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Abstract

We determine a lower bound for the spectral radius of a graph in terms of the number of vertices and the diameter of the graph. For the specific case of graphs with diameter three we give a slightly better bound. We also construct families of graphs with small spectral radius, thus obtaining asymptotic results showing that the bound is of the right order. We also relate these results to the extremal degree/diameter problem.

1 Introduction

In [6], the problem was raised to determine the minimal spectral radius among graphs with given number of vertices and diameter. In [4], we obtained asymptotic results for some cases where the diameter D grows with the number of vertices n. Here we consider the case when D

is fixed, and n grows. We first obtain a general lower bound for the spectral radius of a graph in terms of its number of vertices and its diameter. For the diameter three case, we give a slightly better bound. In the literature we could not find any comparable bounds. Besides the folklore result that the spectral radius is at least the average vertex degree in the graph, the first non-trivial lower bound on the spectral radius of a graph was obtained by Hofmeister [11], who showed that the spectral radius is at least the square root of the average squared vertex degrees, i.e., for a graph with vertex degrees d_v and spectral radius ρ, the bound $\rho^2 \geq \frac{1}{n}\sum_v d_v^2$ holds. Nikiforov [13] generalized this, and obtained a lower bound in terms of the number of certain walks in the graph. An upper bound for the spectral radius in terms of the diameter was recently obtained in [3]: if the graph is not regular, with maximum vertex degree Δ, then $\rho < \Delta - \frac{1}{nD}$.

In Section 3, we construct graphs with small spectral radius, showing that the obtained lower bound is asymptotically of the right order. In the final section we relate our problem to the so-called extremal degree/diameter problem (see [12] for a recent survey on this problem).

Before obtaining the lower bound (in Section 2), we first introduce some terminology as follows. We let $\rho(M)$ denote the spectral radius of a matrix M. The spectral radius of a graph is defined as the spectral radius $\rho(A)$ of its adjacency matrix A. Unless otherwise indicated, for a given graph we let n, D, ρ, and e denote the number of vertices, diameter, spectral radius, and number of edges. Furthermore, we let (d_u) denote the sequence of vertex degrees and Δ the maximum vertex degree.

An ℓ-walk in a graph is a sequence of $\ell+1$ consecutively adjacent vertices (this represents a "walk" of length ℓ along the edges of the graph). By $N_\ell(u)$ we denote the number of ℓ-walks starting in vertex u. Finally, we let $\Gamma_i(u) := \{v \mid d(u,v) = i\}$ be the set of vertices at distance i from u.

2 Lower bounds for the spectral radius

In this section, we shall derive a lower bound for the spectral radius of a graph with given diameter and number of vertices. Then, for the case of diameter three, we shall give a slightly better bound.

2.1 A general lower bound for the spectral radius

We shall show that the spectral radius of a graph with n vertices and diameter D is at least $(n-1)^{1/D}$. This generalizes the following result of Van Dam and Kooij [6] which concerns the case $D = 2$.

Theorem 2.1. *For the spectral radius ρ of a graph with n vertices and diameter two we have that $\rho \geq \sqrt{n-1}$ with equality only for the stars $K_{1,n-1}$, the pentagon, the Petersen graph, the Hoffman-Singleton graph, and putative 57-regular graphs on 3250 vertices.*

In order to prove the general result, we use the following lemma on the number $N_d(u)$ of D-walks starting in an arbitrary vertex u.

Lemma 2.2. *Let Γ be a graph with n vertices and diameter D, and let u be an arbitrary vertex. Then $N_D(u) \geq n-1$. Moreover, $N_D(u) \geq n-1-d_u+d_u^2$ if $D \geq 3$.*

Proof. Let u be a vertex of Γ and v be a different vertex. Let $u = u_0 \sim u_1 \sim u_2 \sim \cdots \sim u_\ell = v$ be a shortest path between u and v. If $\ell < D$, then there exists a D-walk starting with $u_0, u_1, \cdots, u_{\ell-1}, u_\ell, u_{\ell-1}$. If $\ell = D$, then the walk $u = u_0 \sim \cdots \sim u_\ell = v$ is a D-walk. Clearly, each $v \neq u$ gives a different D-walk, which shows that $N_D(u) \geq n - 1$. If $D \geq 3$, then the above d_u walks for $\ell = 1$ can be replaced by the (at least) d_u^2 walks starting with u, v, u, v', which shows the second part of the statement. □

Now we can derive the general lower bound for the spectral radius.

