Bounds on separated pairs of subgraphs, eigenvalues and related polynomials

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Abstract. We give a bound on the sizes of two sets of vertices at a given minimum distance (a separated pair of subgraphs) in a graph in terms of polynomials and the spectrum of the graph. We find properties of the polynomial optimizing the bound. 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 are given, and we find graphs for which the bounds are tight.

1. Introduction

In an earlier paper by Van Dam and Haemers [5], a bound on the sizes of two sets of vertices at a given minimum distance (a separated pair of subgraphs) in a graph in terms of polynomials and the spectrum of the graph was derived. The problem is to choose good polynomials. This problem occured in [3, 5, 8] to bound the diameter of a graph in terms of its eigenvalues. Chung, Faber and Manteuffel [3] and Van Dam and Haemers [5] used Chebyshev polynomials, while Fiol, Garriga and Yebra [8] looked at the best possible polynomials.

Here we also consider the optimal polynomials. They are used to 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, in terms of the Laplace spectrum of the graph. The two bounds are equivalent for regular graphs with four distinct eigenvalues, and here the graphs for which the bounds are tight are characterized.

Other applications are 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. We 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 $Q_{xx} = k_x$, 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 λ_i and its Laplace eigenvalues θ_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 [9]. We frequently use distance-regular graphs, for which we refer to the book by Brouwer, Cohen and Neumaier [1].

2. The tool

The next theorem, which is our main tool, is a theorem by Van Dam and Haemers [5], except that now the Laplace matrix instead of the adjacency matrix is used.

THEOREM 2.1. Let G be a connected graph on v vertices with r distinct Laplace eigenvalues $0 = \theta_1 < \theta_2 < ... < \theta_r$. 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

$$\frac{|X| |Y|}{(v-|X|)(v-|Y|)} \le \max_{i \ne 1} p^{2}(\theta_{i}) .$$

Proof. Let *G* have Laplace matrix *Q*, then $p(Q)_{ij} = 0$ for all vertices $i \in X$ and $j \in Y$. 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

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

Note that *M* is symmetric, has row and column sums equal to 1, and its spectrum is $\{\pm p(\theta_i) \mid i = 1, 2, ..., r\}$ including multiplicities. Let *M* be partitioned symmetrically in the following way.

$$M = \begin{pmatrix} O & \vdots & O & \vdots & \vdots & O \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ O & \vdots & O & \vdots & & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & O & \vdots & O \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ O & \vdots & \vdots & O & \vdots & O \\ \end{pmatrix} \begin{vmatrix} |X| \\ |V-|X| \\ |V-|Y| \\ |V| \end{vmatrix}$$

Let B be 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 $\lambda_1(B) = -\lambda_4(B) = 1$, $\lambda_2(B) = -\lambda_3(B) = \sqrt{\frac{|X||Y|}{(v-|X|)(v-|Y|)}}$. Since the

eigenvalues of B interlace those of M (cf. [9]), we have that

$$\lambda_2(B) \leq \lambda_2(M) \leq \max_{i \neq 1} |p(\theta_i)|$$
,

and the theorem follows.

To obtain the sharpest bound we have to minimize $\max_{i \neq 1} |p(\theta_i)|$ over all polynomials p of degree m such that p(0) = 1. This problem occured in earlier papers [3, 5, 8] 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, Garriga and Yebra [8] the optimal polynomials were investigated. In the next section we shall say some more on these polynomials.

3. The optimal polynomials

Consider the set $P_{m,\mu}$ of all polynomials of degree *m* such that $p(\mu) = 1$. It was proven by Chatelin [2, Thm. 7.1.6] that if we have *r* distinct real numbers $\mu = \mu_1, \mu_2, ..., \mu_r$, and m + 1 < r, then there is a subset *S* of $\{2, ..., r\}$ of size m + 1 such that the polynomial *p* given by

$$p(z) = c_s \sum_{j \in S} \prod_{i \in S \setminus \{j\}} \frac{z - \mu_i}{|\mu_j - \mu_i|} \operatorname{sgn}(\mu - \mu_i) ,$$

where c_s is such that $p(\mu) = 1$, minimizes

$$\max_{i\neq 1} |p(\mu_i)|$$

over all polynomials $p \in P_{m,\mu}$.

