Transactions on Combinatorics
ISSN (print): 2251-8657, ISSN (on-line): 2251-8665
Vol. 14 No. 3 (2025), pp. 157-172.

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MINIMAL GRAPHS WITH RESPECT TO THE MULTIPLICATIVE VERSION OF SOME VERTEX-DEGREE-BASED TOPOLOGICAL INDICES

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Abstract. As a real-valued function, a graphical parameter is defined on the class of finite simple graphs, and remains invariant under graph isomorphism. In mathematical chemistry, vertex-degree-based topological indices are the graph parameters of the general form of $p_\phi(G) = \sum_{uv\in E(G)} \phi(d(u), d(v))$, where ϕ represents a real-valued symmetric function, and $d(u)$ shows the degree of $u \in V(G)$. In this paper, it is proved that if ϕ has certain conditions, then the graph among those with n vertices and m edges, whose difference between the maximum and minimum degrees is at most 1, has the minimal value of p_ϕ. Moreover, it is demonstrated that some well-known topological indices are able to satisfy these certain conditions, and the given indices can be treated in a unified manner.

1. Introduction

In this paper, the notations of [8] are considered. Specifically let $G = (V, E)$ be a finite, simple, connected and undirected graph, having order $n = |V(G)|$ and size $m = |E(G)|$. Such G is called an (n, m)-graph. In particular, if $m = n - 1$, n, or $n + 1$, then G is named a tree, a unicyclic graph or a bicyclic graph, respectively. For each vertex u in $V(G)$, the neighborhood $N(u)$ of u is the set of vertices adjacent to u. The number of vertices in $N(u)$ is further termed the degree of u, and denoted

MSC(2010): Primary: 05C09; Secondary: 05C35.

Keywords: Graph parameter, topological index, General sum connectivity index, multiplicative Zagreb indices, Sombor index; forgotten index.

Article Type: Research Paper.

Communicated by Ebrahim Ghorbani.

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Received: 28 October 2023, Accepted: 24 April 2024, Published Online: 05 May 2024.

Cite this article: M. Eliasi, Minimal graphs with respect to the multiplicative version of some vertex-degree-based topological indices, *Trans. Comb.*, **14** no. 3 (2025) 157-172.

http://dx.doi.org/10.22108/toc.2024.139624.2119 .

by $d(u)$. If $X \subset V(G)$, then $D(X)$ will be exploited to indicate the set of the degrees of all the vertices of X in G. For an edge $uv \in E(G)$, it is represented by $G - uv$ of the subgraph of G, acquired by deleting uv. Likewise, if $u, v \in V(G)$ but $uv \notin E(G)$, then the graph obtained from G by adding uv to $E(G)$ will be denoted by $G + uv$.

A graph parameter, known as a topological index in chemistry, is a real-valued function p from the class of all finite graphs to the real numbers, such that $p(G) = p(H)$, for any two isomorphic graphs G and H. The general reference here is [12], which provides historical information about more than 300 graph parameters as well as approximately 600 references regarding these parameters. In addition, the reader can refer to [25] for characterizing graph parameters obtained as the limits of subgraph densities.

In chemistry, topological indices are extensively used in quantitative structure-activity/property relationship (QASR/QSPR) methods [27, 28], which attempt to express the relationship between the structures of chemical compounds along with their physicochemical properties and biological activities. Whenever standard samples are not available in practice or tests are time-consuming or risky, the QSPR/QSAR method can be further applied to address the problem. This Wiener index is the first topological index to be used in chemistry. The Zagreb indices are also the most studied topological indices of the graph of a chemical compound, proposed by Gutman and Trinajstic [15] in 1975, as topological formulas for total n-electron energy of alternating hydrocarbons. After that, numerous topological indices have been devised and examined by other researchers. In this line, vertex-degree-based (VDB) topological indices are an important class, whose general form is as follows:

$$p_\phi(G) = \sum_{uv \in E(G)} \phi(d(u), d(v)), \tag{1.1}$$

where $\phi(x, y)$ denotes a real-valued symmetric function of x and y.

