Upper Bounds on the Minimum Distance of Spherical Codes

Peter G. Boyvalenkov, Danyo P. Danev, Silvya P. Bumova

Abstract

We use linear programming techniques to obtain new upper bounds on the maximal squared minimum distance of spherical codes with fixed cardinality. Functions $Q_j(n, s)$ are introduced with the property that $Q_j(n, s) < 0$ for some $j > m$ iff the Levenshtein bound $L_m(n, s)$ on $A(n, s) = \max\{|W| : W \text{ is an } (n, |W|, s) \text{ code}\}$ can be improved by a polynomial of degree at least $m+1$. General conditions on the existence of new bounds are presented. We prove that for fixed dimension $n \geq 5$ there exist a constant $k = k(n)$ such that all Levenshtein bounds $L_m(n, s)$ for $m \geq 2k - 1$ can be improved. An algorithm for obtaining new bounds is proposed and discussed.

Index Terms—Spherical codes, Minimum distance, Gegenbauer polynomials.

I. Introduction

An $(n, M, s)$ spherical code is a nonempty finite subset $W$ of $n$-dimensional Euclidean sphere $S^{n-1}$ with cardinality $|W| = M$ and maximal cosine $s = \max\{(x, y) : x, y \in W, x \neq y\}$. The squared minimum distance of an $(n, M, s)$ code is $d = 2(1 - s)$. Bounds on the squared minimum distance $D(n, M) = \max\{d = 2(1 - s) : \text{there exists an } (n, M, s) \text{ code}\}$ and the minimum maximal cosine $s(n, M) = 1 - D(n, M)/2 = \min\{s : \text{there exists an } (n, M, s) \text{ code}\}$ are interesting in view both of combinatorics and coding theory. In particular, the lower bounds on $s(n, M)$ can be used for upperbounding the free distance of trellis codes [11, 25]. The combinatorial problem for finding $D(3, M)$ comes from the classical geometry [19, 13, 14, 26, 27, 10].

The best known upper bounds on $D(n, M)$ are obtained by Levenshtein [21, 22, 23]. In fact, Levenshtein obtains upper bounds on the quantity $A(n, s) = \max\{|W| : W \text{ is an } (n, |W|, s) \text{ code}\}$. These bounds must be reformulated for estimating $s(n, M)$ and then $D(n, M)$.

In [5, 6] the first author describes a method for improving the Levenshtein bounds on $A(n, s)$ in some cases. The linear programming bounds which require appropriate polynomials were used. The polynomials we use are $A_{n,s}$-extremal [6, Section 2.1] (i.e. the best among the polynomials of the same or lower degree). In this paper we adapt this method in order to find improvements on the Levenshtein bounds on $D(n, M)$. Moreover, some conditions for existence of such improvements are considered. In some sense, our approach joins and extends the methods from [22, 23, 5, 6]. Many examples with new bounds and results on the existence of new bounds are given.

In Section II we give some notation and preliminary results. Functions $Q_j(n, s)$ are introduced in Section III. They have the property that $Q_j(n, s) < 0$ for some $j > m$ if and only if the Levenshtein bound $L_m(n, s)$ can be improved by a polynomial of degree at least $m + 1$ (Theorem 3.1). In Section IV we investigate the possibilities for improving the Levenshtein bounds. General results on the sign of $Q_j(n, s)$

\*The authors are with the Institute of Mathematics, Bulgarian Academy of Sciences, 8 G.Bonchev str., 1113 Sofia, Bulgaria

\†This paper was supported in part by Bulgarian NSF under contract MM-502/95

\‡Presented in part at International Workshop on Optimal codes, Sozopol, Bulgaria, May 26 - June 1, 1995
and their corollaries in small cases are presented. In particular, we prove that the even bounds \( L_{2k}(n, s) \) \((k \geq 2)\) can be improved in dimensions \( n = 3, 4, \ldots, k^2 + 2 \) in the whole interval \((\eta_k, \xi_k)\). Furthermore, we show that for fixed dimension \( n \geq 5 \) there exists a constant \( k = k(n) \) such that every Levenshtein bound \( L_m(n, s) \) for \( m \geq 2k - 1 \) can be improved in the whole interval it is valid.

In Section V we describe our method for improving the Levenshtein bounds when this is possible. In fact, we give a general algorithm for computing the new bounds on \( D(n, M) \). Then we consider the key step in detail. In particular, we propose a computer technique for finding the values of the functions \( Q_j(n, s) \). In Section VI we give many examples with new bounds. In three dimensions, the classical Fejes Tóth bound and the Levenshtein bounds on \( D(3, M) \) are improved for \( 13 \leq M \leq 24 \). We show examples in higher dimensions where good codes (we used the tables from [16, 17, 18]) are known. The possibilities for improving the Levenshtein bounds \( L_3(n, s) \) and \( L_5(n, s) \) are studied in detail. The results are summarized in Tables I-IV.

Odlyzko and Sloane [24], [12, Chapter 13] used another method for improving the Levenshtein bounds on the kissing numbers \( \tau_n = A(n, 1/2) \). Their approach can be adapted for obtaining new bounds on \( D(n, M) \) as well. In this case, the preliminary computation of \( Q_j(n, s) \) would show degrees of improving polynomials.

