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The minimal spectral radius of graphs with a given diameter

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Abstract

The spectral radius of a graph (i.e., the largest eigenvalue of its corresponding adjacency matrix) plays an important role in modeling virus propagation in networks. In fact, the smaller the spectral radius, the larger the robustness of a network against the spread of viruses. Among all connected graphs on n nodes the path P_n has minimal spectral radius. However, its diameter D, i.e., the maximum number of hops between any pair of nodes in the graph, is the largest possible, namely $D = n - 1$. In general, communication networks are designed such that the diameter is small, because the larger the number of nodes traversed on a connection, the lower the quality of the service running over the network. This leads us to state the following problem: *which connected graph on n nodes and a given diameter D has minimal spectral radius*? In this paper we solve this problem explicitly for graphs with diameter $D \in \left\{1, 2, \left\lfloor \frac{n}{2} \right\rfloor, n-3, n-2, n-1\right\}$. Moreover, we solve the problem for almost all graphs on at most 20 nodes by a computer search.

AMS classification: 05C50; 05E99; 94C15

Keywords: Graphs; Spectral radius; Diameter; Networks; Virus propagation

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1. Introduction

The theory of the spectra of graphs contains many beautiful results that relate physical properties of a network, such as for instance robustness, diameter, and connectivity, to eigenvalues of matrices associated with the graph, see e.g. [4,13]. Recently it has been shown, see [14], that the spectral radius of a graph (i.e., the largest eigenvalue of its corresponding adjacency matrix) plays an important role in modeling virus propagation in networks. In fact, in [14] the Susceptible-Infected-Susceptible (SIS) infection model is considered. The SIS model assumes that a node in the network is in one of two states: infected and therefore infectuous, or healthy and therefore susceptible to infection. The SIS model assumes instantaneous state transitions. Thus, as soon as a node becomes infected, it becomes infectious and likewise, as soon as a node is cured it is susceptible to re-infection. Epidemiological theory, see for instance [5], predicts the existence of an epidemic threshold τ. If it is assumed that the infection rate along each link is β while the cure rate for each node is δ then the effective spreading rate of the virus can be defined as β/δ. The epidemic threshold can be defined as follows: for effective spreading rates below τ the virus contamination in the network dies out, while for effective spreading rates above τ the virus is prevalent, i.e., a persisting fraction of nodes remains infected. It was shown in [14] that $\tau = 1/\rho(A)$ where $\rho(A)$ denotes the spectral radius of the adjacency matrix A of the graph. If follows from this result that the smaller the spectral radius, the larger the robustness of a network against the spread of viruses.

This naturally leads to the following problem statement: *which connected graph on n nodes has minimal spectral radius*? It can be found for instance in [4] that the path P_n has minimal spectral radius; see also Lemma 1 below.

Although the path P_n has the largest possible epidemic threshold, its diameter D, i.e. the maximum number of hops between any pair of nodes in the graph, is also the largest possible, namely $D = n - 1$. In general, communication networks are designed such that the diameter is small, because the larger the number of nodes traversed on a connection, the lower the quality of the service running over the network. For this reason, we adjust the problem statement above, also taking into account the impact of the diameter of the graph: *which graph on n nodes and a given diameter D has minimal spectral radius*?

As far as we know, the relation between the spectral radius and diameter has so far been investigated by few others: Guo and Shao [7] determined the trees with largest spectral radius among trees of given number of nodes and diameter, while Cioabă et al. [3] gave an upper bound on the spectral radius in terms of the number of nodes, number of links, maximum degree, and diameter. The problem of determining the graphs with maximal spectral radius among the graphs with given diameter is completely solved in [6].

This paper is further organized as follows. In Section 2, we will consider graphs with a large diameter, i.e., $D \in \{n-3, n-2, n-1\}$. In Section 3, we will look at graphs with diameter two and give an explicit expression for the minimal spectral radius of such graphs. In Section 4, we determine the minimal spectral radius of graphs on at most 20 nodes, by using brute computational force. We finish the paper with some concluding remarks in Section 5.

2. Graphs with large diameter

In this section we will explore the relation between the diameter of a connected graph and the minimal spectral radius, in case of a large diameter, i.e., $D \in \{n-3, n-2, n-1\}$. Starting points are the following two well-known results; see for instance [4, p. 21]:

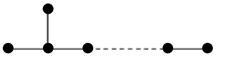

Fig. 1. The graph D_n.

