RELATING GRAPH ENERGY WITH VERTEX-DEGREE-BASED ENERGIES

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Abstract:

Introduction/purpose: The paper presents numerous vertex-degree-based graph invariants considered in the literature. A matrix can be associated to each of these invariants. By means of these matrices, the respective vertex-degree-based graph energies are defined as the sum of the absolute values of the eigenvalues.

Results: The article determines the conditions under which the considered graph energies are greater or smaller than the ordinary graph energy (based on the adjacency matrix).

Conclusion: The results of the paper contribute to the theory of graph energies as well as to the theory of vertex-degree-based graph invariants.

Keywords: energy (of a graph), vertex-degree-based graph invariant, vertex-degree-based graph energy.

Introduction

This paper is concerned with simple graphs, i.e. with graphs without multiple, directed, or weighted edges, and without loops. Let *G* be such a graph with *n* vertices, labeled as $v_1, v_2, \ldots, v_n$. Two vertices connected by an edge are said to be adjacent. The degree of the vertex v_i, denoted by $\deg(v_i)$, is the number of the first neighbors of v_i.

The energy of a graph *G* was defined in 1978 as (Gutman, 1978), (Li et al, 2012)

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. Recall that the adjacency matrix $A(G)$ is a symmetrix square matrix of the order n, whose (i,j)-entry is

$$A(G)_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } v_i \text{ and } v_j \text{ are not adjacent} \\ 0 & \text{if } i = j \end{cases}$$

In the mathematical (Cruz et al, 2015), (Das et al, 2018), (Furtula et al, 2013), (Liu et al, 2019), (Rada & Cruz, 2014), (Zhong & Xu, 2014) and chemical (Todeschini & Consonni, 2009) literature, several dozens of vertex-degree-based graph invariants (usually referred to as "topological indices") have been introduced and extensively studied. Their general formula is

$$VDBI = VDBI(G) = \sum_{1 \le i < j \le n} F\left(\deg(v_i), \deg(v_j)\right)$$

where $F(x, y)$ is some function with the property $F(x, y) = F(y, x)$. In particular,

If $F(x, y) = x + y$, then VDBI = first Zagreb index;

if $F(x, y) = xy$, then VDBI = second Zagreb index;

if $F(x, y) = |x - y|$, then VDBI = Albertson index,

if $F(x, y) = \dfrac{1}{2}\left(\dfrac{x}{y} + \dfrac{y}{x}\right)$, then VDBI = extended index;

if $F(x, y) = (x - y)^2$, then VDBI = sigma index,

if $F(x, y) = 1/\sqrt{xy}$, then VDBI = Randić index;

if $F(x, y) = 2/(x + y)$, then VDBI = harmonic index;

if $F(x, y) = \sqrt{(x + y - 2)/(xy)}$, then VDBI = ABC index;

if $F(x, y) = \sqrt{xy}$, then *VDBI* = reciprocal Randić index;

if $F(x, y) = 1/\sqrt{x + y}$, then *VDBI* = sum-connectivity index;

if $F(x, y) = \sqrt{x + y}$, then *VDBI* = reciprocal sum-connectivity index;

if $F(x, y) = x^2 + y^2$, then *VDBI* = forgotten index;

if $F(x, y) = 2\sqrt{xy} / (x + y)$, then *VDBI* = geometric-arithmetic index;

if $F(x, y) = (x + y) / (2\sqrt{xy})$, then *VDBI* = arithmetic-geometric index; and

if $F(x, y) = xy / (x + y)$, then *VDBI* = inverse sum indeg index.

There are several more such graph invariants; see in (Das et al, 2018), (Kulli, 2020), where also bibliographic data can be found.

For each function $F(x, y)$ and each graph *G,* a symmetric square matrix $\Phi = \Phi(G)$ of the order *n* can be defined, whose (*i,j*)-entry is

$$\Phi(G)_{ij} = \begin{cases} F\left(\deg(v_i), \deg(v_j)\right) & \textit{if } v_i \textit{ and } v_j \textit{ are adjacent} \\ 0 & \textit{if } v_i \textit{ and } v_j \textit{ are not adjacent} \\ 0 & \textit{if } i = j \end{cases}$$

Recall that if v_i and v_j are adjacent, then $\deg(v_i) \geq 1$, $\deg(v_j) \geq 1$.

The respective vertex-degree-based graph energy (of the graph *G*) is equal to the sum of absolute values of the eigenvalues of $\Phi = \Phi(G)$. We will denote it by $E_F = E_F(G)$.

For some of the above given functions $F(x, y)$, the condition $0 < F(x, y) \leq 1$ holds for all $x \geq 1$, $y \geq 1$. Such are the functions pertaining to the Randić, harmonic, sum-connectivity, and geometric-arithmetic indices. For some of the above given functions, $F(x, y) \geq 1$

holds for all $x \geq 1$, $y \geq 1$. Such are those related to the first and second Zagreb, extended, forgotten, and arithmetic-geometric indices, as well as for some reciprocal and inverse indices. For such functions, we prove the following:

Theorem 1.

