Linear Algebra and its Applications 597 (2020) 33–45

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

A bound on the spectral radius of graphs in terms of their Zagreb indices

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A R T I C L E I N F O

Article history:
Received 25 November 2019
Accepted 15 March 2020
Available online 20 March 2020
Submitted by R. Brualdi

MSC:
05C50

Keywords:
Main eigenvalues
Zagreb indices
Number of walks
Rayleigh quotient

A B S T R A C T

The first and the second Zagreb index of a graph, usually defined as the sum of the squares of degrees over all vertices and the sum of the products of degrees of edge endvertices over all edges, respectively, are tightly related to the numbers of walks of length two and three in the graph. We provide here a lower bound on the spectral radius of adjacency matrix A of graph in terms of its Zagreb indices, based on the properties of the least square approximation of the vector A^2j with the vectors Aj and j, where j is the all-one vector. The bound is sharp for all graphs with two main eigenvalues, surpassing the range of sharpness of other bounds among connected graphs.

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https://doi.org/10.1016/j.laa.2020.03.021

1. Introduction

Let $G = (V, E)$ be a simple connected graph with $n = |V|$ vertices and $m = |E|$ edges. The eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of its $(0, 1)$-adjacency matrix A are also said to be the eigenvalues of G. Let $x_1, x_2, \ldots, x_n$ form an orthonormal basis of eigenvectors of A such that x_i is the eigenvector of λ_i for $i = 1, \ldots, n$. The spectral decomposition [26, p. 6] states that

$$A = \sum_{i=1}^{n} \lambda_i x_i x_i^\top. \tag{1}$$

By Perron-Frobenius theorem [26, p. 8], the spectral radius λ_1 is a single eigenvalue with $\lambda_1 \geq |\lambda_i|$, with $\lambda_1 = |\lambda_n|$ if and only if G is bipartite, and x_1 can be chosen to have all its components positive.

Further, let j be the all-one vector indexed by V and let

$$j = \sum_{i=1}^{n} c_i x_i$$

be its representation in the eigenvector basis. A walk W of length k between the vertices u and v in a simple graph G is a sequence of its vertices $W\colon u = w_0, w_1, \ldots, w_k = v$ such that w_i is adjacent to w_{i+1} for $i = 0, \ldots, k-1$. By a folklore result in graph theory, the number of all walks of length k between u and v is equal to $(A^k)_{u,v}$. Hence by the orthonormality of eigenvectors $x_1, x_2, \ldots, x_n$, the number of all walks of length k in G is equal to

$$j^\top A^k j = \sum_{i=1}^{n} \lambda_i^k (j^\top x_i)(x_i^\top j) = \sum_{i=1}^{n} c_i^2 \lambda_i^k.$$

If G is not bipartite, then $\lambda_1 > |\lambda_i|$ for $i = 2, \ldots, n$, so that $\lambda_1 = \lim_{k\to\infty} \sqrt[k]{j^\top A^k j}$. If G is bipartite, then $\lambda_n = -\lambda_1$ and the walks of odd length do not exist, but still

$$\lambda_1 = \lim_{k\to\infty} \sqrt[2k]{j^\top A^{2k} j}. \tag{2}$$

For the vertex u of G let d_u denote the number of vertices adjacent to u in G. The first Zagreb index M_1 and the second Zagreb index M_2 are defined as

$$M_1 = \sum_{u\in V} d_u^2 \quad \text{and} \quad M_2 = \sum_{uv\in E} d_u d_v.$$

These indices were introduced by Gutman and Trinajstić [13] in 1972 within the study of the dependence of total π-electron energy on molecular structure, and were shown to measure branching of the molecular carbon-atom skeleton [14] in 1975. Since for the vector d of vertex degrees holds

$$d = (d_u)_{u \in V} = Aj,$$

we have that

$$M_1 = \sum_{u \in V} d_u^2 = d^\top d = j^\top A^2 j, \tag{3}$$

$$M_2 = \sum_{uv \in E} d_u d_v = \frac{1}{2} d^\top A d = \frac{1}{2} j^\top A^3 j, \tag{4}$$

so that M_1 and M_2 actually count all walks of length two and a half of all walks of length three in G. Taking into account (2), it does not surprise that several results from the literature, mostly in the form of bounds, relate the spectral radius of a graph to the Zagreb indices and other numbers of short walks.