Lemma 1. *Of all connected graphs on n nodes, the path P_n has minimal spectral radius*; $\rho(P_n) = 2\cos\left(\frac{\pi}{n+1}\right)$.

Lemma 2. *Of all connected graphs on n nodes, the complete graph K_n has maximal spectral radius*; $\rho(K_n) = n - 1$.

Among the connected graphs on n nodes the path P_n has the largest diameter ($D = n - 1$) while the complete graph K_n has minimal diameter ($D = 1$). It is clear that the complete graph is also the graph on n nodes with *minimal* spectral radius and diameter $D = 1$. We will next determine the graphs on n nodes with minimal spectral radius and diameter $D = n - 2$ and $D = n - 3$.

Let us first define $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t,p}$ as a path of p nodes ($0 \sim 1 \sim 2 \sim \cdots \sim p - 1$) with pendant paths of n_i links at nodes m_i, for $i = 1, 2, \ldots, t$. Then we define the graph D_n through $D_n = P^1_{1,n-1}$; see Fig. 1. Note that D_n is a graph on n nodes with spectral radius $\rho(D_n) = 2\cos\left(\frac{\pi}{2n-2}\right)$, cf. [4, p. 77].

Theorem 3. *Of all connected graphs on n nodes* ($n \geqslant 4$) *and diameter* $D = n - 2$, *the graph D_n has the minimal spectral radius*; $\rho(D_n) = 2\cos\left(\frac{\pi}{2n-2}\right)$.

For the proof of Theorem 3 we need a classical result by Smith [12].

Lemma 4. *The only connected graphs on n nodes with spectral radius smaller than* 2 *are the path P_n, the graph D_n and the graphs E_6* ($n = 6$), *E_7* ($n = 7$), *and E_8* ($n = 8$) *depicted in Fig.* 2.

Proof of Theorem 3. For the cases $n \in \{4, 5, 9, 10, \ldots\}$ the theorem follows immediately from Lemma 4. For the cases $n \in \{6, 7, 8\}$ we have to determine which of the graphs D_n and E_n has minimal spectral radius. Let $C(G, \lambda)$ denote the characteristic polynomial of the adjacency matrix of the graph G, i.e., $C(G, \lambda) = \det(\lambda I - A(G))$. Let us first consider the case $n = 6$. A straightforward calculation shows that $C(D_6, \lambda) = \lambda^6 - 5\lambda^4 + 5\lambda^2$, while $C(E_6, \lambda) = \lambda^6 - 5\lambda^4 + 5\lambda^2 - 1$. It follows that $C(D_6, \lambda) = C(E_6, \lambda) + 1 > C(E_6, \lambda)$ for all λ, hence $\rho(D_6) < \rho(E_6)$. The case $n = 7$ can be proved in a similar way by using that $C(D_7, \lambda) = \lambda^7 - 6\lambda^5 + 9\lambda^3 - 2\lambda$ and $C(E_7, \lambda) = \lambda^7 - 6\lambda^5 + 9\lambda^3 - 3\lambda$, which implies that $C(D_7, \lambda) = C(E_7, \lambda) + \lambda > C(E_7, \lambda)$ for all $\lambda > 0$, hence $\rho(D_7) < \rho(E_7)$. Finally for the case $n = 8$ we use $C(D_8, \lambda) = \lambda^8 - 7\lambda^6 + 14\lambda^4 - 7\lambda^2$ and $C(E_8, \lambda) = \lambda^8 - 7\lambda^6 + 14\lambda^4 - 8\lambda^2 + 1$, implying that $C(D_8, \lambda) = C(E_8, \lambda) + \lambda^2 - 1 > C(E_8, \lambda)$ for all $\lambda > 1$, hence $\rho(D_8) < \rho(E_8)$. $\square$

Next we define the graph $\widetilde{D}_n$ through $\widetilde{D}_n = P^{1,n-3}_{1,1,n-1}$; see Fig. 3. Note that $\widetilde{D}_n$ is a graph on $n + 1$ nodes.

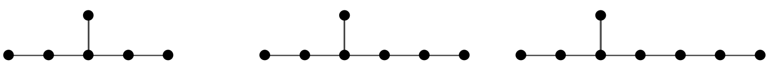

Fig. 2. The graphs E_6, E_7, E_8.

