# Bounds on Special Subsets in Graphs, Eigenvalues and Association Schemes

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**Abstract.**   We give a bound on the sizes of two sets of vertices at a given minimum distance in a graph in terms of polynomials and the Laplace spectrum of the graph. We obtain explicit bounds on the number of vertices at maximal distance and distance two from a given vertex, and on the size of two equally large sets at maximal distance. For graphs with four eigenvalues we find bounds on the number of vertices that are not adjacent to a given vertex and that have $\mu$ common neighbours with that vertex. Furthermore we find that the regular graphs for which the bounds are tight come from association schemes.

**Keywords:**   eigenvalue of graph, association scheme

## 1.   Introduction

In an earlier paper by van Dam and Haemers [6], a bound on the sizes of two sets of vertices at a given minimum distance in a graph in terms of polynomials and the spectrum of the graph was derived. The problem is to choose good polynomials. This problem arose in [3, 6, 10] where the diameter of a graph is bounded in terms of its eigenvalues. Chung et al. [3] and van Dam and Haemers [6] used Chebyshev polynomials, while Fiol et al. [10] looked at the best possible polynomials.

Here we shall use the tool of van Dam and Haemers for other purposes than bounding the diameter of a graph. We shall derive a number of new results, i.e., bounds on special subsets in terms of the Laplace eigenvalues, always by considering the optimal polynomials, thus illustrating the strength of the used technique. We obtain an upper bound on the number of vertices at maximal distance, and a lower bound on the number of vertices at distance two from a given vertex. For graphs with four eigenvalues we prove a more general result. Here we shall bound the number of vertices $n_3$ that are not adjacent to a given vertex and have a fixed number $\mu$ of common neighbours with that vertex, in terms of the spectrum and $\mu$, and we characterize the case of equality. This particular number $n_3$ plays an important role in a characterization of the graphs in a three-class association scheme (cf., [5]), and our bound is evidence for a conjecture on this number.

Another application of our tool gives bounds on the size of two equally large sets of vertices at maximal distance, or distance at least two (i.e., with no edges in between). The latter has applications for the bandwidth of a graph. Here we also find graphs (including some strongly regular graphs) for which the bound is tight.

The Laplace spectrum of a graph is the spectrum of its Laplace matrix. This is a square matrix $Q$ indexed by the vertices, with $Q_{xx} = d_x$, the degree of $x$, and $Q_{xy} = -1$ if $x$ and $y$ are adjacent, and $Q_{xy} = 0$ if $x$ and $y$ are not adjacent. If the graph is regular of degree $k$, then its (adjacency) eigenvalues $\lambda_i$ and its Laplace eigenvalues $\theta_i$ are related by $\theta_i = k - \lambda_i$.

In this paper we use the method of interlacing eigenvalues. For this we refer to the paper by Haemers [11]. For distance-regular graphs and association schemes we refer to the book by Brouwer et al. [1].

## 2. The tools

The next theorem, which is our main tool, is a theorem by van Dam and Haemers [6], except that here the Laplace matrix instead of the adjacency matrix is used.

**Theorem 2.1** *Let $G$ be a connected graph on $v$ vertices with $r + 1$ distinct Laplace eigenvalues $0 = \theta_0 < \theta_1 < \cdots < \theta_r$. Let $m$ be a nonnegative integer and let $X$ and $Y$ be sets of vertices, such that the distance between any vertex of $X$ and any vertex of $Y$ is at least $m + 1$. If $p$ is a polynomial of degree $m$ such that $p(0) = 1$, then*

$$\frac{|X|\,|Y|}{(v - |X|)(v - |Y|)} \leq \max_{i \neq 0} p^2(\theta_i).$$

**Proof:**  Let $G$ have Laplace matrix $Q$, then $p(Q)_{xy} = 0$ for all vertices $x \in X$ and $y \in Y$. Without loss of generality we assume that the first $|X|$ rows of $Q$ correspond to the vertices in $X$ and the last $|Y|$ rows correspond to the vertices in $Y$. Now consider the matrix

$$M = \begin{pmatrix} O & \vdots & P(Q) \\ \cdots & & \cdots \\ p(Q) & \vdots & O \end{pmatrix}.$$

Note that $M$ is symmetric, has row and column sums equal to 1, and its spectrum is $\{\pm p(\theta_i) \mid i = 0, 1, \ldots, r\}$, multiplicities included. Let $M$ be partitioned symmetrically in the following way.

