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Price of SDP relaxations for spherical codes *

Alexey Glazyrin[†]and Oleg R. Musin[‡]

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1 Introduction

Let $\mathcal{C} = \{x_1, \ldots, x_M\} \subset \mathbb{S}^{d-1}$ be a subset of points on the sphere in $\mathbb{R}^d$. We will call $\mathcal{C}$ a spherical φ-code if the angular distance between any two points of $\mathcal{C}$ is not greater than φ. By $A(d, \varphi)$ we denote the maximum cardinality of a φ-code in $\mathbb{S}^{d-1}$. For $\varphi = \pi/3$ the problem of finding $A(d, \pi/3)$ is the kissing number problem. For $d = 3$, the problem of finding d_n, the maximal φ such that $A(3, \varphi) \geq n$ for given n, is the Tammes problem [29] (see [9, Section 1.6: Problem 6]).

The linear programming and semi-definite programming approach is one of the most important methods of analyzing codes. The method was discovered by Delsarte [12, 13] for the Hamming space and then extended to the spherical case [14] and generalized by Kabatyansky and Levenshtein [16]. The key ingredient for Delsarte's method in the spherical case is Schoenberg's theorem [27] (later generalized by Bochner [8]). Let $G_k^{(d)}(t)$ be the classical Gegenbauer polynomial of degree k. Gegenbauer (ultraspherical) polynomials $G_k^{(d)}(t)$ are a special case of Jacobi polynomials $P_k^{(\alpha,\beta)}(t)$ with $\alpha = \beta = \frac{d-3}{2}$ and normalization $G_k^{(d)}(1) = 1$. They may be defined through a recurrence relation:

$$G_0^{(d)}(t) = 1, G_1^{(d)}(t) = t;$$

$$G_k^{(d)}(t) = \frac{2k+d-4}{k+n-3} G_{k-1}^{(d)}(t) - \frac{k-1}{k+d-3} G_{k-2}^{(d)}(t).$$

Consider the $M \times M$ matrix $(G_k^{(d)}(t_{ij}))_{1 \leq i,j \leq M}$ where the matrix elements are the values of $G_k^{(d)}$ evaluated at $t_{ij} = (x_i, x_j), 1 \leq i, j \leq M$. Then the Schoenberg theorem states that

$$(G_k^{(n)}(t_{ij})) \succeq 0 \quad (k = 1, 2, \ldots), \tag{1}$$

i.e. this matrix is positive semidefinite (p.d.) for all $k = 1, 2, \ldots$. Moreover, for any polynomial F of degree k the matrix $F(t_{ij})$ is positive definite for any spherical code $\mathcal{C}$ only if F is a linear combination of the first $k+1$ Gegenbauer polynomials with non-negative coefficients. In particular, $G_1^{(n)}(t) = t$, so Schoenberg's theorem provides a far-reaching extension of the condition on the Gram matrix of $\mathcal{C}$.

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[†]University of Texas at Brownsville.

[‡]University of Texas at Brownsville; Institute for Problems of Information Transmission, Moscow.

The Desarte method uses the relaxed Schoenberg conditions:

$$\sum_{i,j} G_k^{(n)}(t_{ij}) \ge 0 \quad (k = 1, 2, \dots). \tag{2}$$

By means of this inequality it is not difficult to prove the following theorem:

Theorem 1.1 (Delsarte-Goethals-Seidel[14], Kabatyansky-Levenshtein[16]) *For a spherical code $C = \{x_1, \dots, x_M\} \subset \mathbb{S}^{d-1}$, let $f(t)$ be a real polynomial such that $f((x_i, x_j)) \le 0$ for all $i \ne j$ and $f(t)$ has non-negative coefficients in the Gegenbauer basis with a constant coefficient $f_0 > 0$. Then $|C| \le f(1)/f_0$.*

This theorem allows one to find kissing numbers in dimensions 8 and 24 [18, 26], the best asymptotic bounds for kissing numbers [16] (slightly improved in [11]) and the general bound on $A(d, \varphi)$ [18, 19]. Certain strengthening of these linear conditions gives new proofs for the kissing bumber in $\mathbb{R}^3$ [2, 22], solution of the problem in $\mathbb{R}^4$ [25] and the best current bounds for some sphere packing densities [10]. The Delsarte method also accounts for the best known asymptotic bounds in some other spaces [21, 3, 7], thereby representing one of the key tools in extremal problems of distance geometry. The Delsarte method has been recently extended to semidefinite programming bounds that rely on a more detailed version of the positivity constraints and on the corresponding p.d. functions on the space [28, 23, 24, 5, 6, 4].