To state these results, we have to introduce a few further definitions. For a vertex u of G, let the 2-degree $d_{2,u} = \sum_{\{v:\, uv \in E\}} d_v$ be the sum of degrees of the neighbors of u in G, and let $d_{3,u} = \sum_{\{v:\, uv \in E\}} d_{2,v}$ be the sum of 2-degrees of the neighbors of u in G. Therefore, $(d_{2,u})_{u \in V} = A^2 j$ and $(d_{3,u})_{u \in V} = A^3 j$. A graph is regular if its vertices have a constant degree, i.e., if $Aj = rj$ for some integer r. A graph is bipartite semiregular if vertices in the same bipartition have a constant degree. Favaron, Mahéo and Saclé [11] proved the following lower bound, while Berman and Zhang [2] proved the upper bound:

$$\frac{1}{m} \sum_{uv \in E} \sqrt{d_u d_v} \le \lambda_1 \le \max_{uv \in E} \sqrt{d_u d_v}. \tag{5}$$

Favaron, Mahéo and Saclé [11] proved the following bounds as well:

$$\min_{u \in V} \frac{(A^2 j)_u}{(Aj)_u} = \min_{u \in V} \frac{d_{2,u}}{d_u} \le \lambda_1 \le \max_{u \in V} \frac{d_{2,u}}{d_u} = \max_{u \in V} \frac{(A^2 j)_u}{(Aj)_u}; \tag{6}$$

$$\lambda_1 \le \max_{u \in V} \sqrt{d_{2,u}} = \max_{u \in V} \sqrt{(A^2 j)_u}; \tag{7}$$

$$\sqrt{\frac{j^\top A^2 j}{j^\top j}} = \sqrt{\frac{M_1}{n}} \le \lambda_1. \tag{8}$$

Zhou [30] proved the bound

$$\frac{j^\top A^3 j}{j^\top A^2 j} = \frac{2M_2}{M_1} \le \lambda_1. \tag{9}$$

Bound (7) has been proved independently by Cao [4], while bound (8) has been proved independently both by Hofmeister [17] and by Zhou [29]. Note that in each of the bounds

(5), (7) and (8) equality holds if and only if the graph is regular or bipartite semiregular, while equality holds in (6) and (9) if and only if Aj is an eigenvector of A corresponding to λ_1 (in which case graph is also called pseudo-regular).

Yu, Lu and Tian [28] proved the bound

$$\sqrt{\frac{j^\top A^4 j}{j^\top A^2 j}} = \sqrt{\frac{\sum_{u\in V} d_{2,u}^2}{M_1}} \leq \lambda_1 \tag{10}$$

and Hong and Zhang [18] have further proved the bound

$$\sqrt{\frac{j^\top A^6 j}{j^\top A^4 j}} = \sqrt{\frac{\sum_{u\in V} d_{3,u}^2}{\sum_{u\in V} d_{2,u}^2}} \leq \lambda_1. \tag{11}$$

In either of these bounds, equality holds if and only if the ratios of the constituent summands ($d_{2,u}/d_u$ in the first case and $d_{3,u}/d_{2,u}$ in the second case) have a constant value for all vertices of the graph or the graph is bipartite and these ratios have a constant value in each bipartition.

On the other hand, Abdo et al. [1] have shown that

$$\sqrt{\frac{M_2}{m}} = \sqrt{\frac{j^\top A^3 j}{j^\top A j}} \tag{12}$$

is a good approximation of the spectral radius λ_1, sharp for a large set of graphs, although it is neither a lower nor an upper bound for it.

Our goal here is to prove a new lower bound on the spectral radius of a graph in terms of its Zagreb indices and numbers of vertices and edges, that is sharp for a rather large set of graphs—all graphs with two main eigenvalues. While the bound will at the first sight appear to have a rather complicated expression, it will be clear from its proof that this expression follows naturally from the least squares approximation of the vector $A^2 j$ by the vectors Aj and j, where j is the all-one vector.