$$M = \begin{pmatrix} O & \vdots & O & \vdots & & \vdots & O \\ \cdots & & \cdots & & \cdots & & \cdots \\ O & \vdots & O & \vdots & & \vdots & \\ \cdots & & \cdots & & \cdots & & \cdots \\ & \vdots & & \vdots & O & \vdots & O \\ \cdots & & \cdots & & \cdots & & \cdots \\ O & \vdots & & \vdots & O & \vdots & O \end{pmatrix} \begin{matrix} \} & |X| \\ \\ \} & v - |X| \\ \\ \} & v - |Y| \\ \\ \} & |Y| \end{matrix}.$$

Let $B$ be its quotient matrix (the matrix of average row sums in the blocks of this partition), then

$$B = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 - \frac{|Y|}{v-|X|} & \frac{|Y|}{v-|X|} \\ \frac{|X|}{v-|Y|} & 1 - \frac{|X|}{v-|Y|} & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

with eigenvalues $\lambda_0(B) = -\lambda_3(B) = 1$, $\lambda_1(B) = -\lambda_2(B) = \sqrt{\frac{|X||Y|}{(v-|X|)(v-|Y|)}}$. Since the eigenvalues of $B$ interlace those of $M$ (cf., [11]), we have that

$$\lambda_1(B) \leq \lambda_1(M) \leq \max_{i \neq 0} |p(\theta_i)|,$$

and the theorem follows. $\qquad\square$

To obtain the sharpest bound we have to minimize $\max\{|p(\theta_i)| \,|\, i \neq 0\}$ over all polynomials $p$ of degree $m$ such that $p(0) = 1$. This problem occurred in earlier papers [3, 6, 10] to obtain bounds on the diameter of graphs. In the first two papers Chebyshev polynomials were used, which are good but not optimal. In the more recent paper by Fiol et al. [10] the optimal polynomials were investigated. The problem in fact is one from the theory of uniform approximations of continuous functions (cf., [2, 13]).

Let $S$ be a compact set of real numbers and let $C(S)$ be the set of continuous functions on $S$ to the reals. Let $f \in C(S)$, with uniform norm

$$\|f\|_\infty = \max_{z \in S} |f(z)|.$$

Let $W$ be a subspace of $C(S)$ of dimension $n$, then $w^*$ is called a best approximation of $f$ in $W$ if

$$\min_{w \in W} \|f - w\|_\infty = \|f - w^*\|_\infty.$$

The set of critical points of a function is the set $E(f, S) = \{z \in S \mid \|f\|_\infty = |f(z)|\}$. The sign of $z \neq 0$ is defined by $\operatorname{sgn}(z) = z|z|^{-1}$ ($\operatorname{sgn}(0) = 0$). Now we have the following characterization of best approximations (cf., [13]).

**Lemma 2.2** *The function $w^*$ is a best approximation of $f$ if and only if there are distinct points $z_1, \ldots, z_t \in E(f - w^*, S)$, and positive numbers $\alpha_1, \ldots, \alpha_t$ such that for all $w \in W$*

$$\sum_{i=1}^{t} \alpha_i \operatorname{sgn}(f(z_i) - w^*(z_i)) w(z_i) = 0,$$

*where $t \leq n + 1$.*

After substitution of $p(0) = 1$ our problem is to find

$$\min_{p_m, \ldots, p_1} \max_{i \neq 0} \left| p_m \theta_i^m + \cdots + p_1 \theta_i + 1 \right|,$$

so we want a best approximation of the function $-1$ on $S = \{\theta_1, \ldots, \theta_r\}$ from $W = \{w \mid w(z) = p_m z^m + \cdots + p_1 z\}$, which is an $m$-dimensional subspace of $C(S)$. It follows that $p(z)$ is the unique optimal polynomial if and only if there are $z_j \in \{\theta_i \mid i = 1, \ldots, r\}$, $j = 1, \ldots, m+1$, such that $z_1 < z_2 < \cdots < z_{m+1}$, and $p(z_j)$ is alternating $\pm \max\{|p(\theta_i)| \mid i \neq 0\}$ (cf., [13, Theorem 2.8 and 2.10]). It also follows that we must have $z_1 = \theta_1$ and $z_{m+1} = \theta_r$. For $m = 2$, where we have to find the optimal quadratic polynomial, it is easily verified that we have to take $z_2 = \theta_h$, the Laplace eigenvalue closest to $\frac{1}{2}(\theta_1 + \theta_r)$. In the general case it follows (cf., [2, Theorem 7.1.6]) that there is a subset $T$ of $\{1, \ldots, r\}$ of size $m + 1$ such that the polynomial $p$ given by

$$p(z) = c_T \sum_{j \in T} \prod_{i \in T \setminus \{j\}} \frac{z - \theta_i}{|\theta_j - \theta_i|},$$

where $c_T$ is such that $p(0) = 1$, is the unique optimal polynomial. Now let $P_m$ be the set of polynomials of degree $m$ such that $p(0) = 1$, then it follows that $|c_T| = \min_{p \in P_m} \max_{i \neq 0} |p(\theta_i)|$.

