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Original scientific papers

Estimating vertex-degree-based energies

Оценка энергий, онсованных на степени вершин

Процена енергија заснованих на степенима чворова

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Abstract:

Introduction/purpose: In the current literature, several dozens of vertex-degree-based (VDB) graph invariants are being studied. To each such invariant, a matrix can be associated. The VDB energy is the energy (= sum of the absolute values of the eigenvalues) of the respective VDB matrix. The paper examines some general properties of the VDB energy of bipartite graphs.
Results: Estimates (lower and upper bounds) are established for the VDB energy of bipar- tite graphs in which there are no cycles of size divisible by 4, in terms of ordinary graph energy.
Conclusion: The results of the paper contribute to the spectral theory of VDB matrices, especially to the general theory of VDB energy.
Keywords: vertex-degree-based graph invariant, vertex-degree-based matrix, vertex-degree- based energy, energy (of graph).

Резюме:

Введение/цель: В новейшей литературе изучаются десятки инвариантов графов, основанных на степени вершин (VDB). К каждому такому инварианту может присоединиться матрица. Энергия VDB - это энергия (= сумма абсолютных значений собственных значений) соответствующей матрицы VDB. В данной статье исследуются некоторые общие свойства VDB-энергии двудольных графов.
Результаты: Получены оценки (нижней и верхней границы) по энергии VDB двудольных графов, не имеющих циклов величины, кратной 4, в зависимости от обычной энергии графа.
Выводы: Результаты статьи вносят вклад в спектральную теорию матриц VDB, а особенно в общую теорию энергии VDB.
Ключевые слова: инвариант графа, основанный на степени вершины, матрица, основанная на степени вершины, энергия, основанная на степени вершины, энергия (графа).

Abstract:

Увод/циљ: У новијој литератури проучавају се бројне графовске инваријанте засноване на степенима чворова (VDB). Свакој од ових инваријанти може се придружити матрица. VDB енергија је збир апсолутних вредности сопствених вредности одговарајуће VDB матрице. Рад истражује неке опште особине ВДБ енергије бипартитних графова.
Резултати: Добијене су процене (доње и горње границе) за VDB енергију бипартитних графова који немају циколве величине дељиве са 4, а у зависности од обичне графовске енергије.
Закључак: Резултати овог рада доприносе спектралној теорији VDM матрица, а посебно општој теорији VDB енергије.
Keywords: инваријанта заснована на степенима чворова, матрица заснована на стпенима чворова , енергија заснована на степенима чворова, енергија (графа).

Introduction

Let G be a simple graph with the vertex set $\mathbf{V}(G)$ and the edge set $\mathbf{E}(G)$. If the vertices $u, v \in \mathbf{V}(G)$ are adjacent, then the edge connecting them is denoted by uv. The number of edges incident to a vertex v is the degree of that vertex, and is denoted by *d(v)*. The minimum and maximum vertex degrees are denoted by δ and Δ, respectively.

Let $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$. Then the adjacency matrix $\mathbf{A}(G) = [a_{ij}]$ of the graph G is the symmetric matrix of order n, whose elements are (Cvetković et al, 2010):

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{1}$$

If the eigenvalues of $\mathbf{A}(G)$ are $\lambda_1, \ldots, \lambda_n$, then the (ordinary) *energy* of the graph G is defined as

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|\,. \tag{2}$$

The theory of graph energy is nowadays elaborated in due detail (Li et al, 2012; Ramane, 2020).

In the chemical and mathematical literature, a variety of vertex-degree-based (VDB) graph invariants of the form

$$\mathcal{I} = \mathcal{I}(G) = \sum_{uv \in \mathbf{E}(G)} f\big(d(u), d(v)\big) \tag{3}$$

has been considered, where f is a suitably chosen function, with a property $f(x, y) = f(y, x)$ (Kulli, 2020; Todeschini & Consonni, 2009). These are usually referred to as *topological indices*. Of these, we list here a few most popular and best studied ones (Table 1):