(a) If $0 < F(x, y) \leq 1$ holds for all $x \geq 1$, $y \geq 1$, and if G is a bipartite graph, then $E_F(G) \leq E(G)$.

(b) If $F(x, y) \geq 1$ holds for all $x \geq 1$, $y \geq 1$, and if G is a bipartite graph, then $E_F(G) \geq E(G)$.

The equality cases will be considered later.

In order to prove Theorem 1, we need some preparations.

Preliminary considerations

Let

$$P(x) = \sum_{k \geq 0} c_k \, x^{n-k}$$

be a polynomial with all zeros real. Then its energy satisfies (Mateljević et al, 2010)

$$E(P) = \frac{1}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \left[\left(\sum_{k \geq 0} (-1)^k c_{2k} x^{2k} \right)^2 + \left(\sum_{k \geq 0} (-1)^k c_{2k+1} x^{2k+1} \right)^2 \right]$$

If the zeros of $P(x)$ are symmetric w.r.t. $x=0$, i.e., if $c_{2k+1} = 0$ for all $k \geq 0$, then

$$E(P) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} (-1)^k c_{2k} x^{2k}$$

As well known, a graph is bipartite if and only if it does not contain cycles of odd size. The characteristic polynomial of a bipartite graph is of the form

$$\phi(G, x) = \sum_{k \geq 0} c_{2k} x^{n-2k}$$

Analogously, the characteristic polynomial of $\Phi = \Phi(G)$ conforms to the relation

$$\phi_F(G,x) = \sum_{k \geq 0} c_{2k}^{(F)} x^{n-2k}$$

The respective energies are then

$$E(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} (-1)^k c_{2k} x^{2k} \qquad (1)$$

and

$$E_F(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} (-1)^k c_{2k}^{(F)} x^{2k} \qquad (2)$$

Proving Theorem 1

We apply the Sachs coefficient theorem (Cvetković et al, 2010), (Gutman, 2017a). Recall that a Sachs graph is a graph consisting of vertices of degree one and/or two, i.e., all its components are isolated edges and/or cycles.

The application of the Sachs theorem to the coefficients of $\phi_F(G,x)$ yields:

$$c_{2k}^{(F)} = \sum_{s \in S_{2k}(G)} (-1)^{p(s)} 2^{q(s)} w(s)$$

where s is a Sachs graph and $S_{2k}(G)$ is the set of all ($2k$)-vertex Sachs graphs that are as subgraphs contained in the graph G, and where
$p(s)$ = number of components of s,
$q(s)$ = number of cyclic components of s, and
$w(s)$ = weight of s.

The weight of s is equal to the product of the weights of all edges contained in the cycles of s, times the product of the squares of the weights of the isolated edges of s. The weight of a particular edge is equal to the respective element of the matrix $\Phi(G)$. For the proof of

Theorem 1(a), it is only important that $w(s) \leq 1$.

Let *G* be a bipartite graph, and let the Sachs graph $s \in S_{2k}(G)$ contain α isolated edges, β cycles of the size 4*i*+2, and γ cycles of the size 4*i*.Then,

$$p(s) = \alpha + \sum_i \beta_i + \sum_i \gamma_i$$

and

$$2k = 2\alpha + \sum_i (4i+2)\beta_i + \sum_i (4i)\gamma_i \, .$$

Therefore,

$$p(s) + k = 2\left(\alpha + \sum_i (i+1)\beta_i + \sum_i i\gamma_i \right) \alpha + \sum_i \gamma_i$$

implying

$$p(s) + k \equiv \sum_i \gamma_i \pmod 2 \, .$$

In view of the above, the contribution of the Sachs graph *s* to the term

$(-1)^{p(s)} 2^{q(s)} w(s)$ is:

positive if *s* contains no cycles of size divisible by 4,
negative if *s* contains an odd number of cycles of a size divisible by 4, and
positive if s contains an even number of cycles of a size divisible by 4.

Suppose first that $\sum_i \gamma_i$ is zero or even. Then, the contribution of the Sachs graph $s \in S_{2k}(G)$ to $E_F(G)$, Eq. (2), is positive, and because of $w(s) \leq 1$, it is not greater than the respective contribution of *s* to $E(G)$, Eq. (1). In this case, $E_F(G) \leq E(G)$, with equality if all non-zero elements of $\Phi(G)$ are equal to unity.