Multivariate positive definite functions: We consider the multivariate generalization of Schoenberg conditions. Let q be a point on $\mathbb{S}^{d-1}$. A function $F(x, y)$ is p.d. on $\mathbb{S}^{d-1}$ if for any finite configuration of points $C = \{x_1, x_2, \dots, x_M\} \subset \mathbb{S}^{d-1}$ the following matrix

$$(F(t_{ij}, u_i, u_j))_{1 \le i,j \le M}, \quad t_{ij} = (x_i, x_j), u_i = (x_i, q),$$

is positive definite. An explicit characterization of such functions was found in [5], relying on the Bochner theorem; these functions may be written as nonnegative linear combinations of the following trivariate polynomials:

$$G_k^{(d,1)}(t, u, v) = ((1 - u^2)(1 - v^2))^{k/2} G_k^{(d)}\Big(\frac{t - uv}{\sqrt{(1 - u^2)(1 - v^2)}}\Big).$$

The polynomials $G_k^{(d,1)}(t, u, v)$ are proportional to the elements of the zonal matrices that arise under the action of the group $H = O(\mathbb{R}^{d-1})$ that stabilizes a point on $\mathbb{S}^{d-1}$.

Extending this construction to the action of the stabilizer of $m \ge 1$ points, paper [23] constructed a Fourier basis for the space of p.d. functions of $2m + 1$ variables. The corresponding *multivariate Gegenbauer polynomials* have the form

$$G_k^{(d,m)}(t, \boldsymbol{u}, \boldsymbol{v}) = ((1 - |\boldsymbol{u}|^2)(1 - |\boldsymbol{v}|^2))^{k/2} G_k^{(d-m)}\Big(\frac{t - (\boldsymbol{u}, \boldsymbol{v})}{\sqrt{(1 - |\boldsymbol{u}|^2)(1 - |\boldsymbol{v}|^2)}}\Big), \tag{3}$$

where $t, u_1 \dots, u_m, v_1, \dots, v_m$ are real variables. These functions provide a suitable generalization of the Schoenberg theorem to the case of restricted group actions on $\mathbb{S}^{d-1}$.

The meaning of the functions $G_k^{(d,1)}$ is related to Gegenbauer's proof of the "addition formula" for the polynomials $G_k^{(d)}$ [1, pp. 459–462]. Namely, given one reference point q, we project the points x, y on the hyperplane orthogonal to the direction q, scale the picture to put them on the sphere of dimension $d - 1$, and write out Delsarte's conditions for the points on that sphere. A similar procedure is performed for an arbitrary m to yield the functions $G_k^{(d,m)}$. This construction method of the polynomials, put forward in [23], offers a visual perspective of positivity constraints involved in the semidefinite programming (SDP) bounds on spherical codes.

2 SDP relaxations for spherical codes

Any spherical code $x_1, x_2, \ldots, x_M$ in $\mathbb{S}^{d-1}$ can be represented by a Gram matrix T that satisfies the following conditions:

$$T \succeq 0; \quad \mathrm{rank}(T) \leq d; \quad t_{ii} = 1 \ (1 \leq i \leq M), \ \ -1 \leq t_{ij} \leq 1 \ (1 \leq i \neq j \leq M). \tag{4}$$

The rank condition in (4) is difficult to use for computational purposes since it is not linear or semi-definite. Hence often it is replaced by the semi-definite Schoenberg conditions (1) or linear Delsarte conditions (2).

These relaxations enable one to perform explicit calculations of the bounds on codes (after an appropriate symmetrization [4]). In the simplest form (2) the positivity conditions even enable one to compute universal bounds on codes and designs [19, 20]. At the same time, the question of the gap between the exact description of codes (4) and the relaxed conditions (1)-(2) is altogether unexplored.

The convex set of symmetric p.d. matrices with unit main diagonal (*the elliptope*) has been extensively studied in combinatorics and distance geometry [17, 15]. Spherical configurations form a subset of the elliptope isolated by the rank condition. We study properties of the subsets of the elliptope obtained through a sequence of relaxations from the rank condition in (4) to the positivity constraints and Delsarte conditions, and the impact of the relaxations on the bounds on codes.

It appears that for $d = 2$, the Schoenberg conditions (1) are fulfilled if and only if the underlying configuration of points lies on the circle $\mathbb{S}^1$ while the Delsarte conditions (2) miss some non-planar configurations. For $d \geq 3$ even (1) sometimes fails to track the dimension.

For each dimension d it is sufficient to consider only configurations of $d+1$ points. If any subset of $d+1$ points of a spherical code is d-dimensional, then the whole code is d-dimensional.

