

# Linear programming bounds for regular graphs

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## Abstract

Delsarte, Goethals, and Seidel (1977) used the linear programming method in order to find bounds for the size of spherical codes endowed with prescribed inner products between distinct points in the code. In this paper, we develop the linear programming method to obtain bounds for the number of vertices of connected regular graphs endowed with given distinct eigenvalues. This method is proved by some “dual” technique of the spherical case, motivated from the theory of association scheme. As an application of this bound, we prove that a connected  $k$ -regular graph satisfying  $g > 2d - 1$  has the minimum second-largest eigenvalue of all  $k$ -regular graphs of the same size, where  $d$  is the number of distinct non-trivial eigenvalues, and  $g$  is the girth. The known graphs satisfying  $g > 2d - 1$  are Moore graphs, incidence graphs of regular generalized polygons of order  $(s, s)$ , triangle-free strongly regular graphs, and the odd graph of degree 4.

**Key words:** linear programming bound, graph spectrum, expander graph, Ramanujan graph, distance-regular graph, Moore graph.

## 1 Introduction

Delsarte [19] has introduced the linear programming method to find bounds for the size of codes with prescribed distances over finite field. This is called Delsarte’s method, and he stated it for codes in certain special association schemes, so called  $Q$ -polynomial schemes, including the Johnson scheme and the Hamming scheme. Delsarte, Goethals, and Seidel [20] gave the linear programming method on the Euclidean sphere. This is naturally generalized to the compact two-point homogeneous spaces [35]. Delsarte’s method is also extended to various situations like the permutation codes [49], the Grassmannian codes [4], or the ordered codes [8]. The linear programming is very powerful to solve optimization problems, for instance maximizing the size of codes for given distances [43, 41], or maximizing the minimum distance for a fixed cardinality [37, 15]. In the present paper, we develop the linear programming method to find bounds for the order of connected regular graphs with given distinct eigenvalues. This method is not based on Delsarte’s but a kind of “dual” technique of the spherical case inspired from the theory of association schemes.

Let  $X$  be a finite set, and  $R_0, \dots, R_d$  symmetric binary relations on  $X$ . The  $i$ -th adjacency matrix  $\mathbf{A}_i$  is defined to be the matrix indexed by  $X$  whose  $(x, y)$ -entry is 1 if  $(x, y) \in R_i$ ,

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0 otherwise. A configuration  $\mathfrak{X} = (X, \{R_i\}_{i=0}^d)$  is called a *symmetric association scheme* of class  $d$  if  $\{\mathbf{A}_i\}_{i=0}^d$  satisfies the following: (1)  $\mathbf{A}_0 = \mathbf{I}$  (identity matrix), (2)  $\sum_{i=0}^d \mathbf{A}_i = \mathbf{J}$  (all-ones matrix), (3) there exist real numbers  $p_{ij}^k$  such that  $\mathbf{A}_i \mathbf{A}_j = \sum_{k=0}^d p_{ij}^k \mathbf{A}_k$  for all  $i, j \in \{0, 1, \dots, d\}$ . The vector space  $\mathfrak{A}$  spanned by  $\{\mathbf{A}_i\}_{i=0}^d$  over  $\mathbb{C}$  forms a commutative algebra, and it is called the *Bose–Mesner algebra* of  $\mathfrak{X}$ . It is well known that  $\mathfrak{A}$  is semi-simple [6, Section 2.3, II], hence it has the primitive idempotents  $\mathbf{E}_0 = (1/|X|)\mathbf{J}, \mathbf{E}_1, \dots, \mathbf{E}_d$ , which form a basis of  $\mathfrak{A}$ .

We have two remarkable classes of association schemes so called  $P$ -polynomial association schemes and  $Q$ -polynomial association schemes. An association scheme is said to be  $P$ -polynomial if for each  $i \in \{0, 1, \dots, d\}$  there exists a polynomial  $v_i$  of degree  $i$  such that  $\mathbf{A}_i = v_i(\mathbf{A}_1)$ . A  $P$ -polynomial scheme has the relations as the path distances of the graph  $(X, R_1)$ , and  $(X, R_1)$  becomes a distance-regular graph [11]. An association scheme is said to be  $Q$ -polynomial if for each  $i \in \{0, 1, \dots, d\}$  there exists a polynomial  $v_i^*$  of degree  $i$  such that  $|X|\mathbf{E}_i = v_i^*(|X|\mathbf{E}_1^\circ)$ , where  $\circ$  means the multiplication is the entry-wise product. Roughly speaking, the  $P$ -polynomial schemes and the  $Q$ -polynomial schemes correspond to discrete cases of the concepts of two-point homogeneous spaces and rank 1 symmetric spaces, respectively [6, Section 3.6, III], [16, Chapter 9].