TABLE 1

$f(x, y)$	name of index	type
$x + y$	first Zagreb	↑
xy	second Zagreb forgotten	↑
$x^2 + y^2$	Sombor	↑
√x2 + y2	nirmala Randić	↑
√x + y 1/	sum-connectivity	↑
√xy 1/√x	harmonic	↓
+ y 2/(x +	inverse degree	↓
y)	modified Sombor	↓
$1/x^2 + 1/y^2$	atom-bond-connectivity	↓
1/√x2 + y2	Albertson	↓
$[(x + y - 2)/(xy)]^{1/2}$		~
$\lvert x - y \rvert$		~

The parameters x and y (being vertex degrees) always satisfy the condition $x \geq 1$, $y \geq 1$. Bearing this in mind, we immediately recognize that most VDB indices are either monotonically increasing (↑) or monotonically decreasing functions (↓) of the vertex degrees. Only a few such indices do not possess such a monotonicity property (#).

It should be noted that for practically all VDB indices of type ↑ that exist in the literature, the condition $f(x, y) \geq 1$ is satisfied for all values of x and y that occur for the edges of graphs.

Analogously, for practically all VDB indices of type ↓ , $0 < f(x, y) \leq 1$ holds for all values of x and y.

Taking into account Eq (1) and (3) we introduce the VDB matrix

$$\mathbf{A}_{\mathcal{I}}(G) = \left[(a_{\mathcal{I}})_{ij}\right]$$

via

$$(a_{\mathcal{I}})_{ij} = \begin{cases} f\big(d(v_i), d(v_j)\big) & \text{if } v_i v_j \in \mathbf{E}(G) \\ 0 & \text{if } v_i v_j \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases} \tag{4}$$

If its eigenvalues are $\mu_1, \ldots, \mu_n$, then the energy pertaining to the VDB invariant $\mathcal{I}$, Eq. (3), is

$$\mathcal{E}_{\mathcal{I}} = \mathcal{E}_{\mathcal{I}}(G) = \sum_{i=1}^{n} |\mu_i|\,. \tag{5}$$

For recent works on the investigation of this class of graph-spectral invariants see (Das et al, 2018; Gutman, 2020; Gutman, 2021; Gutman et al, 2022; Li & Wang, 2021; Shao et al, 2021).

Main results

A cycle of length p is a cycle consisting of (exactly) p vertices $v_1, v_2, \ldots, v_p$, so that v_i and v_{i+1} are adjacent for $i = 1, 2, \ldots, p-1$, and also v_1 and v_p are adjacent. As it is well known, a graph G is bipartite if and only if all its cycles (if any) are of even length. In this paper, we prove the results valid for bipartite graphs which do not possess cycles of a length divisible by 4. Let G be such a graph. Without loss of generality, we assume that G is connected.

Let the graph energy □ and the VDB energy $\mathcal{E}_{\mathcal{I}}$ be the quantities defined via Eqs. (2) and (5), and let be the function specified in Eq. (3). Let δ ad Δ be the smallest and largest vertex degrees of G.

Theorem 1. Let G be a bipartite graph with no cycle of size divisible by 4. Then

$$f(\delta, \delta)\, \mathcal{E}(G) \leq \mathcal{E}_{\mathcal{I}}(G) \leq f(\Delta, \Delta)\, \mathcal{E}(G)$$

holds for all VDB invariants in which the function f is monotonically increasing and $f(x, y) \geq 1$ for all vertex degrees x and y. Equality on both sides holds if and only if G is a regular graph, in which case $\delta = \Delta$.

The examples of the VDB invariants for Theorem 1 are the above listed first and second Zagreb, forgotten, Sombor, and nirmala indices.

Theorem 2. Let G be a bipartite graph with no cycle of size divisible by 4. Then

$$f(\Delta,\Delta)\,\mathcal{E}(G)\leq\mathcal{E}_{\mathcal{I}}(G)\leq f(\delta,\delta)\,\mathcal{E}(G)$$

holds for all VDB invariants in which the function f is monotonically decreasing and 0 < f (x, y) ≤ 1 for all vertex degrees x and y. Equality on both sides holds if and only if G is a regular graph.

