NEXT LEVELS UNIVERSAL BOUNDS FOR SPHERICAL CODES: THE LEVENSHTEIN FRAMEWORK LIFTED

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ABSTRACT. We introduce a framework based on the Delsarte-Yudin linear programming approach for improving some universal lower bounds for the minimum energy of spherical codes of prescribed dimension and cardinality, and universal upper bounds on the maximal cardinality of spherical codes of prescribed dimension and minimum separation. Our results can be considered as next level universal bounds as they have the same general nature and imply, as the first level bounds do, necessary and sufficient conditions for their local and global optimality. We explain in detail our approach for deriving second level bounds. While there are numerous cases for which our method applies, we will emphasize the model examples of 24 points (24-cell) and 120 points (600-cell) on $\mathbb{S}^3$. In particular, we provide a new proof that the 600-cell is universally optimal, and furthermore, we completely characterize the optimal linear programing polynomials of degree at most 17 by finding two new polynomials, which together with the Cohn-Kumar's polynomial form the vertices of the convex hull that consists of all optimal polynomials. Our framework also provides a conceptual explanation of why polynomials of degree 17 are needed to handle the 600-cell via linear programming.

1. INTRODUCTION

Let $\mathbb{S}^{n-1}$ denote the unit sphere in $\mathbb{R}^n$. We consider finite configurations (codes) $C \subset \mathbb{S}^{n-1}$ of $N \geq 2$ points. Given an (extended real-valued) function $h(t) : [-1, 1] \to [0, +\infty]$, the *h-energy* of C is given by

$$E_h(C) := \sum_{x,y \in C, x \neq y} h(\langle x, y \rangle),$$

where $\langle x, y \rangle$ denotes the usual inner product of x and y. We are interested in lower bounds on the *minimal energy*

$$\mathcal{E}_h(n, N) := \inf_{|C|=N} \{E_h(C)\}, \tag{1}$$

where $|C|$ denotes the cardinality of C.

Delsarte-Yudin's approach [35, 14, 12] for finding such lower bounds by linear programming (LP) is described as follows. Let $A_{n,h}$ denote the *feasible domain* of continuous functions f on $[-1, 1]$:

$$A_{n,h} := \{f : f(t) = \sum_{i=0}^{\infty} f_i P_i^{(n)}(t) \leq h(t),\ t \in [-1, 1],\ f_i \geq 0,\ i = 1, 2, \dots\}, \tag{2}$$

where $\{P_i^{(n)}(t)\}$ are the Gegenbauer polynomials [34] normalized by $P_i^{(n)}(1) = 1$ (see Section 2.1). Then (1) can be estimated by elements of the class (2) by

$$\mathcal{E}_h(n, N) \geq \max_{f \in A_{n,h}} N^2 \left(f_0 - \frac{f(1)}{N} \right). \tag{3}$$

Hereafter we consider only absolutely monotone potentials h.

Date: June 10, 2019.

[1]The research of the first and fifth authors was supported, in part, by a Bulgarian NSF contract DN02/2-2016.

[2]The research of the second author was supported, in part, by a Simons Foundation grant no. 282207.

[3]The research of the third and fourth authors was supported, in part, by the U. S. National Science Foundation under grant DMS-1516400.

Definition 1.1. An extended real-valued function $h(t) : [-1, 1] \to (0, +\infty]$ is called *absolutely monotone* if $h^{(i)}(t) \geq 0$, for every $t \in [-1, 1)$ and every integer $i \geq 0$, and $h(1) = \lim_{t \to 1^-} h(t)$.

Instead of solving the infinite-dimensional linear program on the right-hand side of (3) one may restrict to a subspace $\Lambda \subset C([-1, 1])$ (usually finite-dimensional), namely determining the quantity

$$\mathcal{W}_{h,\Lambda}(n, N) := \sup_{f \in \Lambda \cap A_{n,h}} N^2 \left(f_0 - \frac{f(1)}{N} \right). \tag{4}$$

Definition 1.2. A polynomial $f \in \Lambda \cap A_{n,h}$ is called Λ-LP-*optimal*, if it attains the supremum in (4). If Λ is the space of all real polynomials, then f is called *LP-optimal*.

In our considerations the space Λ depends on n and N. We are interested in a special class of spaces that we call *ULB-spaces* (see subsection 2.3 for the definition).

In [12] we derived *Universal Lower Bounds* (ULB) on energy by finding $\mathcal{W}_{h,\Lambda}(n, N)$ when $\Lambda = \mathcal{P}_m$, the space of polynomials of degree at most $m = \tau(n, N)$ for certain $\tau(n, N)$ (i.e. finding $\mathcal{P}_m$-LP-optimal polynomials; see Theorem 2.8). We now call this ULB a *first level ULB* and proceed further. One of the main goals of this article is to introduce a framework for finding a second level $\mathcal{W}_{h,\Lambda}(n, N)$, where $\Lambda = \mathcal{P}_{\tau(n,N)+4}$. We explain in Section 3 how Λ-LP-optimal polynomials of degree $\tau(n, N) + 4$ can be found in Λ.

We are also interested in the closely related problem of determining the maximal possible cardinality of a spherical code C on $\mathbb{S}^{n-1}$ of prescribed maximal inner product $s(C) := \max\{\langle x, y\rangle : x, y \in C, x \neq y\}$

$$\mathcal{A}(n, s) := \max\{|C| \colon C \subset \mathbb{S}^{n-1}, s(C) = s\}, \tag{5}$$

and the related quantity (also known as the *Tammes problem*)

$$s(n, N) := \min\{s(C) : C \subset \mathbb{S}^{n-1},\ |C| = N\}. \tag{6}$$

Linear programming upper bounds for $\mathcal{A}(n, s)$ are obtained by polynomials from the class

$$B_{n,s} := \{g : g(t) = \sum_{k=0}^{\infty} g_k P_k^{(n)}(t) \leq 0,\ t \in [-1, s],\ g_k \geq 0,\ k = 1, 2, \dots\}, \tag{7}$$

(see Theorem 2.6 below). The first level upper bound $\mathcal{A}(n, s) \leq L(n, s)$, due to Levenshtein [25, 26, 27] (see also [20, 24]), is obtained by polynomials of degree $m = \tau(n, N)$ that belong to the class (7), as explained in Section 2.4 (see (24)). It is important to note an intimate connection between $\mathcal{P}_m$-LP-optimal polynomials that yield our ULB and the Levenshtein polynomials, namely that the first interpolate the potential-interaction function at the zeros of the second. The commonality is given by a special $1/N$-quadrature rule with nodes at these zeros (see Definition 2.2). Even though in most of our applications N denotes the cardinality of a code C, it is beneficial not to restrict N to positive integers, but to positive reals.

Our results yield second level LP bounds for $\mathcal{A}(n, s)$ with polynomials of degree $m+4$ for certain s and $m = \tau(n, L(n, s))$. The second level bounds for $\mathcal{E}_h(n, N)$ and $\mathcal{A}(n, s)$, where $N = L(n, s)$, happen simultaneously and exactly when Λ is a ULB-space. An important $1/N$-quadrature formula serves as the intersecting aspect again, and, exactly as at the first level, its nodes are both roots of the improving polynomials for $\mathcal{A}(n, s)$ as well as interpolation nodes (to the potential-interaction function) of the Λ-LP-optimal polynomials for improving the ULB. Thus, our approach can be viewed as lifting the Levenshtein framework to next level(s).

The paper is organized as follows. In Section 2, following a brief discussion of Gegenbauer polynomials, we define in subsection 2.2 what is meant by a $1/N$-quadrature rule. In subsection 2.3 we introduce the notion of a ULB space. In subsection 2.4 we explain results of Levenshtein and Delsarte, Goethals, and Seidel that are instrumental in defining the first level bounds. Subsections 2.5 and 2.6 are devoted to a general description of the Hermite interpolation problems needed for the proof of Theorem 2.11, which asserts for given dimension n and cardinality N, that $\mathcal{P}_{\tau(n,N)}$ is a ULB space. We define the first level ULB for $\mathcal{E}_h(n, N)$ in Theorem

2.8. Section 3 examines the second level ULB on energy and second-level Levenshtein-type upper bounds on cardinality of codes with fixed maximum inner product. We consider necessary and sufficient conditions on the so-called skip two/add two subspace to be ULB space, with the case when n and N are such that $\tau(n,N)=2k-1$ being considered in more detail. Subsection 3.1 is devoted to a detailed examination on necessary and sufficient conditions for existence and uniqueness of a $1/N$-quadrature rule on the skip two/add two subspace. Section 3.2 considers the existence of a Hermite interpolant on the subspace in question. The second level bounds are presented in subsection 3.3 and in subsection 3.4 we briefly review the case $\tau(n,N)=2k$. Section 4 demonstrates the second level lift with two model examples, $(n,N)=(4,24)$ and $(4,120)$, respectively. In the case of 24 points on $\mathbb{S}^3$ we show that the optimal polynomial solving (4) for $\Lambda=\mathcal{P}_9$ is also a solution of (3). In Section 5 we perform a third level lift of the Levenshtein framework and as a result derive a new proof that the 600-cell is universally optimal. Moreover, we completely characterize the optimal polynomials of degree at most 17 for the Delsarte-Yudin linear programming lower bounds by finding two new polynomials that, together with Cohn-Kumar's polynomial, form the vertices of the convex hull that consists of all optimal polynomials. Our framework provides a conceptual explanation of why polynomials of degree 17 are needed to handle the 600-cell via linear programming. Section 6 presents numerical results, such as graphics illustrating our new bounds, as well as a sample of an extensive list of cases where the lift of the Levenshtein framework is achievable. We display the improved energy bound and the associated separation distance. More comprehensive list may be found on https://my.vanderbilt.edu/edsaff/.

2. Preliminaries

2.1. **Gegenbauer and adjacent polynomials.** We denote by $P_i^{(n)}(t)$ the Gegenbauer polynomials of respective degrees i that are orthogonal with respect to the measure

$$d\mu(t) := \gamma_n (1-t^2)^{\frac{n-3}{2}}\,dt, \quad t\in[-1,1],$$

where $\gamma_n := \Gamma(\frac{n}{2})/\sqrt{\pi}\Gamma(\frac{n-1}{2})$ is a normalizing constant that makes μ a probability measure. We impose the normalization $P_i^{(n)}(1)=1$ for every i, and note that $P_i^{(n)}(t)$ is just the Jacobi polynomial $P_i^{(\frac{n-3}{2},\frac{n-3}{2})}(t)$.

For $a,b\in\{0,1\}$ and $i\geq 0$, we denote by $P_i^{a,b}(t) := P_i^{(a+\frac{n-3}{2},b+\frac{n-3}{2})}(t)$ the corresponding Jacobi polynomial, normalized again by $P_i^{a,b}(1)=1$, which is called an *adjacent polynomial* [27]. The (probability) measure of orthogonality for the sequence of these polynomials is

$$d\nu^{a,b}(t) := c^{a,b}(1-t)^a(1+t)^b d\mu(t), \tag{8}$$

where $c^{a,b}$ is a normalizing constant. Of course, if $a=b=0$ we have the Gegenbauer polynomials where we use instead the (n) indexing. Connections between the Gegenbauer polynomials and their adjacent polynomials are given by the Christoffel-Darboux formulas (see [28, Lemma 5.24]).

We write $\langle f,g\rangle_{a,b}$ to denote the inner product

$$\langle f,g\rangle_{a,b} := \int_{-1}^{1} f(t)g(t)\,d\nu^{a,b}(t),$$

and set $\|f\|_{a,b}^2 := \langle f,f\rangle_{a,b}$, $\|f\|^2 := \langle f,f\rangle$, where $\langle\cdot,\cdot\rangle := \langle\cdot,\cdot\rangle_{0,0}$.

For any real polynomial $f(t)$ of degree r we have for fixed a,b the unique expansion

$$f(t) = \sum_{i=0}^{r} f_i^{a,b} P_i^{a,b}(t)$$

with well-defined coefficients

$$f_i^{a,b} := r_i^{a,b}\int_{-1}^{1} f(t)P_i^{a,b}(t)\,d\nu^{a,b}(t),$$

where

$$r_i^{a,b} \quad := \quad \left(\int_{-1}^{1} \left(P_i^{a,b}(t)\right)^2 \, d\nu^{a,b}(t)\right)^{-1} = \|P_i^{a,b}\|_{a,b}^{-2}$$

(see Lemma 5.24 in [28]) and

$$r_i = r_i^{0,0} = \frac{2i+n-2}{i+n-2}\binom{i+n-2}{i}.$$

For future reference, we write

$$P_i^{a,b}(t) = \sum_{j=0}^{i} a_{i,j}^{a,b} t^j.$$

Definition 2.1. A polynomial $f(t)$ of degree r is called (*strictly*) *positive definite* if $f_i = f_i^{0,0} \geq 0$ for every i (if $f_i > 0$ for every $i = 0, 1, \ldots, r$) in its Gegenbauer expansion.

Similarly, we consider $(1,0)$-positive definite polynomials (note that $(1,0)$-positive definiteness implies positive definiteness since by the Christoffel-Darboux formula $P_i^{1,0}(t) = \sum_{j=0}^{i} r_j P_j^{(n)}(t) / \sum_{j=0}^{i} r_j$ with positive $r_j = r_j^{0,0}$).

We also employ the so-called *Krein condition* and in some cases the *strengthened Krein condition* (see [28, Section 3.3]). Both conditions are satisfied by the Gegenbauer polynomials and their adjacent polynomials since

$$P_i^{(n)}(t) P_j^{(n)}(t) \tag{9}$$

and

$$(t+1) P_i^{1,1}(t) P_j^{1,1}(t) \tag{10}$$

are respectively positive definite and strictly positive definite for any nonnegative integers i, j (see [21], [28, Lemma 3.22]).

2.2. $1/N$**-Quadrature rules and lower bounds for energy on subspaces.** An important ingredient in obtaining LP bounds for $\mathcal{E}_h(n,N)$ and $\mathcal{A}(n,s)$ is the notion of a $1/N$-quadrature rule over subspaces, which we briefly review.

Definition 2.2. A finite sequence of ordered pairs $\{(\alpha_i, \rho_i)\}_{i=1}^{k}$, $-1 \leq \alpha_1 < \alpha_2 < \cdots < \alpha_k < 1$, $\rho_i > 0$ for $i = 1, 2, \ldots, k$, forms a $1/N$*-quadrature rule that is exact for a subspace* $\Lambda \subset C[-1,1]$ if

$$f_0 = \int_{-1}^{1} f(t) d\mu(t) = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i),$$

for all $f \in \Lambda$.

The following results from [12] find frequent utilization in the present work.