Theorem 2.3. *Let Γ be a graph with n vertices, diameter D, and spectral radius ρ. Then*

$$\rho \geq (n-1)^{1/D}$$

with equality if and only if $D = 1$ and Γ is the complete graph K_n, or $D = 2$ and Γ is the star $K_{1,n-1}$, the pentagon, the Petersen graph, the Hoffman-Singleton graph, or a putative 57-regular graph on 3250 vertices.

Proof. Let A be the adjacency matrix of Γ. By Lemma 2.2, the number of D-walks starting in a vertex u is at least $n - 1$. Since $(A^D)_{uv}$ equals the number of D-walks from u to v, the total number of D-walks starting in u is $(A^D\mathbf{1})_u$, where $\mathbf{1}$ is the all-one vector. Thus, $n(n-1) \leq \mathbf{1}^\top A^D \mathbf{1}$. From the Rayleigh quotient, cf. [10, p. 202], we then obtain that

$$n - 1 \leq \frac{\mathbf{1}^\top A^D \mathbf{1}}{n} = \frac{\mathbf{1}^\top A^D \mathbf{1}}{\mathbf{1}^\top \mathbf{1}} \leq \rho(A^D) = \rho(A)^D.$$

We thus have $\rho = \rho(A) \geq (n-1)^{1/D}$. From Lemma 2.2 it follow that equality can only hold for $D \leq 2$. Equality indeed holds trivially for $D = 1$, and then the result follows from Theorem 2.1. □

Note that in the proof of Lemma 2.2 we only counted very specific D-walks. For $D > 3$, it seems to be difficult to count the exact number of D-walks, but for $D = 3$ we are able to do so under some extra conditions. This leads to a better bound for the spectral radius for $D = 3$.

2.2 An improved bound for diameter three

For graphs with diameter $D \geq 3$, the bound $\rho \geq (n-1)^{1/D}$ is not sharp. In this section we derive a slightly better bound for diameter three.

Theorem 2.4. *Let Γ be a graph with n vertices, e edges, diameter three, and spectral radius ρ. Then*

$$\rho^3 - \rho^2 \geq n - 1 - \frac{2e}{n}, \tag{1}$$

with equality if and only if Γ is the heptagon.

Proof. Let A be the adjacency matrix of Γ, then $\rho = \rho(A)$. Lemma 2.2 states that $(A^3\mathbf{1})_u = N_3(u) \geq n - 1 - d_u + d_u^2$. Moreover, equality holds if and only if u is not contained in any

m-cycle for $m = 3, 4, 5, 6$. This follows for example by careful counting and observing that the right hand side of the inequality is equal to $|\Gamma_3(u)| + |\Gamma_2(u)| + |\Gamma_1(u)|^2$. So it follows that

$$\mathbf{1}^\top A^3 \mathbf{1} \geq \sum_u (n - 1 - d_u + {d_u}^2) = n(n-1) - \sum_u d_u + \sum_u {d_u}^2.$$

Because $\sum_u d_u = 2e$ and $\sum_u {d_u}^2 = (A\mathbf{1})^\top (A\mathbf{1}) = \mathbf{1}^\top A^2 \mathbf{1}$, dividing each side by n gives

$$\rho(A^3 - A^2) \geq \frac{\mathbf{1}^\top (A^3 - A^2)\mathbf{1}}{\mathbf{1}^\top \mathbf{1}} = \frac{\mathbf{1}^\top A^3 \mathbf{1} - \mathbf{1}^\top A^2 \mathbf{1}}{\mathbf{1}^\top \mathbf{1}} \geq n - 1 - \frac{2e}{n}.$$

Note that each eigenvector of A with eigenvalue θ is an eigenvector of $A^3 - A^2$ with eigenvalue $\theta^3 - \theta^2$, and hence also that all eigenvalues $A^3 - A^2$ are obtained in this way. This implies that $\rho(A^3 - A^2) = \rho^3 - \rho^2$ because $\theta^3 - \theta^2 < \rho^3 - \rho^2$ for $\theta < \rho$ (since $\rho > 1$). Thus we obtain the required inequality $\rho^3 - \rho^2 \geq n - 1 - \frac{2e}{n}$.