Since for any subset T of $\{2, ..., r\}$ of size m + 1 we have that

$$|c_{T}| = \min_{p \in P_{m,\mu}} \max_{i \in T} |p(\mu_{i})| \le \min_{p \in P_{m,\mu}} \max_{i \neq 1} |p(\mu_{i})| = |c_{S}|,$$

and so

$$|c_{s}| \leq \max_{T \subset \{2,...,r\}, |T|=m+1} |c_{T}| \leq |c_{s}|$$
,

we now find that the minimum equals

$$|c_{S}| = \max_{T \subset \{2,...,r\}, |T| = m+1} \left(\sum_{j \in T} \prod_{i \in T \setminus \{j\}} \frac{|\mu - \mu_{i}|}{|\mu_{j} - \mu_{i}|} \right)^{-1}$$

In the cases that we are interested in, we have that $\mu = \min_{i} \mu_{i}$ or $\mu = \max_{i} \mu_{i}$. It follows from the theory of approximation, and it was also proven by Fiol, Garriga and Yebra [8] that in these cases the optimal polynomial is unique, and it is known that p(x) is the optimal polynomial if and only if there are $x_{j} \in \{\mu_{i} | i = 2,..., r\}$, j = 1,..., m + 1, such that $x_{1} < x_{2} < ... < x_{m+1}$, and $p(x_{j})$ is alternating $\pm \max_{i \neq 1} |p(\mu_{i})|$ (cf. [11, Thm. 2.8 and 2.10]). From this property it follows that, up to a factor (such that $p(\mu) = 1$), the optimal polynomial does not depend on the actual value of μ (as long as $\mu = \min_{i} \mu_{i}$ or $\mu = \max_{i} \mu_{i}$). Together with the fact that the minimum $|c_{s}|$ is smaller than 1 it now follows that we must have $x_{i} = \min_{i} \mu_{i}$ and $x_{i} = \max_{i} \mu_{i}$

1, it now follows that we must have $x_1 = \min_{i \neq 1} \mu_i$ and $x_{m+1} = \max_{i \neq 1} \mu_i$.

In the case m = 2, where we have to find the optimal polynomial of degree two, it is easily verified that we have to take $x_2 = \mu_h$, the number closest to $(x_1 + x_3)/2$.

4. The number of vertices at maximal distance and distance two

It is well known that if a graph has r distinct (Laplace) eigenvalues, then it has diameter at most r - 1. Using the results of the previous section and Theorem 2.1 we find the following.

THEOREM 4.1. Let G be a connected graph on v vertices with r distinct Laplace eigenvalues $0 = \theta_1 < \theta_2 < ... < \theta_r$. Let x be an arbitrary vertex, then for the number of vertices k_{r-1} at distance r - 1 from x we have that

$$k_{r-1} \leq \frac{v}{1 + \frac{1}{c^{2}(v-1)}} , \text{ where } c = \left(\sum_{j \neq 1} \prod_{i \neq 1, j} \frac{\theta_i}{|\theta_j - \theta_j\rangle|}\right)^{-1}$$

Proof. Take $X = \{x\}$, and let Y be the set of vertices at distance r - 1 from x. Now take the optimal polynomial given in the previous section and apply Theorem 2.1, then the bound follows.

In particular, we find that if $v < 1 + c^{-1}$, so that $k_{r-1} < 1$, then the diameter of G is at most r - 2, a result that was already found by Van Dam and Haemers [5, Thm. 2.5].

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. [9]). Therefore

$$p(Q) = \begin{pmatrix} a & \vdots & aj^{T} & \vdots & o^{T} \\ \cdots & \cdots & \cdots & \cdots \\ aj & \vdots & S_{11} & \vdots & S_{12} \\ \cdots & \cdots & \cdots & \cdots \\ o & \vdots & S_{12}^{T} & \vdots & S_{22} \end{pmatrix} \mid v - 1 - k_{r-1} ,$$

where $a = 1/(v - k_{r-1})$, 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 $J - (v - k_{r-1})p(Q)$ is the adjacency matrix of the distance r - 1 graph G_{r-1} of G, and that this graph is a strongly regular $(v, k_{r-1}, \lambda = \mu)$ graph.