By swapping the matrix multiplication  $\cdot$  and the entry-wise multiplication  $\circ$ , the bases  $\{\mathbf{A}_i\}_{i=0}^d$  and  $\{\mathbf{E}_i\}_{i=0}^d$  very similarly behave in the Bose–Mesner algebra. The following are basic equations for the bases [6, Section 2.2, 2.3, II]:

$$\sum_{i=0}^d \mathbf{A}_i = \mathbf{J} = |X|\mathbf{E}_0, \quad \sum_{i=0}^d \mathbf{E}_i = \mathbf{I} = \mathbf{A}_0, \quad (1)$$

$$\mathbf{A}_i \circ \mathbf{A}_j = \delta_{ij} \mathbf{A}_i, \quad \mathbf{E}_i \cdot \mathbf{E}_j = \delta_{ij} \mathbf{E}_i, \quad (2)$$

$$\mathbf{A}_i \cdot \mathbf{A}_j = \sum_{k=0}^d p_{ij}^k \mathbf{A}_k, \quad \mathbf{E}_i \circ \mathbf{E}_j = \frac{1}{|X|} \sum_{k=0}^d q_{ij}^k \mathbf{E}_k, \quad (3)$$

$$\mathbf{A}_i = \sum_{j=0}^d P_i(j) \mathbf{E}_j, \quad \mathbf{E}_i = \frac{1}{|X|} \sum_{j=0}^d Q_i(j) \mathbf{A}_j, \quad (4)$$

$$\mathbf{A}_i \cdot \mathbf{J} = k_i \mathbf{J}, \quad |X|\mathbf{E}_i \circ \mathbf{I} = m_i \mathbf{I}, \quad (5)$$

$$\mathbf{A}_i \circ \mathbf{I} = 0 \ (i \neq 0), \quad \mathbf{E}_i \cdot \mathbf{J} = 0 \ (i \neq 0), \quad (6)$$

$$\tau(\mathbf{A}_i) = |X|k_i, \quad \text{tr}(\mathbf{E}_i) = m_i, \quad (7)$$

$$\text{tr}(\mathbf{A}_i) = 0 \ (i \neq 0), \quad \tau(\mathbf{E}_i) = 0 \ (i \neq 0), \quad (8)$$

$$k_0 = 1, \quad m_0 = 1, \quad (9)$$

where  $\delta_{ij}$  denotes the Kronecker delta,  $\tau(\mathbf{M})$  denotes the summation of all entries in  $\mathbf{M}$ ,  $k_i$  is the degree of the graph  $(X, R_i)$ , and  $m_i$  is the rank of  $\mathbf{E}_i$ . Here  $p_{ij}^k$  is called the *intersection number*, and it is equal to the size of  $\{z \in X \mid (x, z) \in R_i, (z, y) \in R_j\}$  with  $(x, y) \in R_k$ . Naturally  $p_{ij}^k$  is a non-negative integer. On the other hand,  $q_{ij}^k$  is called the *Krein number*, it can be proved that it is a non-negative real number [46]. Such a kind of similar properties obtained by swapping  $\mathbf{A}_i, \mathbf{E}_i$ , multiplications, and corresponding parameters is called a *dual property*. It is obviously seen that the dual concept of  $P$ -polynomial scheme is  $Q$ -polynomial scheme. There are a number of non-trivial dual properties between  $P$ -polynomial schemes and  $Q$ -polynomial schemes [39, 6], and several conjectures are still left [39].

Table 1: Dual properties between regular graph and spherical set

regular graph	spherical set	reason
$\mathbf{A}$ : adjacency matrix	$\mathbf{E}$ : Gram matrix	bases
$k$ : degree	$m$ : dimension	(5),(7)
regular	spherical	(5)
eigenvalues	inner products	(4)
connected	constant weight	(9)
no loop	spherical 1-design	(6)
no multiple edge	spherical 2-design	(2)
$\tau$	tr	(7), (8)
Moore graph	tight spherical design	tightness
$F_i^{(k)}(x)$	$Q_i^{(m)}(x)$	
$\text{tr}(F_i^{(k)}(\mathbf{A})) \geq 0$	$\tau(Q_i^{(m)}(\mathbf{E}^\circ)) \geq 0$	[48, 20]
$\text{tr}(F_i^{(k)}(\mathbf{A})) = 0$ for $1 \leq i \leq g - 1$	$\tau(Q_i^{(m)}(\mathbf{E}^\circ)) = 0$ for $1 \leq i \leq t$	
$\Leftrightarrow$ girth $g$	$\Leftrightarrow$ spherical $t$ -design	[48, 20]