Before we state the main result, let us also briefly introduce main eigenvalues of graphs. An eigenvalue λ of A is called the main eigenvalue of G if its eigenspace is not orthogonal to the all-one vector j [7]. The spectral radius λ_1 is always the main eigenvalue of a connected graph G as its eigenvector x_1 is strictly positive, and Rowlinson [24, Proposition 1.4] showed that regular graphs are the only graphs with exactly one main eigenvalue. Hagos [15] gave the following characterization of the number of the main eigenvalues of a graph.

Theorem 1 *([15]). If k is the maximal integer such that $j, Aj, \dots, A^{k-1}j$ are linearly independent, then G has exactly k main eigenvalues.*

While Cvetković [6] posed the problem of characterization of graphs with a given number of main eigenvalues more than 40 years ago, study of the first nontrivial case—graphs with two main eigenvalues—became an active field of research only after Theorem 1 appeared in 2002. For $k = 2$ it states that a graph has exactly two main eigenvalues if it is not regular and there exist real values α and β such that

$$A^2 j = \alpha A j + \beta j. \tag{13}$$

Many examples of graphs with two main eigenvalues appeared in literature since then. Rowlinson [24] pinpointed cones over regular graphs and strongly regular graphs with one vertex deleted as such examples. General constructions of graphs with two main eigenvalues were described by Hayat et al. [16], Chen and Huang [5], and Huang et al. [22], whose construction may also produce graphs with an arbitrary fixed number of main eigenvalues. Tang and Hou [27] determined integral graphs with spectral radius 3 and two main eigenvalues, while a number of authors [10,19–21,25] managed to characterize unicyclic, bicyclic and tricyclic graphs with two main eigenvalues.

Our main result is as follows.

Theorem 2. *Let G be a nonregular simple graph with n vertices, m edges and the first and the second Zagreb indices M_1 and M_2, respectively, and let*

$$\alpha = \frac{2(nM_2 - mM_1)}{nM_1 - 4m^2} \quad \text{and} \quad \beta = \frac{M_1^2 - 4mM_2}{nM_1 - 4m^2}. \tag{14}$$

The spectral radius λ_1 of G then satisfies

$$\frac{\alpha + \sqrt{\alpha^2 + 4\beta}}{2} \le \lambda_1, \tag{15}$$

with equality if and only if G has exactly two main eigenvalues.

Note that the condition that G is not regular in Theorem 2 is not too restrictive, as if G is regular with all of its vertices having degree r, which is easy to check, then also $\lambda_1 = r$.

The rest of the paper is organised as follows. Proof of the main result is given in Section 2. The approach used in the proof, which is based on the least squares approximation of $A^k j$ via $j, \ldots, A^{k-1} j$ for $k = 2$, is further discussed in Section 3, in particular for $k = 1$ and $k = 3$. Statistical comparison of the lower bound (15) to previously mentioned bounds (5)–(12) on several sets of connected graphs and trees is presented in Section 4, showing that the new bound is comparable to the best among these bounds, at the same time being sharp for larger sets of connected graphs.

2. Proof of Theorem 2

Let us recall that the least squares approximation of the vector $A^2 j$ with a linear combination $\alpha A j + \beta j$ of the vectors Aj and j is performed by projecting $A^2 j$ onto the

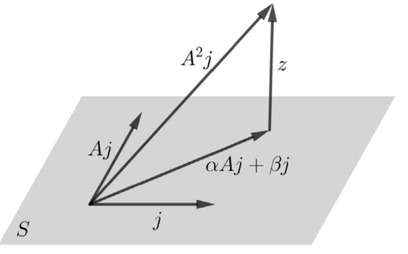

Fig. 1. Illustration of (16).

space $S = \mathrm{span}\{Aj, j\}$, as this minimizes the norm of the difference between A^2j and its approximation $\alpha Aj + \beta j$ (see Fig. 1). Hence we have

$$A^2 j = \alpha Aj + \beta j + z, \quad \text{where } z \perp j \text{ and } z \perp Aj. \tag{16}$$