Theorem 2.3 ([12], Theorems 2.3 and 2.6)**.** *Let* $\{(\alpha_i, \rho_i)\}_{i=1}^{k}$ *be a* $1/N$*-quadrature rule that is exact for a subspace* $\Lambda \subset C([-1,1])$*. If* $f \in \Lambda \cap A_{n,h}$*, then* $\mathcal{E}_h(n,N) \geq N^2 \sum_{i=1}^{k} \rho_i f(\alpha_i)$ *and*

$$\mathcal{W}_{h,\Lambda}(n,N) \leq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i). \tag{11}$$

If there exists an $f \in \Lambda \cap A_{n,h}$ such that $f(\alpha_i) = h(\alpha_i)$ for $i = 1, \dots, k$, then equality holds in (11) (i.e., f is Λ-LP-optimal) which yields the lower bound

$$\mathcal{E}_h(n, N) \geq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i). \tag{12}$$

Furthermore, in this case if $\Lambda' := \Lambda \oplus span\{P_j^{(n)} : j \in \mathcal{I}\}$ for some index set $\mathcal{I} \subseteq \mathbb{N}$ and the quantities

$$Q_j^{(n,N)} := \frac{1}{N} + \sum_{i=1}^{k} \rho_i P_j^{(n)}(\alpha_i) \tag{13}$$

satisfy $Q_j^{(n,N)} \geq 0$ for $j \in \mathcal{I}$, then

$$\mathcal{W}_{h,\Lambda'}(n, N) = \mathcal{W}_{h,\Lambda}(n, N) = N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i);$$

i.e., f is Λ'-LP-optimal. In particular, if $\mathcal{I} = \mathbb{N}$, then f is LP-optimal.

The quantities $Q_j^{(n,N)}$ are called *test functions*[1] and were introduced and investigated in [12] for the Levenshtein quadrature (see (20)-(22)) when $\Lambda = \mathcal{P}_m$, $m \leq \tau(n, N)$, where $\tau(n, N)$ is defined in (18). Observe, that $Q_j^{(n,N)} = 0$, $j = 1, \dots, \tau(n, N)$. It was shown in [10] that both $Q_{\tau(n,N)+1}^{(n,N)} \geq 0$ and $Q_{\tau(n,N)+2}^{(n,N)} \geq 0$ resulting in $\mathcal{W}_{h,\mathcal{P}_{\tau(n,N)}}(n, N) = \mathcal{W}_{h,\mathcal{P}_{\tau(n,N)+2}}(n, N)$. Moreover, a conjecture [12, Conjecture 4.8] tested on numerous occasions states that if $Q_{\tau(n,N)+3}^{(n,N)} \geq 0$ and $Q_{\tau(n,N)+4}^{(n)} \geq 0$, then $Q_j^{(n,N)} \geq 0$ for all j and hence, the ULB is LP-optimal.

Motivated by this we consider in this article cases when at least one of the test functions $Q_{\tau(n,N)+3}^{(n,N)}$ and $Q_{\tau(n,N)+4}^{(n)}$ is strictly negative and consider solving $\mathcal{W}_{h,\Lambda(n,N)}$ for *skip-two add-two* subspaces of

$$\Lambda_{n,k} := \mathcal{P}_{\tau(n,N)} \oplus \ \mathrm{span}\{P_{\tau(n,N)+3}^{(n)}, P_{\tau(n,N)+4}^{(n)}\}, \tag{14}$$

where $k := \lceil \tau(n, N)/2 \rceil$; i.e., $\tau(n, N) = 2k - 1$ or $2k$. In fact, it was also shown in [10] that for each dimension n, there is some $k_0 = k_0(n)$ such that $Q_{2k+3}^{(n,N)} < 0$ for $k \geq k_0$, which yields that for fixed n, if the cardinality N is sufficiently large, we have $\mathcal{W}_{h,\Lambda_{n,k}}(n, N) > \mathcal{W}_{h,\mathcal{P}_{\tau(n,N)}}(n, N)$. In this paper we develop necessary and sufficient conditions for the existence of a $1/N$-quadrature rule that is exact on $\Lambda_{n,k}$ and such that there is an $f \in \Lambda_{n,k} \cap A_{n,h}$ that interpolates h at the nodes of the quadrature for any absolutely monotone h, and thus, provides an improved (or second level) ULB in these cases.

2.3. **ULB-spaces.**

The above theorem motivates the following definition.

Definition 2.4. Let n and N be positive integers. A space $\Lambda \subset C[-1, 1]$ is called a *ULB-space* for dimension n and cardinality N and (12) is called a *universal lower bound (ULB)* if the following two conditions hold:

(i) there exists a $1/N$-quadrature rule that is exact for Λ (see Definition 2.2);

(ii) for any absolutely monotone function h there exists some $f \in \Lambda \cap A_{n,h}$ that agrees with h at the nodes of the $1/N$-quadrature rule from (i).

The following theorem determining a lower bound on the quantity (6) follows directly from the definition.

Theorem 2.5. *Suppose Λ is a ULB-space for given n and N, and let α_k denote the largest node less than 1 in the $1/N$-quadrature rule. Then $s(n, N) \geq \alpha_k$.*

[1] In fact, they coincide with the test functions from [10] (see also [28, Theorem 5.47]) used for investigations of maximal spherical codes.

Proof. Let $\{(\alpha_i,\rho_i)\}_{i=1}^k$, $-1\le\alpha_1<\alpha_2<\cdots<\alpha_k<1$, $\rho_i>0$ for $i=1,2,\ldots,k$, be a $1/N$-quadrature rule for Λ. Let $C\subset\mathbb{S}^{n-1}$ be an optimal code for (6) (also referred to as *best-packing code*), that is a code that minimizes the largest inner product. With $h_a(t):=\exp(at)$, $a>0$, we have the following estimations

$$N(N-1)e^{as(n,N)}\ge E_{h_a}(C)\ge\mathcal{E}_{h_a}(n,N)\ge N^2\sum_{i=1}^k\rho_ie^{a\alpha_i}\ge N^2\rho_ke^{a\alpha_k}.$$

As the inequality holds for all a and ρ_k is independent of a, we conclude that $s(n,N)\ge\alpha_k$. □

We next recall the linear programming upper bound of the quantity $\mathcal{A}(n,s)$ given in (5).

Theorem 2.6. *(LP bound for spherical codes,* [19, 24]*) Let $n\ge2$, $s\in[-1,1)$ and $g(t)=\sum_{i=0}^r g_iP_i^{(n)}(t)\in B_{n,s}$, where $B_{n,s}$ is defined in* (7)*. Then $\mathcal{A}(n,s)\le g(1)/g_0$.*

We note that Definition 2.4 may be extended to positive real $N\ge2$. We use this setting in the maximum cardinality problem (5).

2.4. **Levenshtein's framework and ULB.** Of particular importance is the case when the subspace in subsection 2.2 is $\mathcal{P}_\tau$. For this purpose we briefly introduce Levenshtein's framework (see [28], [6, Chapter 5]). First, we recall two classical notions. The *Delsarte-Goethals-Seidel lower bound* $D(n,\tau)$ on

$$\mathcal{B}(n,\tau):=\min\{|C|:C\subset\mathbb{S}^{n-1}\text{ is a spherical }\tau\text{-design}\}$$

is given by (cf. [19])

$$\mathcal{B}(n,\tau)\ge D(n,\tau):=\binom{n+k-2+\varepsilon}{n-1}+\binom{n+k-2}{n-1},\tag{15}$$

for every $\tau=2k-1+\varepsilon$, $\varepsilon\in\{0,1\}$. Hereafter we use the parameter $\varepsilon\in\{0,1\}$ to present simultaneously the cases of odd $\tau=2k-1$ (where $\varepsilon=0$) and even $\tau=2k$ (where $\varepsilon=1$). Note that

$$D(n,\tau)=p^\varepsilon\sum_{i=0}^{k-1+\varepsilon}r_i,$$

where $p=1-(-1)^kP_k^{1,0}(-1)$ (see [28, Theorem 2.16]).

The *Levenshtein upper bound* on $\mathcal{A}(n,s)$ can be described as follows. Let $t_i^{a,b}$ be the greatest zero of $P_i^{a,b}(t)$, $t_0^{1,1}:=-1$, and denote by I_τ the interval

$$I_\tau:=\left[t_{k-1+\varepsilon}^{1,1-\varepsilon},t_k^{1,\varepsilon}\right].$$

Applying Theorem 2.6 for suitable polynomials (see (24) below) out of the class $B_{n,s,}$, $s\in I_\tau$, defined in (7), Levenshtein (see [28]) proved that

$$\mathcal{A}(n,s)\le L_\tau(n,s):=\left(1-\frac{P_{k-1+\varepsilon}^{1,0}(s)}{P_k^{0,\varepsilon}(s)}\right)\sum_{i=0}^{k-1+\varepsilon}r_i,\quad\forall s\in I_\tau.\tag{16}$$

A very important connection between the bounds (15) and (16) is given by the equalities

$$L_{\tau-1-\varepsilon}(n,t_{k-1-\varepsilon}^{1,1-\varepsilon})=L_{\tau-\varepsilon}(n,t_{k-1-\varepsilon}^{1,1-\varepsilon})=D(n,\tau-\varepsilon)\tag{17}$$

at the ends of the intervals I_τ.

The strict monotonicity in τ of $D(n,\tau)$ implies that for every fixed dimension n and cardinality N there is a unique

$$\tau:=\tau(n,N)\text{ such that }N\in(D(n,\tau),D(n,\tau+1)].\tag{18}$$

Further, with $k = \lceil \frac{\tau+1}{2} \rceil$, let $\alpha_{k+\varepsilon} = s$ be the unique solution of

$$N = L_\tau(n,s),\ \ s \in I_\tau, \tag{19}$$

which exists because of the relations (17) and the strict monotonicity in s of $L_\tau(n,s)$. Then, as described by Levenshtein in [28, Section 5], there exist uniquely determined quadrature nodes

$$-1 \le \alpha_1 < \alpha_2 < \cdots < \alpha_{k+\varepsilon} < 1 \tag{20}$$

and corresponding positive weights

$$\rho_1, \rho_2, \ldots, \rho_{k+\varepsilon}, \tag{21}$$

such that the following $1/N$-quadrature rule (see Definition 2.2) holds:

$$f_0 = \frac{f(1)}{N} + \sum_{i=1}^{k+\varepsilon} \rho_i f(\alpha_i), \quad \forall f \in \mathcal{P}_\tau \tag{22}$$

(this is the first level $1/N$-quadrature rule, exact for $\mathcal{P}_\tau$). The numbers α_i, $i = 1,2,\ldots,k+\varepsilon$, are the roots of the equation

$$(t+1)^\varepsilon \left(P_k^{1,\varepsilon}(t) P_{k-1}^{1,\varepsilon}(\alpha_{k+\varepsilon}) - P_{k-1}^{1,\varepsilon}(t) P_k^{1,\varepsilon}(\alpha_{k+\varepsilon}) \right) = 0. \tag{23}$$

In fact, the nodes $\{\alpha_i\}$ are the roots of the Levenshtein polynomials $f_\tau^{(n,\alpha_{k+\varepsilon})}(t)$ (see [28, Equations (5.81) and (5.82)]) used for obtaining (16); i.e.,

$$f_\tau^{(n,\alpha_{k+\varepsilon})}(t) = (t+1)^\varepsilon \left((P_k^{1,\varepsilon}(t) P_{k-1}^{1,\varepsilon}(\alpha_{k+\varepsilon}) - P_{k-1}^{1,\varepsilon}(t) P_k^{1,\varepsilon}(\alpha_{k+\varepsilon}) \right)^2. \tag{24}$$

The $1/N$-quadrature rule given by (22) is an important ingredient in the derivation and investigation of the ULB from [12] and their test functions (13).

Levenshtein's bound (16) is usually utilized to derive the bound in Theorem 2.5 (see also Theorem 2.11 that establishes that $\mathcal{P}_\tau$ is a ULB-space). The largest solution $\alpha_{k+\varepsilon}$ of the equation $N = L_\tau(n,s)$, $\tau = 2k-1+\varepsilon$, $\varepsilon \in \{0,1\}$, is at most $s(n,N)$;

$$s(n,N) \ge \alpha_{k+\varepsilon} \tag{25}$$

which we refer to as the first-level Levenshtein bound for $s(n,N)$; Theorem 3.17 provides a second-level bound for $s(n,N)$.

2.5. **Hermite interpolation for energy bounds.** Following [35, 14] (see also [15, 12]) we use Hermite interpolation to construct a polynomial f upper bounded by the potential h.

Definition 2.7. Let $T = \{t_1 \le t_2 \le \cdots \le t_\ell\}$ be an interpolation (multi)set in the interval $[-1,1)$. We say that two functions g and h *agree on* T if for each $t \in T$ with multiplicity m_t the j-th order derivatives of g and h exist and agree at t for $j = 0,1,2\ldots,m_t-1$. If g and h agree on T, we write $g|_T = h|_T$. For a polynomial g of degree ℓ with roots T (counted with their multiplicities) in the interval $[-1,1)$ and a sufficiently smooth function h, we denote by $H(h;T) = H(h;g)$ the Hermite interpolating polynomial of degree at most $\ell-1$ to be the unique polynomial of degree at most $\ell-1$ that agrees with h on T (or the roots of g). Further, for a given subspace $\Lambda \subset C([-1,1])$, we denote by $H_\Lambda(h;T) = H_\Lambda(h;g)$ any function in Λ that agrees with h on T (or the roots of g), if such exists.

With the above notation, we remark that the ULB result was obtained in [12] by using the polynomials

$$f = H(h; (\cdot - s) f_\tau^{(n,s)}). \tag{26}$$

Theorem 2.8 ([12], Theorem 3.1)**.** *Let n, N be fixed and h be an absolutely monotone potential on $[-1,1]$. Suppose that $\tau = \tau(n,N) = 2k-1+\varepsilon$ is as in (18) and let the associated $1/N$-quadrature nodes and weights α_i and ρ_i, $i = 1,2,\ldots,k+\varepsilon$, be as in (19)–(23). Then*

$$\mathcal{E}_h(n,N) \geq R_\tau(n,N;h) := N^2 \sum_{i=1}^{k+\varepsilon} \rho_i h(\alpha_i). \tag{27}$$

Moreover, the polynomials $f(t)$ defined by (26) provide the unique optimal solution of the linear program (4) for the subspace $\Lambda = \mathcal{P}_\tau$, and consequently

$$\mathcal{W}_{h,\mathcal{P}_\tau}(n,N) = R_\tau(n,N;h). \tag{28}$$

The optimality property (28) of the polynomials (26) implies that the bound (27) can be improved by linear programming only if the degree of the improving polynomial is at least $\tau+1$. It follows from Theorem 2.3 that for improvements some negative test functions $Q_j^{(n,N)}$, $j \geq \tau+1$, must arise. Furthermore, since $Q_j^{(n,N)} > 0$ for $j \in \{\tau+1, \tau+2\}$ (see Theorem 4.3 in [12]) and every N, any second level ULB for $\mathcal{E}_h(n,N)$ will require polynomials of degree at least $\tau+3$. The same is true for the second level bounds on $\mathcal{A}(n,s)$

In Section 3 we build a framework for the derivation of a second level ULB for the case when the improving polynomial has degree $\tau+4$, where at least one test function $Q_{\tau+3}^{(n,N)}$ or $Q_{\tau+4}^{(n,N)}$ is negative.

2.6. **Positive definite Hermite interpolants.** Let $T = \{t_1 \leq t_2 \leq \cdots \leq t_\ell\}$ be an interpolation (multi)set and

$$g_j(t) = (t-t_1)\cdots(t-t_j),\ j = 1,\ldots,\ell,\quad g_0(t) := 1. \tag{29}$$

We are interested in solutions to Hermite interpolation problems on T for certain subspaces of polynomials. General results can be found in [22, 23, 29].