The matrix  $\mathbf{A}_i$  is regarded as a regular graph. The matrix  $\mathbf{E}_i$  is positive semidefinite with equal diagonals, and it is interpreted as a spherical set. We can observe the dual relationship of  $\mathbf{A}_i$  and  $\mathbf{E}_i$  in the Bose–Mesner algebra, and it shows how properties of graphs dually correspond to those of spherical sets. For example, (4) says that eigenvalues of graphs dually correspond to inner products in spherical sets. Table 1 shows the dual correspondence of the properties of graphs and spherical sets.

We can interpret the Euclidean sphere  $S^{m-1}$  as a continuous case of  $Q$ -polynomial scheme. The polynomial  $v_i^*$  on a  $Q$ -polynomial scheme corresponds to the Gegenbauer polynomial  $Q_i^{(m)}$  on  $S^{m-1}$  [20]. We have fundamental parameters  $s$  and  $t$  for a finite subset  $X$  in  $S^{m-1}$ . The parameter  $s$  is just the number of the Euclidean distances between distinct points in  $X$ . If  $X$  has only  $s$  distances, then we have

$$|X| \leq \binom{m+s-1}{s} + \binom{m+s-2}{s-1}. \quad (10)$$

The other parameter  $t$  is the strength in the sense of spherical design. We call  $X$  a spherical  $t$ -design if for any polynomial  $f$  in  $m$  variables of degree at most  $t$  the following equation holds:

$$\frac{1}{|S^{m-1}|} \int_{S^{m-1}} f(x) dx = \frac{1}{|X|} \sum_{x \in X} f(x),$$

where  $|S^{m-1}|$  is the volume of  $S^{m-1}$ . One of unexpected results is that if  $t \geq 2s - 2$  holds, then  $X$  has the structure of a  $Q$ -polynomial scheme with the relations of distances [20]. For a spherical  $2e$ -design  $X$  in  $S^{m-1}$ , we have an absolute bound [20]:

$$|X| \geq \binom{m+e-1}{e} + \binom{m+e-2}{e-1}.$$

A spherical design is said to be *tight* if it attains this equality. A tight design satisfies  $t = 2s$  [20], and hence it becomes a  $Q$ -polynomial scheme. A tight design also attains the bound (10). Moreover the polynomial  $v_i^*$  of a tight design coincides with  $Q_i^{(m)}$ .

For connected regular graph, we have a very similar situation to the above argument on the sphere. Let  $G$  be a connected  $k$ -regular graph with  $v$  vertices. Throughout this paper, we assume a graph is simple. Since a graph with  $d + 1$  distinct eigenvalues is of diameter at most  $d$ , we can change the assumption of the Moore bound to the number of eigenvalues. Namely if  $G$  has only  $d + 1$  distinct eigenvalues, then we have

$$v \leq 1 + k \sum_{j=0}^{d-1} (k-1)^j.$$

If equality holds, then  $G$  is called a *Moore graph*. Tutte [50] showed that if  $G$  is of girth  $2e + 1$ , then we have

$$v \geq 1 + k \sum_{j=0}^{e-1} (k-1)^j.$$

The graph that attains this equality becomes a Moore graph. It is well known that a Moore graph is distance-regular. Actually we can show that if  $g \geq 2d - 1$  holds, then  $G$  is distance-regular (Theorem 6). Let  $F_i^{(k)}$  be the polynomial of degree  $i$  defined by (11) and (12) in Section 2. The polynomial  $v_i$  of a  $k$ -regular Moore graph coincides with  $F_i^{(k)}$ . Apparently the dual concept of tight spherical design is Moore graph, and the polynomial  $F_i^{(k)}$  dually corresponds to the Gegenbauer polynomial  $Q_i^{(m)}$ .

The linear programming method for spherical codes is essentially based on the positive definiteness of the Gegenbauer polynomials, namely  $\tau(Q_i^{(m)}(\mathbf{E}^\circ)) \geq 0$ , where  $\mathbf{E}$  is the Gram matrix. In this paper, we dually show the linear programming method for connected regular graphs by using the property  $\text{tr}(F_i^{(k)}(\mathbf{A})) \geq 0$ , where  $\mathbf{A}$  is the adjacency matrix.