There remains a case when $\sum_i \gamma_i$ is an odd integer. Then, *s* has at least one cycle whose size is divisible by 4. Let, for the sake of simplicity, this be a single 12-membered cycle, whose edges are $e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9, e_{10}, e_{11}, e_{12}$. Then, in addition to *s*, there exist

two more Sachs graphs $s', s'' \in S_{2k}(G)$ in which instead of the 12-membered cycle, there are 6 isolated edges, $e_1, e_3, e_5, e_7, e_9, e_{11}$ and $e_2, e_4, e_6, e_8, e_{10}, e_{12}$, respectively. The total contribution of the three Sachs graphs $s, s', s'' \in S_{2k}(G)$ is then

$$-2\prod_{i=1}^{12} w(e_i) + \prod_{i=1}^{6} w(e_{2i-1})^2 + \prod_{i=1}^{6} w(e_{2i})^2$$

plus the (necessarily positive) contribution coming from the other (mutually identical) fragments of s, s', s''. The above expression is equal to

$$\left(\prod_{i=1}^{6} w(e_{2n-1}) - \prod_{i=1}^{6} w(e_{2i}) \right)^2$$

which is non-negative. Because of $w(e) \leq 1$, this term is also less than or equal to unity.

Thus, also in this case, the joint contribution of the Sachs graphs s, s', s'' to $E_F(G)$ is positive but not greater than their contribution to $E(G)$.

This completes the proof of Theorem 1(a).

The proof of Theorem 1(b) is analogous. Note that the special case of Theorem 1(b), pertaining to extended energy, was earlier communicated in (Gutman, 2017b).

Discussion

If the graph G is not bipartite, then it contains odd cycles. Then, of course, some Sachs graphs also contain odd cycles. Consequently, some of the coefficients c_{2k+1} and $c_{2k+1}^{(F)}$ are non-zero. Besides, the sign of the coefficients c_{2k} and $c_{2k}^{(F)}$ cannot be predicted in the general case. For these reasons, it is not easy to extend Theorem 1 to non-bipartite graphs, and we leave this for some later moment or some more skilled colleague.

From the definitions of $E(G)$ and $E_F(G)$, it is evident that the equality $E_F(G) = E(G)$ will hold if all non-zero elements of the matrix $\Phi(G)$ are equal to unity. Whether this is an "if and only if" condition remains a (difficult) open problem.

In the case of regular graphs, for which $\deg(v_i) = r$, $i = 1, 2, \ldots, n$, the relation between $E(G)$ and $E_F(G)$ is significantly simplified. $E_F(G) = E(G)$ holds for the extended, geometric-arithmetic, and arithmetic energies. In addition, $E_F(G) = 2rE(G)$ holds for the first Zagreb energy, $E_F(G) = r^2 E(G)$ for the second Zagreb energy, $E_F(G) = 2r^2 E(G)$ for the forgotten energy, $E_F(G) = \dfrac{1}{r} E(G)$ for the Randić and harmonic energies, etc. Interestingly but evidently, the Albertson and sigma energies of regular graphs are equal to zero. On the other hand, for the class of stepwise irregular graphs (Gutman, 2018), the Albertson and sigma matrices coincide with the adjacency matrix, and for such graphs the Albertson and sigma energies are equal to the ordinary graph energy.

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ВЗАИМОСВЯЗЬ ЭНЕРГИИ ГРАФОВ С ЭНЕРГИЕЙ СТЕПЕНИ УЗЛОВ

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Резюме:

Введение/цель: На основании анализа существующей литературы, в статье представлены многочисленные инварианты графов, зависимые от степени узлов. К каждому из этих инвариантов подключается соответствующая матрица, с помощью которой считывается энергия графа, как сумма абсолютных величин собственных значений данных матриц.

Результаты: В статье определены условия, при которых вычисленные энергии графа были больше или меньше средней энергии графа (на основании матрицы смежности).

Выводы: Результаты данной статьи вносят вклад в теорию энергии графов, а также в теорию инвариантов графов, основанных на степени узлов.

Ключевые слова: энергия (графа); инварианты, зависящие от степени узлов; энергия, зависящая от степени узлов.

РЕЛАЦИЈЕ ИЗМЕЂУ ЕНЕРГИЈЕ ГРАФА И ЕНЕРГИЈА ЗАСНОВАНИХ НА СТЕПЕНИМА ЧВОРОВА

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Сажетак:

Увод/циљ: У раду су приказане бројне, у литератури постојеће, графовске инваријанте зависне од степена чворова. Овим инваријантама придружују се одговарајуће матрице, преко којих се израчунава енергија као збир апсолутних вредности сопствених вредности ових матрица.

Резултати: Одређени су услови под којима су испитиване веће, односно мање енергије од обичне енергије графа (засноване на матрици суседства).

Закључак: Рад доприноси теорији графовских енергија, као и теорији графовских инваријанти зависних од степена чворова.

Кључне речи: енергија (графа), инваријанте зависне од степена чворова, енергије зависне од степена чворова.