Pottie and Taylor [25] used sphere-packing arguments to develop upper bounds on the free distance of trellis codes. In particular, they substitute the Levenshtein bound on \( s(n, M) \) to obtain new bounds on the free distance of constant-energy trellis codes. Hence, our improvements can be used in this direction as well.

We notice that the third Levenshtein bound (see below) was asymptotically improved in some cases by Astola [3] by using an argument due to Tietäväinen [31].

II. Preliminaries

We shall need the Gegenbauer polynomials [1, 2]. They are defined by \( P_0^{(n)}(t) = 1, \) \( P_1^{(n)}(t) = t, \) and

\[
(i + n - 2)P_{i+1}^{(n)}(t) = (2i + n - 2)tP_i^{(n)}(t) - iP_{i-1}^{(n)}(t) \quad \text{for} \quad i \geq 1.
\]

It is easy to check that \( P_i^{(n)}(1) = 1, \) the odd (even) polynomials \( P_{2i}^{(n)}(t) \) \((P_{2i-1}^{(n)}(t))\) contain only odd (even) degrees of \( t, \) and the coefficients alternate in sign. We set \( P_i^{(n)}(t) = a_i^{(n)}t^i + a_i^{(n)}t^{-i-2} + \cdots. \)

To any real polynomial \( f(t) = \sum_{i=0}^k a_it^i \) we associate its expansion \( f(t) = \sum_{i=0}^k P_i^{(n)}(t) \) for well-defined Gegenbauer coefficients \( f_i. \) The important coefficient \( f_0 \) can be found by the following explicit formula

\[
f_0 = a_0 + \sum_{i=1}^{[k/2]} \frac{(2i - 1)!a_{2i}}{n(n + 2) \cdots (n + 2i - 2)}.
\]

Upper bounds on \( D(n, M) = 2(1 - s(n, M)) \) can be derived by using the Levenshtein upper bounds [21, 22, 23] on \( A(n, s) \). The explicit form of these bounds is

\[
A(n, s) \leq \begin{cases} 
L_{2k-1}(n, s) = \binom{k + n - 3}{k - 1} \frac{2k + n - 3}{n - 1} - \frac{P_{k-1}^{(n)}(s) - P_k^{(n)}(s)}{(1 - s)P_k^{(n)}(s)} & \text{for} \quad \xi_{k-1} \leq s \leq \eta_k, \\
L_{2k}(n, s) = \binom{k + n - 2}{k} \frac{2k + n - 1}{n - 1} - \frac{(1 + s)(P_k^{(n)}(s) - P_{k+1}^{(n)}(s))}{(1 - s)(P_k^{(n)}(s) + P_{k+1}^{(n)}(s))} & \text{for} \quad \eta_k \leq s \leq \xi_k,
\end{cases}
\]

where \( \xi_k \) and \( \eta_k \) are the greatest zeros of the Jacobi polynomials [1, Chapter 22] \( P_k^{(n, n-2)} \) \((P_k^{(n, n-2)}(t) = P_k^{(n)}(t) + \frac{n+1}{n-1}) \) respectively.
In the papers [7, 8], the possibilities for existence of \((n, L_m(n, s), s)\) codes were investigated. In particular, it is shown that \((n, L_{2k}(n, s), s)\) codes do not exist for \(\eta_k < s < \xi_k\).

We now state the Linear Programming Bound (LPB) for \(A(n, s)\) and \(D(n, M)\).

**Theorem 2.1** (LPB for spherical codes, [15, 20]) Let \(n \geq 3\) and \(f(t)\) be a real polynomial such that

(A1) \(f(t) \leq 0\) for \(-1 \leq t \leq s\), and

(A2) The coefficients in the Gegenbauer expansion \(f(t) = \sum_{i=0}^{k} f_i P_i(t)\) satisfy \(f_0 > 0\), \(f_i \geq 0\) for \(i = 1, \ldots, k\).

Then \(A(n, s) \leq f(1)/f_0\).

The set of suitable polynomials for applying in Theorem 2.1 is denoted by \(A_{n,s}\) [5, 6]. A polynomial \(f(t) \in A_{n,s}\) is called \(A_{n,s}\)-extremal (\(A_{n,s}\)-global extremal) if it gives the best bound on \(A(n, s)\) among the polynomials of the same or lower degree (all polynomials) from \(A_{n,s}\). Sidel’nikov [30] proved that the Levenshtein polynomials are \(A_{n,s}\)-extremal (see also [23, Section 4], [6, Theorem 5.2]).

The following theorem is a reformulation of Theorem 2.1 for bounding \(D(n, M)\).

**Theorem 2.2** (LPB for the minimum distance) If \(f(t) \in A_{n,s}\) \((n \geq 3, 0 < s_0 < 1)\) and \(f(1)/f_0 \leq M\), then \(s \geq s_0\) for any \((n, M, s)\) code and \(D(n, M) \leq 2(1-s_0)\) respectively.

