.387	.390	.393	.394	.395	.394	.392	.388	.384
13	.824	.681	.565	.470	.393	.380	.384	.375	.380	.383	.386	.388	.388	.387	.385	.375	.380	.384	.371	.376	.381	.385	.389	.392	.393	.394	.393	.391	.387	.382
14	.811	.661	.540	.444	.387	.376	.380	.384	.377	.381	.384	.387	.388	.387	.386	.372	.377	.382	.370	.375	.380	.384	.388	.391	.392	.393	.392	.390	.386	.381
15	.799	.642	.517	.419	.386	.386	.377	.381	.384	.378	.382	.385	.387	.387	.386	.370	.375	.380	.384	.374	.379	.383	.387	.390	.391	.392	.391	.389	.385	.380
16	.788	.623	.495	.395	.385	.386	.384	.378	.382	.376	.380	.383	.386	.386	.386	.384	.373	.378	.382	.373	.378	.382	.386	.389	.391	.391	.390	.388	.385	.380
17	.776	.605	.474	.381	.384	.385	.385	.375	.380	.383	.378	.382	.384	.386	.386	.384	.371	.376	.381	.371	.377	.381	.385	.388	.390	.391	.390	.388	.384	.379
18	.764	.587	.453	.378	.382	.384	.385	.383	.377	.381	.376	.380	.383	.385	.385	.384	.382	.374	.379	.370	.376	.380	.384	.387	.389	.390	.389	.387	.383	.378
19	.753	.570	.434	.383	.380	.383	.384	.384	.375	.379	.373	.378	.382	.384	.385	.384	.382	.373	.378	.369	.375	.379	.383	.387	.389	.389	.389	.387	.383	.378
20	.742	.553	.415	.381	.377	.381	.383	.384	.382	.377	.381	.376	.380	.383	.385	.384	.383	.371	.376	.381	.374	.379	.383	.386	.388	.389	.388	.386	.382	.377
21	.731	.537	.397	.379	.382	.379	.382	.383	.383	.375	.379	.374	.379	.382	.384	.384	.383	.369	.375	.379	.373	.378	.382	.385	.388	.388	.388	.386	.382	.377
22	.720	.522	.383	.376	.380	.377	.381	.383	.383	.381	.377	.381	.377	.381	.383	.384	.383	.380	.373	.378	.372	.377	.381	.385	.387	.388	.388	.385	.382	.376
23	.709	.506	.383	.382	.375	.381	.379	.382	.383	.382	.375	.379	.376	.380	.382	.384	.383	.381	.372	.377	.371	.376	.381	.384	.387	.388	.387	.385	.381	.376
24	.699	.492	.382	.382	.376	.380	.377	.381	.382	.382	.373	.378	.374	.378	.381	.383	.383	.381	.371	.376	.370	.375	.380	.384	.386	.387	.387	.385	.381	.375
25	.688	.477	.381	.382	.381	.378	.375	.379	.382	.382	.380	.376	.372	.377	.381	.383	.383	.381	.370	.375	.369	.374	.379	.383	.386	.387	.387	.384	.380	.375
26	.678	.463	.379	.381	.381	.376	.380	.378	.381	.382	.381	.375	.379	.376	.380	.382	.383	.382	.379	.374	.369	.374	.379	.383	.385	.387	.386	.384	.380	.375
27	.668	.450	.377	.380	.381	.380	.378	.376	.380	.381	.381	.373	.377	.375	.379	.381	.382	.382	.379	.373	.378	.373	.378	.382	.385	.386	.386	.384	.380	.375
28	.658	.437	.380	.379	.381	.381	.376	.375	.378	.381	.381	.379	.376	.373	.378	.381	.382	.382	.379	.372	.377	.373	.372	.382	.384	.386	.386	.384	.380	.375
29	.648	.424	.379	.378	.380	.381	.375	.379	.377	.380	.381	.380	.375	.372	.377	.380	.382	.382	.380	.371	.376	.372	.377	.381	.384	.386	.385	.384	.380	.374
30	.639	.411	.377	.376	.379	.381	.379	.377	.376	.379	.381	.380	.373	.378	.376	.379	.381	.382	.380	.370	.375	.372	.377	.381	.384	.385	.385	.383	.379	.374
31	.629	.400	.379	.379	.378	.380	.380	.376	.374	.378	.380	.380	.372	.377	.374	.378	.381	.382	.380	.369	.374	.371	.376	.380	.383	.385	.385	.383	.379	.374
32	.620	.388	.380	.377	.377	.380	.380	.374	.378	.377	.380	.380	.378	.375	.373	.378	.380	.381	.380	.377	.374	.370	.376	.380	.383	.385	.385	.383	.379	.374
33	.611	.379	.380	.376	.375	.379	.380	.378	.377	.376	.379	.380	.379	.374	.372	.377	.380	.381	.380	.371	.373	.370	.375	.379	.383	.384	.385	.383	.379	.374
34	.602	.378	.380	.379	.378	.378	.380	.379	.376	.375	.378	.380	.379	.373	.371	.376	.379	.381	.380	.378	.372	.369	.375	.379	.382	.384	.384	.383	.379	.374
35	.593	.377	.379	.379	.377	.377	.379	.379	.375	.374	.378	.380	.379	.372	.376	.375	.379	.381	.380	.378	.371	.369	.374	.379	.382	.384	.384	.382	.379	.373
36	.584	.375	.379	.379	.376	.375	.378	.379	.373	.377	.377	.379	.379	.377	.376	.374	.378	.380	.380	.378	.371	.376	.374	.378	.382	.384	.384	.382	.379	.373