On the other hand we can prove that if G is a distance-regular graph with diameter r - 1 such that the distance r - 1 graph G_{r-1} of G is a strongly regular $(v, k_{r-1}, \lambda = \mu)$ graph then the bound is tight for every vertex. To do this we have to prove that

$$k_{r-1} = \frac{v}{1 + \frac{1}{c^{2}(v-1)}}$$
, where $c = \max_{i \neq 1} |p(\theta_i)|$,

for some polynomial p of degree r - 2 such that p(0) = 1. This suffices because of the optimality of the bound. Assume that G has degree k, then its Laplace eigenvalues θ_i and its (adjacency) eigenvalues λ_i are related by $\lambda_i = k - \theta_i$. Since G is distance-regular, there is a polynomial q of degree r - 2 such that

$$q(A) = (J - A_{r-1})/(v - k_{r-1}) = (A_{r-2} + \dots + A + I)/(v - k_{r-1}),$$

and then q(k) = 1. Now let p(x) = q(k - x). We have that G_{r-1} is a strongly regular $(v, k_{r-1}, \lambda = \mu)$ graph, and such a graph has (adjacency) eigenvalues k_{r-1} and $\pm \sqrt{k_{r-1}(v - k_{r-1})/(v - 1)}$. From this it follows that

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

which is equivalent to what we want to prove.

Examples are given by all 2-antipodal distance-regular graphs, since they have a disjoint union of edges as G_{r-1} (so with $k_{r-1} = 1$). Other examples are given by the odd graph on 7 points ($k_3 = 18$) and the generalized hexagons GH(q, q) ($k_3 = q^5$).

If G is a connected regular graph with four distinct eigenvalues then the statement can be

reversed, i.e. a tight bound for every vertex implies distance-regularity.

THEOREM 4.2. Let G be a connected regular graph on v vertices with four distinct eigenvalues $k = \lambda_1 > \lambda_2 > \lambda_3 > \lambda_4$. Let x be an arbitrary vertex, then for the number of vertices k_3 at distance 3 from x we have that

$$k_3 \leq \frac{v}{1 + \frac{1}{c^2(v-1)}} , \text{ where } c = \left(\sum_{j \neq 1} \prod_{i \neq 1, j} \frac{|k - \lambda_i|}{|\lambda_j - \lambda_i|}\right)^{-1} ,$$

with equality for every vertex if and only if G is distance-regular such that the distance three graph G_3 of G is a strongly regular (v, k_3 , $\lambda = \mu$) graph.

Proof. What remains to prove is that *G* is distance-regular if the bound is tight for every vertex. In that case we already derived that $A_3 = J - (v - k_3)p(Q)$. Since Q = kI - A and *p* is a polynomial of degree two, it follows that $A_3 \in \langle A^2, A, I, J \rangle$. Since the adjacency matrix A_2 of the distance two graph of *G* follows from $A_3 + A_2 + A + I = J$, and *G* has four eigenvalues, so that (cf. [4])

$$(A - \lambda_2 I)(A - \lambda_3 I)(A - \lambda_4 I) = \frac{(k - \lambda_2)(k - \lambda_3)(k - \lambda_4)}{v} J,$$

we find that we have an association scheme, thus proving that G is distance-regular. \Box

The upper bound for k_3 gives a lower bound for k_2 , the number of vertices at distance 2, since $k_2 = v - 1 - k - k_3$. Van Dam and Haemers [7] conjectured another lower bound for k_2 for connected regular graphs with four distinct eigenvalues in terms of the spectrum of the graph. They characterized the distance-regular graphs with diameter three as the graphs for which equality holds.

Here the lower bound for k_2 generalizes to connected regular graphs with more than four distinct eigenvalues, since we can bound the number of vertices $k_{\geq 3}$ at distance at least three, using the optimal polynomial of degree two (see the last remark of Section 3).

