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Graphs with given diameter maximizing the spectral radius

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Abstract

We determine the graphs with maximal spectral radius among the ones on n nodes with diameter D.

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In this note we determine the graphs with maximal spectral radius among the ones on n nodes with diameter D. This complements the results in [2] on graphs with minimal spectral radius for given number of nodes and diameter. Motivation for this problem comes from virus spreading in networks, cf. [2]. Other related work is done by Guo and Shao [5] who determined the trees with maximal spectral radius for fixed diameter.

Let $M(n, D)$ be the graph obtained from a complete graph on $n - D + 2$ nodes by removing an edge, adding a pendant path of $\lceil \frac{D}{2} \rceil - 1$ edges to one endnode of the removed edge, and adding a pendant path of $\lfloor \frac{D}{2} \rfloor - 1$ edges to its other endnode.

Theorem. *Let n and D be integers, with $1 < D < n$. Then the graph $M(n, D)$ is the graph with maximal spectral radius among all graphs on n nodes with diameter D.*

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The proof of this result will be established in a number of steps. First of all, we need the fact that adding edges to a connected graph increases the spectral radius (cf. [1, p. 19]). This allows us to prove the following.

Lemma 1. *Let n and D be integers, with* $1 < D < n$. *Then a graph with maximal spectral radius among all graphs on n nodes with diameter D is a graph obtained from the path* P_{D+1} *by replacing the nodes by cliques, such that nodes in distinct cliques are adjacent if and only if the corresponding original nodes in the path are adjacent. Moreover, the cliques corresponding to the endnodes have size* 1.

Proof. Consider a graph with maximal spectral radius among the graphs on n nodes with diameter D. Since the diameter of the graph is D, there are nodes v_0 and v_D at distance D. Let N_i be the set of nodes at distance i from v_0, for $i = 0, 1, \ldots, D$. If the graph is not of the claimed form, then one of the sets N_i contains two nodes that are not adjacent, or there is a node in N_i and a node in N_{i+1} that are not adjacent, or the set N_D contains more than one element. In the first two cases this gives a contradiction, since adding the missing edge increases the spectral radius and leaves the diameter the same. In the last case it also does, since adding edges between all but one node of N_D and all nodes of N_{D-2} increases the spectral radius, and leaves the diameter the same. □

Let G now be a graph with maximal spectral radius among all graphs on n nodes with diameter D. According to Lemma 1 it consists of "pathwise adjacent cliques". Let us call these cliques N_i, $i = 0, 1, \ldots, D$, ordered such that all nodes of N_i are adjacent to all nodes of N_{i+1}, for $i = 0, 1, \ldots, D - 1$. Let n_i be the size of N_i, for $i = 0, 1, \ldots, D$. From Lemma 1 we know that $n_0 = n_D = 1$. The following lemma states that there is only one clique N_i of size bigger than 1.

Lemma 2. *There is at most one i such that* $n_i > 1$.

Proof. Consider the partition of the nodes into the sets N_i, and the corresponding quotient matrix of the adjacency matrix of G, i.e., the matrix Q labeled by the sets N_i, where Q_{N_i,N_j} equals the average number of neighbours in N_j, of the nodes in N_i. Since here we have that for all i and j the number of neighbours in N_j is the same for all nodes in N_i (the partition is called regular, or equitable), it follows that the spectral radius of Q is the same as the spectral radius of G (cf. [4, p. 79]). Moreover, Q is the following tridiagonal matrix:

$$Q = \begin{bmatrix} 0 & n_1 & 0 & 0 & \cdots & 0 \\ 1 & n_1 - 1 & n_2 & 0 & \cdots & 0 \\ 0 & n_1 & n_2 - 1 & \ddots & \ddots & \vdots \\ 0 & 0 & n_2 & \ddots & n_{D-1} & 0 \\ \vdots & \vdots & \ddots & \ddots & n_{D-1} - 1 & 1 \\ 0 & 0 & \cdots & 0 & n_{D-1} & 0 \end{bmatrix},$$

and if x is a positive eigenvector of Q corresponding to the spectral radius ρ, then the vector y defined by $y_v = x_i$ if v is a node in N_i is an eigenvector of the adjacency matrix A of G, with eigenvalue ρ. Without loss of generality we normalize x in such a way that y has length

1. Thus $\rho = y^\top Ay$. Moreover, from the eigenvalue equation $Qx = \rho x$ we obtain that $\rho x_i = n_{i-1}x_{i-1} + (n_i - 1)x_i + n_{i+1}x_{i+1}$ for $i = 1, \ldots, D-1$.