Next, we are going to classify the graphs Γ with $n - 1 - \frac{2e}{n} = \rho^3 - \rho^2$. Then all above inequalities must be equalities, from which it follows that Γ has no m-cycles for $m \leq 6$, and that the all-one vector $\mathbf{1}$ is an eigenvector of $A^3 - A^2$. The above observations then imply that $\mathbf{1}$ is also an eigenvector of A, i.e., that Γ is a regular graph.

Because Γ is regular with diameter 3 without m-cycles for $m \leq 6$, it is a Moore graph. However, Bannai and Ito [1] and Damerell [7] showed that a Moore graph with diameter $D > 1$ and valency $k > 2$ must have diameter $D = 2$ (and valency $k \in \{3, 7, 57\}$), hence the valency k of Γ should be 2. Therefore Γ is a heptagon, which finishes the proof. □

The bound of Theorem 2.4 is slightly better than the bound $\rho > \sqrt[3]{n-1}$ of Theorem 2.3 as $\rho^2 \geq \rho \geq \frac{2e}{n}$. Using the latter inequality $\rho \geq \frac{2e}{n}$, for which equality holds if and only if Γ is $\frac{2e}{n}$-regular, we also obtain the following.

Corollary 2.5. *Let Γ be a graph with n vertices, diameter three, and spectral radius ρ. Then*

$$\rho^3 - \rho^2 + \rho \geq n - 1,$$

with equality if and only if Γ is the heptagon.

We note that improved bounds can be obtained by considering more detailed information about the graph. For example, if the graph has t triangles, then one easily obtains that

$$\rho^3 - \rho^2 \geq n - 1 - \frac{2e}{n} + \frac{6t}{n}.$$

We finally remark that in a graph with edge set E, the number of 3-walks can also be expressed as $2\sum_{\{u,v\} \in E} d_u d_v$. We do however not know how to use this expression in our approach.

3 Constructions of graphs with small spectral radius

Next, we shall consider graphs with small spectral radius. First, we define

$$\rho_D(n) := \min\{\ \rho(\Gamma) \mid \Gamma \text{ is a graph with } n \text{ vertices and diameter } D\}.$$

In particular we would like to consider the quotient $\rho_D(n)/\sqrt[D]{n-1}$, for which Theorem 2.3 states that

$$\frac{\rho_D(n)}{\sqrt[D]{n-1}} \geq 1.$$

By constructing graphs with small spectral radius, we would like to find good upper bound for the quotient as well.

We first define some terminology. We say that a partition π of the vertex set $V(\Gamma)$ with cells $\pi_1, \cdots, \pi_r$ is equitable if the number of neighbours in π_j of a vertex u in π_i is a constant b_{ij}, independent of u. The directed graph with the r cells of π as vertices and b_{ij} arcs from the ith to the jth cells of π is called the quotient of Γ over π, and denoted by Γ/π. The adjacency matrix $A(\Gamma/\pi) =: Q(\Gamma)$ of this quotient is called the quotient matrix, and it has the same spectral radius as Γ (cf. [9, p. 79]).

Now, let $a \geq 0$, $b \geq 2$, and $t \geq 1$ be integers. We define $X_t(a,b)$ as the graph with an equitable partition $\pi = \{\pi_0, \pi_1, \cdots, \pi_t\}$, where $|\pi_0| = a+1$, with corresponding quotient matrix

$$A(X_t(a,b)/\pi) = \begin{bmatrix} a & b & & & \\ 1 & 0 & b & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & b \\ & & & 1 & 0 \end{bmatrix}.$$

Note that the graph is completely determined by this information, and has diameter $D = 2t$ if $a = 0$, and $D = 2t+1$ otherwise.

Now we shall consider some sequences of graphs for which $\rho_D(n)/\sqrt[D]{n-1} < 2$, for n large enough. For even diameter we take the trees $X_t(0,b), b \geq 2$ with diameter $D = 2t$, and for odd diameter we take the graphs $X_t(a,a^2), a \geq 2$ with diameter $D = 2t+1$. We shall first determine the spectral radius of these graphs.