Lemma 2.9. *Let Λ be a given subspace of $C([-1,1])$, T a multiset in $[-1,1)$ with finite cardinality ℓ, and g_j the partial product defined in (29) for $j = 0,1,\ldots,\ell$. If for each $j = 0,1,\ldots,\ell$ there exists an interpolant $H_\Lambda(g_j;T)$, then for all sufficiently smooth functions h, the function*

$$H_{\Lambda,T}(h) := \sum_{j=0}^{\ell-1} h[t_1,\ldots,t_j] H_\Lambda(g_j;T), \tag{30}$$

where $h[t_1,\ldots,t_j]$ denotes the divided difference in the listed nodes, agrees with h on T; i.e., $H_{\Lambda,T}(h) = H_\Lambda(h;T)$.

Proof. Considering the standard Newton interpolating polynomial to h in $\mathcal{P}_{\ell-1}$,

$$J_{\ell-1}(t) := \sum_{j=0}^{\ell-1} h[t_1,\ldots,t_j] g_j(t),$$

we note that $J_{\ell-1}(t)|_T = h(t)|_T$. As $g_{j-1}|_T = H_\Lambda(g_{j-1};g_\ell)|_T$, linearity of interpolation yields (30). □

The next theorem provides sufficient conditions for the interpolant defined in (30) to belong to $A_{n,h}$.

Theorem 2.10. *Let Λ be a given subspace of $C([-1,1])$, h be absolutely monotone on $[-1,1]$, T a finite multiset in $[-1,1)$ and g_j as in (29). If $H_\Lambda(g_j;T)$ exist and belong to A_{n,g_j}, $j = 0,1,\ldots,\ell$, then $H_\Lambda(h;T)$ defined by (30) belongs to $A_{n,h}$.*

Proof. Since $h(t)$ is absolutely monotone, the divided differences $h[t_1,\dots,t_j]$ are nonnegative for every j (see, e.g. [18, Cor. 3.4.2]). Hence, the interpolant $H_\Lambda(h;T)$ is positive definite since it is in the positive cone of the interpolants $H_\Lambda(g_j;T)$, $j=0,1,\dots,\ell-1$, which are positive definite by assumption.

We now prove that $H_\Lambda(h;T)\le h(t)$ for every $t\in[-1,1)$. Let, as in Lemma 2.9, $J_{\ell-1}(t)=H(h;g_\ell)$. Then $h(t)\ge J_{\ell-1}(t)$ by consecutive applications of Rolle's theorem (see, for example, [15, Lemma 9]), or, alternatively, by the remainder formula for the Hermite interpolation. Thus it follows from the representation

$$h(t)-H_\Lambda(h;g_\ell)=(h(t)-J_{\ell-1}(t))+(J_{\ell-1}(t)-H_\Lambda(h;T))$$

that it is enough to prove that $J_{\ell-1}(t)-H_\Lambda(h;g_\ell)\ge 0$ for every $t\in[-1,1)$. Since $H_\Lambda(g_{j-1};g_\ell)\in A_{n,g_{j-1}}$ by the assumption, we have

$$(t-t_1)\cdots(t-t_{j-1})-H_\Lambda(g_{j-1};g_\ell)\ge 0.$$

Using again that $h[t_1,\dots,t_j]\ge 0$, the desired result follows from the formula of Lemma 2.9. □

Now the Levenshtein bounds and our ULB can be unified, in a sense.

Theorem 2.11. *Let $n\ge 2$ and τ be positive integers. If $N\in(D(n,\tau),D(n,\tau+1)]$, then $\mathcal{P}_\tau$ is a ULB-space for dimension n and cardinality N.*

Proof. For every $N\in(D(n,\tau),D(n,\tau+1)]$ (even if N is real) we have the Levenshtein $1/N$-quadrature rule (22) with $N=L_\tau(n,s)$. Then the existence and uniqueness of the ULB solution for (ii) follow from Theorem 2.8 (see for details [12]). □

In the next section we develop a framework for proving that certain spaces of polynomials of degrees at most $\tau(n,N)+4$ are also ULB-spaces.

3. Second level ULB: Lifting the Levenshtein framework

We describe in detail our approach in the case when n and N are such that

$$\tau(n,N)=2k-1, \quad \text{and} \quad Q_{2k+2}^{(n,N)}<0 \text{ or } Q_{2k+3}^{(n,N)}<0. \tag{31}$$

In this case the *skip-two/add-two* subspace defined by (14) becomes

$$\Lambda_{n,k}:=\mathcal{P}_{2k-1}\oplus \operatorname{span}\left(P_{2k+2}^{(n)},P_{2k+3}^{(n)}\right). \tag{32}$$

The goal will be to derive conditions on n and N for $\Lambda_{n,k}$ to be a ULB-space (see Definition 2.4). We focus separately on the existence of a $1/N$-quadrature and on an admissible polynomial interpolant in the subspace associated with this quadrature.

3.1. Existence of a $1/N$-quadrature rule for the skip-two/add-two subspace $\Lambda_{n,k}$.

First, we focus on necessary conditions for the existence of a $1/N$-quadrature rule exact on $\Lambda_{n,k}$ under the assumption (31).

Lemma 3.1. *Any $1/N$-quadrature rule that is exact on $\Lambda_{n,k}$ has at least $k+1$ distinct nodes.*

Proof. Let $\{\beta_i,\theta_i\}_{i=1}^{\ell}$ be such a quadrature rule. If $\ell<k$, then $(t-\beta_1)^2\dots(t-\beta_\ell)^2(1-t)\in\Lambda_{n,k}$ and hence

$$\int_{-1}^{1}(t-\beta_1)^2\dots(t-\beta_\ell)^2(1-t)\,d\mu(t)=0,$$

which is absurd. If $\ell=k$, then we are exactly in the condition of the Levenshtein quadrature with $N=L(n,\beta_\ell)$. The remaining nodes $\{\beta_i\}_{i=1}^{k-1}$ are uniquely determined and satisfy (23), and therefore, the quadrature is the Levenshtein quadrature. However, if the Levenshtein quadrature is exact for $P_{2k+2}^{(n)}$ and $P_{2k+3}^{(n)}$, then the test functions $Q_{2k+2}^{(n,N)}$ and $Q_{2k+3}^{(n,N)}$ vanish, which contradicts the hypothesis. □

Suppose now that $\{(\beta_i,\theta_i)\}_{i=1}^{k+1}$ is a $1/N$-quadrature rule with exactly $k+1$ nodes that is exact on the subspace $\Lambda_{n,k}$, namely, $-1\le\beta_1<\cdots<\beta_{k+1}<1$, $\theta_i>0$, $i=1,\dots,k+1$, and

$$f_0=\int_{-1}^1 f(t)d\mu(t)=\frac{f(1)}{N}+\sum_{i=1}^{k+1}\theta_i f(\beta_i) \tag{33}$$

holds for every polynomial from the subspace $\Lambda_{n,k}$ defined in (32). We define the *partial products* associated with the $1/N$-quadrature rule as

$$q_j(t):=(t-\beta_1)\cdots(t-\beta_j),\quad j=1,2,\dots,k+1,\quad q_0(t)\equiv 1. \tag{34}$$

The following theorem provides some insight on how to determine this quadrature and its relation to the Levenshtein $1/N$-quadrature $\{(\alpha_i,\rho_i)\}_{i=1}^{k}$.

Theorem 3.2. *If $\{(\beta_i,\theta_i)\}_{i=1}^{k+1}$ is a $1/N$-quadrature rule exact on the subspace $\Lambda_{n,k}$, then there are constants c_1, c_2, and c_3 such that (compare to* (23) *with $\varepsilon=0$)*

$$a_{k+1,k+1}^{1,0}q_{k+1}(t)=P_{k+1}^{1,0}(t)+c_1P_k^{1,0}(t)+c_2P_{k-1}^{1,0}(t)+c_3P_{k-2}^{1,0}(t), \tag{35}$$

where $a_{k+1,k+1}^{1,0}$ denotes the leading coefficient of the polynomial $P_{k+1}^{1,0}(t)$. Moreover, $(\beta_i)_{i=1}^{k+1}$ interlace with the nodes $(\alpha_i)_{i=1}^{k}$ of the Levenshtein quadrature for $\mathcal{P}_{2k-1}$ given in (20)-(22)*; i.e.,*

$$-1\le\beta_1<\alpha_1<\cdots<\beta_k<\alpha_k<\beta_{k+1}<1. \tag{36}$$

Proof. Since the degrees of the polynomials $q_{k+1}(t)(1-t)P_i^{1,0}(t)$ for $i=0,1,\dots,k-3$ do not exceed $2k-1$, these polynomials belong to $\Lambda_{n,k}$. As they annihilate the quadrature, we obtain that $q_{k+1}(t)$ is orthogonal to the adjacent polynomials $P_i^{1,0}(t)$, $i=0,1,\dots,k-3$, with respect to the adjacent measure $d\nu^{1,0}(t):=(1-t)d\mu(t)$ (see (8)). Therefore, the expansion of $q_{k+1}(t)$ in terms of the polynomials $P_i^{1,0}$ has at most four non-zero terms and (35) follows.

To prove the interlacing property (36) of the nodes, we use suitable polynomials of degree $2k-1$ simultaneously in the quadratures (22) and (33). We first prove that $\beta_{k+1}>\alpha_k$ and $\beta_1<\alpha_1$. Applying (22) and (33) to the Levenshtein polynomial

$$f_{2k-1}^{(n,\alpha_k)}(t)=(t-\alpha_1)^2(t-\alpha_2)^2\cdots(t-\alpha_{k-1})^2(t-\alpha_k)$$

yields that

$$\sum_{i=1}^{k+1}\theta_i f_{2k-1}^{(n,\alpha_k)}(\beta_i)=0.$$

If $\beta_{k+1}\le\alpha_k$, then the last sum consists of $k+1$ nonpositive terms and they cannot be all equal to zero (otherwise $\{\beta_1,\beta_2,\dots,\beta_{k+1}\}\subseteq\{\alpha_1,\alpha_2,\dots,\alpha_k\}$, which is impossible). Thus, the sum is negative, a contradiction that yields $\beta_{k+1}>\alpha_k$.

Similarly, (22) and (33) applied to the polynomial $f_1(t):=(t-\alpha_k)f_{2k-1}^{(n,\alpha_k)}(t)/(t-\alpha_1)$ shows that

$$\sum_{i=1}^{k+1}\theta_i f_1(\beta_i)=0,$$

implying a contradiction if $\beta_1\ge\alpha_1$; i.e., we have $\beta_1<\alpha_1$.

We proceed with separating $\beta_2,\dots,\beta_k$ to interlace $\alpha_1,\dots,\alpha_k$ as follows. Consider the polynomial

$$f_2(t):=\frac{(t-\beta_1)(t-\alpha_k)f_{2k-1}^{(n,\alpha_k)}(t)}{(t-\alpha_1)(t-\alpha_2)}.$$

Applying both (22) and (33) to $f_2(t)$ we conclude as above that there is some β_i, $i \in \{2,3,\ldots,k\}$, in the interval (α_1,α_2). Continuing this way (consecutively getting β_i's in intervals (α_j,α_{j+1})) we conclude that every interval (α_i,α_{i+1}), $i=1,2,\ldots,k-1$, contains some β_j. Since the number of β_j's to be placed that way is equal to the number of the intervals for placing them, the proof of the interlacing is completed. □

For arbitrary real numbers c_1, c_2, c_3, set

$$r_{k+1}(t) := P_{k+1}^{1,0}(t) + c_1 P_k^{1,0}(t) + c_2 P_{k-1}^{1,0}(t) + c_3 P_{k-2}^{1,0}(t). \tag{37}$$

We seek necessary conditions on the coefficients c_1, c_2, and c_3 in (35), so that a $1/N$-quadrature (33) exists. Consider polynomials of degree $2k+3$ that lie in the subspace $\Lambda_{n,k}$ and have the form

$$L(t) := r_{k+1}(t)(1-t)\left[d_0 P_{k+1}^{1,0}(t) + d_1 P_k^{1,0}(t) + d_2 P_{k-1}^{1,0}(t) + d_3 P_{k-2}^{1,0}(t)\right] \in \Lambda_{n,k}, \tag{38}$$

where d_i, $i=0,1,2,3$, are chosen so that the required inclusion holds. Since $\Lambda_{n,k} \perp \operatorname{span}(P_{2k}^{(n)}, P_{2k+1}^{(n)})$, we have

$$\langle L, P_{2k}^{(n)} \rangle = \langle L, P_{2k+1}^{(n)} \rangle = 0. \tag{39}$$

We use the two equations from (39) to express the coefficients d_2 and d_3 as functions of d_0 and d_1; i.e., we obtain $d_2 = d_2(d_0,d_1)$ and $d_3 = d_3(d_0,d_1)$. Since this procedure is applicable to all polynomials $L(t)$ in (38), we can substitute $(d_0,d_1)=(1,0)$ and $(0,1)$ to find

$$d_2^{(1)} := d_2(1,0),\ d_3^{(1)} := d_3(1,0),\ d_2^{(2)} := d_2(0,1),\ d_3^{(2)} := d_3(0,1). \tag{40}$$

Note that (40) gives $d_i^{(j)}$ as functions of c_1, c_2, and c_3.

Should the roots of $r_{k+1}(t)$ be all simple and lie in $[-1,1)$, we can apply the quadrature (33) to $L(t)$ with these $d_i^{(j)}$ to obtain the equations

$$\|P_{k+1}^{1,0}\|_{1,0}^2 + c_2 d_2^{(1)} \|P_{k-1}^{1,0}\|_{1,0}^2 + c_3 d_3^{(1)} \|P_{k-2}^{1,0}\|_{1,0}^2 = 0, \tag{41}$$

and

$$c_1 \|P_k^{1,0}\|_{1,0}^2 + c_2 d_2^{(2)} \|P_{k-1}^{1,0}\|_{1,0}^2 + c_3 d_3^{(2)} \|P_{k-2}^{1,0}\|_{1,0}^2 = 0. \tag{42}$$

Further, we apply the $1/N$-quadrature (33) to the polynomial $r_{k+1}(t)$ to get the linear equation

$$I_{k+1} + c_1 I_k + c_2 I_{k-1} + c_3 I_{k-2} = \frac{1+c_1+c_2+c_3}{N}, \tag{43}$$

where

$$I_j := \int_{-1}^{1} P_j^{1,0}(t)\,d\mu(t) = \left(\sum_{i=0}^{j} r_i\right)^{-1}$$

from the Christoffel-Darboux formula.

Thus, we obtain the equations (41)-(43) for the coefficients c_1, c_2, and c_3. We first express c_1 as a linear function of c_2 and c_3 from (43). Then c_2 is derived uniquely as a function of c_3. The final polynomial equation for c_3 has degree 6. This also allows us to conclude via interval analysis the existence of exact solutions close to numerical ones. There are multiple choices for c_3 and we check all of them to obtain a polynomial $r_{k+1}(t)$. In general, the roots of $r_{k+1}(t)$ need not be all real, there are some cases when there is a complex conjugate pair (as the lemma below shows, there can be no more than one such pair). If the roots are all real and simple, and belong to $[-1,1)$, then these may serve as $1/N$-quadrature nodes $\beta_1,\beta_2,\ldots,\beta_{k+1}$.

Given the nodes $\{\beta_i\}_{i=1}^{k+1}$, the corresponding weights $\theta_1, \theta_2, \ldots, \theta_{k+1}$ can be computed using in (33) the Lagrange basis polynomials

$$\ell_i(t) = (t-1)\prod_{j\neq i}(t-\beta_j) = \frac{(t-1)q_{k+1}(t)}{a^{1,0}_{k+1,k+1}(t-\beta_i)},$$

as follows

$$\theta_i = \frac{1}{\ell_i(\beta_i)}\int_{-1}^{1}\ell_i(t)d\mu(t), \quad i=1,2,\ldots,k+1. \tag{44}$$

If the weights are all positive, then the roots of $r_{k+1}(t)$ serve indeed as $1/N$-quadrature nodes. We summarize the discussion in the following theorem.