We can apply the linear programming method for determining the graph maximizing the spectral gap. The *spectral gap* of a graph is the difference between the first and second largest eigenvalues of the graph. The *edge expansion ratio*  $h(G)$  of a  $k$ -regular graph  $G = (V, E)$  is defined as

$$h(G) = \min_{S \subset V, |S| \leq |V|/2} \frac{|\partial S|}{|S|},$$

where  $\partial S = \{\{u, v\} \mid u \in S, v \in V \setminus S, \{u, v\} \in E\}$ . By the spectral gap  $\tau$  of  $G$ , we have  $\tau/2 \leq h(G) \leq \sqrt{2k\tau}$  [2, 3, 21]. This implies that a graph with large spectral gap has high connectivity. The second-largest eigenvalue cannot be much smaller than  $2\sqrt{k-1}$  [2]. Ramanujan graphs have an asymptotically smallest possible second-largest eigenvalue (see [33]). Several regular graphs with very small second-largest eigenvalues are determined (see [36]).

The dual concept of the graphs maximizing the spectral gap is well known as optimal spherical code in the sense of maximizing the minimum distance. The optimal configurations of  $n$  points on  $S^2$  are known only for  $n \leq 13$ , and  $n = 24$  [22, Chapter 3], [42]. For higher dimensions, the linear or semidefinite programming bound determined many optimal codes [37, 15, 5]. In particular, we have a strong theorem using the parameters  $s$  and  $t$ , namely if  $t \geq 2s - 1$  holds, then the set is optimal [37, 15]. In the present paper, as the dual theorem of it, we prove that a connected  $k$ -regular graph satisfying  $g \geq 2d$  has the minimum second-largest eigenvalue of all  $k$ -regular graphs of the same size, where  $d$  is the number of distinct non-trivial eigenvalues, and  $g$  is the girth.

## 2 Linear programming method

In the present section, we give the linear programming bounds for connected regular graphs. First let us introduce certain polynomials  $F_i^{(k)}(x)$  which play a key role in the linear programming method. Indeed  $F_i^{(k)}(x)$  is the polynomial attached to the homogeneous tree of degree  $k$ , which is an infinite distance-regular graph.

A graph  $G = (V, E)$  is said to be *locally finite* if the degree of any vertex is finite. We also consider an infinite graph here. A *path* in a graph is a sequence of vertices, where any two consecutive vertices are connected. Let  $d(x, y)$  be the shortest path distance from  $x \in V$  to  $y \in V$ . The  *$i$ -th distance matrix*  $\mathbf{A}_i$  of  $G$  is defined to be the matrix indexed by  $V$  whose  $(x, y)$ -entry is 1 if  $d(x, y) = i$ , 0 otherwise. In particular  $\mathbf{A}_1$  is called the *adjacency matrix* of  $G$ .

A locally finite graph  $G = (V, E)$  is called a *distance-regular graph* if for any choice of  $x, y \in V$  with  $d(x, y) = k$ , the number of vertices  $z \in V$  such that  $d(x, z) = i$ ,  $d(z, y) = j$  is independent of the choice  $x, y$ . For  $x, y \in V$  with  $d(x, y) = k$ , the number  $p_{ij}^k = |\{z \in V \mid d(x, z) = i, d(z, y) = j\}|$  is called the *intersection number* of a distance-regular graph. We use the notation  $a_i = p_{1,i}^i$ ,  $b_i = p_{1,i+1}^i$ , and  $c_i = p_{1,i-1}^i$ . The *intersection array* of a distance-regular graph is defined to be

$$\begin{pmatrix} * & c_1 & c_2 & \cdots \\ a_0 & a_1 & a_2 & \cdots \\ b_0 & b_1 & b_2 & \cdots \end{pmatrix}.$$

The matrix  $\mathbf{A}_i$  of a distance-regular graph can be written as the polynomial  $v_i$  in  $\mathbf{A}_1$  of degree  $i$  [11, page 127], where  $v_i$  is defined by

$$\begin{aligned} v_0(x) &= 1, & v_1(x) &= x, \\ c_{i+1}v_{i+1}(x) &= (x - a_i)v_i(x) - b_{i-1}v_{i-1}(x) & (i = 1, 2, \dots). \end{aligned}$$