Fig. 3. The graph $\widetilde{D}_n$.

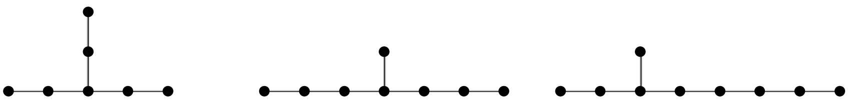

Fig. 4. The graphs $\widetilde{E}_6$, $\widetilde{E}_7$, $\widetilde{E}_8$.

Theorem 5. *Among all connected graphs on n nodes* $(n \geqslant 5)$ *and diameter* $D = n - 3$, *the minimal spectral radius equals* $\rho = 2$. *For* $n \geqslant 8$, *the minimal spectral radius only occurs for the graph* $\widetilde{D}_{n-1}$. *For* $n = 5$, *the minimal spectral radius occurs both for the cycle graph* C_5 *and the star with four leaves* $K_{1,4} = \widetilde{D}_4$. *For* $n = 6$, *the minimal spectral radius occurs both for the cycle graph* C_6 *and the graph* $\widetilde{D}_5$. *For* $n = 7$, *the minimal spectral radius occurs both for the graph* $\widetilde{D}_6$ *and the graph* $\widetilde{E}_6$ *depicted in Fig.* 4.

For the proof of Theorem 5 we again need results from Smith [12].

Lemma 6. *The only connected graphs on n nodes with spectral radius equal to* 2 *are the cycle graph* C_n, *the graph* $\widetilde{D}_{n-1}$ *depicted in Fig.* 3 *and the graphs* $\widetilde{E}_6$ $(n = 7)$, $\widetilde{E}_7$ $(n = 8)$, *and* $\widetilde{E}_8$ $(n = 9)$ *depicted in Fig.* 4.

Theorem 5 follows directly from Lemmas 4 and 6, as does the following theorem:

Theorem 7. *Among all connected graphs on n nodes* $(n \geqslant 5)$ *and diameter* $D = \lfloor \frac{n}{2} \rfloor$, *the minimal spectral radius equals* $\rho = 2$. *For* $n \geqslant 7$, *the minimal spectral radius only occurs for the cycle graph* C_n. *For* $n = 5$, *the minimal spectral radius occurs both for the cycle graph* C_5 *and the star with four leaves* $K_{1,4} = \widetilde{D}_4$. *For* $n = 6$, *the minimal spectral radius occurs both for the cycle graph* C_6 *and the graph* $\widetilde{D}_5$.

Based on the results so far, namely that certain trees minimize the spectral radius for graphs on n nodes and diameter D, for $D \geqslant n - 3$, and the computational results of Section 4, we conjecture the following:

Conjecture 8. *For fixed* e, *the graph* $P^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}$ *has minimal spectral radius among the graphs on n nodes and diameter* $D = n - e$, *for n large enough.*

We finish this section with a qualitative result on the minimal spectral radius for connected graphs on n nodes as a function of the diameter.

Theorem 9. *For connected graphs on n nodes* $(n \geqslant 9)$, *the minimal spectral radius is not a monotonically decreasing function of the diameter of the graph.*

Proof. The diameters of the graphs C_n and $\widetilde{D}_{n-1}$ are $\lfloor \frac{n}{2} \rfloor$ and $n - 3$, respectively, while $\rho(C_n) = \rho(\widetilde{D}_{n-1}) = 2$. For $n \geqslant 9$ there is at least one integer m satisfying $\lfloor \frac{n}{2} \rfloor < m < n - 3$. The minimal spectral radius for connected graphs on n nodes and diameter m must be larger than 2, because for all graphs mentioned in Lemmas 4 and 6, the diameter D satisfies $D = \lfloor \frac{n}{2} \rfloor$ or $D \geqslant n - 3$. □

3. Graphs with diameter two

From the previous section it follows that we know the minimal spectral radius of connected graphs on n nodes and diameter $D \in \{1, \lfloor \frac{n}{2} \rfloor, n-3, n-2, n-1\}$. In this section we consider the case of connected graphs on n nodes with diameter two. In fact, we shall prove that for these graphs $\sqrt{n-1}$ is the minimal spectral radius.