If $T'$ is an arbitrary subset of $\{1, \ldots, r\}$ of size $m + 1$, then

$$|c_{T'}| = \min_{p \in P_m} \max_{i \in T'} |p(\theta_i)| = \left( \sum_{j \in T'} \prod_{i \in T' \setminus \{j\}} \frac{\theta_i}{|\theta_j - \theta_i|} \right)^{-1}.$$

Now it follows that $|c_{T'}| \leq |c_T|$, and so $|c_T| \leq \max_{T' \subset \{1, \ldots, r\}, |T'| = m+1} |c_{T'}| \leq |c_T|$. Thus we find that the required minimum equals

$$|c_T| = \max_{T' \subset \{1, \ldots, r\}, |T'| = m+1} \left( \sum_{j \in T'} \prod_{i \in T' \setminus \{j\}} \frac{\theta_i}{|\theta_j - \theta_i|} \right)^{-1}.$$

## 3. The number of vertices at maximal distance and distance two

It is well known that if a graph has $r + 1$ distinct adjacency eigenvalues, then it has diameter at most $r$. The same holds for the Laplace spectrum, and this result can be derived quite easily from Theorem 2.1. Using the results of the previous section we find a bound on the number of vertices that are at maximal distance $r$ from a fixed vertex. By $G_i$ we denote the distance $i$ graph of $G$.

**Theorem 3.1** *Let $G$ be a connected graph on $v$ vertices with $r + 1$ distinct Laplace eigenvalues $0 = \theta_0 < \theta_1 < \cdots < \theta_r$. Let $x$ be an arbitrary vertex, and let $k_r$ be the number*

*of vertices at distance r from x. Then*

$$k_r \le \frac{v}{1 + \frac{\gamma^2}{v-1}}, \quad \text{where } \gamma = \sum_{j \ne 0} \prod_{i \ne 0, j} \frac{\theta_i}{|\theta_j - \theta_i|}.$$

*If equality holds for every vertex, then $G_r$ is a strongly regular $(v, k_r, \lambda, \lambda)$ graph. If $G$ is a distance-regular graph with diameter $r$ such that $G_r$ is a strongly regular $(v, k_r, \lambda, \lambda)$ graph then the bound is tight for every vertex.*

**Proof:** Take $X = \{x\}$, and let $Y$ be the set of vertices at distance $r$ from $x$. Now take the optimal polynomial of degree $r - 1$ given in the previous section, with $\gamma = |c_T|^{-1}$ and apply Theorem 2.1, then the bound follows. If the bound is tight, then it follows that in the proof of Theorem 2.1 we have tight interlacing, and so the partition of $M$ is regular (cf., [11]). Therefore,

$$p(Q) = \begin{pmatrix} a & \vdots & a\underline{1}^T & \vdots & \underline{0}^T \\ \cdots & & \cdots & & \cdots \\ a\underline{1} & \vdots & S_{11} & \vdots & S_{12} \\ \cdots & & \cdots & & \cdots \\ \underline{0} & \vdots & S_{12}^T & \vdots & S_{22} \end{pmatrix} \begin{matrix} \} & 1 \\ \\ \} & v-1-k_r, \\ \\ \} & k_r \end{matrix}$$

where $a = 1/(v - k_r)$, is regularly partitioned with $S_{12}$ and $S_{22}$ having the same row sums. If the bound is tight for every vertex, then it follows that $J - (v - k_r)p(Q)$ is the adjacency matrix of $G_r$, and that this graph is a strongly regular $(v, k_r, \lambda, \lambda)$ graph.

On the other hand, if $G$ is a distance-regular graph with diameter $r$ such that $G_r$ is a strongly regular $(v, k_r, \lambda, \lambda)$ graph then we shall show that

$$k_r = \frac{v}{1 + \frac{\gamma^2}{v-1}}, \quad \text{where } \gamma^{-1} = \max_{i \ne 0} |p(\theta_i)|,$$

for some polynomial $p$ of degree $r - 1$ such that $p(0) = 1$. Because of the optimality of the bound this suffices to prove that the bound is tight for every vertex. Now assume that $G$ has degree $k$, then its Laplace eigenvalues $\theta_i$ and its adjacency eigenvalues $\lambda_i$ are related by $\lambda_i = k - \theta_i$. Furthermore, let $A$ be the adjacency matrix of $G$, and let $A_i$ be the adjacency matrix of the distance $i$ graph $G_i$ of $G$. Since $G$ is distance-regular, there is a polynomial $q$ of degree $r - 1$ such that

$$q(A) = (J - A_r)/(v - k_r) = (A_{r-1} + \cdots + A + I)/(v - k_r),$$

and then $q(k) = 1$. Now, let $p(z) = q(k - z)$. We have that $G_r$ is a strongly regular $(v, k_r, \lambda, \lambda)$ graph, and such a graph has (adjacency) eigenvalues $k_r$ and $\pm\sqrt{k_r(v - k_r)/(v - 1)}$.