We follow some notations from [23]. So the numbers \(\alpha_0 < \alpha_1 < \cdots < \alpha_{k-1} = s\ (-1 \leq \alpha_0)\) are all different zeros of the Levenshtein polynomial \(f_{2k-1}^{(s)}(t) = (t-s)(K_{k-1}^{1,0}(t, s))^2\) used for obtaining the bound \(A(n, s) \leq L_{2k}(n, s)\) (Levenshtein sets \(\alpha_k = 1\)). The positive weights \(\rho_i, i = 0, 1, \ldots, k\) have been defined in [23, Theorem 4.1]. For any real polynomial \(f(t)\) of degree at most \(2k-1\) the equality

\[
  f_0 = \sum_{i=0}^{k} \rho_i f(\alpha_i)
\]

holds [23, Theorem 4.1]. Moreover, for \(\xi_{k-1} \leq s \leq \eta_k\) we have \(L_{2k-1}(n, s) = 1/\rho_k\).

Correspondingly, the numbers \(-1 = \beta_0 < \beta_1 < \cdots < \beta_k = s\) are all different zeros of the Levenshtein polynomial \(f_{2k}^{(s)}(t) = (t+1)(t-s)(K_{k-1}^{1,1}(t, s))^2\) used for obtaining the bound \(A(n, s) \leq L_{2k}(n, s)\). The positive weights are \(\gamma_i, i = 0, 1, \ldots, k+1\) and \(\beta_{k+1} = 1\). We have \(L_{2k}(n, s) = 1/\gamma_{k+1}\) for \(\eta_k \leq s \leq \xi_k\) and

\[
  f_0 = \sum_{i=0}^{k+1} \gamma_i f(\beta_i)
\]

for any real polynomial \(f(t)\) of degree at most \(2k\) [23, Theorem 4.2].

The next lemma gives an useful relation between the parameters \(\rho_i\) and \(\alpha_i, i = 0, 1, \ldots, k\); \(\gamma_i\) and \(\beta_i, i = 0, 1, \ldots, k+1\). We denote by \(S_l\) simultaneously the power sums \(\sum_{i=0}^{k} \rho_i \alpha_i^l\) and \(\sum_{i=0}^{k+1} \gamma_i \beta_i^l\).

**Lemma 2.3** (Sidel’nikov [28, 29]) The numbers \(\rho_i\) and \(\alpha_i, i = 0, 1, \ldots, k\) \((\gamma_i\) and \(\beta_i, i = 0, 1, \ldots, k+1)\) satisfy the system of \(2k\) \((2k+1)\) equations

\[
  S_l = \begin{cases} 
    0 & \text{for odd } l, \\
    \frac{(v-1)!}{n^l(n+2)\ldots(n+2l-2)} & \text{for even } l.
  \end{cases}
\]

for \(0 \leq l \leq 2k-1\) \((0 \leq l \leq 2k)\).

**Proof.** We set consecutively \(f(t) = 1, t, \ldots, t^{2k-1}\) \((1, t, \ldots, t^{2k})\) in (1) and (2).

**Lemma 2.4** For any integer \(m > 0\) we have

\[
  \sum_{i=0}^{m} \frac{(2i-1)!!}{n(n+2)\ldots(n+2i-2)} a^{(n)}_{m,2i} = 0. \quad (4)
\]
The next theorem shows the important role these functions have to play in our investigations.

For any integer \( k \geq 0 \) we have \((k + 1)(t^2 - 1)P_k^{(n+2)}(t) = (n-1)[P_k^{(n)}(t) - tP_k^{(n)}(t)].\)

Proof. By induction.

III. The functions \( Q_j(n, s) \)

We introduce the following functions in \( III. \) The functions \( Q_j(n, s) \) by induction.

Lemma 2.5

We uniquely determine the coefficients \( \{22, 23\} \). Let \( h \) (for the last inequality we use \( g \)).

Proof. Theorem 3.1

We introduce the following functions in \( III. \) The functions \( Q_j(n, s) \) by induction.

\[
Q_j(n, s) = \begin{cases} 
\sum_{i=0}^{k} \rho_i P_i^{(n)}(\alpha_i) & \text{for } \xi_{k-1} \leq s \leq \eta_k, \\
\sum_{i=1}^{\eta_k} \gamma_i P_i^{(n)}(\beta_i) & \text{for } \eta_k \leq s \leq \xi_k. 
\end{cases}
\]

(5)

It follows by Lemmas 2.3 and 2.4 that \( Q_j(n, s) = 0 \) for \( 1 \leq j \leq 2k - 1 \) and \( \xi_{k-1} \leq s \leq \eta_k \) and for \( 1 \leq j \leq 2k \) and \( \eta_k \leq s \leq \xi_k, \) So we assume \( j \geq 2k \) when \( \xi_{k-1} \leq s \leq \eta_k \) and \( j \geq 2k + 1 \) when \( \eta_k \leq s \leq \xi_k. \)

The next theorem shows the important role these functions have to play in our investigations.