Lemma 3.1. *Let $t \geq 1$, $a \geq 2$, and $b \geq 2$. Then $\rho(X_t(0,b)) = 2\sqrt{b}\cos\left(\frac{\pi}{t+2}\right)$ and $\rho(X_t(a,a^2)) = 2a\cos\left(\frac{\pi}{2t+3}\right)$.*

Proof. It is easy to see that the quotient matrix $Q(X_t(a,b))$ is similar to $\sqrt{b}Q(X_t(\frac{a}{\sqrt{b}},1))$, hence $\rho(X_t(a,b)) = \sqrt{b}\rho(X_t(\frac{a}{\sqrt{b}},1))$, at least when $\frac{a}{\sqrt{b}}$ is integer.

Now consider the graph $X_t(0,b)$. From the fact that $X_t(0,1)$ is the path P_{t+1}, which has spectral radius $2\cos\left(\frac{\pi}{t+2}\right)$, cf. [5, p. 73], we obtain that $\rho(X_t(0,b)) = \sqrt{b}\rho(X_t(0,1)) = \sqrt{b}\rho(P_{t+1}) = 2\sqrt{b}\cos\left(\frac{\pi}{t+2}\right)$.

Because the graph $X_t(1,1)$ is the path P_{2t+2}, it follows that $\rho(X_t(a,a^2)) = a\rho(X_t(1,1)) = a\rho(P_{2t+2}) = 2a\cos\left(\frac{\pi}{2t+3}\right)$. □

Using this, we determine the limits of the quotients under consideration. Let n_b and n_a be the numbers of vertices of the graphs $X_t(0,b)$ and $X_t(a,a^2)$, respectively.

Proposition 3.2. *Let $t \geq 1$. Then*

$$\lim_{b\to\infty} \frac{\rho(X_t(0,b))}{\sqrt[2t]{n_b-1}} = 2\cos\left(\frac{\pi}{t+2}\right) \quad \textit{and} \quad \lim_{a\to\infty} \frac{\rho(X_t(a,a^2))}{\sqrt[2t+1]{n_a-1}} = 2\cos\left(\frac{\pi}{2t+3}\right).$$

Proof. Because $n_b = 1 + b + b^2 + \cdots + b^t$, it follows that

$$\frac{\rho(X_t(0,b))}{\sqrt[2t]{n_b - 1}} = \frac{2\sqrt{b}\cos\left(\frac{\pi}{t+2}\right)}{\sqrt[2t]{b + b^2 + \cdots + b^t}} = \frac{2\cos\left(\frac{\pi}{t+2}\right)}{\sqrt[2t]{1 + b^{-1} + \cdots + b^{1-t}}} \to 2\cos\left(\frac{\pi}{t+2}\right) \quad (b \to \infty).$$

The other result follows similarly from the fact that $n_a = (a+1)(1 + a^2 + a^4 + \cdots + a^{2t})$. □

Proposition 3.2 immediately implies that $\liminf_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} < 2$. We shall now show that $\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} < 2$ as well. First consider the even diameter case. Let $\mathcal{T}_{2t}(n)$ be a tree with n vertices and diameter $2t$ which is an induced subgraph of $X_t(0,b)$ containing a subgraph $X_t(0,b-1)$. It follows that

$$\frac{\rho(\mathcal{T}_{2t}(n))}{\sqrt[2t]{n-1}} \le \frac{\rho(X_t(0,b))}{\sqrt[2t]{n-1}} = \frac{2\sqrt{b}\cos\left(\frac{\pi}{t+2}\right)}{\sqrt[2t]{n-1}} \le \frac{2\sqrt{b}\cos\left(\frac{\pi}{t+2}\right)}{\sqrt[2t]{n_{b-1}-1}}.$$

Letting $b \to \infty$, we obtain

$$\limsup_{n\to\infty} \frac{\rho(\mathcal{T}_{2t}(n))}{\sqrt[2t]{n-1}} \le 2\cos\left(\frac{\pi}{t+2}\right).$$

The odd diameter case can be handled similarly. Therefore we obtain the following.