From this it follows that

$$\max_{i \neq 0} |p(\theta_i)| = \max_{i \neq 0} |q(\lambda_i)| = \sqrt{\frac{k_r}{(v-1)(v-k_r)}},$$

which proves the claim.                                                                                          □

A side result of Theorem 3.1 is that if $v < 1 + \gamma$, so that $k_r < 1$, then the diameter of $G$ is at most $r - 1$, which was already found by van Dam and Haemers [6, Theorem 2.5].

Examples of graphs for which the bound is tight for every vertex are given by the two-antipodal distance-regular graphs, with $k_r = 1$ ($G_r$ being a disjoint union of edges). Other examples are given by the Odd graph on seven points ($k_3 = 18$) and the generalized hexagons $GH(q,q)(k_3 = q^5)$. If $G$ is a connected regular graph with four eigenvalues then we can also prove that a tight bound for every vertex implies distance-regularity, but we shall prove this in more generality in the next section.

**Remark** By taking $r = 2$ in Theorem 3.1, we see that the bound is tight for strongly regular $(v, k, \lambda', \lambda' + 2)$ graphs. Using results from [7, Theorem 2.1], it is not hard to show that for any connected graph with three Laplace eigenvalues the bound also follows from the parameter restrictions of such a graph. It is interesting to note that the bound is tight for *some* vertex if and only if $G$ comes from a polarity in a symmetric design with at least one absolute point. The absolute points correspond to the vertices for which the bound is tight.

For graphs with four eigenvalues, the upper bound for $k_3$ gives a lower bound for $k_2$, the number of vertices at distance 2 from $x$, since $k_2 = v - 1 - d_x - k_3$, where $d_x$ is the vertex degree of $x$. This lower bound generalizes to graphs with more than four eigenvalues, since we can bound the number of vertices $k_{3+}$ at distance at least three, using the optimal quadratic polynomial. By $G_{1,2}$ we denote the graph on the same vertices as $G$, where two vertices are adjacent if they have distance 1 or 2 in $G$.

**Theorem 3.2** *Let $G$ be a connected graph on $v$ vertices with $r + 1 \geq 4$ distinct Laplace eigenvalues $0 = \theta_0 < \theta_1 < \cdots < \theta_r$, and let $\theta_h$ be an eigenvalue unequal to $\theta_1$ and $\theta_r$, which is closest to $\frac{1}{2}(\theta_1 + \theta_r)$. Let $x$ be an arbitrary vertex with vertex degree $d_x$, and let $k_{2,x}$ be the number of vertices at distance 2 from $x$. Then*

$$k_{2,x} \geq v - 1 - d_x - \frac{v}{1 + \frac{\gamma^2}{v-1}}, \quad \text{where } \gamma = \sum_{j=1,h,r} \prod_{\substack{i=1,h,r \\ i \neq j}} \frac{\theta_i}{|\theta_j - \theta_i|}.$$

*If equality holds for every vertex, then the distance 1 or 2 graph $G_{1,2}$ of $G$ is a strongly regular $(v, d_x + k_{2,x}, \lambda', \lambda' + 2)$ graph. If $G$ is a distance-regular graph such that the distance 1 or 2 graph $G_{1,2}$ of $G$ is a strongly regular $(v, k + k_2, \lambda', \lambda' + 2)$ graph then the bound is tight for every vertex.*

**Proof:** The proof is similar to the proof of Theorem 3.1. Here equality for every vertex implies that "the distance at least 3 graph" $G_{3+}$ is a strongly regular $(v, k_{3+}, \lambda, \lambda)$ graph,

and so $G_{1,2}$ is a strongly regular $(v, d_x + k_{2,x}, \lambda', \lambda' + 2)$ graph. Note that in that case $G$ must have diameter 3 or 4.                                                                                   □

Examples for $r = 3$ for which this bound is tight were already given above. We do not know of any graph with more than four eigenvalues for which the bound is tight.