Let us now determine α and β from (16). From the conditions $z \perp j$ and $z \perp Aj$ we get the system:

$$\begin{aligned} 0 &= j^\top z = j^\top A^2 j - \alpha j^\top Aj - \beta j^\top j, \\ 0 &= (Aj)^\top z = j^\top A^\top A^2 j - \alpha j^\top A^\top Aj - \beta j^\top A^\top j. \end{aligned}$$

The adjacency matrix A is symmetric as G is an undirected graph, so that we actually have

$$\begin{aligned} \alpha j^\top Aj + \beta j^\top j &= j^\top A^2 j, \\ \alpha j^\top A^2 j + \beta j^\top Aj &= j^\top A^3 j, \end{aligned}$$

whose solution by the Cramer's rule is given by

$$\alpha = \frac{\begin{vmatrix} j^\top A^2 j & j^\top j \\ j^\top A^3 j & j^\top Aj \end{vmatrix}}{\begin{vmatrix} j^\top Aj & j^\top j \\ j^\top A^2 j & j^\top Aj \end{vmatrix}} \quad \text{and} \quad \beta = \frac{\begin{vmatrix} j^\top Aj & j^\top A^2 j \\ j^\top A^2 j & j^\top A^3 j \end{vmatrix}}{\begin{vmatrix} j^\top Aj & j^\top j \\ j^\top A^2 j & j^\top Aj \end{vmatrix}}$$

Recalling that

$$j^\top j = n, \quad j^\top Aj = 2m, \quad j^\top A^2 j = M_1 \text{ and } j^\top A^3 j = 2M_2,$$

we obtain

$$\alpha = \frac{2(nM_2 - mM_1)}{nM_1 - 4m^2} \quad \text{and} \quad \beta = \frac{M_1^2 - 4mM_2}{nM_1 - 4m^2}. \tag{17}$$

As already shown in [23, Theorem 2.1], the Cauchy-Schwarz inequality applied to the vectors j and $d = Aj$ yields

$$nM_1 = \sum_{u\in V} 1^2 \sum_{u\in V} d_u^2 \geq \left(\sum_{u\in V} 1\cdot d_u\right)^2 = 4m^2,$$

with equality if and only if $d = rj$ some integer r, namely if and only if G is a regular graph. As G is assumed not to be regular, this means that $nM_1 - 4m^2 > 0$, so that α and β are well-defined in (17).

Next, we would like to find a pair (μ, x) of a pseudoeigenvalue μ and a pseudoeigenvector x of A in S having the form

$$x = Aj + \gamma j$$

for some real γ such that

$$Ax = \mu x + z. \tag{18}$$

Using (16) this implies

$$Ax = A^2 j + \gamma Aj = (\alpha+\gamma)Aj + \beta j + z = \mu(Aj + \gamma j) + z.$$

Since G is not regular, it has at least two main eigenvalues, so that by Theorem 1 the vectors Aj and j are linearly independent. The last equality above then implies

$$\alpha + \gamma = \mu, \tag{19}$$

$$\beta = \mu\gamma. \tag{20}$$

Multiplying (19) by μ and replacing $\mu\gamma$ from (20) yields the quadratic equation

$$\alpha\mu + \beta = \mu^2,$$

for which we will choose the solution with the plus sign:

$$\mu = \frac{\alpha + \sqrt{\alpha^2 + 4\beta}}{2}, \tag{21}$$

so that

$$\gamma = \frac{\beta}{\mu} = \frac{2\beta}{\alpha + \sqrt{\alpha^2 + 4\beta}}.$$

Now we can finally apply the Rayleigh quotient to the vector x to deduce the lower bound for the spectral radius λ_1 of A:

$$\lambda_1 \geq \frac{x^\top Ax}{x^\top x} = \frac{x^\top(\mu x + z)}{x^\top x} = \mu + \frac{x^\top z}{x^\top x} = \mu, \tag{22}$$

since

$$x^\top z = (Aj)^\top z + \gamma j^\top z = 0$$

as $z \perp j$ and $z \perp Aj$. Combining (22), (21) and (17) now proves the lower bound in Theorem 2. Equality holds in (22) if and only if x is an eigenvector of A, which by (18) holds if and only if $z = 0$, which further by (16) holds if and only if $A^2 j$ is linearly dependent on Aj and j, and which by Theorem 1 holds if and only if G has exactly two main eigenvalues. □