Theorem 3.1

The bound \( L_m(n, s) \) can be improved by a polynomial from \( A_{n,s} \) of degree at least \( m + 1 \) if and only if \( Q_j(n, s) < 0 \) for some \( j \geq m + 1. \) Moreover, if \( Q_j(n, s) < 0 \) for some \( j \geq m + 1, \) then \( L_m(n, s) \) can be improved by a polynomial from \( A_{n,s} \) of degree \( j. \)

Proof. We give a proof for \( m = 2k - 1. \) Let us have \( Q_j(n, s) \geq 0 \) for all \( j \geq 2k. \) For a polynomial \( f(t) \in A_{n,s} \) with \( \deg(f) = r \geq 2k \) we write

\[
f(t) = g(t) + \sum_{i=2k}^{r} f_i P_i^{(n)}(t),
\]

(6)

where \( \deg(g) \leq 2k - 1. \) Then by (1) for \( g(t), \) (5) and (6) we have

\[
f_0 = g_0 = \sum_{i=0}^{k} \rho_i g(\alpha_i) = \sum_{i=0}^{k} \rho_i [f(\alpha_i) - \sum_{j=2k}^{r} f_j P_j^{(n)}(\alpha_i)]
\]

\[
= \sum_{i=0}^{k} \rho_i f(\alpha_i) - \sum_{j=2k}^{r} f_j Q_j(n, s) \leq \rho_k f(1).
\]

(7)

(8)

(for the last inequality we use \( f(t) \in A_{n,s} \) and \( Q_j(n, s) \geq 0) \). Therefore \( f(1)/f_0 \geq 1/\rho_k = L_{2k-1}(n, s), \) i.e. \( f(t) \) does not improve the Levenshtein bound.

Conversely, let us have \( Q_j(n, s) < 0 \) for some \( j \geq 2k. \) We consider polynomials

\[
f(t) = g(t) + P_j^{(n)}(t) = h_1(t)h_2(t) = \sum_{i=0}^{j} f_i P_i^{(n)}(t),
\]

where \( \deg(g) \leq 2k - 1, \) \( h_1(t) = f_2k-1(t) = \sum_{i=0}^{2k-1} f_i' P_i^{(n)}(t) \in A_{n,s} \). We have \( f_i' > 0 \) for \( 0 \leq i \leq 2k - 1 \) \[22, 23] \). Let \( h_2(t) = a_0 t^{j-2k+1} + a_1 t^{j-2k} + \cdots + a_{j-2k+1}. \) We have to choose \( h_2(t) \) in such a way that \( f(t) \in A_{n,s} \) (obviously, \( f(1)/f_0 < L_{2k-1}(n, s) \) as in (7)–(8)).

We uniquely determine the coefficients \( a_0, a_1, \ldots, a_{j-2k} \) by the triangular system \( f_{2k} = f_{2k+1} = \cdots = f_{j-1} = 0, f_j = 1. \) So we find the polynomial \( h_3(t) = a_0 t^{j-2k+1} + a_1 t^{j-2k} + \cdots + a_{j-2k} t = h_2(t) - a_{j-2k+1}. \) It remains to choose \( a_{j-2k+1} \) such that \( f(t) \in A_{n,s}. \)

The polynomial \( g(t) = P_j^{(n)}(t) - h_1(t)h_3(t) = a_{j-2k+1} h_1(t) - g(t) = \sum_{i=0}^{2k-1} f_i' P_i^{(n)}(t) \) has degree at most \( 2k - 1. \) Since \( f(t) = P_j^{(n)}(t) + a_{j-2k+1} h_2(t) - g(t), \) we obtain \( f_i = a_{j-2k+1} f_i' - f_i'' \) for \( i = 0, 1, \ldots, 2k - 1. \)

So we must have \( a_{j-2k+1} > f_i'/f_i'' \) for \( i = 0, 1, 2, \ldots, 2k - 1. \) Since \( h_1(t) \leq 0 \) for \( t \in [-1, 1] \) we need
\[ a_{j-2k+1} \geq \varepsilon = -\min\{b_3(t) : t \in [-1, s]\} \] to obtain \( h_2(t) = h_3(t) + a_{j-2k+1} \geq 0 \) for \( t \in [-1, s] \). Thus we must take
\[ a_{j-2k+1} > \max\{\varepsilon, f'_0, f'_1, \ldots, f'_{2k-1}\} \]
to obtain \( f(t) \in A_{n,s} \). This completes the proof.

**Corollary 3.2** The Levenshtein polynomial \( f_m^{(k)}(t) \) is \( A_{n,s} \)-global extremal iff \( Q_j(n, s) \geq 0 \) for all \( j \geq m + 1 \).

Using a similar argument, if \( Q_j(n, s) > 0 \), then one can find "good" polynomials \( f(t) = g(t) - P_j^{(n)}(t) = h_1(t)h_2(t) \notin A_{n,s} \) such that \( f(1)/f_0 < L_{2k-1}(n, s) (L_{2k}(n, s) \text{ resp.}) \) Such polynomials are used in [6, Theorems 3.1,3.2] to prove that \( f_j = 0 \) for \( A_{n,s} \)-extremal polynomials. Indeed, better results are obtained by polynomials \( f(t) = g(t) - f_j \cdot P_j^{(n)}(t) + P_j^{(n)}(t) = h_1(t)h_2(t) \notin A_{n,s} \), where \( f_j > 0, Q_j(n, s) > 0, Q_{j_2}(n, s) < 0, \) and \( m < j_1 < j_2 \).