THEOREM 4.3. Let G be a connected regular graph on v vertices with $r \ge 4$ distinct eigenvalues $k = \lambda_1 > \lambda_2 > ... > \lambda_r$, and let λ_h be the eigenvalue unequal to λ_2 and λ_r , which is closest to $(\lambda_2 + \lambda_r)/2$. Let x be an arbitrary vertex, then for the number of vertices k_2 at distance 2 from x we have that

$$k_{2} \geq v - 1 - k - \frac{v}{1 + \frac{1}{c^{2}(v-1)}}, \text{ where } c = \left(\sum_{\substack{j=2,h,r \ i \neq j}} \prod_{\substack{i=2,h,r \ i \neq j}} \frac{|k - \lambda_{i}|}{|\lambda_{j} - \lambda_{i}|}\right)^{-1}.$$

Similarly as before, equality for every vertex implies that $G_{\geq 3}$ is a strongly regular

 $(v, k_{\geq 3}, \lambda = \mu)$ graph, and so $G_{1,2}$ is a strongly regular $(v, k + k_2, \lambda' = \mu' - 2)$ graph. Vice versa, if G is a distance-regular graph, such that $G_{1,2}$ is a strongly regular $(v, k + k_2, \lambda' = \mu' - 2)$ graph, then the bound is tight for every vertex. Note that G must have diameter 3 or 4. We do not know any graph with more than four distinct eigenvalues for which the bound is tight.

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 distinct Laplace eigenvalues $0 = \theta_1 < \theta_2 < ... < \theta_r$. Let X_1 and X_2 be sets of vertices of size κ , such that the distance between any vertex of X_1 and any vertex of X_2 is r - 1, then

$$\kappa \leq \frac{v}{1 + \frac{1}{c}} , \text{ where } c = \left(\sum_{j \neq 1} \prod_{i \neq 1, j} \frac{\theta_i}{|\theta_j - \theta_i|} \right)^{-1} .$$

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

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

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

$$\kappa' \leq v(\theta_r - \theta_2)/(2\theta_r).$$

This bound on the size of two equally large sets of size κ' with no edges in between, holds for any connected graph with *r* distinct Laplace eigenvalues. Here we have to use the first degree polynomial $p(x) = 1 - 2x/(\theta_2 + \theta_r)$. This method was used by Haemers [9] to find a bound due to Helmberg, Mohar, Poljak and Rendl [10] on the bandwidth of a graph.

If the bound on κ' is tight, then it follows that the Laplace matrix Q is regularly

partitioned with quotient matrix

$$\begin{pmatrix} \theta_2 & -\theta_2 & 0\\ \frac{1}{2}(\theta_2 - \theta_r) & \theta_r - \theta_2 & \frac{1}{2}(\theta_2 - \theta_r)\\ 0 & -\theta_2 & \theta_2 \end{pmatrix}.$$

Thus a necessary condition for tightness is that $\theta_r - \theta_2$ is even.

Connected graphs with three distinct Laplace eigenvalues have a nice combinatorial characterization. They are the connected graphs with constant μ and $\overline{\mu}$, that is, any two vertices that are not adjacent have μ common neighbours, and in the complement of the graph any two vertices that are not adjacent have $\overline{\mu}$ common neighbours (cf. [6]). Moreover, in such a graph only two vertex degrees can occur, and the regular ones are precisely the strongly regular graphs.

Families of (strongly regular) graphs for which we have a tight bound are given by the multipartite complete graphs $K_{m\times n}$ for even *n*, with $\kappa \le n/2$, the triangular graphs T(n) for even *n*, with $\kappa \le \binom{n/2}{2}$, and the lattice graphs OA(*n*, 2) for even *n*, with $\kappa \le (n/2)^2$. Besides these, the only connected graphs with three distinct 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

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

where

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

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 OA(4, 2). 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 $\kappa \leq 3$.

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 $\kappa \leq 6$ 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 are cospectral with and 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 8-cycle have a tight bound, the one that is obtained from switching with respect to 8-cycle and a 5-cycle not.

Now consider the connected regular graphs with four distinct eigenvalues. Whenever *G* is a 2-antipodal distance-regular graph with diameter 3, so that it has eigenvalues $k > \lambda_2 > -1 > \lambda_4$, with $\lambda_2 \lambda_4 = -k$, then $G \oplus J_n$ (the graph with vertex set $V \times \{1, ..., n\}$, 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 distinct eigenvalues (cf. [4]), for which the bound $\kappa \leq n$ is tight.

The only other examples of regular graphs with four distinct 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 three 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) design.

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