Following [14], the multiplicative version of topological indices has thus far attracted much attention. Similar to Equation (1.1), the multiplicative version of a VDB index is defined by:

$$\Pi_\phi(G) = \prod_{uv \in E(G)} \phi(d(u), d(v)). \tag{1.2}$$

Of note, $\ln \Pi_\phi(G) = \sum_{uv \in E(G)} \ln \phi(d(u), d(v))$, as a VDB index, is achieved by taking the logarithm of both sides of Equation (1.2). It is worth recalling that the forgotten index, which was first introduced in [15] and reinvented in [11], is described as:

$$F(G) = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2) = \sum_{u \in V(G)} d(u)^3.$$

A multiplicative version of the forgotten index, viz. the product of cubes of vertex degrees, was further defined in [31]. Note that $\prod_{u \in V(G)} d(u)^3 = [\prod_{u \in V(G)} d(u)]^3$. Since the extremal properties of $\prod_{u \in V(G)} d(u)$, known as the Narumi-Katayama index [26], have been investigated by many researchers

http://dx.doi.org/10.22108/toc.2024.139624.2119

[3, 4, 14, 16, 20], this version of the forgotten index is not taken into account in this paper; instead, the following multiplicative version of this index is reflected:

$$\Pi_F^* = \prod_{uv \in E(G)} (d(u)^2 + d(v)^2).$$

Current literature reveals a great deal of research on determining extremal graphs with respect to various VDB topological indices in different classes [5, 18, 22, 23, 30]. Surprisingly, the extremal values often have the same properties, and it does not matter what index is chosen. This, in turn, conveys the idea that the functions utilized in defining indices probably have some common properties. The motivation behind the present work goes back to [2], with an attempt to identify the mentioned properties for (n, m)-graphs. Upon examining different methods of obtaining minimum graphs in various classes, it is concluded that the technique used for $\phi(x, y) = \sqrt{x^2 + y^2}$ in [1] can disclose some properties. Indeed, it is proved that if ϕ satisfies some particular conditions, then the difference between the maximum and minimum degrees of the minimal (n, m)-graph with respect to the p_ϕ index is is at most 1. The value of this idea becomes apparent once the results of different studies are obtained as a unified approach. Moreover, new results can be driven, and some open problems are then proposed to shed light on future research. Some VDB indices together with the logarithm of their multiplicative version in the present paper are listed in Table 1.

Table 1. VDB indices considered in the present paper.

function $\phi(x,y)$	equation corresponds to	symbol
$(x+y)^\beta$	general sum connectivity index [32]: $0 < \beta < 1$	χ_β
$\sqrt{x^2+y^2}$	sombor index [13]	SO
$\ln\sqrt{x^2+y^2}$	the log. of multiplicative Sombor index [21]	$\ln \Pi_{SO}$
$\ln(x^2+y^2)$	the log. of multiplicative forgotten index	$\ln \Pi_F^*$
$\ln(x+y)$	the log. of multiplicative first Zagreb index [9]	$\ln \Pi_1^*$
$\ln(xy)$	the log. of multiplicative second Zagreb index [14]	$\ln \Pi_2$

2. Preliminaries

We denote by P_n and C_n the path and the cycle with n vertices, respectively. The number $\delta(G) := \min\{d(v) | v \in V(G)\}$ is the minimum degree of G and the number $\Delta(G) := \max\{d(v) | v \in V\}$ its maximum degree. The following theorem is needed throughout the paper.