A homogeneous tree of degree  $k$  is an infinite distance-regular graph with intersection numbers

$$b_0 = k, \quad b_i = k - 1 (i = 1, 2, \dots), \quad c_i = 1 (i = 1, 2, \dots), \quad a_i = 0 (i = 0, 1, 2, \dots).$$

Let  $F_i^{(k)}$  denote a polynomial of degree  $i$  defined by:

$$F_0^{(k)}(x) = 1, \quad F_1^{(k)}(x) = x, \quad F_2^{(k)}(x) = x^2 - k, \quad (11)$$

and

$$F_i^{(k)}(x) = xF_{i-1}^{(k)}(x) - (k-1)F_{i-2}^{(k)}(x) \quad (12)$$

for  $i \geq 3$ . Let  $q = \sqrt{k-1}$ . The polynomials  $F_i^{(k)}$  form a sequence of orthogonal polynomials with respect to the weight

$$w(x) = \frac{\sqrt{4q^2 - x^2}}{k^2 - x^2} \quad (13)$$

on the interval  $[-2q, 2q]$  (see [34, Section 4]). Note that  $F_i^{(k)}(k) = k(k-1)^{i-1}$  for any  $i \geq 1$ .

A path  $u_0 \sim u_1 \sim \cdots \sim u_p$  is said to be *reducible* if any sequence  $u_i \sim u_j \sim u_i$  appears [48]. A path is said to be *irreducible* if the path is not reducible.

**Theorem 1** ([48]). *Let  $G$  be a connected  $k$ -regular graph with adjacency matrix  $\mathbf{A}$ . Then the  $(u, v)$ -entry of  $F_i^{(k)}(\mathbf{A})$  is the number of irreducible paths of length  $i$  from  $u$  to  $v$ .*

By Theorem 1, the following is obvious.

**Corollary 1.** *Let  $G$  be a connected  $k$ -regular graph with adjacency matrix  $\mathbf{A}$ . Then the following are equivalent.*

- (1)  $\text{tr}(F_i^{(k)}(\mathbf{A})) = 0$  for each  $1 \leq i \leq g - 1$ , and  $\text{tr}(F_g^{(k)}(\mathbf{A})) \neq 0$ .
- (2)  $G$  is of girth  $g$ .

The following is the linear programming bound for connected regular graphs.

**Theorem 2.** *Let  $G$  be a connected  $k$ -regular graph with  $v$  vertices. Let  $\tau_0 = k, \tau_1, \dots, \tau_d$  be the distinct eigenvalues of  $G$ . Suppose there exists a polynomial  $f(x) = \sum_{i \geq 0} f_i F_i^{(k)}(x)$  such that  $f(k) > 0$ ,  $f(\tau_i) \leq 0$  for any  $i \geq 1$ ,  $f_0 > 0$ , and  $f_i \geq 0$  for any  $i \geq 1$ . Then we have*

$$v \leq \frac{f(k)}{f_0}. \quad (14)$$

*Proof.* Let  $\mathbf{A}$  be the adjacency matrix of  $G$ . From the spectral decomposition  $\mathbf{A} = \sum_{i=0}^d \tau_i \mathbf{E}_i$ , we have

$$\sum_{i=0}^d f(\tau_i) \mathbf{E}_i = f(\mathbf{A}) = \sum_{i \geq 0} f_i F_i^{(k)}(\mathbf{A}) = f_0 \mathbf{I} + \sum_{i \geq 1} f_i F_i^{(k)}(\mathbf{A}). \quad (15)$$

Taking the traces in (15), we have

$$f(k) = \text{tr}(f(k) \mathbf{E}_0) \geq \text{tr}\left(\sum_{i=0}^d f(\tau_i) \mathbf{E}_i\right) = \text{tr}(f_0 \mathbf{I} + \sum_{i \geq 1} f_i F_i^{(k)}(\mathbf{A})) \geq \text{tr}(f_0 \mathbf{I}) = v f_0.$$

Therefore we have  $v \leq f(k)/f_0$ . □

**Remark 1.** We can normalize  $f_0 = 1$  in Theorem 2.

**Remark 2.** Let  $f$  be a polynomial which satisfies the condition in Theorem 2. The equality holds in (14) if and only if  $f_i \text{tr}(F_i^{(k)}(\mathbf{A})) = 0$  for any  $i = 1, \dots, \deg(f)$ , and  $f(\tau_i) = 0$  for any  $i = 1, \dots, d$ . In particular, if  $f_i > 0$  for any  $i$ , then the girth of  $G$  is at least  $\deg(f) + 1$  by Corollary 1.