3. Discussion of the proof approach

The approach used in the proof of Theorem 2: finding the coefficients of the projection of the vector $A^k j$ to the space S spanned by the vectors $j, \dots, A^{k-1}j$, using these coefficients to determine a pseudoeigenvalue μ and a pseudoeigenvector x of A satisfying $Ax = \mu x + z$, where z is the difference between $A^k j$ and its projection on S, and then applying the Rayleigh quotient to show that $\lambda_1 \geq \mu$, may be also applied to values of k different from two.

The case $k = 1$ is trivial, as the projection step and the pseudoeigenvalue equality step overlap, both requiring $Aj = \mu j + z$, with j forced to being a pseudoeigenvector. The condition $z \perp j$ yields $0 = j^\top z = j^\top (Aj - \mu j) = 2m - \mu n$, i.e., $\mu = \frac{2m}{n}$, which recreates a classical lower bound $\lambda_1 \geq \frac{2m}{n}$ with equality if and only if the graph is regular with j as its true eigenvector.

We will now apply this approach to the case $k = 3$ as a more illustrative example. To simplify notation, let $w_i = j^\top A^i j$ denote the number of all walks of length i in the graph. Setting the projection equality

$$A^3 j = \alpha A^2 j + \beta A j + \gamma j + z,$$

the condition $z \perp \{j, Aj, A^2 j\}$ yields the system:

$$\begin{aligned} \alpha w_2 + \beta w_1 + \gamma w_0 &= w_3 \qquad (\text{from } j^\top z = 0), \\ \alpha w_3 + \beta w_2 + \gamma w_1 &= w_4 \qquad (\text{from } (Aj)^\top z = 0), \\ \alpha w_4 + \beta w_3 + \gamma w_2 &= w_5 \qquad (\text{from } (A^2 j)^\top z = 0), \end{aligned}$$

whose solution is given by

$$\alpha = \frac{\begin{vmatrix} w_3 & w_1 & w_0 \\ w_4 & w_2 & w_1 \\ w_5 & w_3 & w_2 \end{vmatrix}}{\begin{vmatrix} w_2 & w_1 & w_0 \\ w_3 & w_2 & w_1 \\ w_4 & w_3 & w_2 \end{vmatrix}}, \qquad \beta = \frac{\begin{vmatrix} w_2 & w_3 & w_0 \\ w_3 & w_4 & w_1 \\ w_4 & w_5 & w_2 \end{vmatrix}}{\begin{vmatrix} w_2 & w_1 & w_0 \\ w_3 & w_2 & w_1 \\ w_4 & w_3 & w_2 \end{vmatrix}}, \qquad \gamma = \frac{\begin{vmatrix} w_2 & w_1 & w_3 \\ w_3 & w_2 & w_4 \\ w_4 & w_3 & w_5 \end{vmatrix}}{\begin{vmatrix} w_2 & w_1 & w_0 \\ w_3 & w_2 & w_1 \\ w_4 & w_3 & w_2 \end{vmatrix}}.$$

Note that this solution is unique if we assume that G has at least three main eigenvalues, so that the vectors j, Aj and A^2j are linearly independent.

Next, we set up the pseudoeigenvalue equality

$$Ax = \mu x + z \tag{23}$$

assuming x to have the form $x = A^2j + \delta Aj + \varepsilon j$. Replacing x in (23) yields the equation

$$Ax = A^3j + \delta A^2j + \varepsilon Aj = (\alpha + \delta)A^2j + (\beta + \varepsilon)Aj + \gamma j + z = \mu(A^2j + \delta Aj + \varepsilon j) + z.$$

Since A^2j, Aj and j are assumed to be linearly independent, the above equation leads to the system:

$$\begin{aligned} \alpha + \delta &= \mu, \\ \beta + \varepsilon &= \mu\delta, \\ \gamma &= \mu\varepsilon. \end{aligned}$$