http://dx.doi.org/10.22108/toc.2024.139624.2119

Theorem 2.1. *Let $\phi(x,y)$ be a symmetric nonnegative real-valued function that satisfies the following conditions:*
(1) $\frac{\partial\phi}{\partial x}>0$ *and* $\frac{\partial\phi}{\partial y}>0$*, for* $x,y\in[1,+\infty)$.
(2) $\frac{\partial\phi}{\partial x}$ *is decreasing in* y *and* $\frac{\partial\phi}{\partial y}$ *is decreasing in* x.
(3) $t[\phi(t,t)-\phi(t-1,t)]-s[\phi(s+1,s)-\phi(s,s)]>0$*, where* $t>s+1$ *and* $t,s\geq 1$.
(4) *If* $0\leq d\leq c<b\leq a$*, then* $\phi(a,b)+\phi(c,d)\leq\phi(a,c)+\phi(b,d)$.
Suppose that G is an (n,m)-graph with minimum p_ϕ index. Then $\Delta(G)-\delta(G)\leq 1$.

Proof. Assume the assertion of the lemma is false and $\Delta(G)-\delta(G)\geq 2$. Then, there exist vertices $p,q\in V(G)$ such that $d(p)=\delta(G)<\Delta(G)=d(q)$. Since $d(p)<d(q)$, we conclude that $N(q)-N(p)\neq\emptyset$. Let $w\in N(q)-N(p)$ and define $G^*=G-qw+pw$. Obviously, G^* is also an (n,m)-graph. Let S denote the set of all edges in G which are incident with p or q. We consider two following cases according to the the adjacency of p and q.

1. $pq\notin E(G)$. Suppose that $D(N(p))=\{c_1,c_2,\ldots,c_\delta\}$ and $D(N(q))=\{d_1,d_2,\ldots,d_\Delta\}$. There is no loss of generality in assuming $d_\Delta=d(w)$. The difference between the values of p_ϕ indices of G and G^* is,
$p_\phi(G)-p_\phi(G^*)$

$$\begin{aligned}
&= \sum_{uv\in E(G)\setminus S}\phi(d(u),d(v))+\sum_{i=1}^{\Delta}\phi(\Delta,d_i)+\sum_{j=1}^{\delta}\phi(\delta,c_j)\\
&\quad -[\sum_{uv\in E(G)\setminus S}\phi(d(u),d(v))+\sum_{i=1}^{\Delta-1}\phi(\Delta-1,d_i)+\sum_{j=1}^{\delta}\phi(\delta+1,c_j)\\
&\quad +\phi(\delta+1,d_\Delta)]\\
&= \sum_{i=1}^{\Delta-1}[\phi(\Delta,d_i)-\phi(\Delta-1,d_i)]-\sum_{j=1}^{\delta}[\phi(\delta+1,c_j)-\phi(\delta,c_j)]\\
&\qquad +[\phi(\Delta,d_\Delta)-\phi(\delta+1,d_\Delta)]\\
&= \sum_{i=1}^{\Delta-1}[\phi(\Delta,d_i)-\phi(\Delta-1,d_i)]-\sum_{j=1}^{\delta}[\phi(\delta+1,c_j)-\phi(\delta,c_j)]\\
&\quad +[\phi(\Delta,d_\Delta)-\phi(\delta+1,d_\Delta)]+[\phi(\Delta,d_\Delta)-\phi(\Delta-1,d_\Delta)]\\
&\qquad -[\phi(\Delta,d_\Delta)-\phi(\Delta-1,d_\Delta)]\\
&= \sum_{i=1}^{\Delta}[\phi(\Delta,d_i)-\phi(\Delta-1,d_i)]-\sum_{j=1}^{\delta}[\phi(\delta+1,c_j)-\phi(\delta,c_j)]\\
&\quad +[\phi(\Delta-1,d_\Delta)-\phi(\delta+1,d_\Delta)].
\end{aligned}$$