Theorem 3.3. *Suppose c_1, c_2, and c_3 are real solutions to the system* (41)-(43)*, where $d_2^{(i)}, d_3^{(i)}$, $i=1,2$ are found utilizing* (39) *and* (40)*. Then $r_{k+1}(t)$ defined in* (37) *has at least $k-1$ distinct real roots, of which at least $k-2$ are in the interval $[-1,1)$. If all of its roots are real and simple, belong to $[-1,1)$, and if the associated weights* (44) *are all positive, then the collection $\{(\beta_i,\theta_i)\}_{i=1}^{k+1}$ forms a $1/N$-quadrature rule for $\Lambda_{n,k}$.*

Proof. We first show that $r_{k+1}(t)$ has at least $k-2$ sign changes in $[-1,1)$. Indeed, if it has less, then there is a polynomial p_{k-3} of degree at most $k-3$ that has the same sign changes. But then $r_{k+1}(t)p_{k-3}(t)(1-t)$ does not change sign in $[-1,1]$, and hence

$$\int_{-1}^{1} r_{k+1}(t)p_{k-3}(t)(1-t)\,d\mu(t) \neq 0.$$

This is a contradiction since $r_{k+1}(t)$ is orthogonal to $p_{k-3}(t)$ with respect to $d\nu^{1,0}(t)$ (see (8) and (37)). Hence, $r_{k+1}(t)$ has at most one pair of complex conjugate roots. As the total number of roots, counting multiplicity, is exactly $k+1$, and as we already have at least $k-2$ sign changes in $[-1,1]$, we conclude that r_{k+1} has at least $k-1$ distinct real roots.

Suppose now that all roots of $r_{k+1}(t)$ are real and simple and lie in $[-1,1)$, and that the weights (44) are all positive. Let $f(t)\in\Lambda_{n,k}$ be arbitrary. We want to show that the $1/N$-quadrature (33) holds. We first observe, that by the choice of the weights θ_i from (44) and the condition (43) the $1/N$-quadrature rule (33) holds for the Lagrange basis polynomials of degree $k+1$ associated with the nodes $\{\beta_1,\ldots,\beta_{k+1},1\}$, and hence it holds for all polynomials in $\mathcal{P}_{k+1}$. We expand $f(t)$

$$f(t) = (1-t)r_{k+1}(t)u_{k+1}(t) + v_{k+1}(t) \tag{45}$$

for some $u_{k+1}, v_{k+1}\in\mathcal{P}_{k+1}$. Consider the two polynomials

$$y_1(t) := P^{1,0}_{k+1}(t) + d_2^{(1)}P^{1,0}_{k-1}(t) + d_3^{(1)}P^{1,0}_{k-2}(t), \quad y_2(t) := P^{1,0}_{k}(t) + d_2^{(2)}P^{1,0}_{k-1}(t) + d_3^{(2)}P^{1,0}_{k-2}(t).$$

Observe that by the choice of $d_i^{(j)}$ and (39) we have

$$\langle(1-t)r_{k+1}(t)y_j(t), P_{2k}(t)\rangle = 0, \quad \langle(1-t)r_{k+1}(t)y_j(t), P_{2k+1}(t)\rangle = 0, \quad j=1,2, \tag{46}$$

or $(1-t)r_{k+1}(t)y_j(t)\in\Lambda_{n,k}$ for $j=1,2$. We can express $u_{k+1}(t)$ as

$$u_{k+1}(t) = Ay_1(t) + By_2(t) + CP^{1,0}_{k-1}(t) + DP^{1,0}_{k-2}(t) + w_{k-3}(t),$$

for some $w_{k-3}\in\mathcal{P}_{k-3}$. From $\langle f, P_{2k+1}\rangle = 0$ and (46) we have that

$$0 = \langle r_{k+1}(t)(1-t)(CP^{1,0}_{k-1}(t) + DP^{1,0}_{k-2}(t) + w_{k-3}(t)), P_{2k+1}(t)\rangle = C\int_{-1}^{1} P^{1,0}_{k+1}(t)P^{1,0}_{k-1}(t)P_{2k+1}(t)(1-t)\,d\mu(t).$$

Since $P_{k+1}^{1,0}(t)P_{k-1}^{1,0}(t)(1-t)$ is of exact degree $2k+1$ and has nonzero leading coefficient, the integral is non-zero and we conclude that $C=0$. Similarly $\langle f, P_{2k}\rangle = 0$ and (46) imply that $D=0$. Equations (41) and (42) now yield that

$$\int_{-1}^{1}(1-t)r_{k+1}(t)u_{k+1}(t)\,d\mu(t)=0.$$

Utilizing this equation, the fact that the first term in the sum on the right-hand side of (45) annihilates the quadrature sum, and that the quadrature holds for v_{k+1}, we conclude (33), which completes the proof. □

3.2. **Existence of Hermite interpolant to $h(t)$ in the skip-two/add-two subspace $\Lambda_{n,k}$.** We shall use Lemma 2.9 and Theorem 2.10 to determine sufficient conditions for the existence of a $\Lambda_{n,k}$-LP-extremal polynomial

$$f^h(t)=f_{2k+3}^hP_{2k+3}^{(n)}(t)+f_{2k+2}^hP_{2k+2}^{(n)}(t)+\sum_{i=0}^{2k-1}f_i^hP_i^{(n)}(t)\in\Lambda_{n,k}\cap A_{n,h} \tag{47}$$

that interpolates the potential function $h(t)$ at the nodes $\{\beta_i\}_{i=1}^{k+1}$.

Lemma 3.4. *Suppose h is an absolutely monotone function on $[-1,1)$ and T is a multiset on $(-1,1)$*

$$T=\{\beta_1,\beta_1,\beta_2,\beta_2,\ldots,\beta_{k+1},\beta_{k+1}\}$$

with $q_{k+1}(t)=(t-\beta_1)\ldots(t-\beta_{k+1})$ (see (34)). If

$$\langle tq_{k+1}^2(t),P_{2k}^{(n)}(t)\rangle\cdot\langle q_{k+1}^2(t),P_{2k+1}^{(n)}(t)\rangle\neq\langle tq_{k+1}^2(t),P_{2k+1}^{(n)}(t)\rangle\cdot\langle q_{k+1}^2,P_{2k}^{(n)}(t)\rangle, \tag{48}$$

then there exists a unique polynomial $f^h\in\Lambda_{n,k}$ denoted

$$f^h(t):=H_{\Lambda_{n,k}}(h;q_{k+1}^2) \tag{49}$$

that interpolates $h(t)$ at the nodes of the multiset T.

Proof. We first prove the uniqueness. If $F_1^h(t)$ and $F_2^h(t)$ are two such interpolants, then the nodes of the multiset are zeros of the difference, and therefore

$$F_1^h(t)-F_2^h(t)=q_{k+1}^2(t)(At+B). \tag{50}$$

Since each $F_i^h(t)$, $i=1,2$ is orthogonal to $P_{2k}^{(n)}(t)$ and $P_{2k+1}^{(n)}(t)$, the constants A and B satisfy the linear system

$$\begin{aligned}A\langle tq_{k+1}^2(t),P_{2k}^{(n)}(t)\rangle+B\langle q_{k+1}^2(t),P_{2k}^{(n)}(t)\rangle&=\quad 0,\\ A\langle tq_{k+1}^2(t),P_{2k+1}^{(n)}(t)\rangle+B\langle q_{k+1}^2(t),P_{2k+1}^{(n)}(t)\rangle&=\quad 0.\end{aligned} \tag{51}$$

Equation (48) now yields that (51) has only the trivial solution, which implies the uniqueness.

To prove the existence, as $H_{\Lambda_{n,k}}(g_j;g_{2k+2})=g_j(t)$ for all $j\leq 2k-1$, by the definition (32) of the subspace $\Lambda_{n,k}$, it is enough to establish the existence of the interpolants $H_{\Lambda_{n,k}}(g_j;g_{2k+2})$ for $j=2k$ and $2k+1$ and apply Lemma 2.9 (note that $g_{2k}(t)=q_k^2(t)$, $g_{2k+1}(t)=q_k(t)q_{k+1}(t)$, and $g_{2k+2}(t)=q_{k+1}^2(t)$). Similar to (50) we find

$$\begin{aligned}H_{\Lambda_{n,k}}(q_k^2;q_{k+1}^2)-q_k^2(t)=&\quad q_{k+1}^2(t)(A_1t+B_1),\\ H_{\Lambda_{n,k}}(q_kq_{k+1};q_{k+1}^2)-q_k(t)q_{k+1}(t)=&\quad q_{k+1}^2(t)(A_2t+B_2),\end{aligned} \tag{52}$$

where the parameters A_i, B_i can be determined by the orthogonality conditions (39). As in (51) we get that A_1 and B_1 satisfy the linear system

$$\begin{aligned} A_1\langle tq_{k+1}^2(t), P_{2k}^{(n)}(t)\rangle + B_1\langle q_{k+1}^2(t), P_{2k}^{(n)}(t)\rangle &= -\langle q_k^2(t), P_{2k}^{(n)}(t)\rangle, \\ A_1\langle tq_{k+1}^2(t), P_{2k+1}^{(n)}(t)\rangle + B_1\langle q_{k+1}^2(t), P_{2k+1}^{(n)}(t)\rangle &= -\langle q_k^2(t), P_{2k+1}^{(n)}(t)\rangle. \end{aligned}$$

The constants A_2 and B_2 satisfy similar system, the only difference being the right-hand side. By (48) this system has non-zero determinant, which implies the existence (and uniqueness) of the constants A_i, B_i, $i = 1, 2$. ☐

The proof, and in particular, the equation (52) imply the following corollary.

Corollary 3.5. *In the context of Lemma 3.4, suppose that*

$$\max\{A_i + B_i, B_i - A_i\} \le 0, \quad i = 1, 2, \tag{53}$$

where A_i, B_i are defined in (52)*. Then*

$$H_{\Lambda_{n,k}}(q_k^2; q_{k+1}^2) \le q_k^2(t), \quad H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2) \le q_k(t)q_{k+1}(t).$$

Subsequently, if $h(t)$ is absolutely monotone potential, then $f^h(t) = H_{\Lambda_{n,k}}(h; q_{k+1}^2) \le h(t)$.

Proof. Since $A_i t + B_i$ in (52) are linear functions, both will be non-positive on $[-1, 1]$ if and only if (53) holds. The conclusion $H_{\Lambda_{n,k}}(h; q_{k+1}^2) \le h(t)$ for absolutely monotone potentials now follows from (30). ☐

To apply Theorem 2.10 for f^h defined in (49) we need to show the positive definiteness of the interpolants $H_{\Lambda_{n,k}}(g_{j-1}; g_{2k+2})$ for $j = 1, \ldots, 2k+2$. For $j \in \{2k+1, 2k+2\}$, the special polynomial $H_{\Lambda_{n,k}}(q_k^2; q_{k+1}^2)$ and $H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2)$ can be written using (52) as

$$H_{\Lambda_{n,k}}(q_k^2; q_{k+1}^2) = q_k^2(t) + q_{k+1}^2(t)(A_1 t + B_1) = q_k^2(t)(1 + (t - \beta_{k+1})^2(A_1 t + B_1)),$$

$$H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2) = q_k(t)q_{k+1}(t) + q_{k+1}^2(t)(A_2 t + B_2) = q_k(t)q_{k+1}(t)(1 + (t - \beta_{k+1})(A_2 t + B_2)).$$

Then we can verify the positive definiteness of $H_{\Lambda_{n,k}}(q_k^2; q_{k+1}^2)$ and $H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2)$ directly (in particular, $A_1 > 0$ and $A_2 > 0$ are necessary conditions) which along with Corollary 3.5 gives

$$H_{\Lambda_{n,k}}(q_k^2; q_{k+1}^2) \in A_{n,q_k^2}, \quad H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2) \in A_{n,q_k q_{k+1}}.$$

For $j = 1, \ldots, 2k$ we have that $H_{\Lambda_{n,k}}(g_{j-1}; g_{2k+2}) = g_{j-1}(t)$. Therefore, it is enough to focus on deriving sufficient conditions that guarantee the $(1, 0)$-positive definiteness of the partial products q_i, $i \le k$; i.e., to have nonnegative coefficients in their expansion in terms of the adjacent polynomials $P_i^{1,0}(t)$. Recall that $(1, 0)$-positive definiteness implies positive definiteness. Since $g_{2j}(t) = q_j^2(t), g_{2j+1}(t) = q_j(t)q_{j+1}(t)$, $j = 0, 1, \ldots, k-1$ (see (29) and (34)), the Krein condition (9) will imply that the hypothesis conditions in Theorem 2.10 hold.

The $(1, 0)$-positive definiteness of $q_{k+1}(t)$ is equivalent to the non-negativity of the constants c_1, c_2, c_3 in Theorem 3.3. The next two lemmas provide sufficient conditions for the $(1, 0)$-positive definiteness of $q_k(t)$ and $q_{k-1}(t)$.

Lemma 3.6. *In the context of Lemma 3.4, let $d_0 := \theta_{k+1}(1 - \beta_{k+1})q_k(\beta_{k+1})$ (note that $d_0 > 0$). If*

$$c_3 > -\frac{d_0 a_{k+1,k+1}^{1,0} a_{k-2,k-2}^{1,0} r_{k-2}^{1,0} P_{k-1}^{1,0}(\beta_{k+1})}{a_{k-1,k-1}^{1,0}}, \tag{54}$$

then the polynomial $q_k(t)$ is $(1, 0)$-positive. In particular, since the right-hand side of (54) *is negative, non-negativity of c_3 implies that* (54) *is satisfied.*

Proof. Let $q_k(t)=\sum_{i=0}^k d_i P_i^{1,0}(t)$. First, note that $d_k=1/a_{k,k}^{1,0}>0$. For any $\ell\le k-2$ the degree of the polynomial $q_k(t)P_\ell^{1,0}(t)(1-t)$ is $k+\ell+1\le 2k-1$ and this polynomial belongs to $\Lambda_{n,k}$. Thus, we apply (33) to get

$$d_\ell\|P_\ell^{1,0}(t)\|^2=\int_{-1}^1 q_k(t)P_\ell^{1,0}(t)(1-t)d\mu(t)=\theta_{k+1}q_k(\beta_{k+1})P_\ell^{1,0}(\beta_{k+1})(1-\beta_{k+1})=d_0P_\ell^{1,0}(\beta_{k+1})$$

(all other terms are equal to 0; note d_0 as in the condition). Since all factors are positive (observe that $\beta_{k+1}>\alpha_k>t_k^{1,0}>t_\ell^{1,0}$) we have $d_\ell>0$.

