On the spectral radius of VDB graph matrices

Ivan Gutman
University of Kragujevac, Faculty of Science,
Kragujevac, Republic of Serbia,
e-mail: gutman@kg.ac.rs,
ORCID ID: https://orcid.org/0000-0001-9681-1550
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Abstract:
Introduction/purpose: Vertex-degree-based (VDB) graph matrices form a
special class of matrices, corresponding to the currently much investigated
vertex-degree-based (VDB) graph invariants. Some spectral properties of
these matrices are investigated.
Results: Generally valid sharp lower and upper bounds are established for
the spectral radius of any VDB matrix. The equality cases are
characterized. Several earlier published results are shown to be special
cases of the presently reported bounds.
Conclusion: The results of the paper contribute to the general spectral
theory of VDB matrices, as well as to the general theory of VDB graph
invariants.

Keywords: Vertex-degree-based matrix, VDB matrix, vertex-degree-
based graph invariant, VDB graph invariant, spectral radius (of matrix).

Introduction
This paper concerns simple connected graphs. Let $G$ be such a
graph. Its vertex and edges sets are $V(G)$ and $E(G)$, respectively,
whereas its order (number of vertices) and size (number of edges) are
$|V(G)| = n$ and $|E(G)| = m$, respectively. By $uv \in E(G)$, we denote
the edge of $G$ connecting the vertices $u$ and $v$. 
The degree (= number of first neighbors) of a vertex \( u \in V(G) \) is denoted by \( d_u \). If \( d_u = r \) for all \( u \in V(G) \), then \( G \) is said to be a regular graph of the degree \( r \). If \( d_u = n - 1 \) for all \( u \in V(G) \), then \( G \) is the complete graph (of the order \( n \)), denoted by \( K_n \).

For other graph-theoretical notions, the readers are referred to standard textbooks (Harary, 1969; Bondy & Murthi, 1976).

In the present-day mathematical and chemical literature, a large number, well over hundred, of degree-based graph invariants of the form

\[
TI(f;G) = \sum_{uv \in E(G)} f(d_u, d_v)
\]

are being studied, where \( f(x, y) \) is an appropriately chosen function with the property \( f(x, y) = f(y, x) \) and \( f(x, y) \geq 0 \) for all \( x, y = d_u, d_v \).

In chemistry, molecular physics, pharmacology, and elsewhere, these graph invariants found a great variety of applications, and are usually referred to as „topological indices“ or „molecular structure-descriptors“ (Gutman, 2013; Todeschini & Consonni, 2009; Kulli, 2020). Instead of „vertex-degree-based“ the abbreviation VDB is often used (Rada, 2014; Li et al, 2021; Monsalve & Rada, 2022).

Let the vertices of the graph \( G \) be labelled as \( v_1, v_2, \ldots, v_n \). Then, to each VDB graph invariant \( TI(f;G) \), a symmetric square matrix \( M(f;G) \) of the order \( n \) can be associated, whose \((i,j)\)-element is equal to \( f(d_{v_i}, d_{v_j}) \) if the vertices \( v_i \) and \( v_j \) are adjacent, i.e. if \( v_i, v_j \in E(G) \), and is equal to zero otherwise. In particular,

\[
TI(f;G)_{ii} = 0 \quad \text{for all } i = 1, 2, \ldots, n.
\]

As it is well known in linear algebra (Brualdi & Cvetković, 2008), the eigenvalues of \( M(f;G) \) are real-valued numbers, forming the spectrum of the matrix \( M(f;G) \). Further on, they will be denoted by \( \lambda_1, \lambda_2, \ldots, \lambda_n \) so that \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \). Then \( \lambda_i \geq |\lambda_i| \), \( i = 2, 3, \ldots, n \), and therefore \( \lambda_1 \) is called the spectral radius of the corresponding VDB graph matrix (Stevanović, 2015).
In order to prove our main result, Theorem 1, we need an auxiliary lemma.

**Lemma 1.** Let \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) be the eigenvalues of the VDB matrix \( M(f;G) \). Then,

\[
\sum_{i=1}^{n} \lambda_i = 0 \tag{2}
\]

and

\[
\sum_{i=1}^{n} \lambda_i^2 = 2TI(f^2;G) \tag{3}
\]

*Proof.* By definition of the matrix \( M(f;G) \), its diagonal elements are always equal to zero. From this, Eq. (2) follows straightforwardly.

In order to arrive at Eq. (3), note that the sum of \( k \)-th powers of the eigenvalues is equal to the trace (sum of diagonal elements) of the \( k \)-th power of the respective matrix. Thus,

\[
\sum_{i=1}^{n} \lambda_i^2 = Tr M(f;G)^2 = \sum_{i=1}^{n} \left( M(f;G)^2 \right)_{ii} = \sum_{i=1}^{n} \sum_{j=1}^{n} M(f;G)_{ij} M(f;G)_{ji} = \sum_{i=1}^{n} \sum_{j=1}^{n} \left( M(f;G)_{ij} \right)^2 = 2 \sum_{uv \in E(G)} (f(d_u,d_v))^2 = 2TI(f;G)
\]

where we used the above specified definition of the elements of the VDB matrix \( M(f;G) \).

Note that the above lemma is a direct generalization of Lemma 1 in (Gutman, 2021), stated for a special case of the function \( f \) in Eq. (1), namely for \( f = \sqrt{x^2 + y^2} \).