## 4. Special subsets in graphs with four eigenvalues

In a graph with four eigenvalues being at distance 3 is the same as being nonadjacent and having no common neighbours. The purpose of this section is to generalize the bound on the number of vertices $k_3$ at distance 3 from a vertex $x$ to a bound on the number of vertices $n_3$ that are not adjacent to $x$ and have $\mu$ common neighbours with $x$. Here the reader should keep in mind the analogue of the generalization of distance-regular graphs with diameter three to three-class association schemes. The question of bounding $n_3$ was raised after we characterized, among the regular graphs with four eigenvalues, the graphs in a three-class association scheme as those graphs for which $n_3$ equals $g(\Sigma, \mu)$, for every vertex, for some $\mu$. Here $g(\Sigma, \mu)$ is a (rather complicated) function of the spectrum $\Sigma$ of the graph and $\mu$ [5]. This result in fact is a generalization of a characterization of distance-regular graphs with diameter 3 [8]. Furthermore, it turned out that if $g(\Sigma, \mu)$ is a nonnegative integer then $n_3$ is at most $g(\Sigma, \mu)$. We think that the integrality condition can be dropped, but are (so far) unable to prove so. Still, our bound is close, giving some evidence for the conjecture.

Let us define $G_\mu$ as the graph on the same vertices as $G$, where two vertices are adjacent if in $G$ they are not adjacent, and have $\mu$ common neighbours. Let $G_{\neg\mu}$ be the graph with two vertices being adjacent if in $G$ they are not adjacent, and do not have $\mu$ common neighbours.

**Theorem 4.1**    *Let $G$ be a connected graph on $v$ vertices with four distinct Laplace eigenvalues $0 = \theta_0 < \theta_1 < \theta_2 < \theta_3$. Let $\mu$ be a nonnegative integer, let $x$ be an arbitrary vertex, and let $n_3$ be the number of vertices that are not adjacent to $x$ and have $\mu$ common neighbours with $x$. Then*

$$
n_3 \leq \frac{v}{1 + \frac{\gamma^2}{v-1}}, \quad \text{where } \gamma = \begin{cases} \dfrac{2(\theta_1\theta_3 - v\mu)}{(\theta_3 - \theta_2)(\theta_2 - \theta_1)} + 1 & \text{if } v\mu \leq \theta_1\theta_2 \text{ or } \theta_2\theta_3 < v\mu, \\[2ex] \dfrac{2(\theta_2\theta_3 - v\mu)}{(\theta_3 - \theta_1)(\theta_1 - \theta_2)} + 1 & \text{if } \theta_1\theta_2 < v\mu \leq \theta_1\theta_3, \\[2ex] \dfrac{2(\theta_1\theta_2 - v\mu)}{(\theta_2 - \theta_3)(\theta_3 - \theta_1)} + 1 & \text{if } \theta_1\theta_3 < v\mu \leq \theta_2\theta_3. \end{cases}
$$

*If equality holds for every vertex, then $G_\mu$ is a strongly regular $(v, n_3, \lambda, \lambda)$ graph. If $G$ is regular then equality holds for every vertex if and only if $G$, $G_\mu$ and $G_{\neg\mu}$ form a three-class association scheme and $G_\mu$ is a strongly regular $(v, n_3, \lambda, \lambda)$ graph.*

**Proof:** Here we use a slight variation to the interlacing technique we used before. Let $p(z) = p_2 z^2 + p_1 z + p_0$ be a quadratic polynomial such that $p(0) = 1 + p_2 v\mu$. Let $Q$ be the Laplace matrix of $G$, then $(p_2(Q^2 - \mu J) + p_1 Q + p_0 I)_{xy} = 0$ for all vertices $y$ that are not adjacent to $x$ and have $\mu$ common neighbours with $x$. If we replace $p(Q)$ by $p_2(Q^2 - \mu J) + p_1 Q + p_0 I$ in the proof of Theorem 2.1, then the matrix $M$ has row and column sums equal to 1, and spectrum $\{\pm 1\} \cup \{\pm p(\theta_i) \mid i = 1, 2, 3\}$ with corresponding multiplicities. Now it follows that

$$n_3 \leq \frac{v}{1 + \frac{\gamma^2}{v-1}}, \quad \text{where } \gamma^{-1} = \max_{i \neq 0} |p(\theta_i)|.$$

So here the sharpest bound is obtained by minimizing $\max\{|p(\theta_i)| \mid i \neq 0\}$ over all polynomials $p(z) = p_2 z^2 + p_1 z + p_0$ such that $p(0) = 1 + p_2 v\mu$. For $\mu = 0$ we know the solution: there is a unique optimal polynomial $p$, and $p(\theta_1) = -p(\theta_2) = p(\theta_3)$. In general the situation is more complicated. We shall see that the polynomial is not always unique anymore. However, we can use Lemma 2.2 to optimize our bound explicitly. Note that in order to characterize the case of equality, we need to be sure that the bound we find is indeed derived with the best possible polynomial. After substitution of $p(0) = 1 + p_2 v\mu$ our problem becomes to find

$$\min_{p_2, p_1} \max_{i \neq 0} \left| p_2(\theta_i^2 + v\mu) + p_1 \theta_i + 1 \right|,$$

so we are looking for a best approximation of the function $-1$ on $S = \{\theta_1, \theta_2, \theta_3\}$ from $W = \{w \mid w(z) = p_2(z^2 + v\mu) + p_1 z\}$, which is a two-dimensional subspace of $C(S)$.