Theorem 10. *For the spectral radius ρ of a graph with diameter two on n nodes we have $\rho \geqslant \sqrt{n-1}$ with equality only for the stars $K_{1,n-1}$, the cycle graph C_5, the Petersen graph Pe_{10}, the Hoffman-Singleton graph H_{50}, and putative 57-regular graphs on 3250 nodes.*

For the proof of Theorem 10 we need two lemmas.

Lemma 11. *Let G be a graph with diameter two on node set N of n nodes, with degrees $d_v,\ v \in N$. Then $n - 1 \leqslant \frac{1}{n}\sum_{v \in N} d_v^2$ with equality only if G is a star $K_{1,n-1}$, the cycle graph C_5, the Petersen graph Pe_{10}, the Hoffman-Singleton graph H_{50}, or a putative 57-regular graph on 3250 nodes.*

Proof. We count induced paths of two links (on three nodes) in two different ways. First, since the diameter of the graph is two and hence each pair of nodes that is not linked is contained in at least one such induced path, the number of induced paths of length two is at least $\frac{n(n-1)}{2} - e$, where e is the number of links in the graph. Second, each node v can be the middle node of at most $\frac{d_v(d_v-1)}{2}$ induced paths of two links, hence there are at most $\sum_{v \in V} \frac{d_v(d_v-1)}{2}$ such induced paths. The claimed inequality now follows.

Equality is possible only if the graph contains no triangles, and any two non-adjacent nodes have a unique common neighbour, and this is only the case in the stated graphs. Indeed, consider in such a graph two non-adjacent nodes. These nodes must have the same number of neighbours, since any neighbour of one of them is either also a neighbour of the other, or adjacent to one neighbour of the other. Thus the graph is regular or its complement is disconnected. In the latter case it is a star $K_{1,n-1}$; in the first case, the graph is a (regular) Moore graph of diameter two. For such Moore graphs, i.e., k-regular graphs (hence having spectral radius k) on $k^2 + 1$ nodes with diameter two, it was already shown in 1960 [8] that $k \in \{2, 3, 7, 57\}$. The case $k = 2$ is realized by the cycle graph C_5, the case $k = 3$ is realized by the Petersen graph Pe_{10}; see Fig. 5, and the case $k = 7$ by the Hoffman-Singleton graph H_{50}; see [8]. For a nice graphical representation of the Hoffman-Singleton graph we refer to [15]. Whether or not a 57-regular graph with diameter two consisting of 3250 nodes exists is a famous open problem. □

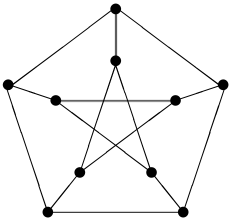

Fig. 5. The Petersen graph.

The following lemma is a result by Hofmeister [9]:

Lemma 12. *Let G be a graph on node set N of n nodes, with degrees d_v, $v \in N$, and spectral radius ρ. Then $\rho^2 \geqslant \frac{1}{n}\sum_{v\in N} d_v^2$. If G is connected, then equality holds if and only if G is regular or bipartite with constant degrees on each of the two parts.*

Theorem 10 now follows directly from Lemmas 11 and 12.

4. Graphs on at most 20 nodes

By computer we determined the minimal spectral radius for graphs on n nodes and diameter D, for almost all D and $n \leqslant 20$. The results are given in Tables 1 and 2. (The names of the graphs are explained below.)

For given n and given number of links e, we first generated all connected graphs on n nodes and with e links using *nauty* [10]. We then determined the graphs among those that minimize the spectral radius for each possible D; and then compared the results over all possible e. This comparison was done by increasing e; for the following reason. If for some combination of n and D the minimal ρ found by searching among the connected graphs with at most e links satisfied $\rho < 2(e+1)/n$ then this ρ was the definite minimum, and e did not have to be increased further. Indeed, because of the general bound $\rho \geqslant 2e/n$ (the average degree) we would only find graphs with spectral radius larger than the minimum so far.

For almost all cases the search was limited to e being increased to at most $n+2$. Exceptions were the cases $[D = 3, n \geqslant 12]$ and $[D = 4, n \geqslant 16]$.

In the cases $n = 20$ we could not increase e further for computational (capacity) reasons. Thus for $n = 20$ we obtained the minimal spectral radius for $D \geqslant 6$, and upper bounds for $D = 4, 5$. The upper bound for $D = 3$ is attained by an extremal 3-regular graph constructed by Alegre et al. [1]. It would not surprise us if this gives the minimal spectral radius in this case.