The examples of the VDB invariants for Theorem 2 are the above listed Randi´c, sum-connectivity, harmonic, and modified Sombor indices, as well as the inverse degree.

A tree is a connected graph with no cycles. Therefore, Theorems 1 and 2 apply to trees. For any tree δ = 1, but Theorems 1 and 2 can be slightly strengthened.

Theorem 3. Let T be a tree with n ≥ 3 vertices. Then

$$f(1,2)\,\mathcal{E}(T)\leq\mathcal{E}_{\mathcal{I}}(T)<f(\Delta,\Delta)\,\mathcal{E}(T)$$

holds for all V DB invariants in which the function f is monotonically increasing and f (x, y) ≥ 1 for all x, y. Equality on the left-hand side holds if and only if n = 3.

Theorem 4. Let T be a tree with n ≥ 3 vertices. Then

$$f(\Delta,\Delta)\,\mathcal{E}(T)<\mathcal{E}_{\mathcal{I}}(T)\leq f(1,2)\,\mathcal{E}(T)$$

holds for all VDB invariants in which the function f is monotonically decreasing and 0 < f (x, y) ≤ 1 for all x, y. Equality on the right-hand side holds if and only if n = 3.

In addition to trees, Theorems 1 and 2 are applicable to various classes of cycle- containing graphs. Of these, of particular interest may be the hexagonal systems (molecular graphs of benzenoid hydrocarbons) (Gutman & Cyvin, 1989). All their vertices are of degrees 2 and 3. The so-called catacondesned hexagonal systems (= hexagonal systems having no internal vertices) are known to possess only cycles of size 4p + 2. For these molecular graphs

$$f(2,2)\,\mathcal{E}(G)<\mathcal{E}_{\mathcal{I}}(G)<f(3,3)\,\mathcal{E}(G)\,. \tag{6}$$

or

$$f(3,3)\,\mathcal{E}(G)<\mathcal{E}_{\mathcal{I}}(G)<f(2,2)\,\mathcal{E}(G)\,. \tag{7}$$

depending on whether f (x, y) monotonically increases or decreases.

Hexagonal systems possessing internal vertices have cycles of size 4p, p = 3, 4, etc., and thus Theorems 1 and 2 are not applicable. We nevertheless conjecture that estimates (6) and (7) are valid for all hexagonal systems.

In order to prove the above theorems, we need an auxiliary result, stated below as Lemma 3.

Energy of a weighted bipartite graph

The main part of the results outlined in this section was reported in (Gutman et al, 2021). These are repeated here (in an abbreviated form) in order to maintain completeness. Also, a few errors committed in (Gutman et al, 2021) are corrected.

Let G be a bipartite graph with n vertices. Let G_w be obtained from G by associating weighs to its edges, so that wij is the weight of the edge ij. Then the characteristic polynomial of G_w is of the form (Cvetković et al, 2010)

$$\phi(G_w,\lambda) = \lambda^n + \sum_{k\geq 1}(-1)^k\, c(G_w,k)\, \lambda^{n-2k} \tag{8}$$

whereas the energy of G_w satisfies the equality (Gutman, 1977), (Gutman, 2020), (Li et al, 2012)

$$\mathcal{E}(G_w) = \frac{2}{\pi}\int_0^{+\infty}\frac{dx}{x^2}\,\ln\left[1+\sum_{k\geq 1} c(G_w,k)\,x^{2k}\right]. \tag{9}$$

Note that □(G_w) is a monotonically increasing function of any of the coefficients $c(G_w,k)$.

According to the Sachs theorem (Cvetković et al, 2010).

$$(-1)^k\, c(G_w,k) = \sum_{\sigma\in\mathcal{S}_{2k}(G_w)} (-1)^{p(\sigma)}\, 2^{c(\sigma)}\, w(\sigma) \tag{10}$$

where $S_k(G_w)$ is the set of all Sachs graphs of G_w possessing exactly $2k$ vertices, and where σ is an element of $S_{2k}(G_w)$, containing $p(\sigma)$ components, of which $c(\sigma)$ are cycles. The weight of the Sachs graph σ is equal to the product of the weights of its components.