Now suppose we have a best approximation $w^*$ (these always exist), and suppose that it has one critical point ($t = 1$), say $\theta_i$. Then it follows from the lemma that for all $w \in W$, $w(\theta_i) = 0$, which implies that $\theta_i = 0$, a contradiction.

Now suppose that it has two critical points $\theta_i$ and $\theta_j$, with $s_i = \text{sgn}(w^*(\theta_i) + 1)$ and $s_j = \text{sgn}(w^*(\theta_j) + 1)$. Then there are $\alpha_i, \alpha_j > 0$ such that for all $p_2$ and $p_1$ we have

$$\alpha_i s_i \left( p_2(\theta_i^2 + v\mu) + p_1 \theta_i \right) + \alpha_j s_j \left( p_2(\theta_j^2 + v\mu) + p_1 \theta_j \right) = 0.$$

Setting $p_2 = 0$ gives $\alpha_i s_i \theta_i + \alpha_j s_j \theta_j = 0$, from which we find that $s_i = -s_j$. Then we also find by setting $p_1 = 0$ and using the derived equation, that $(\theta_i^2 + v\mu)\theta_j = (\theta_j^2 + v\mu)\theta_i$, which is equivalent to $v\mu = \theta_i \theta_j$. Using that $w^*(\theta_i) + 1 = -(w^*(\theta_j) + 1)$, we find that in this case the optimal value of our problem equals

$$\frac{|\theta_i - \theta_j|}{\theta_i + \theta_j}.$$

Note that here the optimal polynomial is not unique, in fact there are infinitely many.

Next, consider the case that all three eigenvalues $\theta_i$ are critical points with $s_i = \text{sgn}(w^*(\theta_i) + 1)$. Then it follows from Lemma 2.2 that there are $\alpha_i > 0$ such that

$$\sum_{i=1}^{3} \alpha_i s_i (\theta_i^2 + v\mu) = 0, \quad \text{and} \quad \sum_{i=1}^{3} \alpha_i s_i \theta_i = 0,$$

which is equivalent to

$$\alpha_1 s_1 (\theta_3 - \theta_1)(\theta_1 \theta_3 - v\mu) + \alpha_2 s_2 (\theta_3 - \theta_2)(\theta_2 \theta_3 - v\mu) = 0,$$
$$\alpha_3 s_3 (\theta_3 - \theta_1)(\theta_1 \theta_3 - v\mu) + \alpha_2 s_2 (\theta_2 - \theta_1)(\theta_1 \theta_2 - v\mu) = 0.$$

So it follows that if $v\mu < \theta_1 \theta_2$ or $v\mu > \theta_2 \theta_3$, then $s_1 = -s_2 = s_3$. Now the optimal polynomial is uniquely determined giving optimal value

$$\frac{(\theta_3 - \theta_2)(\theta_2 - \theta_1)}{|2(\theta_1 \theta_3 - v\mu) + (\theta_3 - \theta_2)(\theta_2 - \theta_1)|}.$$

Similarly we find that if $\theta_1 \theta_2 < v\mu < \theta_1 \theta_3$, then $-s_1 = s_2 = s_3$ and if $\theta_1 \theta_3 < v\mu < \theta_2 \theta_3$, then $s_1 = s_2 = -s_3$, giving similar expressions as above for the optimal value. It is no surprise that the optimal value is a continuous function of $\mu$. Thus we find the "optimal" bound.

If for every vertex the bound is tight, then it follows (similarly as before) that $J - (v - n_3)(p_2(Q^2 - \mu J) + p_1 Q + p_0 I)$ is the adjacency matrix of $G_\mu$ and that this graph is a strongly regular $(v, n_3, \lambda, \lambda)$ graph. Moreover, if $G$ is regular, then we have to prove that we have a three-class association scheme. To show this, suppose that $G$ is regular with degree $k$ and adjacency matrix $A$. Furthermore, let $A_3$ be the adjacency matrix of $G_\mu$, and $A_2 = J - I - A - A_3$ be the adjacency matrix of $G_{\neg\mu}$. As $Q = kI - A$, it follows that $A_3, A_2 \in \langle A^2, A, I, J \rangle$, the adjacency algebra $\mathbf{A}$ of $G$. Since $G$ is regular with four eigenvalues, it follows that $A^3 \in \mathbf{A}$. This implies that $\langle A_3, A_2, A, I \rangle = \mathbf{A}$, and so $G, G_\mu$ and $G_{\neg\mu}$ form a three-class association scheme.