**Remark 3.** Theorem 2 can be expressed as the following linear programming problem and its dual.

$$v \leq \max_{m_i} \left\{ 1 + m_1 + \dots + m_d \mid \begin{array}{l} -\sum_{i=1}^d m_i F_j^{(k)}(\tau_i) \leq F_j^{(k)}(k), \quad j = 1, \dots, u, \\ m_i \geq 0, \quad i = 1, \dots, d \end{array} \right\},$$

$$v \leq \min_{f_j} \left\{ 1 + f_1 F_1^{(k)}(k) + \dots + f_u F_u^{(k)}(k) \mid \begin{array}{l} -\sum_{j=1}^u f_j F_j^{(k)}(\tau_i) \geq 1, \quad i = 1, \dots, d, \\ f_j \geq 0, \quad j = 1, \dots, u \end{array} \right\},$$

where  $u$  is the degree of  $f$ ,  $m_i$  is the multiplicity of  $\tau_i$  and  $f_0 = 1$ .

**Remark 4.** Delsarte, Goethals, and Seidel [20] gave the linear programming bounds for spherical codes by using inner products and Gegenbauer polynomials, instead of eigenvalues and  $F_i^{(k)}$ . This is the dual version of Theorem 2.

### 3 Minimizing the second-largest eigenvalue

For fixed  $v$  and  $k$ , a graph  $G$  is said to be *extremal expander* if  $G$  has the minimum second-largest eigenvalue in all  $k$ -regular graphs of order  $v$ . A disconnected graph is not extremal expander, because the first and second largest eigenvalues are equal. In the present section, we obtain extremal expander graphs for several  $v$  and  $k$  by applying the linear programming method. First we give several results related to  $F_i^{(k)}(x)$ .

**Theorem 3.** *Let  $F_i^{(k)}(x)F_j^{(k)}(x) = \sum_{l=0}^{i+j} p_l(i, j)F_l^{(k)}(x)$  for real numbers  $p_l(i, j)$ . Then we have  $p_0(i, j) = F_i^{(k)}(k)\delta_{ij}$  and  $p_l(i, j) \geq 0$  for all  $l, i, j$ . Moreover  $p_l(i, j) > 0$  if and only if  $|i - j| \leq l \leq i + j$  and  $l \equiv i + j \pmod{2}$ .*

*Proof.* Let  $T_k$  be a homogeneous tree of degree  $k$ . Let  $\mathbf{A}_i$  be the  $i$ -th distance matrix of  $T_k$ , and  $p_{ij}^k$  the intersection number of  $T_k$ . Since  $F_i^{(k)}(x)$  is the polynomial attached to  $T_k$ , we have

$$\sum_{l=0}^{i+j} p_l(i, j)\mathbf{A}_l = \sum_{l=0}^{i+j} p_l(i, j)F_l^{(k)}(\mathbf{A}_1) = F_i^{(k)}(\mathbf{A}_1)F_j^{(k)}(\mathbf{A}_1) = \mathbf{A}_i\mathbf{A}_j = \sum_{l=0}^{i+j} p_{ij}^l\mathbf{A}_l. \quad (16)$$

Clearly  $p_l(i, j) = p_{ij}^l$  holds. This theorem now follows by a counting argument.  $\square$

Since  $F_{i+1}^{(k)}(k) - (k-1)F_i^{(k)}(k) = 0$  holds, let  $G_i^{(k)}(x)$  denote the polynomial of degree  $i$

$$G_i^{(k)}(x) = \frac{F_{i+1}^{(k)}(x) - (k-1)F_i^{(k)}(x)}{x - k}$$

for any  $i \geq 1$ , and  $G_0^{(k)}(x) = 1$ . By the three-term recurrence relation (12), it holds that

$$G_i^{(k)}(x) = \sum_{j=0}^i F_j^{(k)}(x).$$

From Lemmas 3.3, 3.5 in [15],  $G_0, G_1, \dots$  are monic orthogonal polynomials with respect to the positive weight  $u(x) = (k-x)w(x)$  on the interval  $[-2q, 2q]$ , where  $w(x)$  is defined in (13).

**Theorem 4** ([15, Theorem 3.1]). *Let  $p_0, p_1, \dots$  be monic orthogonal polynomials with  $\deg(p_i) = i$ . Then for any  $\alpha \in \mathbb{R}$ , the polynomial  $p_n + \alpha p_{n-1}$  has  $n$  distinct real roots  $r_1 < \dots < r_n$ . Moreover for  $k < n$ ,  $\prod_{i=1}^k (x - r_i)$  has positive coefficients in terms of  $p_0(x), p_1(x), \dots, p_k(x)$ .*

The following is a key theorem.