**IV. Conditions for improving the Levenshtein bounds**

In this section we consider the possibilities for improving the Levenshtein bounds. By the next theorem we give a formula for \( Q_j(n, s) \) in terms of the power sums \( S_i \), and the coefficients of the Gegenbauer polynomials.

**Theorem 4.1** For \( m \geq k \) we have
\[ Q_{2m}(n, s) = \sum_{i=0}^{k} \rho_i P_{2m}(\alpha_i) = \sum_{l=k}^{m} \left[ S_{2l} - \frac{(2l-1)!}{n(n+2)\ldots(n+2l-2)} \right] a_{2m,2l}^{(n)} \]
\[ Q_{2m+1}(n, s) = \sum_{i=0}^{k} \rho_i P_{2m+1}(\alpha_i) = \sum_{l=k}^{m} S_{2l+1} a_{2m+1,2l+1}^{(n)} \]

**Proof.** Use (3) and Lemma 2.4.

We omit the technical (and long) proof of the following lemma.

**Lemma 4.2** a) If \( \xi_{k-1} < s < \eta_k \), then \( Q_j(n, s) > 0 \) for \( j = 2k \) and \( j = 2k + 1 \) (i.e. the bound \( L_{2k-1}(n, s) \) cannot be improved by polynomials of degree at most \( 2k + 1 \)).

b) If \( \eta_k < s < \xi_k \), then \( Q_{2k+1}(n, s) > 0 \) (i.e. the bound \( L_{2k}(n, s) \) cannot be improved by polynomials of degree at most \( 2k + 1 \)).

In general, the analytical computation of the functions \( Q_j(n, s) \) seems to be very difficult. In Section V we shall give an algorithm for computer calculations of \( Q_j(n, s) \) for given \( n \) and \( s \). The next theorem gives formulae for \( Q_{2k+3}(n, s) \) which turn out to be sufficient for our purposes in this section.

**Theorem 4.3** a) \( Q_{2k+3}(n, s) = S_{2k+1} \left[ a_{2k+3,2k+3}^{(n)}(\alpha_0^2 + \alpha_1^2 + \cdots + \alpha_k^2) + a_{2k,3,2k+1}^{(n)} \right] \) for \( \xi_{k-1} \leq s \leq \eta_k \).

b) \( Q_{2k+3}(n, s) = S_{2k+1} \left[ a_{2k+3,2k+3}^{(n)}(1 + \beta_1^2 + \cdots + \beta_k^2) + a_{2k,3,2k+1}^{(n)} \right] \) for \( \eta_k < s \leq \xi_k \).

**Proof.** a) We consider two linear systems with the equations \( S_{2k+1} = \sum_{i=0}^{k} \rho_i \alpha_i^{2k+1} \) and \( S_{2k+3} = \sum_{i=0}^{k} \rho_i \alpha_i^{2k+3} \) as \((k+1)\)-th equations together with the \( k \) "odd" equations (these with zeroth right-hand side) from (3). Resolving these two systems with respect to \( \rho_k \) and equating the results we obtain \( S_{2k+3} = (\alpha_0^2 + \alpha_1^2 + \cdots + \alpha_k^2) S_{2k+1} \). Now by (10) for \( m = k + 1 \) we have the desired formula. As a matter of fact, \( S_{2k+1} > 0 \) and therefore \( Q_{2k+1}(n, s) > 0 \) by (10) for \( m = k \).

b) Analogously.

We have \( S_{2k+1} > 0 \) by Lemma 4.2. Then Theorem 4.3, \( \alpha_k = 1, \) and \( a_{2k+3,2k+1}^{(n)}/a_{2k+3,2k+3}^{(n)} = -(2k^2 + 5k + 3)/(n + 4k + 2) \) imply the following:
Corollary 4.4 a) If $\xi_{k-1} < s < \eta_k$, then $Q_{2k+3}(n, s) < 0$ if and only if
\[
\sum_{i=0}^{k-1} \alpha_i^2 - \frac{2k^2 + k + 1 - n}{n + 4k + 2} < 0.
\]

b) If $\eta_k < s < \xi_k$, then $Q_{2k+3}(n, s) < 0$ if and only if
\[
\sum_{i=1}^{k} \beta_i^2 - \frac{2k^2 + k + 1 - n}{n + 4k + 2} < 0.
\]

Corollary 4.5 a) $(k = 2)$ $Q_7(n, s) < 0$ for $\xi_1 < s < \eta_2$ if and only if
\[
\frac{(1 + s)^2}{(1 + ns)^2} + s^2 < \frac{11 - n}{n + 10}
\]

b) $(k = 3)$ $Q_9(n, s) < 0$ for $\xi_2 < s < \eta_3$ if and only if
\[
\frac{(2s(1 + s)^2}{(n + 2)s^2 + 2s - 1} - \frac{2(3 - (n + 2)s^2)}{(n + 2)(n + 2)s^2 + 2s - 1} + s^2 < \frac{22 - n}{n + 14}
\]