Theorem 3.3. *Let $D \ge 1$. Then*

$$\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} \le \begin{cases} 2\cos\left(\frac{\pi}{2+D/2}\right) & \text{if } D \text{ is even;} \\ 2\cos\left(\frac{\pi}{2+D}\right) & \text{if } D \text{ is odd.} \end{cases}$$

In particular,

$$\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} < 2.$$

We conjecture however that the lower bound of the previous section is closer to the truth than this upper bound.

Conjecture 3.4. *Let $D \ge 1$. Then*

$$\lim_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} = 1.$$

4 The degree/diameter problem

Our problem is related to the well-known degree/diameter problem, i.e., the problem to determine graphs with maximum degree Δ and diameter D and with as many vertices as possible, for given Δ and D, cf. [12]. The maximum number of vertices of such graphs is denoted by $n_{\Delta,D}$. An obvious and well-known bound is the so-called Moore bound:

$$n_{\Delta,D} = \sum_{i=0}^{D} |\Gamma_i(v)| \le 1 + \Delta + \Delta(\Delta-1) + \ldots + \Delta(\Delta-1)^{D-1} = 1 + \Delta\frac{(\Delta-1)^D - 1}{\Delta - 2},$$

where we have assumed that $\Delta \geq 3$ to avoid trivialities. Related to the number $n_{\Delta,D}$ is the parameter

$$\mu_D := \liminf_{\Delta\to\infty} \frac{n_{\Delta,D}}{\Delta^D},$$

which was introduced by Delorme [8]. From the Moore bound it follows that $\mu_D \leq 1$. It is known that $\mu_D = 1$ for $D = 1, 2, 3$, and 5, and that $\mu_4 \geq \frac{1}{4}$, cf. [12]. Moreover, Bollobás [2, p. 213] conjectured that $\mu_D = 1$ for $D \geq 3$.

To relate the degree/diameter problem to ours, we introduce $m_{\Delta,D}$ as the maximum number of vertices of a graph with diameter D and spectral radius $\rho \leq \Delta$, for given Δ and D. Similar as for the degree/diameter problem, we introduce the parameter

$$\tilde{\mu}_D := \liminf_{\Delta\to\infty} \frac{m_{\Delta,D}}{\Delta^D}.$$

Because $\rho(\Gamma) \leq \Delta(\Gamma)$ for any graph Γ, it follows that $n_{\Delta,D} \leq m_{\Delta,D}$, and hence that $\mu_D \leq \tilde{\mu}_D$. The relation of the parameter $\tilde{\mu}_D$ to the earlier results in this paper is the following.

Lemma 4.1. *Let $D \geq 1$. Then*

$$\tilde{\mu}_D = \left(\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} \right)^{-D}.$$

Proof. Because $\rho_D(m_{\Delta,D}) \leq \Delta$, we obtain that $\frac{m_{\Delta,D}}{\Delta^D} \leq \frac{m_{\Delta,D}}{\rho_D(m_{\Delta,D})^D}$. From this it follows that

$$\tilde{\mu}_D \leq \liminf_{n\to\infty} \frac{n}{\rho_D(n)^D} = \left(\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} \right)^{-D}.$$

On the other hand, from the definition of $m_{\Delta,D}$ it follows that $\rho_D(m_{\Delta,D}+1) > \Delta$, so

$$\limsup_{\Delta\to\infty} \frac{\Delta}{\sqrt[D]{m_{\Delta,D}}} \leq \limsup_{\Delta\to\infty} \frac{\rho_D(m_{\Delta,D}+1)}{\sqrt[D]{m_{\Delta,D}+1-1}} \leq \limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}},$$

and hence $\tilde{\mu}_D \geq \left(\limsup_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} \right)^{-D}$. □

From the results in Section 3 it now follows that $2^{-D} < \tilde{\mu}_D \leq 1$. The more specific bound for $D = 4$ implies that $\tilde{\mu}_4 \geq \frac{1}{4}$, which also follows from the fact that $\mu_4 \geq \frac{1}{4}$.

Moreover, if $\mu_D = 1$, then also $\tilde{\mu}_D = 1$, and hence $\lim_{n\to\infty} \frac{\rho_D(n)}{\sqrt[D]{n-1}} = 1$. Thus Conjecture 3.4 is true for $D = 1, 2, 3, 5$, and it is true in general if Bollobás' conjecture is true.

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