Multiplying the second equation by μ, replacing $\mu\varepsilon$ in it by γ, and then multiplying the first equation by μ^2, and replacing $\mu^2\delta$ in it by $\beta\mu + \gamma$ yields the cubic equation with μ as the only unknown:

$$\alpha\mu^2 + \beta\mu + \gamma = \mu^3.$$

Numerical algorithms, such as MPSolve [3] or Eigensolve [12], may then be used to find the largest real solution of this equation, which will be a lower bound for the spectral radius λ_1 by the Rayleigh quotient. However, it is questionable whether this would yield any advantage over applying the Lanczos algorithm directly to A to estimate its spectral radius. The apparent conclusion that this discussion imposes is that the case $k \geq 3$ ceases to produce nice closed-form expressions compared to the case $k = 2$ that was used to obtain Theorem 2.

4. Statistical comparison

We show the results of simple statistical comparison of the estimates in (5)–(12) and the new bound (15) in Fig. 3. We calculated the root-mean-square deviation between the values of the spectral radius λ_1 and these estimates for the sets of connected graphs from four to ten vertices (a total of 11,989,760 graphs; the upper left diagram in Fig. 3) and the sets of trees from 10 to 20 vertices (a total of 1,345,929 trees; the lower left diagram), as well as the ratio of the numbers of graphs in these sets for which these estimates are sharp (the upper right diagram for the sets of connected graphs and the lower right diagram for the sets of trees). Here the value of an estimate was deemed to be sharp if it was within 10^{-8} of the spectral radius of adjacency matrix, as calculated by the Lanczos algorithm.

Diagrams clearly indicate that the root-mean-square deviation of an estimate is related to the highest power of A appearing in its definition: the best performing estimate is (11), combining the sixth and the fourth powers of A, followed by (10) which combines the fourth and the second powers of A. The estimates (15), from our main theorem, and (12), which both depend on the third power of A, behave rather similarly, especially within the sets of connected graphs, and substantially better than the estimate (9), which combines the third and the second power of A. Reflecting on this, one should certainly expect even smaller root-mean-square deviation from the estimates employing even higher powers of A, such as, e.g.,

$$\lambda_1 \geq \sqrt{\frac{j^\top A^8 j}{j^\top A^6 j}}.$$

However, such estimates lose their methodological benefit, as it takes almost the same effort to calculate them as it takes to call an implementation of the Lanczos algorithm in any of the modern software matrix tools and libraries. Hence one should not aim higher than the third power of A, which is still recognizable in the literature disguised as the second Zagreb index, when looking for new estimates for the spectral radius of A.

While the root-mean-square deviations tend to change at a constant rate, the ratios of the numbers of graphs for which these estimates are sharp apparently drop exponentially with increase in the number of vertices. From the upper right diagram of Fig. 3, it is evident that the bound (15) from Theorem 2 is superior to other estimates in the numbers of connected graphs for which it is sharp. For example, among connected graphs on ten vertices, the bound (15) is sharp for 1,117 graphs, followed by the estimate (12) which is sharp for 369 graphs, with the remaining estimates being sharp for between 173 and 238 such graphs. The situation with sharpness ratios changes significantly when we switch to trees, as the conditions for equality in these estimates are usually expressed in various terms of regularity, which are much harder satisfied for trees (for example, the bounds in (6) and (9) are never sharp for trees, and the star is usually the only tree satisfying equality in other estimates). The exception here is the estimate (12), which is, let us repeat, neither a lower nor an upper bound for the spectral radius. This estimate is sharp for semiharmonic graphs [9] that satisfy $A^3 j = \lambda_1^2 A j$, but also for certain non-semiharmonic graphs [1]. Semiharmonic graphs can be found easily among trees: according to [8], a tree is semiharmonic if and only if for some $a, b \in \mathbb{N}$ it contains a central vertex v of degree a, every neighbor w of v has degree b and every neighbor of w distinct from v is a leaf. However, computational results show that the estimate (12) is sharp for non-semiharmonic trees as well, two examples of which are shown in Fig. 2.