On the other hand, if $G$ is a graph with four eigenvalues such that $G, G_\mu$ and $G_{\neg\mu}$ form a three-class association scheme and $G_\mu$ is a strongly regular $(v, n_3, \lambda, \lambda)$ graph then the bound is tight for every vertex. The proof is similar to the situation in the previous section. Here we have to show that the bound is tight for some polynomial $p(z) = p_2 z^2 + p_1 z + p_0$ such that $p(0) = 1 + p_2 v\mu$. Now there are $q_2, q_1$ and $q_0$ such that $(J - A_3)/(v - n_3) = q_2(A^2 - \mu J) + q_1 A + q_0 I$. If we now take $q(z) = q_2 z^2 + q_1 z + q_0$, then it follows by taking row sums in the matrix equation that $q(k) = 1 + q_2 v\mu$, and by taking $p(z) = q(k - z)$, we find the required polynomial (note that $p_2 = q_2$). It gives a tight bound, which is proven similarly as in the proof of Theorem 3.1.                                           □

Examples of graphs for which the bound is tight, and $\mu \neq 0$, are given by the line graph of the Petersen graph ($\mu = 1, n_3 = 8$), the Johnson graph $J(7, 3)$ ($\mu = 4, n_3 = 18$), the distance two graph of the generalized hexagon $GH(q, q)$ ($\mu = q^3 + q^2 - q - 1, n_3 = q^5$) and several graphs in the association schemes that are obtained by Hoffman-colorings in strongly regular $(v, n_3, \lambda, \lambda)$ graphs (cf., [5]).

The bound, in general, does not prove the conjecture mentioned in the beginning of this section. For example, suppose we have a regular graph with spectrum $\{[5]^1, [\sqrt{5}]^7, [-1]^5, [-\sqrt{5}]^7\}$. After rounding the numbers, the bound gives $n_3 \leq 2, 15, 3, 1, 0, 0$ for $\mu = 0, 1, 2, 3, 4, 5$, respectively. The conjectured bounds, however, are $2, 14, 2, 0, 0, 0$, respectively. There is precisely one graph with the given spectrum (cf., [9]), for which every vertex has $n_3 = 1, 12, 1, 0, 0, 0$, respectively.

## 5.   Equally large sets at maximal distance

In case we have two equally large sets at maximal distance, we derive the following from Theorem 2.1.

**Theorem 5.1**  *Let G be a connected graph on v vertices with $r + 1$ distinct Laplace eigenvalues $0 = \theta_0 < \theta_1 < \cdots < \theta_r$. Let $X_1$ and $X_2$ be sets of vertices of size $\kappa$, such that the distance between any vertex of $X_1$ and any vertex of $X_2$ is $r$. Then*

$$\kappa \leq \frac{v}{1 + \gamma}, \quad \text{where } \gamma = \sum_{j \neq 0} \prod_{i \neq 0, j} \frac{\theta_i}{|\theta_j - \theta_i|}.$$

If the bound is tight then again we must have tight interlacing in Theorem 2.1, and so the partition of $M$ is regular. It now follows that the partition of $p(Q)$ induced by the partition of the vertices into $X_1$, $X_2$ and the set of remaining vertices is regular with quotient matrix

$$\begin{pmatrix} \frac{\kappa}{v-\kappa} & 1 - \frac{\kappa}{v-\kappa} & 0 \\ \frac{\kappa}{v-\kappa} & 1 - \frac{2\kappa}{v-\kappa} & \frac{\kappa}{v-\kappa} \\ 0 & 1 - \frac{\kappa}{v-\kappa} & \frac{\kappa}{v-\kappa} \end{pmatrix}.$$

If we have only three Laplace eigenvalues then Theorem 5.1 states that if we have two sets of vertices of size $\kappa'$, such that there are no edges between the two sets, then

$$\kappa' \leq \frac{1}{2} v (1 - \theta_1/\theta_r).$$

This bound on the size of two equally large sets of size $\kappa'$ with no edges in between, holds for any connected graph with $r + 1$ distinct Laplace eigenvalues. Here we have to use the first degree polynomial $p(z) = 1 - 2z/(\theta_1 + \theta_r)$. This method was used by Haemers [11] to find a bound due to Helmberg et al. [12] on the bandwidth of a graph. If the bound on $\kappa'$ is tight, then it follows that the Laplace matrix $Q$ is regularly partitioned with quotient matrix

$$\begin{pmatrix} \theta_1 & -\theta_1 & 0 \\ \frac{1}{2}(\theta_1 - \theta_r) & \theta_r - \theta_1 & \frac{1}{2}(\theta_1 - \theta_r) \\ 0 & -\theta_1 & \theta_1 \end{pmatrix}.$$

Thus a necessary condition for tightness is that $\theta_r - \theta_1$ is an even integer.