Finally, for the last remaining d_{k-1} we consider (as in [14])

$$I:=\int_{-1}^1\frac{q_{k+1}(t)\left(P_{k-1}^{1,0}(t)-P_{k-1}^{1,0}(\beta_{k+1})\right)}{t-\beta_{k+1}}d\nu^{1,0}(t).$$

Comparing coefficients, we obtain

$$\frac{P_{k-1}^{1,0}(t)-P_{k-1}^{1,0}(\beta_{k+1})}{t-\beta_{k+1}}=\frac{a_{k-1,k-1}^{1,0}}{a_{k-2,k-2}^{1,0}}P_{k-2}^{1,0}(t)+\cdots,$$

whence $I=c_3a_{k-1,k-1}^{1,0}\|P_{k-2}^{1,0}\|_{1,0}^2/(a_{k+1,k+1}^{1,0}a_{k-2,k-2}^{1,0})$. On the other hand,

$$\begin{aligned}
&I=\int_{-1}^1 q_k(t)\left(P_{k-1}^{1,0}(t)-P_{k-1}^{1,0}(\beta_{k+1})\right)d\nu^{1,0}(t),\\
\iff\quad&\int_{-1}^1 q_k(t)P_{k-1}^{1,0}(t)d\nu^{1,0}(t)=I+P_{k-1}^{1,0}(\beta_{k+1})\int_{-1}^1 q_k(t)d\nu^{1,0}(t)\\
\iff\quad&d_{k-1}\|P_{k-1}^{1,0}\|_{1,0}^2=I+P_{k-1}^{1,0}(\beta_{k+1})d_0>0
\end{aligned}$$

and we conclude that $d_{k-1}>0$. □

Lemma 3.7. *In the context of Lemma 3.4, if*

$$P_j^{1,0}(\beta_k)>-\frac{\theta_{k+1}q_{k-1}(\beta_{k+1})(1-\beta_{k+1})P_j^{1,0}(\beta_{k+1})}{\theta_kq_{k-1}(\beta_k)(1-\beta_k)}\tag{55}$$

for every $j\le k-2$, then the polynomial $q_{k-1}(t)$ is $(1,0)$-positive definite.

Proof. Let $q_{k-1}(t)=\sum_{i=0}^{k-1}e_iP_i^{1,0}(t)$. It is clear that $e_{k-1}>0$. For $j\le k-2$ we have

$$\begin{aligned}
e_j&=\int_{-1}^1 q_{k-1}(t)P_j^{1,0}(t)d\nu^{1,0}(t)\\
&=\int_{-1}^1 q_{k-1}(t)P_j^{1,0}(t)(1-t)d\mu(t)\\
&=\theta_kq_{k-1}(\beta_k)P_j^{1,0}(\beta_k)(1-\beta_k)+\theta_{k+1}q_{k-1}(\beta_{k+1})P_j^{1,0}(\beta_{k+1})(1-\beta_{k+1})>0
\end{aligned}$$

using (33). □

Remark 3.8. For small N the requirement (55) can be replaced with the weaker $\beta_k>t_j^{1,0}$. For example, in three dimensions the last is satisfied for each $j\le k-2$ and $N\le 14$, for each $j\le k-3$ and $N\le 44$, etc.

To analyze the remaining partial products $q_i(t)$, $i\le k-2$, we adapt the approach from [14, Section 3] utilizing the $1/N$-quadrature rule (33). We consider the signed measure $\mu_j(t)$ defined by

$$d\mu_j(t)\;=\;(\beta_{k+1}-t)(\beta_k-t)\dots(\beta_{k-j+2}-t)(1-t)d\mu(t)$$

(of course, $\mu_0 = \mu$; the cases $j = 0$ and $j = 1$ were considered above).

Definition 3.9. A signed Borel measure η on $\mathbb{R}$ for which all polynomials are integrable is called *positive definite up to degree* m if for all real polynomials $p \not\equiv 0$ of degree at most m we have $\int p(t)^2 d\eta(t) > 0$.

Lemma 3.10. *For* $2 \leq j \leq k$*, the signed measure* $\mu_j(t)$ *is positive definite up to degree* $k - j$*.*

Proof. If $f(t)$ is arbitrary polynomial of degree at most $k - 1 - j/2 \geq k - j$ for $j \geq 2$, then

$$\begin{aligned} \int_{-1}^{1} f^2(t) d\mu_j(t) &= \int_{-1}^{1} f^2(t)(\beta_{k+1} - t)(\beta_k - t) \dots (\beta_{k-j+2} - t)(1 - t) d\mu(t) \\ &= \sum_{i=1}^{k-j+1} \theta_i f^2(\beta_i)(\beta_{k+1} - \beta_i)(\beta_k - \beta_i) \dots (\beta_{k-j+2} - \beta_i)(1 - \beta_i) \geq 0, \end{aligned}$$

where we used that $f^2(t)(\beta_{k+1} - t)(\beta_k - t) \dots (\beta_{k-j+2} - t)(1 - t) \in \Lambda_{n,k}$ and therefore the quadrature (33) can be applied. The equality can be attained if and only if $f(\beta_i) = 0$ for $i = 1, 2, \dots, k - j + 1$, which means that $f(t) \equiv 0$ when $\deg(f) \leq k - j$. This completes the proof for $j \geq 2$. □

Lemma 3.11. ([14, Lemma 3.5]) *Let the measure* $\eta(t)$ *be positive definite up to degree* M*. Then there are unique monic polynomials* $p_0, p_1, \dots, p_{M+1}$ *such that* $\deg(p_i) = i$ *for each* i *and*

$$\int p_i(t) p_j(t) d\eta(t) = 0$$

for $i \neq j$*. For each* i*,* p_i *has* i *distinct real roots, and the roots of* p_i *and* p_{i-1} *are interlaced.*

Proof. The proof adopts standard Gramm-Schmidt orthogonalization and can be found in [14] or [33]. □

Combining Lemmas 3.10 and 3.11, we denote by

$$q_{j,0}(t), q_{j,1}(t), \dots, q_{j,k-j+1}(t)$$

the unique monic polynomials that are orthogonal with respect to $\mu_j(t)$ and enjoy the properties

(a) for each i, $q_{j,i}$ has i distinct real roots;
(b) the roots of $q_{j,i}$ and $q_{j,i-1}$ are interlaced.

For $j < k+1$, the monic polynomial $q_j(t)$ of degree j is orthogonal to all polynomials of degree at most $j-1$ with respect to the signed measure $\mu_j(t)$ (this follows from the quadrature (33); see also the paragraph just before Lemma 3.3 in [14]). Since such a polynomial is unique, we conclude that it coincides with $q_{j,k-j+1}(t)$, i.e.

$$q_{j,k-j+1}(t) = (t - \beta_1) \dots (t - \beta_{k-j+1}) =: q_{k-j+1}(t)$$

for every $j \leq k$. This and the fact that the roots are interlaced, imply, again as in [14], that for $i < k - j + 1$, the largest root of $q_{j,i}(t)$ is less than β_{k-j+1}. Therefore, $q_{j-1,i}(\beta_{k-j+2}) \neq 0$ for every $i \leq k - j + 1$. Note that in fact $q_{j-1,i}(\beta_{k-j+2}) > 0$ (we need this below). Then there are constants $\alpha_{j,i}$ such that for $i \leq k - j + 1$,

$$q_{j,i}(t) = \frac{q_{j-1,i+1}(t) + \alpha_{j,i} q_{j-1,i}(t)}{t - \beta_{k-j+2}}.$$

Lemma 3.12. *For* $1 \leq j \leq k + 1$ *and* $i \leq k - j + 1$*, the polynomial* $q_{j,i}$ *is a positive linear combination of the polynomials* $q_{j-1,0}, \dots, q_{j-1,i}$*.*

Proof. We argue as in the end of the proof of Lemma 3.6. Define $d_0, \dots, d_i$ so that

$$q_{j,i}(t) = \sum_{\ell=0}^{i} d_\ell q_{j-1,\ell}(t).$$

For every $\ell \le i$, we have by orthogonality

$$\int_{-1}^{1} (q_{j-1,i+1}(t) + \alpha_{i,j} q_{j-1,i}(t)) \cdot \frac{q_{j-1,\ell}(t) - q_{j-1,\ell}(\beta_{k-j+2})}{t - \beta_{k-j+2}} d\mu_{j-1}(t) = 0,$$

since the polynomial $\frac{q_{j-1,\ell}(t) - q_{j-1,\ell}(\beta_{k-j+2})}{t - \beta_{k-j+2}}$ has degree $\ell - 1 \le i - 1$. This and the formula for $q_{j,i}(t)$ imply that

$$\int_{-1}^{1} q_{j,i}(t) q_{j-1,\ell}(t) d\mu_{j-1}(t) = q_{j-1,\ell}(\beta_{k-j+2}) \int_{-1}^{1} q_{j,i}(t) d\mu_{j-1}(t).$$

Therefore

$$d_\ell \int_{-1}^{1} q_{j-1,\ell}(t)^2 d\mu_{j-1}(t) = d_0 q_{j-1,\ell}(\beta_{k-j+2}) \int_{-1}^{1} d\mu_{j-1}(t).$$

Because $\ell \le i \le k - j + 1$, both integrals are positive. The largest root of $q_{j-1,\ell}(t)$ is less than β_{k-j+2}, so $q_{j-1,\ell}(\beta_{k-j+2}) > 0$. Thus, $d_0, \dots, d_i$ all have the same sign, which is positive because $d_i > 0$ (this follows also from $d_0 > 0$ by the quadrature). □

We summarize the above work on the positive definiteness of the partial products $q_j(t)$.

Theorem 3.13. *In the context of Lemma 3.4, all polynomials $q_j(t) = (t - \beta_1) \dots (t - \beta_j)$, $j = 0, 1, \dots, k-2$, are positive definite. The polynomials $q_{k-1}(t)$, $q_k(t)$, and $q_{k+1}(t)$ are $(1,0)$-positive definite if* (55), (54) *and $c_i \ge 0$ are fulfilled, respectively.*

Now Theorem 3.13 and the Krein condition (9) imply the following.

Theorem 3.14. *In the context of Lemma 3.4, if* (55) *and $c_i \ge 0$, $i = 1, 2, 3$, hold, then the polynomial f^h expands with nonnegative Gegenbauer coefficients; i.e., $f_i^h \ge 0$ for every i.*

Remark 3.15. In general, the condition $c_i \ge 0$ is not necessary to verify the regular positive definiteness of q_{k+1}, q_k, q_{k-1}. However, in the extensive numerical computations we have not observed a case where f^h is positive definite, while this condition fails.

3.3. **Second level bounds on $\Lambda_{n,k}$.** We can combine the subsections 3.1 and 3.2 into the following theorem extending Theorem 2.8, which we shall refer to as second level ULB.

Theorem 3.16. *In the context of Theorem 3.3 and Lemma 3.4, if* (55) *and $c_i \ge 0$, $i = 1, 2, 3$, are satisfied, then the Hermite interpolant $f^h(t)$ defined by* (47) *belongs to the class $\Lambda_{n,k} \cap A_{n,h}$. The following second level universal lower bound holds*

$$\mathcal{E}_h(n, N) \ge S_\tau(n, N; h) := N^2 \sum_{i=1}^{k+1} \theta_i h(\beta_i). \tag{56}$$

Moreover, $f^h(t)$ is the unique optimal polynomial that yields (see (4)*)*

$$N^2 f_0^h - N f^h(1) = \mathcal{W}_{h,\Lambda_{n,k}}(n, N) = S_\tau(n, N; h).$$

Proof. Corollary 3.5 shows that $f^h \le h(t)$ for all $t \in [-1, 1)$ and Theorem 3.14 says that f^h is positive definite. Therefore $f^h \in A_{n,h}$, yielding immediately that $f^h \in \Lambda_{n,k} \cap A_{n,h}$.

The calculation of the second level ULB (56) produced by f^h is straightforward by the $1/N$-quadrature rule (33). We have

$$N^2 f_0^h - N f^h(1) = N^2 \sum_{i=1}^{k+1} \theta_i f^h(\beta_i) = N^2 \sum_{i=1}^{k+1} \theta_i h(\beta_i)$$

(we used $f^h(\beta_i) = h(\beta_i)$ from the interpolation). Now Theorem 2.3 shows the optimality of f^h. □

The inclusion $P_\tau \subset \Lambda_{n,k}$ implies that $S_\tau(n,N;h) > R_\tau(n,N;h)$ (see also the proof of the sufficiency of Theorem 4.1 in [12]).

We proceed with explanation of the second level bound on $\mathcal{A}(n,s)$ improving on the first level; i.e. on the Levenshtein bounds.

Methods for obtaining better than the Levenshtein bounds utilizing polynomials of degrees $m+3$ and $m+4$ (in our terminology – for finding second level bounds) were developed previously. For example, in [32] Odlyzko and Sloane discretized the constraint $f(t) \leq 0$ in $[-1,1/2]$ and applied the simplex method to target the so-called kissing number problem; in [9] Boyvalenkov proposed a computational method to approximate optimal polynomials of degree $\tau(n,N)+3$ and $\tau(n,N)+4$; and Lagrange multipliers were applied in some cases for utilization of the conditions $f_i = 0$ by Nikova and Nikov in [31].

Our second level bound for $\mathcal{A}(n,s)$ is obtained by the *second level Levenshtein-type polynomial*

$$g(t) := H_{\Lambda_{n,k}}(0; q_{k+1}q_k). \tag{57}$$

Indeed, the conditions for existence and uniqueness of g and its belonging to $\Lambda_{n,k} \cap B_{n,\beta_{k+1}}$ are the same as these for $f^h \in \Lambda_{n,k} \cap A_{n,h}$. Thus, $g(t) \in \Lambda_{n,k} \cap B_{n,\beta_{k+1}}$ can be applied in Theorem 2.6 to give the second level bound on $\mathcal{A}(n,s)$. Moreover, as the monotonicity of the Levenshtein bound implies the lower bound (25) on the quantity $s(n,N)$, we obtain similarly a second level bound on $s(n,N)$ which inproves on (25). The discussion of this paragraph is summarized in the next theorem.

Theorem 3.17. *In the context of Theorem 3.3 and Lemma 3.4, if* (55) *and* $c_i \geq 0$*,* $i=1,2,3$*, are satisfied, then the polynomial* $g(t)$ *defined by* (57) *belongs to the class* $\Lambda_{n,k} \cap B_{n,\beta_{k+1}}$*. The following second level universal bound hold*

(a) $\mathcal{A}(n,\beta_{k+1}) \leq g(1)/g_0 = N < L_{2k-1}(n,\beta_{k+1})$,

(b) $s(n,N) \geq \beta_{k+1} > \alpha_k$.

Moreover, there exist no polynomials in $\Lambda_{n,k} \cap B_{n,\beta_{k+1}}$ *which give better bound than* $\mathcal{A}(n,\beta_{k+1}) \leq N$.

Proof. As discussed above, we have $g \in \Lambda_{n,k} \cap B_{n,\beta_{k+1}}$ and therefore $\mathcal{A}(n,\beta_{k+1}) \leq g(1)/g_0$. Then the $1/N$-quadrature rule (33) gives $g_0 N = g(1)$; i.e., $\mathcal{A}(n,\beta_{k+1}) \leq N$. The strict monotonicity of the Levenshtein bound and $\alpha_k < \beta_{k+1}$ from Theorem 3.2 imply the strict inequality in (a) since $N = L_{2k-1}(n,\alpha_k)$. The optimality of $g(t)$ follows from (33).

The proof of Theorem 2.5 can be adapted to derive (b). It can be verified also whenever the ULB-space $\Lambda_{n,k}$ comes for an interval $[N_1,N_2] \subset (D(2k-1,n), D(2k,n)]$. □

Note that the value N in our new bound $\mathcal{A}(n,\beta_{k+1}) \leq N$ is set well before we actually find what we do improve (i.e., the number β_{k+1} and then the bound $L(n,\beta_{k+1})$). Since $\mathcal{A}(n,\beta_{k+1}) \leq \lfloor N \rfloor$, one would prefer to have in this setting N slightly less than an integer.