For $d = 2$ the Gram matrix has the form

$$T = \begin{pmatrix} 1 & \cos\alpha & \cos\beta \\ \cos\alpha & 1 & \cos\gamma \\ \cos\beta & \cos\gamma & 1 \end{pmatrix}. \tag{5}$$

The Gegenbauer polynomials for $d = 2$ are the Chebyshev polynomials of the first kind, $G_k^{(2)}(t) = \cos k(\arccos t)$, and therefore (2) is equivalent to

$$\cos k\alpha + \cos k\beta + \cos k\gamma \geq -\frac{3}{2} \tag{6}$$

It is easy to see that (6) does not guarantee that $\mathrm{rank}(T) = 2$. For instance the values $\alpha = \beta = \frac{2}{3}\pi, \gamma = \frac{1}{3}\pi$ satisfy this inequality for all positive integer k, while $\mathrm{rank}(T) = 3$. At the same time, using (1) points out that this is not a valid configuration on $\mathbb{S}^{(1)}$: for instance, $\det(G_3^{(2)}(T)) = -4 < 0$, so these conditions do not hold for $k = 3$. The fact that such k exists is not accidental: we proved that if $\mathrm{rank}(T) = 3$ then there always is a value of k such that $G_k^{(2)}(T) \not\succeq 0$.

Theorem 2.1 *For $\alpha, \beta, \gamma \in [0, \pi]$, the matrix*

$$\begin{pmatrix} 1 & \cos k\alpha & \cos k\beta \\ \cos k\alpha & 1 & \cos k\gamma \\ \cos k\beta & \cos k\gamma & 1 \end{pmatrix}.$$

is positive semidefinite for all $k = 0, 1, \ldots,$ if and only if there are three points x_1, x_2, x_3 on a unit circle such that $x_1 \cdot x_2 = \cos\gamma, x_2 \cdot x_3 = \cos\alpha,$ $x_3 \cdot x_1 = \cos\beta$.

Things become more involved for larger dimensions. As an example, let $d = 3$ and consider configurations of 4 points on the 3-sphere such that all the inner products t_{ij} except two of them are 0, and $t_{12} = u, t_{34} = v$. This gives a Gram matrix of the form

$$T = \begin{pmatrix} 1 & u & 0 & 0 \\ u & 1 & 0 & 0 \\ 0 & 0 & 1 & v \\ 0 & 0 & v & 1 \end{pmatrix}.$$

To see how much we lose by replacing the rank condition with the positivity constraints, we evaluate the matrices $G_k^{(3)}(T), k = 1, 2, \dots$, (the $G_k^{(3)}$ are the Legendre polynomials) and check whether the resulting matrices are p.d. Since $\det T = (1-u^2)(1-v^2)$, the corresponding section of the elliptope is a square $(0 \le u \le 1, 0 \le v \le 1)$. It is not hard to show that for $u = v = 0.9$ all Gegenbauer matrices are still positive definite but the dimension of this configuration (rank of the matrix) is not 3.

3 Discussion

1. Let $Q = \{q_1, \dots, q_m\} \subset \mathbb{S}^{d-1}$ to be the set of reference points on the sphere. Paper [23] proves that any spherical set of points $\mathcal{C} = \{x_1, \dots, x_M\}$ satisfies

$$(G_k^{(d,m)}(t_{ij}, \boldsymbol{u}_i, \boldsymbol{u}_j))_{1\le i,j\le M} \succeq 0 \quad (k = 1, 2, \dots), \tag{7}$$

where the functions $G_k^{(d,m)}$ are defined above (3), and $t_{ij} = (x_i, x_j), \boldsymbol{u}_i = (u_{i,1}, \dots, u_{i,m}), \boldsymbol{u}_j = (u_{j,1}, \dots, u_{j,m})$, $u_{p.l} = (x_p, q_l), p = 1, 2$; $l = 1, \dots, m$. In particular, with $m = 1$ we recover the positivity conditions of [5], while $Q = \emptyset$ corresponds to the classical Schoenberg's theorem.

As a direct corollary of the statement for two-dimensional codes that we proved, for $m = d-2$, inequalities (7) are able to substitute the rank condition. It would be interesting to find the minimal m satisfying this condition.

For $m = 1$, the main problem is to find out when inequalities (7) fail to confirm the rank, and therefore to determine how strong is the method employed in [5].

2. It would be interesting to investigate the impact of SDP relaxations (1)-(2) for spherical codes and to estimate the maximum distance between matrices T that satisfy (1) and the rank condition in (4). Based on the outcome of this research, it is possible to estimate the accuracy of the bounds on codes derived from SDP problems.

3. Finally, it would be interesting to provide a complete description of point sets on $\mathbb{S}^1$ that are isolated by the Delsarte conditions (2). This will provide a characterization of $M \times M$ matrices $T = (t_{ij})$ for which the conditions $\{(G_k^{(d,d-2)}(t_{ij}, \boldsymbol{u}_i, \boldsymbol{u}_j))_{1\le i,j\le M} \succeq 0,\ k = 1, 2, \dots\}$ are equivalent to the rank condition in (4). Such matrices correspond to valid point configurations on the sphere $\mathbb{S}^{d-1}$.

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