Since $\Delta-\delta\geq 2$, $\delta+1\leq\Delta-1$ and ϕ is increasing in x ($\frac{\partial\phi}{\partial x}\geq 0$), we have $\phi(\Delta-1,d_\Delta)-\phi(\delta+1,d_\Delta)>0$. For $0\leq b\leq a$, define $\Psi_{a,b}(y)=\phi(a,y)-\phi(b,y)$. Taking the derivative with

respect to y gives $\frac{d\Psi_{a,b}}{dy}(y) = \frac{\partial\phi}{\partial y}(a,y) - \frac{\partial\phi}{\partial y}(b,y)$. Since $\frac{\partial\phi}{\partial y}$ is decreasing in the first variable, $\Psi_{a,b}(y)$ is decreasing on the interval $(0,+\infty)$. Hence
$p_\phi(G) - p_\phi(G^*)$

$$\begin{aligned}
&\geq \sum_{i=1}^{\Delta}[\phi(\Delta,d_i) - \phi(\Delta-1,d_i)] - \sum_{j=1}^{\delta}[\phi(\delta+1,c_j) - \phi(\delta,c_j)] \\
&= \sum_{i=1}^{\Delta}\Psi_{\Delta,\Delta-1}(d_i) - \sum_{j=1}^{\delta}\Psi_{\delta+1,\delta}(c_j) \\
&\geq \sum_{i=1}^{\Delta}\Psi_{\Delta,\Delta-1}(\Delta) - \sum_{j=1}^{\delta}\Psi_{\delta+1,\delta}(\delta) \\
&= \Delta[\phi(\Delta,\Delta) - \phi(\Delta-1,\Delta)] - \delta[\phi(\delta,\delta+1) - \phi(\delta,\delta)],
\end{aligned}$$

which is positive by the hypothesis of the theorem. This yields $P_\phi(G) > P_\phi(G^*)$, a contradiction.

2. $pq \in E(G)$. Suppose that $D(N(p)\backslash\{q\}) = \{c_1, c_2, \ldots, c_{\delta-1}\}$ and $D(N(q)\backslash\{p\}) = \{d_1, d_2, \ldots, d_{\Delta-1}\}$. With no loss of generality, assume that $d_{\Delta-1} = d(w)$. The difference between the values of p_ϕ indices of G and G^* is equal to $p_\phi(G) - p_\phi(G^*)$

$$\begin{aligned}
&= [\sum_{uv\in E(G)\backslash S}\phi(d(u),d(v)) + \sum_{i=1}^{\Delta-1}\phi(\Delta,d_i) + \sum_{j=1}^{\delta-1}\phi(\delta,c_j) \\
&\quad +\phi(\Delta,\delta)] - [\sum_{uv\in E(G)\backslash S}\phi(d(u),d(v)) + \sum_{i=1}^{\Delta-2}\phi(\Delta-1,d_i) \\
&\quad +\sum_{j=1}^{\delta-1}\phi(\delta+1,c_j) + \phi(\delta+1,d_{\Delta-1}) + \phi(\Delta-1,\delta+1)] \\
&= \sum_{i=1}^{\Delta-2}[\phi(\Delta,d_i) - \phi(\Delta-1,d_i)] - \sum_{j=1}^{\delta-1}[\phi(\delta+1,c_j) - \phi(\delta,c_j)] \\
&\quad +[\phi(\Delta,d_{\Delta-1}) - \phi(\delta+1,d_{\Delta-1})] + [\phi(\Delta,\delta) - \phi(\Delta-1,\delta+1)] \\
&= \sum_{i=1}^{\Delta-1}[\phi(\Delta,d_i) - \phi(\Delta-1,d_i)] - \sum_{j=1}^{\delta-1}[\phi(\delta+1,c_j) - \phi(\delta,c_j)] \\
&\quad +[\phi(\Delta-1,d_{\Delta-1}) - \phi(\delta+1,d_{\Delta-1})] + [\phi(\Delta,\delta) - \phi(\Delta-1,\delta+1)].
\end{aligned}$$