Suppose now that $n_s > 1$ and $n_t > 1$, where $s \neq t$. Without loss of generality we may assume that $x_s \geqslant x_t$. Consider then the graph G' obtained from G by moving one node from clique N_t to clique N_s. Then G' has the same number of nodes and diameter as G (and it is of similar form, as in Lemma 1). If A' is the adjacency matrix of G' with spectral radius ρ', then it follows that if s and t differ by more than one, then $\rho' \geqslant y^\top A'y = y^\top Ay + 2x_t(n_{s-1}x_{s-1} + n_s x_s + n_{s+1}x_{s+1} - n_{t-1}x_{t-1} - (n_t - 1)x_t - n_{t+1}x_{t+1}) = \rho + 2x_t(x_s + \rho(x_s - x_t)) > \rho$. Since G has maximal spectral radius, this gives a contradiction. If s and t differ by one, then we find similarly that $\rho' \geqslant y^\top A'y = \rho + 2x_t(\rho + 1)(x_s - x_t) \geqslant \rho$. This implies that $\rho' = \rho$, and that y is also an eigenvector of A' with eigenvalue ρ. It then follows that $Ay = A'y$, which gives a contradiction by considering the entry of a node in N_{s-1} or N_{s+1} (depending on whether s is smaller or larger than t) in these vectors. Thus the made assumption is not true, and the statement is proven. □

From now on, consider graphs of the form in Lemma 1 where at most one of the cliques, say N_a, has size bigger than one. Let $m = n_a$ be fixed in the remainder, and let $b = D - a$. Notice that these are graphs obtained from a complete graph on $m + 2 = n - D + 2$ nodes by removing an edge, adding a pendant path of $a - 1$ edges to one endnode of the removed edge, and adding a pendant path of $b - 1$ edges to its other endnode. Thus we have proven the theorem if we can show that a and b differ by at most one in a graph with maximal spectral radius.

Let $C_{a,b}$ be the characteristic polynomial of the quotient matrix Q of the above graph (on $n = a + m + b$ nodes and with diameter $D = a + b$), i.e., $C_{a,b}(\lambda) = \det(\lambda I - Q)$. Also, let P_k be the characteristic polynomial of the path on k nodes.

Lemma 3. *If* $a > b + 1 \geqslant 1$, *then* $C_{a,b}(\lambda) - C_{a-1,b+1}(\lambda) = (m-1)(\lambda+1)P_{a-b-2}(\lambda)$.

Proof. If $b > 0$ then it follows from expansion of the determinant that $C_{a,b}(\lambda) = \lambda C_{a-1,b}(\lambda) - C_{a-2,b}(\lambda)$ and that $C_{a-1,b+1}(\lambda) = \lambda C_{a-1,b}(\lambda) - C_{a-1,b-1}(\lambda)$, and hence it follows that $C_{a,b} - C_{a-1,b+1} = C_{a-1,b-1} - C_{a-2,b}$. Thus it follows by induction that $C_{a,b} - C_{a-1,b+1} = C_{a-b,0} - C_{a-b-1,1}$.

Now let $T_c = C_{c,0} - C_{c-1,1}$ for $c > 0$. From expansion of the determinants in $C_{c,0}$ and $C_{c-1,1}$ it follows that $T_c(\lambda) = \lambda T_{c-1}(\lambda) - T_{c-2}(\lambda)$ for $c > 2$. Thus T_c satisfies the same recurrence relation as the characteristic polynomials of the paths. Since $T_1 = C_{1,0} - C_{0,1} = 0$ and since it can be shown that $T_2(\lambda) = C_{2,0}(\lambda) - C_{1,1}(\lambda) = (m-1)(\lambda+1) = (m-1)(\lambda+1)P_0(\lambda)$, it now readily follows that $T_c(\lambda) = (m-1)(\lambda+1)P_{c-2}(\lambda)$. The claimed statement now follows. □

To finish the proof of the theorem, suppose that a and b differ by more than 1 in a graph with maximal spectral radius. Without loss of generality we may assume that $a > b + 1$. Since the theorem is trivially true for $D = n - 1$ ($m = 1$), we also assume that $m \geqslant 2$. Then the graph contains a triangle, and hence its spectral radius is at least 2. Since the roots of the characteristic polynomial of a path are all less than 2, it follows from Lemma 3 that the largest root of $C_{a-1,b+1}$ is strictly larger than the largest root of $C_{a,b}$, which is a contradiction, and which completes the proof of the theorem.

Note. After writing this paper, the author was informed about two other papers. Hansen and Stevanović [6] (see [7] for an extended abstract) obtained the same result in a different manner. Feng [3] claims the same result, however with an incomplete proof.

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