**Theorem 5.** *Let  $G$  be a connected  $k$ -regular graph of girth  $g$ . Assume the number of distinct eigenvalues of  $G$  is  $d+1$ . If  $g \geq 2d$  holds, then  $G$  is an extremal expander graph.*

*Proof.* Let  $\tau_0 = k > \tau_1 > \dots > \tau_d$  be the distinct eigenvalues of  $G$ . We show the polynomial

$$f(x) = (x - \tau_1) \prod_{i=2}^d (x - \tau_i)^2 = \sum_{i=0}^{2d-1} f_i F_i^{(k)}(x)$$

satisfies the condition in Theorem 2. It trivially holds that  $f(k) > 0$ , and  $f(\tau_i) = 0$  for any  $i = 1, \dots, d$ .

Let  $\mathbf{A}$  be the adjacency matrix of  $G$ . If the diameter of  $G$  is greater than  $d$ , then the number of distinct eigenvalues is greater than  $d + 1$ . Thus the diameter of  $G$  is at most  $d$ . Since  $g \geq 2d$  holds, the diameter is exactly  $d$ . Then  $G$  partially has the structure of a homogeneous tree around any vertex, namely  $F_i^{(k)}(\mathbf{A}) = \mathbf{A}_i$  for any  $i = 0, 1, \dots, d - 1$ . Because the Hoffman polynomial [31] of  $G$  is of degree  $d$ , there exists a natural number  $e$  such that

$$\sum_{i=0}^{d-1} F_i^{(k)}(\mathbf{A}) + \frac{1}{e} F_d^{(k)}(\mathbf{A}) = \mathbf{J},$$

where  $\mathbf{J}$  is the all-ones matrix. Note that the roots of the Hoffman polynomial  $P(x) = \sum_{i=0}^{d-1} F_i^{(k)}(x) + (1/e)F_d^{(k)}(x)$  are the non-trivial distinct eigenvalues of  $G$  [31].

For some positive constant number  $c$ , the polynomial  $f(x)$  can be expressed as

$$f(x) = \frac{cP(x)^2}{x - \tau_1} = \frac{c}{e} \frac{G_d^{(k)}(x) - (1 - e)G_{d-1}^{(k)}(x)}{x - \tau_1} P(x).$$

By Theorem 4,  $g(x) = (G_d^{(k)}(x) - (1 - e)G_{d-1}^{(k)}(x))/(x - \tau_1)$  has positive coefficients in terms of  $G_0^{(k)}(x), G_1^{(k)}(x), \dots, G_{d-1}^{(k)}(x)$ . This implies that  $g(x)$  has positive coefficients in terms of  $F_0^{(k)}(x), F_1^{(k)}(x), \dots, F_{d-1}^{(k)}(x)$ . By Theorem 3, it is shown that  $f(x)$  has positive coefficients in terms of  $F_0^{(k)}(x), F_1^{(k)}(x), \dots, F_{2d-1}^{(k)}(x)$ . Thus  $f(x)$  satisfies the condition in Theorem 2.

By Remark 2,  $G$  attains the linear programming bound obtained from  $f(x)$ . Assume there exists a graph  $G'$  such that its second-largest eigenvalue is smaller than  $\tau_1$ , and it has the same number of vertices as  $G$ . Then  $G'$  also attains the linear programming bound obtained from  $f(x)$ . By Remark 2,  $G'$  has only  $d$  distinct eigenvalues, and the girth of  $G'$  is at least  $2d$ . Therefore  $G'$  is of diameter at least  $d$ , it contradicts that the number of distinct eigenvalues of  $G'$  is greater than  $d$ . Thus  $G$  is an extremal expander graph.  $\square$

**Remark 5.** Levenshtein [37] proved that a spherical  $s$ -distance set of strength  $t$  satisfying  $t \geq 2s - 1$  is an optimal spherical code in the sense of maximizing the minimum distance. This result is the dual version of Theorem 5. Cohn and Kumar [15] extended this result to universally optimal codes.

We characterize connected regular graphs satisfying  $g \geq 2d$  as follows.