Proof. a) Holds by $\alpha_0 = -(1 + s)/(1 + ns)$ and Theorem 4.3 a).

b) Here $\alpha_0$ and $\alpha_1$ are the roots of $(n + 2)(n + 2)s^2 + 2s - 1) = 2s(s + 1)(n + 2)t + 3 - (n + 2)s^2 = 0$. We now consider the possibilities for improving the bounds $L_{2k}(n, s)$ and $L_{2k-1}(n, s)$ by polynomials of degree $2k + 3$. To use Corollary 4.4 b) we need formulae for $(\sum_i^{k} \beta_i)$ and $\sum_{1 \leq i < j \leq k} \beta_i \beta_j$.

Lemma 4.6 For every $s \in [\eta_k, \xi_k]$, $k \geq 2$, the numbers $\beta_1, \beta_2, \ldots, \beta_k$ satisfy the equalities
\[
\sum_{i=1}^{k} \beta_i = \frac{(n + k - 1)P_k^{1,1}_k(s)}{(n + 2k - 2)P_k^{1,1}_k(s)}.
\]

(11)

\[
\sum_{1 \leq i < j \leq k} \beta_i \beta_j = -\frac{k(k - 1)}{2(n + 2k - 2)}.
\]

(12)

Proof. This is a consequence of the fact that the numbers $\beta_1, \beta_2, \ldots, \beta_k$ are all roots of the equation $(t - s)K^{1,1}_{k-1}(t) = P_k^{(n+2)}(t)P_k^{(n+2)}(s) - P_k^{(n+2)}(s)P_k^{(n+2)}(t) = 0$. We use the Viète formulæ.

Lemma 4.7 For $k \geq 1$ we have
\[
P_k^{(n+2)}(\eta_k) = \frac{k}{n + k - 1}P_k^{(n+2)}(\eta_k).
\]

Proof. We use $P_k^{(n)}(\eta_k) = P_k^{(n)}(\eta_k)$ [22, 23], the recurrence relation for the Gegenbauer polynomials and Lemma 2.5.

By (11) and (12) we obtain in Corollary 4.4 b)
\[
H(n, s) = \sum_{i=1}^{k} \beta_i^2 - \frac{2k^2 + k + 1 - n}{n + 4k + 2} = \left[ \frac{(n + k - 1)P_k^{1,1}_k(s)}{(n + 2k - 2)P_k^{1,1}_k(s)} \right]^2 + \frac{k(k - 1)}{n + 2k - 2} - \frac{2k^2 + k + 1 - n}{n + 4k + 2}.
\]
The function $H(n, s)$ is decreasing in $s$ in the interval $[\eta_k, \xi_k]$ because $P_k^{1,1}(s)/P_k^{1,1}(s)$ is increasing and negative in this interval [23, Corollary 2.1]. Thus, we need to consider the functions $\psi_1(n) = H(n, \eta_k)$ and $\psi_2(n) = H(n, \xi_k)$ (because $\psi_1(n) > H(n, s) > \psi_2(n)$ for all $s \in (\eta_k, \xi_k)$).

**Lemma 4.8** For $k \geq 2$ we have

\[
\psi_1(n) = \frac{(n-2)(n+2k-1)(n-k^2-2)}{(n+4k+2)(n+2k-2)^2},
\]

\[
\psi_2(n) = \frac{n^2-(k^2+3)n+2-2k}{(n+4k+2)(n+2k-2)}.
\]

**Proof.** Use Lemma 4.7 for (13) and $P_k^{1,1}(\xi_k) = 0$ for (14).

We are now in a position to state the main theorem concerning $Q_{2k+3}(n, s)$ for the even bounds. The proof follows by (13), (14), and Theorem 4.3 b).

**Theorem 4.9** The function $Q_{2k+3}(n, s)$ ($s \in [\eta_k, \xi_k]$) has the following properties:

1) $Q_{2k+3}(n, \xi_k) = 0$ and $Q_{2k+3}(n, s) \leq 0$ for $s \in [\eta_k, \xi_k]$ and $3 \leq n \leq k^2+1$;

2) $Q_{2k+3}(k^2+2, \eta_k) = 0$ and $Q_{2k+3}(k^2+2, s) < 0$ for $s \in (\eta_k, \xi_k)$;

3) There exists $s_0 = s_0(k) \in (\eta_k, \xi_k)$ such that $Q_{2k+3}(k^2+3, s) > 0$ for $s \in [\eta_k, s_0)$, $Q_{2k+3}(k^2+3, s_0) = 0$, and $Q_{2k+3}(k^2+3, s) < 0$ for $s \in (s_0, \xi_k)$;

4) $Q_{2k+3}(n, s) > 0$ for $s \in [\eta_k, \xi_k)$ and $n \geq k^2+4$.

