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Gutman, Ivan

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On the spectral radius of VDB graph matrices

О спектральном радиусе матриц графов ВДБ

Спектрални радијус ВДБ графовских матрица

Ivan Gutman ^a

University of Kragujevac, Serbia

gutman@kg.ac.rs

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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).

Р е з ю м е :

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 опубликованные 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.

К л ю ч е в ы е с л о в а : матрица основанная на степени вершин, матрица ВДБ, инвариант графа, основанный на степени вершин, инвариант графа ВДБ, спектральный радиус (матрицы).

ABSTRACT:

Увод/циљ: На степенима чворова засноване, ВДБ графовске матрице образују класу специјалних матрица које одговарају, данас често истраживаним, на степенима чворова заснованим, ВДБ графовским инваријантама. Испитиване су неке спектралне особине ових матрица.

Резултати: Добијене су општеважеће доње и горње границе за спектрални радијус ВДБ матрица. Окарактерисани су и случајеви када важе једнакости. За неколико раније публикованих резултата је показано да су специјални случајеви сада у наведеним границама.

Закључак: Резултати изложени у раду представљају допринос општој спектралној теорији ВДБ матрица, као и општој теорији ВДБ графовских инваријанти.

KEYWORDS: графовске матрице засноване на степенима чворова, ВДБ матрице, графовске инваријанте засноване на степенима чворова, ВДБ графовске инваријанте, спектрални радијус (матрице).

AUTHOR NOTES

^a University of Kragujevac, Faculty of Science, Kragujevac, Republic of Serbia

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 $uv \in (G)$, 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

$$TI(f; G) = \sum_{uv \in E(G)} f(d_u, d_v) \quad (1)$$

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 $v_1, v_2, \dots, v_n$. 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, $TI(f; G)_{ii} = 0$ for all $i = 1, 2, \dots, n$.

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 $\lambda_1, \lambda_2, \dots, \lambda_n$ so that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Then $\lambda_1 \geq |\lambda_i|$, $i = 2, 3, \dots, n$, and therefore λ_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 $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of the VDB matrix $M(f; G)$. Then

$$\sum_{i=1}^n \lambda_i = 0 \quad (2)$$

and

$$\sum_{i=1}^n \lambda_i^2 = 2 TI(f^2; G).$$

(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,

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

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 λ_1 be the spectral radius of its VDB matrix $M(f;G)$. Then λ_1 is bounded as:

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

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 $\Omega = (1, 1, \dots, 1)^T$,

$$\frac{\Omega^T M(f;G) \Omega}{\Omega^T \Omega} \leq \lambda_1 \quad (5)$$

with equality if and only if $\Omega = (1, 1, \dots, 1)^T$ is an eigenvector of $M(f;G)$, corresponding to the eigenvalue λ_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

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

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 $\lambda_2 = \lambda_3 = \dots = \lambda_n$, 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 $n-1, -1, -1, \dots, -1$ (Cvetković et al, 2010), the VDB-eigenvalues of the complete graph satisfy $\lambda_2 = \lambda_3 = \dots = \lambda_n = -f(n-1, n-1)$. 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).

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ADDITIONAL INFORMATION

FIELD: mathematics (mathematics subject classification: primary 05C50, secondary 05C07, 05C09)

ARTICLE TYPE: original scientific paper

EDITORIAL NOTE: The author of this article, Ivan Gutman, is a current member of the Editorial Board of the Military Technical Courier. Therefore, the Editorial Team has ensured that the double blind reviewing process was even more transparent and more rigorous. The Team made additional effort to maintain the integrity of the review and to minimize any bias by having another associate editor handle the review procedure independently of the editor – author in a completely transparent process. The Editorial Team has taken special care that the referee did not recognize the author's identity, thus avoiding the conflict of interest.

КОММЕНТАРИЙ РЕДКОЛЛЕГИИ: Автор данной статьи Иван Гутман является действующим членом редколлегии журнала «Военно-технический вестник». Поэтому редколлегия провела более открытое и более строгое двойное слепое рецензирование. Редколлегия приложила дополнительные усилия для того чтобы сохранить целостность рецензирования и свести к минимуму предвзятость, вследствие чего второй редактор-сотрудник управлял процессом рецензирования независимо от редактора-автора, таким образом процесс рецензирования был абсолютно прозрачным. Редколлегия во избежание конфликта интересов позаботилась о том, чтобы рецензент не узнал кто является автором статьи.

РЕДАКЦИЈСКИ КОМЕНТАР: Аутор овог чланка Иван Гутман је актуелни члан Уређивачког одбора Војнотехничког гласника. Због тога је уредништво спровело транспарентнији и ригорознији двоструко слепи процес рецензије. Уложило је додатни напор да одржи интегритет рецензије и

необјективност сведе на најмању могућу меру тако што је други уредник сарадник водио процедуру рецензије независно од уредника аутора, при чему је тај процес био апсолутно транспарентан. Уредништво је посебно водило рачуна да рецензент не препозна ко је написао рад и да не дође до конфликта интереса.

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