Connected graphs with three Laplace eigenvalues have a nice combinatorial characterization. They are the connected graphs with constant $\mu$ and $\bar{\mu}$, that is, any two vertices that are not adjacent have $\mu$ common neighbours, and in the complement of the graph any two vertices that are not adjacent have $\bar{\mu}$ common neighbours. Moreover, in such a graph only two vertex degrees can occur, and the regular ones are precisely the strongly regular graphs (cf., [7]).

Families of (strongly regular) graphs for which we have a tight bound are given by the complete multipartite graphs $K_{m \times n}$ for even $n$, with $\kappa \le \frac{1}{2}n$, the triangular graphs $T(n)$ for even $n$, with $\kappa \le \binom{\frac{1}{2}n}{2}$, and the lattice graphs $L_2(n)$ for even $n$, with $\kappa \le (\frac{1}{2}n)^2$. Checking the list of feasible parameter sets in [7], it follows that besides the mentioned graphs, the only connected graphs with three Laplace eigenvalues on at most 27 vertices for which the bound can be tight are the graphs obtained from polarities in 2-(15, 8, 4), 2-(16, 6, 2) and 2-(21, 5, 1) designs. A symmetric design has a polarity if and only if it has a symmetric incidence matrix, and then we consider the graph which has the incidence matrix minus its diagonal as adjacency matrix. For example, the matrices given by

$$
\begin{pmatrix}
D_1 & & I\,I & I\,P & O\,O \\
 & I\,I & I\,I & P\,I & O\,O \\
I\,I & D_2 & O\,O & I\,P \\
I\,I & & O\,O & P\,I \\
I\,P & O\,O & D_3 & I\,I \\
P\,I & O\,O & & I\,I \\
O\,O & I\,P & I\,I & D_4 \\
O\,O & P\,I & I\,I &
\end{pmatrix}
, \quad \text{with } D_i \in \left\{ \begin{pmatrix} O & J \\ J & O \end{pmatrix}, \begin{pmatrix} J & O \\ O & J \end{pmatrix} \right\},
$$

where

$$
O = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad J = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
$$

are incidence matrices of 2-(16, 6, 2) designs with a polarity, and we obtain graphs with Laplace spectrum $\{[8]^m, [4]^{15-m}, [0]^1\}$ for $m = 5, 6, 7, 8,$ and 9. For these graphs we have $\kappa \le 4$, and the bound is tight, as we can see from the matrices. The regular graphs in this example are the Clebsch graph and the lattice graph $L_2(4)$. The only other regular graph obtained from a 2-(16, 6, 2) design with a polarity is the Shrikhande graph, and also here the bound is tight. The triangular graph $T(6)$ is an (the only regular) example obtained from a 2-(15, 8, 4) design with a polarity, and it has tight bound $\kappa \le 3$. Furthermore, there are precisely two graphs that can be obtained from a polarity in the 2-(21, 5, 1) design (the projective plane of order 4), and for both graphs the bound $\kappa \le 6$ is tight.

Besides the graphs we already mentioned, there are only two other strongly regular graphs on at most 35 vertices for which the bound is tight: these are two of the three Chang graphs. These graphs have the same spectrum as and are obtained from switching in the triangular graph $T(8)$. The one that is obtained from switching with respect to a 4-coclique and the one that is obtained from switching with respect to an 8-cycle have a tight bound, the one that is obtained from switching with respect to the union of a 3-cycle and a 5-cycle not.

Next, consider the connected regular graphs with four eigenvalues. Whenever $G$ is a 2-antipodal distance-regular graph with diameter 3, so that it has eigenvalues $k > \lambda_1 >$

$\lambda_2 = -1 > \lambda_3$, with $\lambda_1\lambda_3 = -k$, then $G \circledast J_n$ (the graph with vertex set $V \times \{1, \ldots, n\}$, where $V$ is the vertex set of $G$, and where two distinct vertices $(v, i)$ and $(w, j)$ are adjacent if and only if $v = w$ or $v$ and $w$ are adjacent in $G$) is a connected regular graph with four eigenvalues (cf., [4]), for which the bound $\kappa \leq n$ is tight. Checking the list of feasible parameter sets in [9], it follows that the only other examples of regular graphs with four eigenvalues on at most 30 vertices, for which the bound is tight, are given by the four incidence graphs of 2-(15, 8, 4) designs, which all have a tight bound $\kappa \leq 3$. The problem of finding two sets of size 3 at distance 3 is equivalent to finding three points all of which are incident with three blocks in the corresponding complementary 2-(15, 7, 3) designs.

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