For $[D = 3, n = 12]$, also the graphs with $e = 15$ were considered, and for $[D = 3, n = 13]$, the ones with $e = 16$ and 17 were checked. For $[D = 3, n = 14]$, also the graphs with $e = 17$ and 18 were considered. Moreover, here also the graphs with $e = 19$ and maximal degree 4 were taken into account. The latter restriction can be made by using the inequality in Lemma 12: a node of degree at least 5 implies that $\rho \geqslant \sqrt{8}$. Similarly, for $[D = 3, n = 15]$, also the graphs with $e = 18$ and 19 were checked, and the graphs with $e = 20$ and node degrees only 2 and 3. For $[D = 3, n = 16]$, also the graphs with $e = 19$, with $e = 20$ and node degrees at most 7, with $e = 21$ and node degrees at most 6, and with $e = 22$ and node degrees at most 5 were checked. From Lemma 12 it follows that it was not necessary to check the graphs with $e = 23$. For these cases with $D = 3$ we used a special routine to generate graphs with diameter 3, written by Kris Coolsaet (private communication). It was also used to check the graphs with $[D = 3, n = 17]$ with $e = 24$ and node degrees at most 5. This gave the upper bound in this case. In the case $[D = 3, n = 18]$ the upper bound is attained by a 3-regular graph, cf. [11]. In the case $[D = 3, n = 19]$ the upper bound is attained by the graph obtained by contraction of one of the links in the 3-regular graph on 20 nodes.

For $[D = 4, n = 16]$, also the graphs with $e = 19$ were considered, while for $[D = 4, n = 17]$, the graphs with $e = 20$, and the ones with $e = 21$ and node degrees 2 and 3 were also checked. For the cases $[D = 4, n = 18, 19, 20]$ we obtained only upper bounds.

Table 1
Minimal spectral radius among graphs on n nodes with diameter D

$D \backslash n$	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
2		1.4142	1.7321	2	2.2361	2.4495	2.6458	2.8284	3	3.1623	3.3166	3.4641	3.6056	3.7417	3.8730	4	4.1231	4.2426	4.3589
3			1.6180	1.8478	2	2	2.3028	2.2784	2.4728	2.4860	2.5616	2.6970	2.7817	2.7321	2.8779	$\leqslant$2.9755	$\leqslant$3	$\leqslant$3.0742	$\leqslant$3
4				1.7321	1.9021	2	2	2	2.2361	2.2361	2.2230	2.3686	2.3778	2.3989	2.4303	2.5335	$\leqslant$2.7024	$\leqslant$2.7498	$\leqslant$2.7913
5					1.8019	1.9319	2	2.0840	2	2	2.1701	2.2105	2.1987	2.1907	2.3028	2.3167	2.3228	2.3536	$\leqslant$2.4605
6						1.8478	1.9499	2	2.0743	2.0743	2	2	2.1463	2.1940	2.1829	2.1753	2.1701	2.2688	2.2723
7							1.8794	1.9616	2	2.0684	2.1067	2.0684	2	2	2.1285	2.1693	2.1723	2.1649	2.1598
8								1.9021	1.9696	2	2.0647	2.1010	2.1010	2.0647	2	2	2.1149	2.1505	2.1649
9									1.9190	1.9754	2	2.0623	2.0912	2.1149	2.0912	2.0623	2	2	2.1056
10										1.9319	1.9796	2	2.0608	2.0840	2.1120	2.1120	2.0840	2.0608	2
11											1.9419	1.9829	2	2.0598	2.0785	2.1054	2.1183	2.1054	2.0785
12												1.9499	1.9854	2	2.0592	2.0743	2.1010	2.1169	2.1169
13													1.9563	1.9874	2	2.0588	2.0710	2.0981	2.1111
14														1.9616	1.9890	2	2.0586	2.0684	2.0962
15															1.9659	1.9904	2	2.0584	2.0664
16																1.9696	1.9915	2	2.0583
17																	1.9727	1.9924	2
18																		1.9754	1.9932
19																			1.9777