If the isolated edge ij is a component of σ, then its weight is $\mathrm{w}_{\mathrm{ij}}^2$. If a cycle Z is a component of σ, then its weight is the product of weights of the edges contained in Z.

Lemma 1. (Gutman et al, 2021) *If the Sachs graph σ # $S_{2k}(G_w)$ ≠ # does not contain cycles whose size is divisible by 4, then*

$(-1)^k\,(-1)^{p(\sigma)}\,2^{c(\sigma)} > 0$.

Proof. The Sachs graph σ has $p(\sigma)$ components. Let among them be $r_0 \geq 0$ isolated edges, whose total number of vertices is $2r_0$. Let σ contain $r_1 \geq 0$ cycles, whose total number of vertices is $4x + 2\,r_1$ for some integer x. Thus, $2k = 2r_0 + 4x + 2\,r_1$.

Case 1: $2k$ is not divisible by 4. Then $(-1)^k = -1$ whereas $r_0 + r_1 = p(\sigma)$ is odd.

Therefore, $(-1)^k (-1)^{p(\sigma)} > 0$ and the claim of Lemma 1 holds.

Case 2: $2k$ is divisible by 4. Then $(-1)^k = +1$ whereas $r_0 + r_1 = p(\sigma)$ is even, implying, again, $(-1)^k (-1)^{p(\sigma)} > 0$.

Lemma 1 has the following noteworthy consequences:

Lemma 2.

(a) Let G_w be an edge-weighted bipartite graph whose all cycles (if any) have size not divisible by 4, and let the weights of all its edges be positive-valued. Then for any Sachs graph σ # $S_{2k}(G_w)$ ≠ #,

$(-1)^k (-1)^{p(\sigma)} 2^{c(\sigma)} w(\sigma) > 0$.

(b) Therefore, because of Eq. (10), the coefficients $c(G_w, k)$ in Eq. (8) are non-negative and are the monotonically increasing functions of the edge-weights.

(c) Therefore, because of Eq. (9), the energy of the graphs G_w is a monotonically increas- ing function of the edge-weights.

From Lemma 2(c), we obtain the result needed for our proofs:

Lemma 3. Let G_w be an edge-weighted bipartite graph whose all cycles (if any) have size not divisible by 4.

(a) If for all edges ij # $\mathbf{E}(G_w)$, the condition $w_{ij} \geq 1$ holds, then □ $(G_w) \geq$ □ (G).

If $w_{ij} > 1$ for at least one edge ij, then □ $(Gw) >$ □ (G).

(b) If for all edges ij # $\mathbf{E}(G_w)$, the condition $w_{ij} \leq 1$ holds, then □ $(G_w) \leq$ □ (G).

If $w_{ij} < 1$ for at least one edge ij, then □ $(Gw) <$ □ (G).

(c) If in both cases (a) and (b), $w_{ij} = w$ holds for all edges ij # $\mathbf{E}(G_w)$, *then* □ $(G_w) = w$ □ (G).

Proof of Theorems 1-4

The adjacency matrix $A_{\mathcal{I}}(G)$, Eq. (4), could be viewed as the ordinary adjacency matrix of an edge-weighted modification of the graph G. Therefore, if the condition f (dvi, dvj) >

Therefore, if the condition $f(dv_i, dv_j > 1)$ holds, and if $f(x, y)$ is an increasing function for $x \geq 1$ and y ≥ 1, then the lower bound of Theorem 1 follows by Lemma 3 if all $f(x, y)$ are replaced by $f(\delta, \delta)$.

The upper bound is obtained if all $f(x, y)$ are replaced by $f(\Delta, \Delta)$.

The proof of Theorem 2 is analogous.

Theorems 3 and 4 are based on the fact that no tree with $n \geq 3$ vertices is a regular graph. The only tree having two adjacent degree-one vertices is the two-vertex tree. Therefore, for trees with 3 or more vertices, the minimal (resp. maximal) value of $f(x, y)$ is $f(1, 2)$.

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