**Theorem 6.** *Let  $G$  be a connected  $k$ -regular graph of girth  $g$ , and with only  $d + 1$  distinct eigenvalues. If  $g \geq 2d - 1$  holds, then  $G$  is a distance-regular graph of diameter  $d$ .*

*Proof.* Brouwer and Haemers [12] proved that a graph with the spectrum of a distance-regular graph with diameter  $D$  and girth at least  $2D - 1$ , is such a graph. The proof in [12] used the fact that regularity, connectedness, girth, and diameter of a graph are determined by the spectrum. Therefore the theorem of Brouwer and Haemers is interpreted as that a connected regular graph with  $g \geq 2D - 1$  is distance-regular. In general we have  $d \geq D$ . Therefore in our condition,  $g \geq 2d - 1 \geq 2D - 1$  holds, and  $G$  is distance-regular. Since  $G$  is distance-regular,  $d$  is equal to the diameter [11, Section 4.1].  $\square$

Abiad, Van Dam, and Fiol [1] proved Theorem 6 independently.



Table 2: Extremal expander graphs

$v$	$k$	$g$	Eigenvalues	Name
$g$	2	$g$	$2 \cos(2k\pi/n); 1 \leq k \leq n-1$	$g$ -cycle $C_g$
$k+1$	$k$	3	0	complete $K_{k+1}$
$2k$	$k$	4	$0, -k$	comp. bipartite $K_{k,k}$
$2 \sum_{i=0}^2 q^i$	$q+1$	6	$\pm\sqrt{q}, -(q+1)$	inc. graph of $PG(2, q)$ [48, 11]
$2 \sum_{i=0}^3 q^i$	$q+1$	8	$\pm\sqrt{2q}, 0, -(q+1)$	inc. graph of $GQ(q, q)$ [9, 11]
$2 \sum_{i=0}^5 q^i$	$q+1$	12	$\pm\sqrt{3q}, \pm\sqrt{q}, 0, -(q+1)$	inc. graph of $GH(q, q)$ [9, 11]
10	3	5	$1^5, (-2)^4$	Petersen [32]
50	7	5	$2^{28}, (-3)^{21}$	Hoffman–Singleton [32]
35	4	6	$2^{14}, (-1)^{14}, (-3)^6$	Odd graph [40]
16	5	4	$1^{10}, (-3)^5$	Clebsch [47, 25]
56	10	4	$2^{35}, (-4)^{20}$	Gewirtz [12, 25]
77	16	4	$2^{55}, (-6)^{21}$	$M_{22}$ [30, 25]
100	22	4	$2^{77}, (-8)^{22}$	Higman–Sims [30, 25]

$PG(2, q)$ : projective plane,  $GQ(q, q)$ : generalized quadrangle,

$GH(q, q)$ : generalized hexagon,  $q$ : prime power

**Remark 6.** Delsarte, Goethals, and Seidel [20] proved that a spherical  $s$ -distance set of strength  $t$  satisfying  $t \geq 2s - 2$  has the structure of a  $Q$ -polynomial association scheme. This result is the dual version of Theorem 6.

The distance-regular graph with  $g \geq 2d$  is called a *Moore polygon* [18] and it has the following intersection array:

$$\begin{pmatrix} * & 1 & 1 & \cdots & 1 & c \\ 0 & 0 & 0 & \cdots & 0 & k-c \\ k & k-1 & k-1 & \cdots & k-1 & * \end{pmatrix},$$

where  $c$  is a natural number. If  $c = 1$ , then the graph is a Moore graph and it does not exist for  $d \geq 3$  (with  $k \geq 3$ ) [7, 17]. If  $c = k$ , then the graph is an incidence graph of a regular generalized polygon of order  $(s, s)$  [11, Section 6.9], and it does not exist for  $d \geq 7$  (with  $k \geq 3$ ) [23]. If  $c \neq 1, k$ , then the graph is called a *non-trivial* Moore polygon, and it does not exist for  $d \geq 6$  [18]. Strongly regular graphs of girth 4 are non-trivial Moore polygons.

Table 2 shows known examples of extremal expander graphs satisfying  $g \geq 2d$ . The following graphs are unique: Petersen graph [32], Hoffman–Singleton graph [32], Odd graph [40], Clebsch graph [26, Theorem 10.6.4], Gewirtz graph [24],  $M_{22}$  graph [10], Higman–Sims graph [24],  $PG(2, q)$  for  $q \leq 8$  [38, 27, 29],  $GQ(q, q)$  for  $q \leq 4$  [44, 45], and  $GH(2, 2)$  [14]. For  $PG(2, 9)$ , there are four non-isomorphic graphs [28, 51]. The uniqueness of other examples in Table 2 is open.

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