Table 2
Graphs with minimal spectral radius on n nodes with diameter D

$D \backslash n$	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	P_2 $= K_2$	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}	K_{13}	K_{14}	K_{15}	K_{16}	K_{17}	K_{18}	K_{19}	K_{20}
2		P_3 $= K_{1,2}$	D_4 $= K_{1,3}$	$\widetilde{D}_4$ $= K_{1,4}$ C_5	$K_{1,5}$	$K_{1,6}$	$K_{1,7}$	$K_{1,8}$	$K_{1,9}$ Pe_{10}	$K_{1,10}$	$K_{1,11}$	$K_{1,12}$	$K_{1,13}$	$K_{1,14}$	$K_{1,15}$	$K_{1,16}$	$K_{1,17}$	$K_{1,18}$	$K_{1,19}$
3			P_4	D_5	$\widetilde{D}_5$ C_6	C_7	$Q_{3,3,3}$ $DS_{3,3}$	$Q_{3,3,4}$	Fig. 6	Fig. 6	Fig. 6	Fig. 6	Fig. 7	Fig. 7	Fig. 7	?	?	?	?
4				P_5	D_6	$\widetilde{D}_6$ $\widetilde{E}_6$	C_8	C_9	$T_4(1,1,1)$	$Q_{4,4,4}$	$Q_{4,4,5}$	Fig. 8	Fig. 8	Fig. 8	Fig. 8	Fig. 8	?	?	?
5					P_6	D_7	$\widetilde{D}_7$	C_8^0 $P^{1,3}_{1,2,6}$	C_{10}	C_{11}	$C_9^{0,3,6}$	$Q_{4,5,5}$	$Q_{5,5,5}$	$Q_{5,5,6}$	Fig. 9	Fig. 9 (2*)	Fig. 9	Fig. 9	?
6						P_7	D_8	$\widetilde{D}_8$	$P^3_{3,7}$ $P^{1,4}_{1,2,7}$	C^0_{10}	C_{12}	C_{13}	$C^{0,4,8}_{11}$	$Q_{4,6,6}$	$Q_{5,6,6}$	$Q_{6,6,6}$	$Q_{6,6,7}$	Fig. 10	Fig. 10
7							P_8	D_9	$\widetilde{D}_9$	$P^{1,5}_{1,2,8}$	$P^{1,4}_{1,3,8}$ C^{+2}_{10}	C^0_{12}	C_{14}	C_{15}	$C^{0,4,8}_{13}$	$C^{0,3,5,8}_{13}$	$Q_{5,7,7}$	$Q_{6,7,7}$	$Q_{7,7,7}$
8								P_9	D_{10}	$\widetilde{D}_{10}$	$P^{1,6}_{1,2,9}$	$P^{1,5}_{1,3,9}$ $P^{2,6}_{2,2,9}$ $P^4_{4,9}$	$C^{0,6}_{12}$ C^{+2}_{12}	C^0_{14}	C_{16}	C_{17}	$C^{0,5,10}_{15}$	$C^{0,3,6,9}_{15}$	$Q_{5,8,8}$
9									P_{10}	D_{11}	$\widetilde{D}_{11}$	$P^{1,7}_{1,2,10}$	$P^{2,7}_{2,2,10}$	$P^{1,5}_{1,4,10}$ C^{+3}_{12}	$C^{0,7}_{14}$	C^0_{16}	C_{18}	C_{19}	$C^{0,6,12}_{17}$
10										P_{11}	D_{12}	$\widetilde{D}_{12}$	$P^{1,8}_{1,2,11}$	$P^{2,8}_{2,2,11}$	$P^{1,6}_{1,4,11}$ $P^{2,7}_{2,3,11}$ $P^5_{5,11}$	C^{+3}_{14} $C^{+1,+2}_{14}$	$C^{0,8}_{16}$	C^0_{18}	C_{20}

(*continued on next page*)

Table 2 (*continued*)