A similar argument can be used for a close examination of the possibilities for improving $L_{2k-1}(n, s)$ by polynomials of degree $2k+3$. We omit the details and formulate the final result. For $n \geq 5$ we let $k(n) = (2n - 4 + \sqrt{2n^4 - 9n^2 + 4n + 16})/(n - 4)$. The first few values of $k(n)$ are $k(5) = 14$, $k(6) = 11$, $k(7) = 10$, $k(8) = 9$.

**Theorem 4.10** The function $Q_{2k+3}(n, s)$ is negative in the whole interval $[\xi_{k-1}, \eta_k]$ for $n \geq 5$ and $k \geq k(n)$.

Combining Theorems 4.9 and 4.10 we have the following

**Theorem 4.11** If $n \geq 5$ and $m \geq 2k(n) - 1$, then the Levenshtein bound $L_m(n, s)$ can be improved in the whole interval of its validity.

V. A method for obtaining new bounds on $D(n, M)$

We begin this section with a general algorithm for finding new upper bounds on $D(n, M)$.

**Algorithm**

1. Given $n$ and $M$, compute $s_L$ by the equation $M = L_m(n, s_L)$.

2. Compute $Q_j(n, s_L)$ for $j = m+3, m+4$.

3. If $Q_{m+3}(n, s_L) < 0$ or $Q_{m+4}(n, s_L) < 0$, then find (by the method from [5, 6]) the new bound $A(n, s) \leq K(n, s) \leq L_m(n, s_L) = M$.

4. Increase $s := s_L + h$ until $K(n, s) \leq M$.

5. Compute the new bound $D(n, M) \leq d = 2(1 - s)$.

The choice of the parameter $m$ in Step 1 can be easily made by using the very impressive form of the Levenshtein bounds $L_{2k-1}(n, \eta_k) = L_{2k}(n, \eta_k) = \binom{n+k-1}{n-1} + \binom{n+k-2}{n-2}$, and $L_{2k}(n, \xi_k) = L_{2k+1}(n, \xi_k) = 2\binom{n+k}{n-1}$. Thus, we need only to compare the integer number $M$ with these (integer) bounds. We omit the details.

The method for improving (if possible) the Levenshtein bounds $L_m(n, s)$ by polynomials of degrees $m+3$ and $m+4$ has been described in [5, 6]. Thus, we need only to consider the key Step 2 in detail. In fact,
we propose a general procedure for computing \( Q_j(n, s) \) for \( j \geq m + 1 \). In the algorithm below we use results from [22, 23] and from the previous section. The parameters \( n \) and \( s \) are fixed.

**Algorithm for computing the \( Q_j(n, s) \)’s**

1. Calculate the necessary coefficients of the Gegenbauer polynomials by the defining recurrent relation.
2. Find the “adjacent” [22, 23] polynomials \( P_{k}^{1,0}(t) = \sum_{i=0}^{k} r_i t^i P_{i}^{(n)}(t) \) and \( P_{k}^{1,1}(t) = \sum_{i=0}^{k-1} r_i t^i P_{i}^{(n+2)}(t) \), where [23, Eq. 1.12] \( r_i = \frac{n+2i-2}{i} \binom{n+i-3}{i} \).
3. Find the polynomials \( h_1(t) = P_{k}^{1,0}(t)P_{k-1}^{1,0}(s) - P_{k}^{1,0}(s)P_{k-1}^{0,0}(t) \) for the odd bounds \( L_{2k-1}(n, s) \), and \( h_2(t) = (t + 1)[P_{k}^{1,1}(t)P_{k-1}^{1,1}(s) - P_{k}^{1,1}(s)P_{k-1}^{1,1}(t)] \) for the even bounds \( L_{2k}(n, s) \). We denote \( h_i(t) = \sum_{i=0}^{k} a_i^{(i)} t^i \) for \( i = 1, 2 \).
4. Calculate (see Lemma 2.3)
   \[
   b_i = \begin{cases} 
   1 & \text{for } i = 0, \\
   0 & \text{for } i \geq 1 \text{ odd}, \\
   \frac{(2p-1)!!}{n(n+2)...(n+2p-2)} & \text{for } i = 2p.
   \end{cases}
   \]
5. Calculate
   \[
   \rho_k = \frac{\sum_{i=0}^{k} a_i^{(1)} b_i}{h_1(1)} = \frac{1}{L_{2k-1}(n, s)},
   \]
   \[
   \gamma_{k+1} = \frac{\sum_{i=0}^{k} a_i^{(2)} b_i}{h_2(1)} = \frac{1}{L_{2k}(n, s)}.
   \]
6. Calculate \( \sigma_i^{(1)} = b_l - \rho_k, \ l = 0, 1, \ldots, 2k - 1 \) for \( L_{2k-1}(n, s) \), and \( \sigma_i^{(2)} = b_l - \gamma_{k+1}, \ l = 0, 1, \ldots, 2k \) for \( L_{2k}(n, s) \).
7. Calculate
   \[
   \sigma_i^{(1)} = -\frac{\sum_{p=0}^{k-1} n_p}{} a_k \sigma_{i-k+l}^{(1)}, \ l \geq 2k \quad \text{for } L_{2k-1}(n, s);
   \]
   \[
   \sigma_i^{(2)} = -\frac{\sum_{p=0}^{k} n_p}{} a_k \sigma_{i-k+l}^{(2)}, \ l \geq 2k + 1 \quad \text{for } L_{2k}(n, s).
   \]
8. Calculate \( S_l = \sigma_l^{(1)} + \rho_k, \ l \geq 2k \) for \( L_{2k-1}(n, s) \), and \( S_l = \sigma_l^{(2)} + \gamma_{k+1}, \ l \geq 2k + 1 \) for \( L_{2k}(n, s) \).
9. Compute \( Q_j(n, s) \) by the formulae (9) and (10) from Theorem 4.1.