Remark 3.18. Having defined the second level $1/N$-quadrature rule (33) we can construct second level test functions (13) from Theorem 2.3. Investigation of their signs will give, as its first level counterpart does, necessary and sufficient conditions for existence of further improvements by linear programming.

3.4. Lifting the Levenshtein framework, even case $\tau(n,N) = 2k$ (sketch).

The even case $\tau(n,N) = 2k$ is quite similar. Let n and N be such that $Q_{2k+3}^{(n,N)} < 0$ (the sign of $Q_{2k+4}^{(n)}$ can be arbitrary). Now the *skip-two/add-two* subspace (14) is

$$\Lambda_{n,k} = \mathcal{P}_{2k} \oplus \operatorname{span}\left(P_{2k+3}^{(n)}, P_{2k+4}^{(n)}\right)$$

and our target is a $\Lambda_{n,k}$-LP-extremal polynomial

$$f^h(t) = f^h_{2k+4}P^{(n)}_{2k+4}(t) + f^h_{2k+3}P^{(n)}_{2k+3}(t) + \sum_{i=0}^{2k} f^h_i P^{(n)}_i(t) \in \Lambda_{n,k} \cap A_{n,h}.$$

The $1/N$ quadrature rule exact for $\Lambda_{n,k}$ is

$$f_0 = \frac{f(1)}{N} + \theta_0 f(-1) + \sum_{i=2}^{k+2} \theta_i f(\beta_i),$$

where $\beta_1 = -1$ and the nodes $\beta_2, \beta_3, \dots, \beta_{k+2}$ are the roots of the equation

$$P^{1,1}_{k+1}(t) + d_1 P^{1,1}_k(t) + d_2 P^{1,1}_{k-1}(t) + d_3 P^{1,1}_{k-2}(t) = 0 \tag{58}$$

(compare to (23) with $\varepsilon = 1$). The interlacing now is $\alpha_1 = \beta_1 = -1$ and $\beta_i < \alpha_i < \beta_{i+1}$ for $i = 2, 3, \dots, k+1$.

Exactly as in the Levenshtein framework for the first level, in the even case $\tau(n, N) = 2k$ the strengthened Krein condition (10) should be used instead of (9).

The second level Hermite interpolant to h is

$$f^h := H_{\Lambda_{n,k}}(h; (\cdot + 1)s^2_{k+1}) \in \Lambda_{n,k} \cup A_{n,h},$$

where $s_{k+1}(t)$ is the polynomial in the LHS of (58). The Levenshtein bound is improved as in Theorem 3.17.

4. Two special examples of the second level lift – the 24-cell and the 600-cell on $\mathbb{S}^3$

As our approach yields next-level necessary and sufficient conditions for existence of better bounds, it is particularly illustrative to consider the cases $(n, N) = (4, 24)$ and $(n, N) = (4, 120)$. Both fall in the case of subsection 3.1. Moreover, for these parameters there are prominent codes, namely the 24-cell and the 600-cell, whose properties are widely investigated in the literature [1, 2, 7, 8, 13, 14, 16, 17].

4.1. **The 24-cell.** The $(4, 24)$-codes take prominence in the literature ([9, 32, 30]). In particular, the 24-cell code (derived from the D_4 root system) solving the kissing number problem [30], is suspected to be a maximal code, but is not universally optimal (see [13]). In this case $\tau = 5$, $k = 3$, $\varepsilon = 0$, the Levenshtein nodes and weights are approximately $\{\alpha_1, \alpha_2, \alpha_3\} = \{-0.817352, -0.257597, 0.47495\}$, $\{\rho_1, \rho_2, \rho_3\} = \{0.138436, 0.433999, 0.385897\}$. This defines the corresponding 1/24-quadrature rule (22).

The first seven test functions associated with the Levenshtein 1/24-quadrature rule (22) are shown approximately in Table 1. Two of them, namely $Q^{(4,24)}_8$ and $Q^{(4,24)}_9$, are negative.

Table 1. Approximations of the first seven non-zero test functions for the Levenshtein 1/24-quadrature rule

$Q^{(4,24)}_6$	$Q^{(4,24)}_7$	$Q^{(4,24)}_8$	$Q^{(4,24)}_9$	$Q^{(4,24)}_{10}$	$Q^{(4,24)}_{11}$	$Q^{(4,24)}_{12}$
0.0857	0.1600	−0.0239	−0.0204	0.0642	0.0368	0.0598

The next assertion is a $(4, 24)$-code version of Theorem 2.3.

Theorem 4.1. *The collection of nodes and weights* $\{(\beta_i, \theta_i)\}_{i=1}^4$

$$\begin{aligned} \{\beta_1, \beta_2, \beta_3, \beta_4\} &= \{-0.86029..., -.0.48984..., -0.19572..., .0.478545...\} \\ \{\theta_1, \theta_2, \theta_3, \theta_4\} &= \{0.09960..., 0.14653..., 0.33372..., 0.37847...\}, \end{aligned} \tag{59}$$

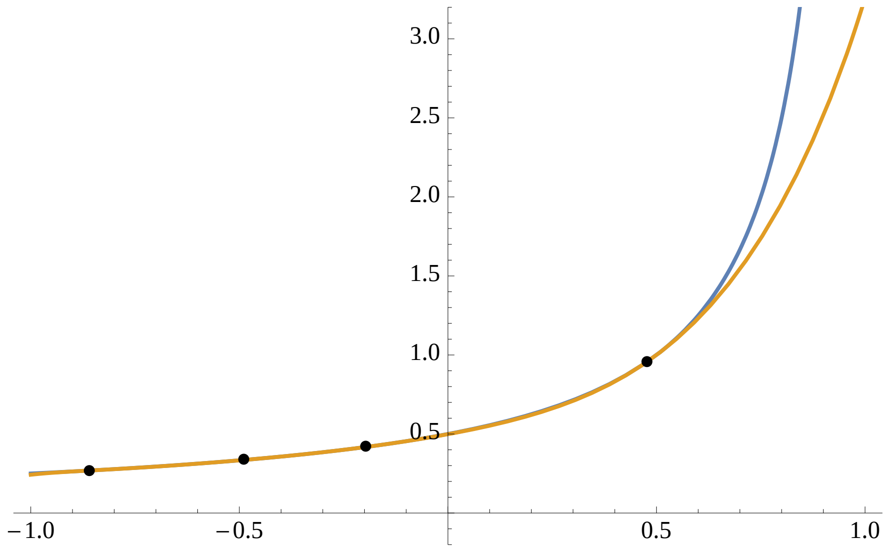

FIGURE 1. The $(n,N)=(4,24)$ case optimal interpolant – Newton potential

define $1/24$*-quadrature rule* (33) *that is exact for the subspace* $\Lambda_{4,3} := \mathcal{P}_5 \oplus \mathrm{span}\left(P_8^{(4)}, P_9^{(4)}\right)$. *For every absolutely monotone* h *the Hermite interpolant* $f^h(t) = H_{\Lambda_{4,3}}(h; q_4^2)$ *exists and belongs to* $\Lambda_{4,3} \cap A_{4,h}$. *Subsequently,* $\Lambda_{4,3}$ *is a ULB-space and the following universal lower bound (and an improvement of* (27)*) holds*

$$\mathcal{E}_h(4,24) \geq S_5(4,24;h) = 24^2 \sum_{i=1}^{4} \theta_i h(\beta_i).$$

The test functions $Q_j^{(4,24)}$ *associated with the second-level* $1/24$*-quadrature rule* (33) *with nodes and weights* (59) *are positive for all* $j \in \mathbb{N} \setminus \{1,2,3,4,5,8,9\}$ *and therefore* $f^h(t)$ *is LP-optimal* (*see Figure 1*).

Proof. Following the procedure in subsection 3.1 we arrive at the equations (41)-(43):

$$6776c_1^2c_3 - 2200c_1c_2 - 2233c_1c_3 - 7425c_2c_3 + 875c_1 + 675c_2 - 1134c_3 = 0,$$

$$195657c_1^2c_3 - 698775c_1c_2c_3 - 63525c_1c_2 - 83006c_1c_3 + 226875c_2^2 + 889350c_3^2 + 61600c_2 + 76538c_3 + 36750 = 0,$$

$$77c_1 - 275c_2 - 1463c_3 + 217 = 0,$$

respectively. We obtain

$$c_1 = 0.909977..., \; c_2 = 0.501716..., \; c_3 = 0.101911... \tag{60}$$

Resolving the equation $q_4(t) = 0$ we get distinct zeros $\beta_1, \beta_2, \beta_3, \beta_4$, all in $(-1,1)$. The weights $\theta_1, \theta_2, \theta_3, \theta_4$ are all positive, hence by Theorem 3.3 we obtain that (59) defines the unique $1/24$-quadrature on $\Lambda_{4,3}$ (observe the interlacing of the first and second level quadrature nodes as described in Theorem 3.2).

The conditions of Theorem 2.10 are also checked directly with the interpolation set $T = \{\beta_1, \beta_1, \ldots, \beta_4, \beta_4\}$. With the constants from (60) we have that (48) holds, which implies the existence and uniqueness of the Hermite interpolant $H_{\Lambda_{4,3}}(h; q_4^2)$ on the subspace $\Lambda_{4,3}$. Computing $(A_1, B_1) \approx (1.2197, -1.7419)$ and $(A_2, B_2) \approx (1.5983, -2.7379)$ yields that condition (53) holds so the inequality $H_{\Lambda_{4,3}}(h; q_4^2) \leq h(t)$ follows from Corollary 3.5. We can verify the positive definiteness of the partial products directly or via Theorem

3.13. Theorem 3.14 extends this property to $H_{\Lambda_{4,3}}(h;q_4^2)$.Therefore, $H_{\Lambda_{4,3}}(h;q_4^2) \in \Lambda_{4,3} \cap A_{4,h}$ for every absolutely monotone h.

The signs of the second level test functions $Q_j^{(4,24)}$, $j \in \mathbb{N} \setminus \{1,2,3,4,5,8,9\}$, can be investigated as in [12, Section 4.3]. In this case the parameter $j_0 = j_0(4,24)$ from that article is equal to 15. □

The typical behaviour of the second level energy bounds with respect to the first level ULB and actual energies is well illustrated by the situation with $h(t)$ being the Newton potential. In this case the first level energy bound is 333, the second level is ≈ 333.15 and the best known energy is 334 – the energy of the 24-cell [5]. The second level bound on maximal codes is better understood by observing that starting with $24-\epsilon$, where $\epsilon > 0$ is very small will result in a second level bound $\mathcal{A}(4,s) \leq 23$ instead of $\mathcal{A}(4,s) \leq 24$, where s is slightly smaller than β_4. With a few exceptions, all second level results for integer $N = \mathcal{A}(n, \beta_{k+1})$ can be treated this way.

The LP-optimality of the second level polynomial implies that the 24-cell can not be shown to be optimal for any particular absolutely monotone potential by linear programming. In fact, it was proved in [13] that the 24-cell is not universally optimal.

We note also that the second level Levenshtein polynomial (57) for $(n,N) = (4,24)$ (along with $(n,N) = (4,25)$) was derived first by Arestov and Babenko in [4].

4.2. **The 600-cell.** In the case $\tau(4,120) = 11$ the first level ULB is provided by the Hermite interpolant to the potential function at the Levenshtein nodes $(\alpha_i)_{i=1}^6 \approx (-0.9356, -0.7266, -0.3810, 0.04406, 0.4678, 0.8073)$. Since $Q_{12}^{(4,120)} > 0$, $Q_{13}^{(4,120)} > 0$, $Q_{14}^{(4,120)} < 0$, and $Q_{15}^{(4,120)} < 0$, we apply the technique from Section 3.1.

To prove that $\Lambda_{4,6} = \mathcal{P}_{11} \oplus \operatorname{span}\left(P_{14}^{(4)}, P_{15}^{(4)}\right)$ is a ULB-space we proceed similarly to subsection 4.1. The equations (41)-(43) are too long to be stated here. We find

$$(c_1, c_2, c_3) = (0.944..., 0.532..., 0.318...).$$

This leads us to a 1/120-quadrature with 7 internal nodes

$$(\beta_i)_{i=1}^7 = (-0.9819..., -0.7965..., -0.4765..., -0.1654..., 0.0977..., 0.4754..., 0.8079...).$$

The corresponding weights $\{\theta_i\}_{i=1}^7$ are all positive, and by Theorem 3.3 we conclude the 1/120-quadrature is exact in the space $\Lambda_{4,6}$. In a similar fashion as in subsection 4.1 we verify that the Hermite interpolant to the potential function h at these nodes exists, stays underneath the potential, and is positive definite, i.e. $H_{\Lambda_{4,6}}(h;q_7^2) \in \Lambda_{4,6} \cap A_{4,h}$. Actually, the new test functions of order 12 and 13 are positive and hence, $H_{\Lambda_{4,6}}(h;q_7^2)$ is $\mathcal{P}_{15}$-LP-optimal.

We note that with the Newton potential the first level ULB is 10786.8 while the second level gives 10788.2. This is still below the actual Newton energy 10790 of the 600-cell which is going to be achieved by a third level lift in the next section.

5. The universal optimality of the 600-cell revisited - third level lift

5.1. **Universal optimality of the 600-cell.** We start with a general result about generation of $1/N$-quadrature rules by (good) codes. We define the i-th moment of a spherical code $C = \{x_1, x_2, \ldots, x_N\}$ by

$$M_i(C) := \sum_{j,\ell=1}^{N} P_i^{(n)}(\langle x_j, x_\ell \rangle).$$

It is well known that $M_i(C) \geq 0$ with equality if and only if $\sum_{j=1}^{N} Y(x_j) = 0$ for all spherical harmonics $Y \in \mathrm{Harm}(i)$. The set

$$\mathcal{I}(C) := \{i \in \mathbb{N} \colon M_i(C) = 0\}$$

is called the *index set* of C. Hence, C is a spherical τ-design if and only if $\{1, 2, \ldots, \tau\} \subseteq \mathcal{I}(C)$.

It is straightforward to see that the identity

$$E_f(C) = f_0 N^2 - f(1)N + \sum_{i=1}^{r} f_i M_i(C) \tag{61}$$

holds for any polynomial $f(t) = \sum_{i=0}^{r} f_i P_i^{(n)}(t)$.

A key component of the proof of Theorem 5.2 below is that an N-point code $C \subset \mathbb{S}^{n-1}$ provides a $1/N$-quadrature rule that is exact on the subspace spanned by $P_i^{(n)}$ for i in the index set $\mathcal{I}(C)$.