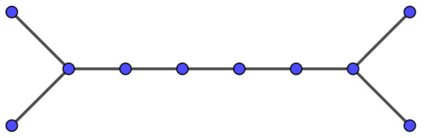

Fig. 2. Two non-semiharmonic trees on ten vertices for which $\lambda_1 = \sqrt{M_2/m}$ holds. The left tree is one of the Smith graphs with $\lambda_1 = 2$ and $M_2 = 36$, while the right tree has $\lambda_1 = \sqrt{5}$ and $M_2 = 45$.

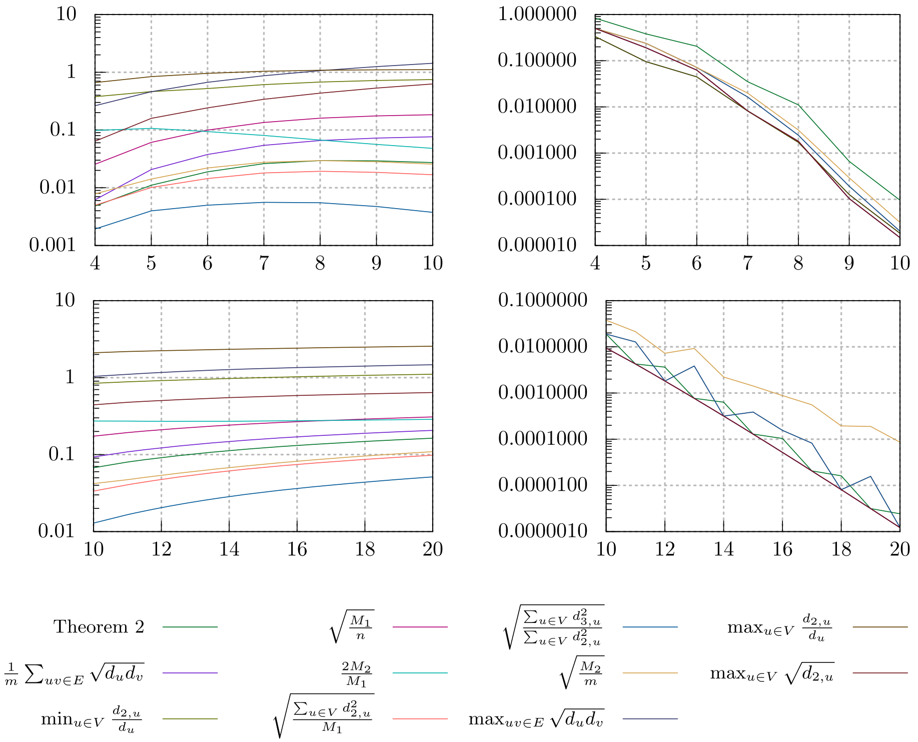

Fig. 3. Diagrams of simple statistical analysis of various estimates for the spectral radius of graphs: upper left) oot-mean-square deviation between the spectral radius and the estimates from (5)–(12) and (15) for the sets of connected graphs from four to ten vertices; upper right) ratio of the number of connected graphs for which these estimates are sharp; lower left) root-mean-square deviation between the spectral radius and the estimates for the sets of trees from 10 to 20 vertices; lower right) ratio of the number of trees for which the estimates are sharp. Note that the upper right and the lower right diagram have a number of lines overlapping entirely, as the respective estimates are sharp for exactly the same sets of graphs, so that only one of the overlapping lines is visible. In particular, the line for $\max_{u\in V}\sqrt{d_{2,u}}$ represents the sharpness of all estimates in (5), (7) and (8), the line for $\max_{u\in V} d_{2,u}/d_u$ represents also the sharpness of lower bounds in (6) and (9, and the line for $\sqrt{\sum_{u\in V} d_{3,u}^2/\sum_{u\in V} d_{2,u}^2}$ represents also the sharpness of $\sqrt{\sum_{u\in V} d_{2,u}^2/M_1}$. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

Declaration of competing interest

No potential conflict of interest was reported by the authors.

Acknowledgements

LF was supported by NSFC (No. 11671402, 11871479), Hunan Provincial Natural Science Foundation (2016JJ2138, 2018JJ2479) and Mathematics and Interdisciplinary Sciences Project of Central South University. DS was partly supported by Grant ON174033 of the Serbian Ministry of Education, Science and Technological Development.

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