In many cases we obtain \( Q_j(n, s) < 0 \) not only for \( j = m + 3 \) or \( m + 4 \). However, the computer investigations suggest the following

**Conjecture 5.1** If \( Q_j(n, s) \geq 0 \) for \( j = m + 3 \) and \( j = m + 4 \), then \( Q_j(n, s) \geq 0 \) for all \( j \geq m + 1 \).

For \( n \) and \( s \) fixed and when \( j \) tends to infinity, the sum in the defining formula (5) tends to \( 1/L_m(n, s) > 0 \).

Thus, we have the following:

**Theorem 5.2** For \( n, s \) fixed there exist constant \( j_0 = j_0(n, s) \) such that \( Q_j(n, s) > 0 \) for all \( j \geq j_0 \).

**VI. Some examples with new bounds**

Examples with new bounds on \( D(n, M) \) were presented in [9].

The problem for finding \( D(3, M) \) belongs mainly to the classical geometry. The optimal configurations of \( M \) points on \( S^2 \) are known only for \( M \leq 12 \) and \( M = 24 \). (For \( M = 3, 4, 6, 12 \) see Fejes Tóth [19], for \( M = 5, 7, 8, 9 \) – Schütte-van der Waerden [27], for \( M = 10, 11 – 12 \) Danzer [14], for \( M = 24 – 12 \) Robinson [26].) The classical Fejes Tóth bound gives

\[
D \leq d_{FT} = 4 - \frac{1}{\sin^2 \frac{\pi M}{6(M-2)}}.
\]
Example 6.1 In Table I we show improvements on $d_{FT}$ and the Levenshtein bound which our method gives for $13 \leq M \leq 24$. Interestingly, in a few cases the Fejes Tóth bound lies between the two linear programming bounds, which are extremal in the sense of [30, 23, 6]. We improve bounds $L_5(3, s_L)$, $L_6(3, s_L)$, and $L_7(3, s_L)$ for the corresponding $s_L$.

Example 6.2 To give new bounds in higher dimensions we used the selected cases in Tables VI and VII by Ericson-Zinoviev [17] and the tables from [16]. Nine examples are shown in Table II. In fact, we have improved 23 out of 45 entries with upper bounds in Table VI and 66 out of 80 entries with upper bounds in Table VII in [17].

The next two examples follow by a close examination of the inequalities in Corollary 4.5 and computations of $Q_6(n, s)$ and $Q_8(n, s)$.

Example 6.3 It is not difficult to prove that the inequality in Corollary 4.5 a) is possible in dimensions $n = 3, 4, 5$ only. In these three cases, the equation

$$h(s) = \frac{(1 + s)^2}{(1 + ns)^2} + s^2 - \frac{11 - n}{n + 10} = 0$$

has a unique root $s_0(n) \in [0, 1/(1 + \sqrt{n + 3})] = [\xi_1, \eta_2]$. We have $h(s) < 0$ for $s_0(n) < s \leq \eta_2$. Thus, the bound $L_3(n, s)$ can be improved by a polynomial of degree 7 for $n = 3, 4, 5$ and $s_0(n) < s \leq \eta_2$. The values of $s_0(n)$ and $\eta_2$ are given in Table III. Notice that $A(5, 1/5) = L_3(5, 1/5) = 16$. The computation of $Q_6(n, s)$ gives that $L_3(n, s)$ can be improved by a polynomial of degree 6 in dimensions 3 and 4 only. The improvements are possible in intervals $s_1(n) < s < s_2(n)$, $n = 3, 4$. The values of $s_1(n)$ and $s_2(n)$ are shown in Table III.

Example 6.4 The examination of the inequality in Corollary 4.5 b) shows that the bound $L_5(n, s)$ can be improved by a polynomial of degree 9 when $n = 3, 4, \ldots, 10$ and $s_0(n) < s \leq \eta_3$. Further, $Q_6(n, s) < 0$ in dimensions $n = 3, 4, \ldots, 8$ for $s_1(n) < s < s_2(n)$. In particular, $L_5(n, s)$ can be improved in the whole interval $(\xi_2, \eta_3]$ for $n = 3$ (the icosahedron shows that $A(3, \xi_2 = 1/\sqrt{5}) = 12$). These results are summarized in Table IV. We omit simultaneously $s_2(n)$ and $s_0(n)$ when $s_0(n) < s_2(n)$, i.e. when $L_5(n, s)$ can be improved in the interval $(s_1(n), \eta_3]$

Acknowledgment. The authors thank Stefan Dodunekov for helpful discussions.

References