$D \backslash n$	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
11											P_{12}	D_{13}	$\widetilde{D}_{13}$	$P^{1,9}_{1,2,12}$	$P^{2,9}_{2,2,12}$	$P^{2,8}_{2,3,12}$	$P^{1,6}_{1,5,12}$ C^{+4}_{14}	$C^{+1,+2}_{16}$	$C^{0,9}_{18}$
12												P_{13}	D_{14}	$\widetilde{D}_{14}$	$P^{1,10}_{1,2,13}$	$P^{2,10}_{2,2,13}$	$P^{2,9}_{2,3,13}$	$P^{6}_{6,13}$ $P^{1,7}_{1,5,13}$ $P^{2,8}_{2,4,13}$ $P^{3,9}_{3,3,13}$	C^{+4}_{16} $C^{+1,+3}_{16}$ $C^{+2,+2}_{16}$
13													P_{14}	D_{15}	$\widetilde{D}_{15}$	$P^{1,11}_{1,2,14}$	$P^{2,11}_{2,2,14}$	$P^{2,10}_{2,3,14}$	$P^{3,10}_{3,3,14}$
14														P_{15}	D_{16}	$\widetilde{D}_{16}$	$P^{1,12}_{1,2,15}$	$P^{2,12}_{2,2,15}$	$P^{2,11}_{2,3,15}$
15															P_{16}	D_{17}	$\widetilde{D}_{17}$	$P^{1,13}_{1,2,16}$	$P^{2,13}_{2,2,16}$
16																P_{17}	D_{18}	$\widetilde{D}_{18}$	$P^{1,14}_{1,2,17}$
17																	P_{18}	D_{19}	$\widetilde{D}_{19}$
18																		P_{19}	D_{20}
19																			P_{20}

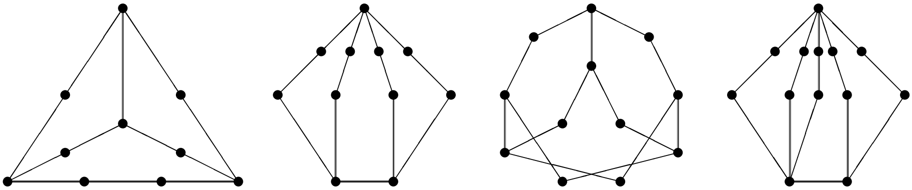

Fig. 6. Graphs with minimal spectral radius and diameter 3; $n = 10, 11, 12, 13$.

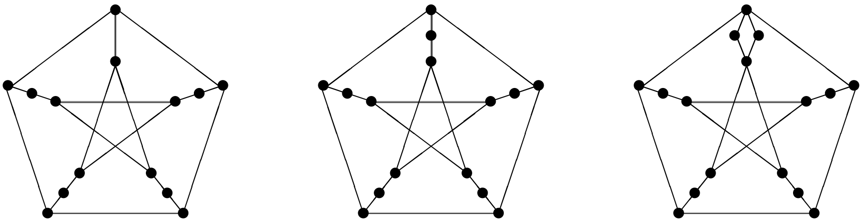

Fig. 7. Graphs with minimal spectral radius and diameter 3; $n = 14, 15, 16$.

To explain Table 2, we need to define the following graphs. The graph $Q_{n_1,n_2,\ldots,n_t}$ consists of two nodes connected by t disjoint paths of $n_1, n_2, \ldots, n_t$ links. The graph $C_m^{m_1,\ldots,m_t}$ is defined as a cycle of m nodes $(0 \sim 1 \sim 2 \sim \cdots \sim m-1 \sim 0)$ with pendant links at nodes $m_1, \ldots, m_t$. Also, let C_m^{+t} be an m-cycle with a pendant path of t links. For even m, let $C_m^{+t,+s}$ be a cycle of m nodes $(0 \sim 1 \sim 2 \sim \cdots \sim m-1 \sim 0)$ with a pendant path of t links at node 0, and a pendant path of s links at node $m/2$. The tree $T_4(1, 1, 1)$ is as defined by Woo and Neumaier [16]; it consist of a node which is adjacent to three other nodes, which each in turn is adjacent to two endnodes. The Double Star $DS_{3,3}$ is a tree consisting of two adjacent nodes which each are adjacent to three endnodes.

An interesting feature of Table 1 is that, as far as our computations show, for fixed diameter $D \geqslant 3$ the minimal spectral radius ρ for $n = D + 3 + i$ is the same as for $n = 2D - i$, for $i = 0, 1, \ldots, D - 3$. For $i = 0$ this clearly follows from the results in Section 2; however we have no general explanation.

Besides Conjecture 8, we could make some other guesses on which graphs minimize the spectral radius for particular values of n and D. From Table 2 it for example seems that the graph C_{2D-2}^0 minimizes the spectral radius for $n = 2D - 1$, $D \geqslant 5$. It also seems that the graph $Q_{D,D,D+1}$ is the optimal graph for $n = 3D$, and similar graphs are optimal for slightly smaller n. Notice also the pattern for $n = 3D + 1$ from Figs. 8–10.