We are now prepared to state our main result.
Theorem 1. Let $G$ be a connected graph of the order $n$, and let $\lambda_1$ be the spectral radius of its VDB matrix $M(f; G)$. Then $\lambda_1$ is bounded as:

$$\frac{2TI(f; G)}{n} \leq \lambda_1 \leq \sqrt{\frac{2(n-1)}{n}TI(f^2; G)}.$$  \hspace{1cm} (4)

The equality on the left-hand side holds if and only if $G$ is regular. The equality on the right-hand side holds if $G \cong K_n$.

Proof of Theorem 1

**Lower bound.** We proceed in an analogous manner as in the proof of Lemma 2 in (Gutman, 2021). Thus, in view of the Rayleigh-Ritz variational principle, for an $n$-dimensional column-vector $\Omega = (1,1,...,1)^T$,

$$\frac{\Omega^TM(f; G)\Omega}{\Omega^T\Omega} \leq \lambda_1$$ \hspace{1cm} (5)

with equality if and only if $\Omega = (1,1,...,1)^T$ is an eigenvector of $M(f; G)$, corresponding to the eigenvalue $\lambda_1$. As it is well known (Brualdi & Cvetković, 2008; Cvetković et al, 2010), this happens if and only if the graph $G$ is regular.

The lower bound for the spectral radius follows directly from Eq. (5).

**Upper bound.** Eq. (2) can be rewritten as

$$\lambda_1 = -\sum_{i=2}^{n} \lambda_i \quad \text{i.e.,} \quad \lambda_1^2 = \left( \sum_{i=2}^{n} \lambda_i \right)^2$$

Using the Cauchy-Schwarz inequality, we get

$$\left( \sum_{i=2}^{n} \lambda_i \times 1 \right)^2 \leq \sum_{i=2}^{n} \lambda_i^2 \sum_{i=2}^{n} 1^2 = (n-1)\sum_{i=2}^{n} \lambda_i^2$$ \hspace{1cm} (6)

implying

$$\lambda_1^2 \leq (n-1) \left[ \sum_{i=1}^{n} \lambda_i^2 - \lambda_1^2 \right] \quad \text{and} \quad n\lambda_1^2 \leq (n-1)\sum_{i=1}^{n} \lambda_i^2$$
i.e.,

\[ \lambda_1 \leq \sqrt{\frac{n-1}{n} \sum_{i=1}^{n} \lambda_i^2}. \]

The upper bound for the spectral radius is followed by Eq. (3).

The equality in (6) happens if and only if \( \lambda_2 = \lambda_3 = \cdots = \lambda_n \), which is the case only for the complete graph \( K_n \). Recall that the complete graph is an \((n-1)\)-regular graph, and therefore its VDB matrix is equal to \( f(n-1,n-1)A(K_n) \) where \( A(G) \) stands for the ordinary adjacency matrix of the graph \( G \). Since the ordinary eigenvalues of \( K_n \) are \( n-1,-1,-1,\ldots,-1 \) (Cvetković et al, 2010), the VDB-eigenvalues of the complete graph satisfy \( \lambda_2 = \lambda_3 = \cdots = \lambda_n = -f(n-1,n-1) \). The complete graph is the only connected graph whose all eigenvalues, except the spectral radius, are mutually equal.

As already mentioned, the special case of the lower bound in Theorem 1 for \( f = \sqrt{x^2 + y^2} \) was reported in (Gutman, 2021). The same special case for the upper bound was recently communicated in (Lin et al, 2023).

References


О спектральном радиусе матриц графов ВДБ

Иван Гутман

Крагуевацкий университет, естественно-математический факультет,
г. Крагуевац, Республика Сербия

РУБРИКА ГРНТИ: 27.29.19 Краевые задачи и задачи на собственные значения для обыкновенных дифференциальных уравнений и систем уравнений

ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Матрицы графа, основанные на вершинных степенях (ВДБ), образуют особый класс матриц, соответствующих в настоящее время широко исследованным инвариантам графа, основанным на вершинных степенях (ВДБ). В данной статье исследованы некоторые спектральные свойства подобных матриц.

Результаты: Получены общепринятые нижняя и верхняя границы спектрального радиуса матриц ВДБ. Также представлены случаи, в которых применяются равенства. В статье показано, что ранее
популикованные результаты являются частными случаями пределов, которые теперь более подробно описаны.

Выводы: Результаты настоящей работы вносят вклад в общую спектральную теорию матриц ВДБ, а также в общую теорию инвариантов графов ВДБ.

Ключевые слова: матрица основанная на степени вершин графа ВДБ, ванвариант графа, основанный на степени вершин графа ВДБ, спектральный радиус (матрицы).
Team has taken special care that the referee did not recognize the author’s identity, thus avoiding the conflict of interest.

**COMMENTS OF THE EDITORIAL BOARD:** The author of this article Ivan Gutman is a member of the editorial board of the journal “Military Technical Courier.” Therefore, the editorial board conducted more open and more rigorous double-blind peer review. The editorial board made additional efforts to maintain the integrity of the review and minimize bias, so that the second editor—a colleague—acted independently of the author-editor, thus the review process was absolutely transparent. The editorial board took special care that the reviewer did not recognize the author’s identity, thus avoiding the conflict of interest.

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