Theorem 5.1. *Let $C \subset \mathbb{S}^{n-1}$ be an N-point code and*

$$\{-1 \leq \alpha_1 < \cdots < \alpha_m < 1\} := \{\langle x, y\rangle \colon x \neq y \in C\}, \tag{62}$$

be the set of inner products with

$$\rho_\ell := \frac{\left|\{(i,j) \colon \langle x_i, x_j\rangle = \alpha_\ell\}\right|}{N^2}, \qquad \ell = 1, \ldots, m, \tag{63}$$

the relative frequency of occurrence of α_ℓ. If

$$\Lambda(C) := \mathrm{span}\{1, P_j^{(n)}(t) \colon j \in \mathcal{I}(C)\},$$

then $\{(\alpha_\ell, \rho_\ell)\}_{\ell=1}^m$ is a $1/N$-quadrature rule exact for $\Lambda(C)$ and for any $f \in \Lambda(C)$

$$E_f(C) = N^2 \sum_{\ell=1}^{m} \rho_\ell f(\alpha_\ell) = N^2(f_0 - f(1)/N). \tag{64}$$

Proof. Suppose $f \in \Lambda(C)$ is a polynomial of the form $f = \sum_{j=0}^{n} f_i P_i^{(n)}$ with $f_i \neq 0$ if and only if $i \in \mathcal{I}(C) \cup \{0\}$. The first equality in (64) holds from the definitions (62) and (63) (in fact for any function $f \in \Lambda(C)$). The second equality in (64) follows from (61) and also shows that $\{(\alpha_\ell, \rho_\ell)\}_{\ell=1}^m$ is exact for $\Lambda(C)$. □

We now turn to a third level lift and apply it to derive an alternative proof of the 600-cell W_{120} universal optimality. The 16-th degree second level test function associated with the new nodes being negative prompts us to seek a 1/120-quadrature with the parameters of the 600-cell: eight nodes

$$(\gamma_i)_{i=1}^8 = \left\{-1, \frac{-1-\sqrt{5}}{4}, -\frac{1}{2}, \frac{1-\sqrt{5}}{4}, 0, \frac{\sqrt{5}-1}{4}, \frac{1}{2}, \frac{1+\sqrt{5}}{4}\right\}$$

occurring with corresponding relative frequencies (weights)

$$\{\nu_1, \ldots, \nu_8\} = \left\{\frac{1}{120}, \frac{1}{10}, \frac{1}{6}, \frac{1}{10}, \frac{1}{4}, \frac{1}{10}, \frac{1}{6}, \frac{1}{10}\right\}.$$

By direct computation (or see [3, Section 3], [11, Theorem 5.1]) one may verify that the index set of W_{120} contains $\{0, 1, 2, \ldots, 19\} \setminus \{12\}$ and $\{(\gamma_i, \nu_i)\}_{i=1}^8$ form a (third level) 1/120-quadrature rule exact on the subspace $\mathcal{P}_{19} \cap \{P_{12}^{(4)}\}^\perp$. The problem is then to establish that for a given h absolutely monotone on $[-1, 1]$ there exists some positive definite polynomial f of degree at most 19 with $f_{12} = 0$ and such that $h(t) \geq f(t)$, $t \in [-1, 1)$, with equality if $t \in \{\gamma_1, \ldots, \gamma_8\}$. Cohn and Kumar [14] consider the subspace

$$\Lambda_3 := \mathcal{P}_{10} \oplus \mathrm{span}\left(P_{14}^{(4)}, P_{15}^{(4)}, P_{16}^{(4)}, P_{17}^{(4)}\right)$$

TABLE 2. The nonzero values of A_j^k and B_j^k in (??).

k	A_k^1	B_k^1	A_k^2	B_k^2
11	$-\frac{128}{13}$	$\frac{352}{39}$	0	0
12	$-\frac{4(87+16\sqrt{5})}{13}$	$\frac{16(59+11\sqrt{5})}{39}$	$-\frac{220}{29}$	$\frac{192}{29}$
13	$-\frac{2(210+79\sqrt{5})}{13}$	$\frac{4(279+107\sqrt{5})}{39}$	$-\frac{2(234+55\sqrt{5})}{29}$	$\frac{16(25+6\sqrt{5})}{29}$
14	$\frac{-725-301\sqrt{5}}{26}$	$\frac{4(235+99\sqrt{5})}{39}$	$\frac{-965-413\sqrt{5}}{58}$	$\frac{16(25+11\sqrt{5})}{29}$
15	$\frac{-471-185\sqrt{5}}{52}$	$\frac{271+115\sqrt{5}}{39}$	$\frac{-983-345\sqrt{5}}{116}$	$\frac{2(93+35\sqrt{5})}{29}$

and show there is a unique $f \in \Lambda_3$ to the interpolation problem $f(-1) = h(-1)$, $f(\gamma_i) = h(\gamma_i)$, and $f'(\gamma_i) = h'(\gamma_i)$ for $i = 2, 3, \ldots 8$ and, furthermore, that f is positive definite and stays below h; i.e., that $f \in A_{4,h} \cap \Lambda_3$. We find two other subspaces, namely,

$$\Lambda_1 := \mathcal{P}_{10} \oplus \text{span}\left(P_{13}^{(4)}, P_{14}^{(4)}, P_{15}^{(4)}, P_{16}^{(4)}, P_{17}^{(4)}\right)$$

and

$$\Lambda_2 := \mathcal{P}_{11} \oplus \text{span}\left(P_{14}^{(4)}, P_{15}^{(4)}, P_{16}^{(4)}, P_{17}^{(4)}\right)$$

either of which yields a simpler proof of the universal optimality of W_{120}.

Theorem 5.2. *The 600-cell W_{120} is universally optimal. If h is strictly absolutely monotone in $[-1,1]$ and C_{120} is any 120-point code on $\mathbb{S}^3$ not isometric to W_{120}, then*

$$E_h(W_{120}) < E_h(C_{120}).$$

Proof. Let $T = \{\gamma_1, \gamma_1, \ldots, \gamma_8, \gamma_8\} = \{t_0, t_1, \ldots, t_{15}\}$ and $g(t) = \prod_{i=1}^{8}(t-\gamma_i)^2$. For $i = 1$ or 2, we define

$$p_j(\Lambda_i, T; t) := g_j(t) + (A_j^i + B_j^i t)g(t), \qquad j = 0, 1, \ldots, 15,$$

where $g_j(t)$ is defined in (29) and A_j^i and B_j^i are the unique values so that $p_j(\Lambda_i, T; \cdot)$ is orthogonal to $P_{11}^{(4)}$ and $P_{12}^{(4)}$ if $i = 1$ and to $P_{12}^{(4)}$ and $P_{13}^{(4)}$ if $i = 2$. Note that $A_j^i = B_j^i = 0$ for $j = 0, \ldots, 10$ in the case $i = 1$ and for $j = 0, \ldots, 11$ in the case $i = 2$. Observe that we have $p_j(\Lambda_i, T; t) = H_{\Lambda_i}(g_j; g)$.

By explicit computation aided by a computer algebra system (CAS), we compute the nonzero values of A_j^i and B_j^i shown in Table 2. Observing (see (53)) that $B_j^i \geq 0$ and $A_j^i + B_j^i \leq 0$ for all $0 \leq j \leq 15$ and $i = 1, 2$ shows that $(A_j^i + B_j^i t) \leq 0$ for $t \in [-1, 1]$ and so

$$p_j(\Lambda_i, T; t) \leq g_j(t) \qquad j = 0, 1, \ldots, 15, \tag{65}$$

for $t \in [-1, 1]$.

Exact CAS computations show that the coefficients in the Gegenbauer expansion of $p_j(\Lambda_i, T; t)$ are nonnegative and therefore $p_j(\Lambda_i, T; t)$ is positive semi-definite for $j = 0, 1, \ldots, 15$ and $i = 1, 2$. Let h be absolutely monotone on $[-1, 1)$ and, for $i = 1$ or 2, let

$$H_{\Lambda_i}(h; g) := \sum_{j=0}^{15} h[t_0, t_1, \ldots, t_j] p_j(\Lambda_i, T; t).$$

By (65) and the non-negativity of the divided differences $h[t_0, t_1, \ldots, t_j]$, we have $H_{\Lambda_i}(h; g) \leq H(h; g)(t)$ for $t \in [-1, 1]$. Additionally, we may use the remainder formula for the Hermite interpolation to write

$$h(t) - H(h; g)(t) = h[\gamma_1, \gamma_1, \ldots, \gamma_8, \gamma_8, t] \prod_{i=1}^{8} (t - \gamma_i)^2 \geq 0.$$

showing $H(h; g)(t) \leq h(t)$ for $t \in [-1, 1)$. We have therefore established that $H_{\Lambda_i}(h; g) \in A_{4,h} \cap \Lambda_i$, $i = 1, 2$, and since $H_{\Lambda_i}(h; g)(\gamma_j) = H(h; g)(\gamma_j) = h(\gamma_j)$ for $j = 1, \ldots, 8$ and $i = 1, 2$, it follows from Theorem 2.3, Theorem 5.1, and the above discussion concerning $H_{\Lambda_i}(h; g)$ that $E_h(W_{120}) = \mathcal{E}_h(4, 120)$ and therefore that W_{120} is universally optimal. □

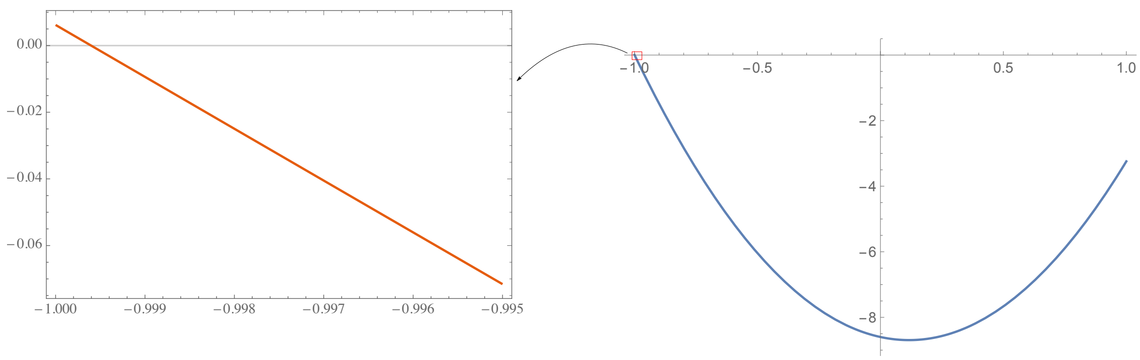

FIGURE 2. Right: plot of $A^0_{14} + B^0_{14}t + C^0_{14}t^2$ on $[-1, 1]$. Left: Blowup of graph for $t \in [-1, -.995]$.

It is interesting to consider why this approach does not work for Λ_3. In this case, the interpolation set $T_0 = \{\gamma_1, \gamma_2, \gamma_2, \ldots, \gamma_8, \gamma_8\}$ has $\gamma_1 = -1$ with multiplicity 1 and so the regular interpolant is a polynomial of degree at most 14. Since there are 3 orthogonality conditions, we consider

$$p_j(\Lambda_3, T_0; t) := p_j(T_0; t) + (A^0_j + B^0_j t + C^0_j t^2)(t + 1) \prod_{i=2}^{8} (t - \gamma_i)^2, \qquad j = 0, 1, \ldots, 14, \tag{66}$$

and again compute A^0_j, B^0_j, and C^0_j using exact CAS computations. In this case we verify that $p_j(\Lambda_3, T_0; t)$ for all $j = 0, \ldots, 14$ are positive semi-definite and that $p_j(\Lambda_3, T_0; t) \leq p_j(T_0; t)$ for $j = 0, \ldots, 13$. For $j = 14$ we have $A^0_{14} = \frac{-27-11\sqrt{5}}{6}$, $B^0_{14} = \frac{-27-\sqrt{5}}{18}$, and $C^0_{14} = \frac{4(3+\sqrt{5})}{3}$ and the quadratic term $A^0_{14} + B^0_{14}t + C^0_{14}t^2$ has a zero at $t = t^* = \frac{1}{48}\left(19 - 6\sqrt{5} - \sqrt{2413 + 204\sqrt{5}}\right) \approx -.999603$ and $p_{14}(\Lambda_3, T_0; t) > 0$ for $t \in [-1, t^*)$ as shown in Figure 2. Cohn and Woo [15] proceed by replacing the quadratic term in (66) for $j = 14$ with a cubic term resulting in a degree eighteen generalized partial product that is positive semi-definite and negative on $[-1, 1]$.

5.2. **Third level lift – quadrature nodes of the 600-cell.** It is noteworthy to say that as the 600-cell is almost a 19-design, its inner products $\{\gamma_i\}$ and relative frequencies $\{\nu_i\}$ form a (third level) 1/120-quadrature rule exact on the subspace $\mathcal{P}_{19} \cap \{P^{(4)}_{12}\}^{\perp}$. Therefore, unlike the second level lift, we din't need to perform the necessary work to determine the quadrature nodes in subsection 5.1. Below we sketch briefly an adaptation of the computational framework described in subsection 3.1 to determine the quadrature nodes for the third level lift in the $(n, N) = (4, 120)$ case. Namely, we seek the eight nodes $\{\delta_i\}_{i=1}^{8}$ as roots of a polynomial (compare with (37))

$$q_8(t) = P^{1,0}_8(t) + c_1 P^{1,0}_7(t) + c_2 P^{1,0}_6(t) + c_3 P^{1,0}_5(t) + c_4 P^{1,0}_4(t) + c_5 P^{1,0}_3(t).$$

Similar to (38), we require that

$$L(t) = (1-t)q_8(t)\left(d_0P_8^{1,0}(t) + d_1P_7^{1,0}(t) + d_2P_6^{1,0}(t) + d_3P_5^{1,0}(t) + d_4P_4^{1,0}(t) + d_5P_3^{1,0}(t)\right) \in \Lambda_2,$$

where we use the orthogonality conditions

$$\langle L, P_{12}^{(n)}\rangle = \langle L, P_{13}^{(n)}\rangle = 0$$

to express

$$d_4 = d_4(d_0, d_1, d_2, d_3), \quad d_5 = d_5(d_0, d_1, d_2, d_3).$$

Substituting (d_0, d_1, d_2, d_3) with $(1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, and $(0,0,0,1)$, respectively, we obtain four equations of degree at most 3 in the variables c_0, c_1, c_2, c_4, c_5. Together with the linear equation (see (43))

$$I_8 + c_1I_7 + c_2I_6 + c_3I_5 + c_4I_4 + c_5I_3 = \frac{1 + c_1 + c_2 + c_3 + c_4 + c_5}{120},$$

we find

$$c_1 = 0.8947\ldots, c_2 = 0.7894\ldots., c_3 = 0.6842\ldots, c_4 = 0.2315\ldots, c_5 = 0.1894\ldots.$$

As expected, the roots $\{\delta_i\}_{i=1}^8$ of $q_8(t)$ coincide with the inner products of the 600-cell.

If we require that $L(t) \in \Lambda_1$, in which case the orthogonality conditions used are

$$\langle L, P_{11}^{(n)}\rangle = \langle L, P_{12}^{(n)}\rangle = 0,$$

we arrive again at the same nodes.

5.3. **Characterization of LP-optimal polynomials of minimal degree.** We conclude this section with a characterization of all polynomials $f \in \mathcal{P}_{17}$ that are LP-optimal for $(n, N) = (4, 120)$ and a given h absolutely monotone on $[-1, 1]$. For $i = 1, 2$, let $f_{h,\Lambda_i}(t)$ denote the LP-optimal polynomial in Λ_i constructed above and let $f_{h,\Lambda_3}(t)$ be the LP-optimal polynomial whose existence is proved in [14].