Note further that Brouwer and Neumaier [2] classified all graphs with spectral radius between 2 and $\sqrt{2+\sqrt{5}} \approx 2.0582$. All these graphs have diameter $D = n - 2$ or $D = n - 3$, and from the results in Section 2 it thus follows that none of them has minimal spectral radius given the diameter and number of nodes.

Woo and Neumaier [16] show that a graph with spectral radius between 2 and $\frac{3}{2}\sqrt{2} \approx 2.1312$ is either a tree with maximum degree 3 such that all nodes of degree 3 lie on a path; or is a connected graph of maximum degree 3 such that all nodes of degree 3 lie on a cycle, and this is the only cycle in the graph; or it consists of a path one of whose endnodes has 3 pendant links. Indeed, we encounter some of these graphs in Table 2.

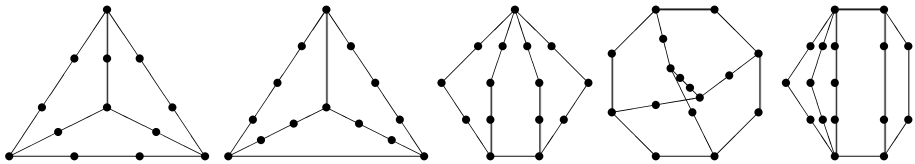

Fig. 8. Graphs with minimal spectral radius and diameter 4; $n = 13, 14, 15, 16, 17$.

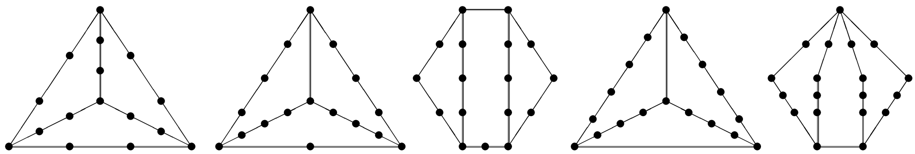

Fig. 9. Graphs with minimal spectral radius and diameter 5; $n = 16, 17(2*), 18, 19$.

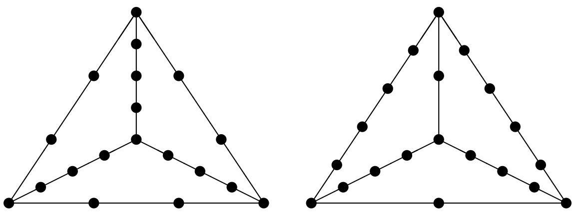

Fig. 10. Graphs with minimal spectral radius and diameter 6; $n = 19, 20$.

5. Conclusions

In this paper we have tackled the following problem: *which graph on n nodes and a given diameter D has minimal spectral radius*? This problem was inspired by the fact that the smaller the spectral radius of a graph, the larger the robustness of the network against the spread of viruses.

We have solved the problem stated above explicitly for graphs with diameter $D \in \{1, 2, \lfloor \frac{n}{2} \rfloor, n-3, n-2, n-1\}$. In addition, for almost all graphs on at most 20 nodes we have founds the graphs minimizing the spectral radius by a computer search.

Interesting issues for further research include the following items:

- determine the graphs with minimal spectral radius for the cases: $[D = 3, 17 \leqslant n \leqslant 20]$, $[D = 4, 18 \leqslant n \leqslant 20]$, $[D = 5, n = 20]$;
- prove Conjecture 8; probably a good starting point is the case $e = 4$, for which the conjecture becomes: *for* $n \geqslant 9$ *the graph* $P^{1,n-6}_{1,2,n-3}$ *has minimal spectral radius among the graphs on n nodes and diameter* $D = n - 4$;
- show that the graph C^0_{2D-2} minimizes the spectral radius for $n = 2D - 1$, $D \geqslant 5$, that the graph $Q_{D,D,D+1}$ is the optimal graph for $n = 3D$, $D \geqslant 3$, etc.;
- prove that for fixed diameter $D \geqslant 3$ the minimal spectral radius ρ for $n = D + 3 + i$ is the same as for $n = 2D - i$, for $i = 0, 1, \ldots, D - 3$;
- can sharp lower and upper bounds be formulated for the minimal spectral radius for diameter $D \geqslant 3$? A good starting point is the case $D = 3$; an idea is to use the Moore bound to obtain a lower bound for the minimal spectral radius.

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