37	.575	.378	.378	.379	.374	.374	.378	.379	.378	.376	.376	.379	.379	.378	.375	.373	.377	.380	.380	.379	.370	.375	.373	.378	.381	.384	.384	.382	.379	.373
38	.567	.376	.376	.379	.378	.377	.377	.379	.378	.375	.375	.378	.379	.378	.374	.373	.377	.380	.380	.379	.369	.375	.373	.378	.381	.383	.384	.382	.378	.373
39	.559	.375	.375	.378	.379	.376	.376	.378	.378	.374	.374	.377	.379	.378	.373	.372	.376	.379	.380	.379	.376	.374	.372	.377	.381	.383	.384	.382	.378	.373
40	.550	.378	.377	.377	.379	.375	.375	.378	.379	.373	.373	.377	.379	.378	.372	.376	.376	.379	.380	.379	.376	.374	.372	.377	.381	.383	.383	.382	.378	.373
41	.542	.379	.376	.376	.378	.377	.377	.377	.378	.377	.376	.376	.378	.379	.376	.376	.375	.378	.380	.379	.376	.373	.372	.376	.380	.383	.383	.382	.378	.373
42	.534	.378	.375	.375	.378	.378	.376	.376	.378	.377	.375	.375	.378	.379	.377	.375	.374	.378	.380	.379	.376	.372	.371	.376	.380	.382	.383	.382	.378	.373
43	.526	.378	.378	.374	.377	.378	.375	.375	.378	.378	.374	.374	.378	.379	.377	.374	.374	.377	.379	.379	.377	.372	.371	.376	.380	.382	.383	.381	.378	.373
44	.518	.377	.378	.376	.377	.378	.374	.374	.377	.378	.373	.373	.377	.378	.377	.373	.373	.377	.379	.379	.377	.371	.370	.375	.379	.382	.383	.381	.378	.372
45	.510	.377	.378	.375	.376	.378	.377	.373	.377	.378	.372	.372	.376	.378	.378	.372	.372	.376	.379	.379	.377	.371	.370	.375	.379	.382	.383	.381	.378	.372
46	.503	.376	.378	.374	.375	.378	.377	.376	.376	.378	.376	.376	.376	.378	.378	.372	.371	.376	.379	.379	.377	.370	.370	.375	.379	.382	.382	.381	.378	.372
47	.495	.374	.377	.377	.374	.377	.377	.375	.376	.378	.377	.375	.375	.378	.378	.371	.371	.375	.378	.379	.377	.370	.369	.375	.379	.381	.382	.381	.378	.372
48	.488	.376	.377	.377	.376	.376	.377	.374	.375	.377	.377	.374	.374	.377	.378	.376	.375	.375	.378	.379	.378	.369	.369	.374	.378	.381	.382	.381	.378	.372
49	.481	.375	.376	.377	.375	.376	.377	.373	.374	.377	.377	.373	.374	.377	.378	.376	.374	.374	.378	.379	.378	.369	.374	.374	.378	.381	.382	.381	.377	.372
50	.474	.374	.375	.377	.374	.375	.377	.376	.373	.377	.377	.372	.373	.377	.378	.376	.374	.374	.377	.379	.378	.374	.374	.374	.378	.381	.382	.381	.377	.372
60	.408	.375	.376	.376	.374	.376	.374	.375	.376	.373	.374	.376	.376	.374	.375	.377	.376	.373	.374	.377	.378	.376	.370	.371	.376	.379	.381	.380	.377	.371
70	.376	.374	.376	.375	.375	.373	.375	.375	.372	.375	.375	.372	.375	.375	.373	.374	.376	.375	.373	.374	.377	.377	.374	.369	.374	.378	.380	.379	.376	.371
80	.375	.374	.374	.374	.374	.374	.374	.373	.375	.373	.375	.374	.372	.375	.375	.373	.375	.376	.373	.371	.375	.377	.375	.370	.372	.377	.379	.379	.376	.371
90	.373	.374	.374	.374	.373	.374	.373	.374	.372	.374	.373	.374	.374	.372	.375	.374	.372	.375	.375	.371	.373	.376	.376	.372	.371	.375	.378	.379	.376	.370
100	.373	.374	.373	.373	.374	.372	.374	.372	.374	.372	.374	.373	.374	.373	.373	.374	.371	.373	.375	.373	.371	.375	.376	.373	.369	.374	.378	.378	.376	.370
110	.372	.372	.374	.373	.372	.374	.372	.374	.372	.373	.372	.374	.372	.374	.372	.374	.374	.370	.374	.374	.371	.373	.375	.374	.371	.373	.377	.378	.375	.370
120	.373	.373	.373	.373	.373	.372	.373	.372	.373	.373	.373	.373	.373	.373	.373	.371	.374	.372	.373	.374	.372	.372	.375	.374	.370	.373	.376	.377	.375	.370
130	.373	.373	.372	.372	.373	.373	.372	.373	.373	.371	.373	.373	.373	.372	.373	.370	.373	.373	.371	.374	.373	.370	.374	.375	.371	.372	.376	.377	.375	.370

TABLE 2. Table of improvement factors to δ_n via spherical codes using angles θ between 61° and 90° when comparing to Cohn–Zhao [CZ14]. Contains the information of maximal δ.

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