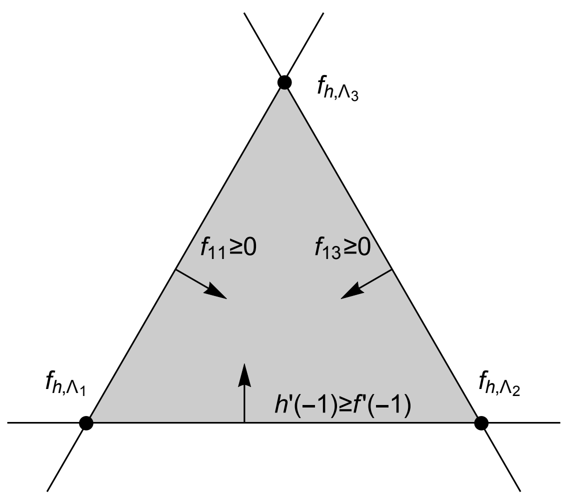

FIGURE 3. Set of LP-optimal polynomials for 600-cell and given h as in Theorem 5.3.

Theorem 5.3. *Let h be an absolutely monotone function on $[-1, 1)$. Then $f \in \mathcal{P}_{17}$ is LP-optimal for $(n, N) = (4, 120)$ if and only if f is a convex combination of f_{h,Λ_3}, f_{h,Λ_1}, and f_{h,Λ_2}.*

Remark 5.4. In his proof that the 600-cell W_{120} is a maximal code [1], Andreev utilizes the counterpart of Figure 4 triangle's (polynomial) vertex f_{h,Λ_2} that corresponds to the maximal cardinality problem (5) and notes that the counterpart of the whole segment $h'(-1) = f'(-1)$ works. In a subsequent article [2, Theorem 2] Andreev also proves that W_{120} minimizes the Newton energy among all configurations of 120 points by using a polynomial that lies in the interior of the side of the triangle (with $h(t) = 1/(1-t)$) determined by the condition $h'(-1) = f'(-1)$.

Proof. Theorem 5.2 implies that any LP-optimal f in $\mathcal{P}_{17}$, $(n,N) = (4,120)$, must satisfy the necessary conditions:

(a) $f_{12} = 0$ and $f_j \geq 0$, $j = 0,1,\ldots,17$,
(b) $f(\gamma_j) = h(\gamma_j)$, $j = 1,2,\ldots 8$,
(c) $f'(-1) \leq h'(-1)$ and $f'(\gamma_j) = h'(\gamma_j)$, $\quad j = 2,3,\ldots,8$.

Suppose $f, g \in \mathcal{P}_{17}$ both satisfy conditions (a), (b), and (c). The equality constraints in (b) and (c) imply

$$f(t) - g(t) = (t+1)\prod_{j=2}^{8}(t-\gamma_j)^2(A + Bt + Ct^2),$$

for some constants A, B, C. Further, from $f_{12} = g_{12} = 0$, a direct computation gives $5A = -6(B+C)$ and so

$$f(t) - g(t) = (t+1)\prod_{j=2}^{8}(t-\gamma_i)^2(B(t-6/5) + C(t^2-6/5)). \tag{67}$$

Then, exact computations give

$$\begin{aligned} f'(-1) - g'(-1) = \lambda_{1,2}(B,C) &:= -\frac{15(113B+83C)}{4096}, \\ (f-g)_{11} = \lambda_{1,3}(B,C) &:= -\frac{\pi(12B+7C)}{2621440}, \\ (f-g)_{13} = \lambda_{2,3}(B,C) &:= \frac{\pi(11C-24B)}{18350080}. \end{aligned}$$

Let $g := f_{h,\Lambda_1}$ and $f_{B,C}$ denote the polynomial defined by (67) for given B and C. Also, let $\alpha := g_{13} = (f_{h,\Lambda_1})_{13}$. Since $g'(-1) = h'(-1)$ and $g_{11} = 0$, it follows that if $f_{B,C}$ is optimal, then (B,C) must lie in the intersection Δ of the half-spaces $\lambda_{1,2}(B,C) \leq 0$, $\lambda_{1,3}(B,C) \geq 0$, and $\lambda_{2,3}(B,C) \geq -\alpha$. Let $L_{1,2}$, $L_{1,3}$, and $L_{2,3}$ denote the lines $\lambda_{1,2}(B,C) = 0$, $\lambda_{1,3}(B,C) = 0$, and $\lambda_{2,3}(B,C) = -\alpha$, respectively. Let (B_1,C_1), (B_2,C_2), (B_3,C_3) be the intersection points $\{(B_1,C_1)\} = \{(0,0)\} = L_{1,2} \cap L_{1,3}$, $\{(B_2,C_2)\} = L_{1,2} \cap L_{2,3}$, and $\{(B_3,C_3)\} = L_{1,3} \cap L_{2,3}$ and observe that $f_{B_k,C_k} = f_{h,\Lambda_k}$. Then $f_{B,C}$ is a convex combination of f_{h,Λ_3}, f_{h,Λ_1}, and f_{h,Λ_2} if and only if $(B,C) \in \Delta$. Since any LP-optimal polynomial $f \in \mathcal{P}_{17}$, $(n,N) = (4,120)$, is of the form $f = f_{B,C}$, the proof is completed. □

We remark that if $\alpha = 0$ in the above proof then $\Delta = \{(0,0)\}$ and $f_{h,\Lambda_1} = f_{h,\Lambda_2} = f_{h,\Lambda_3}$ is the only LP-optimal polynomial in $\mathcal{P}_{17}$, $(n,N) = (4,120)$. Otherwise, if $\alpha > 0$ then Δ forms a non-degenerate triangle.

6. Numerical illustration of the second level ULB

In this section we give examples of second level bounds which illustrate well the typical behaviour in the framework of Section 3.

Figure 4 illustrates the first and second level ULB for $\mathcal{E}_h(12,N)$ (on the left) for Newton potential, and the first and second level bounds for $\mathcal{A}(12,s)$ (on the right) in the particular case $(n,\tau) = (12,9)$.

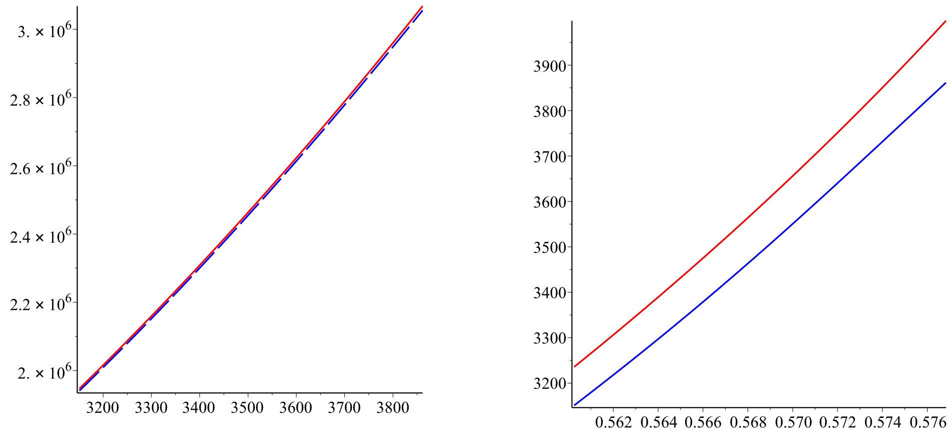

FIGURE 4. First and second level ULB (for Newton potential) and Levenshtein bounds for $(n,\tau)=(12,9)$

TABLE 3. First and second level ULB optimality for $n=8$, $90 \le N \le 990$.

$\tau(8,N)$	$[D(8,\tau),D(8,\tau+1)]$	ULB1-LP	No ULB2	ULB2-LP	ULB2	No ULB2
5	$[72,156]$	$[72,79],[91,102]$	$[80,90]$			[103,155]
6	$[156,240]$		$[156,167]$	$[168,239]$		
7	$[240,450]$	240		$[241,316]$		$[317,449]$
8	$[450,660]$			$[450,532]$	$[533,625]$	$[626,659]$

Even though the two ULB bounds look very close, as numerical comparison in [12, Table 1] reveals, the actual energy and the first level ULB are very close to start with. The juxtaposition of the Levenshtein bound and its second level lift illustrates a significant change. In fact the parameters $n=12$ and $\tau=9$ are chosen to illustrate the improvement on $\mathcal{A}(n,s)$ since in small dimensions it may look insignificant.

In Tables 3 and 4 we show how different situations arise in dimension $n=8$ and for $\tau(8,N)\in\{5,6,7,8\}$ and $n=9$ and for $\tau(9,N)\in\{5,6,7,8\}$ respectively. No test functions are negative for $\tau(8,N)\le 4$ and $\tau(9,N)\le 4$; i.e., the first level bounds are LP-optimal in these cases. In the columns ULB1-LP and ULB2-LP we show the intervals where the first and second level bounds are LP-optimal, respectively. The columns No ULB2 collect intervals where some of the necessary conditions from Section 3 is not satisfied. Finally, the column ULB2 shows intervals where the second level bounds exist but are not optimal.

More extensive data for $3\le n\le 12$ and $3\le N\le 1007$ can be found at https://my.vanderbilt.edu/edsaff/.

In Table 5 we present examples of bounds for small dimensions and cardinalities which behave typically. For each pair (n,N) we give the values of the corresponding parameters α_k, β_{k+1} and the best known maximal inner product $s(C)$ (i.e., an upper bound on $s(n,N)$). The first level and second level ULBs are shown in the fifth and seventh column, respectively, and the best known Newton energies are shown in the ninth column. The value of the corresponding Levenshtein bound is shown in the last column only if it is improved by our second level bound (equal to N). The data for eighth and ninth columns is taken from [5] (see https://aimath.org/data/paper/BBCGKS2006/).

TABLE 4. First and second level ULB optimality for $n = 9$, $90 \leq N \leq 990$.

$\tau(9,N)$	$[D(9,\tau),D(9,\tau+1)]$	ULB1-LP	No ULB2	ULB2-LP	ULB2	No ULB2
5	$[90,210]$	$[90,141]$	$[142,209]$			
6	$[210,330]$		$[210,232]$	$[233,284]$		$[285,329]$
7	$[330,660]$	$[330,332]$	$[333,338]$	$[339,439]$		$[440,659]$
8	$[660,990]$			$[660,850]$	$[851,929]$	$[930,989]$

The case $(3,12)$ corresponds, of course, to the icosahedron – a universally optimal code (indicated with superscript $^{\blacktriangle}$). The empty cells for ULB2 mean that some of the necessary conditions from Section 3 is not satisfied (the positive definiteness of the Hermite interpolant $H_{\Lambda_{n,k}}(q_k q_{k+1}; q_{k+1}^2)$ fails first). The superscripts $^{\diamond}$ and * mean that ULB1 and ULB2 are LP-optimal, respectively. The superscripts of the cardinalities show the signs of the test-functions $Q_{\tau(n,N)}+3$ and $Q_{\tau(n,N)}+4$, respectively.

In conclusion we formulate the following conjecture.

Conjecture 6.1. *For every dimension n the values $N \in [D(n,\tau), D(n,\tau+1)]$ for which second level bounds exist form an interval.*

Acknowledgements The research of the first and fifth authors was supported, in part, by a Bulgarian NSF contract DN02/2-2016. The research of the second author was supported, in part, by a Simons Foundation grant no. 282207. The research of the third and fourth authors was supported, in part, by the U. S. National Science Foundation under grant DMS-1516400. The first author is also with Technical Faculty, South-Western University, Blagoevgrad, Bulgaria. The research for this article was concluded while four of the authors were in residence at Oberwolfach Research Institute for Mathematics under the "Research in Pairs" program in May-June 2019.

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TABLE 5. First and second level ULBs vs. harmonic energy for a sample of cases $3 \leq n \leq 5$.

n	N	$\tau(n,N)$	α_k	ULB1	β_{k+1}	ULB2	$s(C)$	Energy	$L_\tau(n,\beta_{k+1})$
$3^\blacktriangle$	12	5	0.44721	98.33050	$---$	$---$	0.44721	98.33050	$---$
3	13^{-+}	5	0.48937	117.50227	0.49320	117.52252	0.61129	117.70646	13.10104
3	14^{--}	5	0.52401	138.43302	0.52767	138.45874	0.60367	138.61272	14.11861
3	15^{+-}	5	0.55223	161.12063			0.65309	161.34048	
3	16^{-+}	6	0.57531	185.56365	0.57655	185.57396	0.65689	185.82331	16.04667
3	17^{-+}	6	0.60000	211.85442	0.60253	211.88210	0.64134	212.10080	17.11170
3	18^{--}	6	0.62115	239.93234	0.62358	239.96600	0.67514	240.16893	18.12579
3	19^{--}	6	0.63921	269.79600	0.64099	269.82637	0.70822	270.17893	19.10762
3	20^{-+}	7	0.65465	301.44437			0.69348	301.76313	
4	14^{-+}	4	0.27429	98.00000			0.33921	98.52459	
4^*	15^{-+}	4	0.30620	114.95833	0.30901	115.00000	0.35355	115.23320	15.09646
4^*	16^{-+}	4	0.33333	133.33333	0.33668	133.39481	0.43652	133.89967	16.13540
4	17^{-+}	4	0.35645	153.12500	0.35921	153.18839	0.47650	153.96222	17.13061
4	18^{-+}	4	0.37627	174.33333	0.37792	174.38060	0.48480	175.23235	18.09042
4	19^{-+}	4	0.39337	196.95833			0.48797	197.90580	
$4^\diamond$	20	5	0.40824	221.00000	$---$	$---$	0.44168	221.59853	$---$
4^*	21^{-+}	5	0.42720	246.75000	0.42895	246.80226	0.52049	247.47325	21.09675
4^*	22^{-+}	5	0.44461	274.00000	0.44767	274.10417	0.54446	275.03231	22.18545
4^*	23^{-+}	5	0.46050	302.75000	0.46399	302.88662	0.57524	304.08398	23.23343
4^*	24^{--}	5	0.47495	333.00000	0.47854	333.15757	0.50000	334.00000	24.26443
4	25^{--}	5	0.48807	364.75000			0.60167	365.97676	
4	26^{+-}	5	0.50000	398.00000			0.56449	399.38498	
4	27^{+-}	5	0.51084	432.75000			0.64815	434.30824	
4	28^{+-}	5	0.52072	469.00000			0.64237	470.79842	
4	29^{+-}	5	0.52973	506.75000			0.62694	508.75066	
4	30^{-+}	6	0.53798	546.00000	0.53982	546.12516	0.63014	548.37233	30.18048
$5^\diamond$	30	5	0.37796	398.22942			0.41665	400.57973	
5	31^{-+}	5	0.38810	429.26411			0.49636	431.73992	
5^*	32^{-+}	5	0.39779	461.55489	0.39870	461.65839	0.44721	463.22759	32.09565
5^*	33^{-+}	5	0.40702	495.10289	0.40860	495.29351	0.52494	498.25726	33.17595
5^*	34^{-+}	5	0.41580	529.90910	0.41781	530.17012	0.55380	533.83563	34.23704
5^*	35^{-+}	5	0.42413	565.97439	0.42637	566.28683	0.57230	570.72828	35.27872
5^*	36^{--}	5	0.43202	603.29953	0.43436	603.64803	0.51722	607.97487	36.30722
5^*	37^{--}	5	0.43950	641.88518	0.44196	642.26961	0.57729	647.27793	37.34082
5	38^{--}	5	0.44659	681.73194			0.56512	687.15114	
5	39^{+-}	5	0.45330	722.84035			0.58602	728.31676	
5	40^{+-}	5	0.45965	765.21089			0.56248	769.75044	

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