Since $\delta+1 \leq \Delta-1$ and ϕ is increasing in x, we conclude that $\phi(\Delta-1,d_{\Delta-1}) - \phi(\delta+1,d_{\Delta-1}) \geq 0$. For $0 \leq b \leq a$, define $\Psi_{a,b}(y) = \phi(a,y) - \phi(b,y)$. Then $\Psi_{a,b}(y)$ is decreasing on the interval $(0,+\infty)$. Indeed, $\frac{d\Psi_{a,b}}{dy}(y) = \frac{\partial\phi}{\partial y}(a,y) - \frac{\partial\phi}{\partial y}(b,y)$ and $\frac{\partial\phi}{\partial y}$ decreases in the first variable. Hence,

$$\begin{aligned}
p_\phi(G) - p_\phi(G^*) & \\
&\geq \sum_{i=1}^{\Delta-1}[\phi(\Delta, d_i) - \phi(\Delta-1, d_i)] - \sum_{j=1}^{\delta-1}[\phi(\delta+1, c_j) - \phi(\delta, c_j)] \\
&\quad +[\phi(\Delta, \delta) - \phi(\Delta-1, \delta+1)] \\
&= \sum_{i=1}^{\Delta-1}\Psi_{\Delta,\Delta-1}(d_i) - \sum_{j=1}^{\delta-1}\Psi_{\delta+1,\delta}(c_j) + [\phi(\Delta, \delta) - \phi(\Delta-1, \delta+1)] \\
&\geq \sum_{i=1}^{\Delta-1}\Psi_{\Delta,\Delta-1}(\Delta) - \sum_{j=1}^{\delta-1}\Psi_{\delta+1,\delta}(\delta) + [\phi(\Delta, \delta) - \phi(\Delta-1, \delta+1)] \\
&= (\Delta-1)[\phi(\Delta, \Delta) - \phi(\Delta-1, \Delta)] - (\delta-1)[\phi(\delta+1, \delta) - \phi(\delta, \delta)] \\
&\quad [\phi(\Delta, \delta) - \phi(\Delta-1, \delta+1)] \\
&= \Delta[\phi(\Delta, \Delta) - \phi(\Delta-1, \Delta)] + \delta[\phi(\delta, \delta) - \phi(\delta, \delta+1)] + \\
&\quad \phi(\Delta-1, \Delta) - \phi(\Delta, \Delta) + \phi(\delta+1, \delta) - \phi(\delta, \delta) \\
&\quad +\phi(\Delta, \delta) - \phi(\Delta-1, \delta+1).
\end{aligned}$$

By the hypotheses of theorem, we know that

$$\Delta[\phi(\Delta, \Delta) - \phi(\Delta-1, \Delta)] + \delta[\phi(\delta, \delta) - \phi(\delta, \delta+1)] > 0.$$

Thus, we get

$$\begin{aligned}
p_\phi(G) - p_\phi(G^*) & \\
&\geq \phi(\Delta-1, \Delta) - \phi(\Delta, \Delta) + \phi(\delta+1, \delta) - \phi(\delta, \delta) + \phi(\Delta, \delta) \\
&\quad -\phi(\Delta-1, \delta+1).
\end{aligned} \tag{2.1}$$

We show that the right side of (2.1) is not negative. By the hypotheses of theorem we also know that if $a \geq b > c \geq d \geq 0$, then

$$\phi(a, c) + \phi(b, d) \geq \phi(a, b) + \phi(c, d).$$

Let $a = \Delta$, $b = \Delta$, $c = \Delta - 1$ and $d = \delta$. Then,

$$\begin{aligned}
\phi(\Delta, \Delta-1) + \phi(\Delta, \delta) + \phi(\delta+1, \delta) &\geq \phi(\Delta, \Delta) + \phi(\Delta-1, \delta) \\
&\quad +\phi(\delta+1, \delta).
\end{aligned} \tag{2.2}$$

Similarly, by choosing $a = \Delta - 1$, $b = \delta + 1$, $c = \delta$ and $d = \delta$ we conclude that,

$$\begin{aligned}
-\phi(\Delta-1, \delta+1) - \phi(\delta, \delta) - \phi(\Delta, \Delta) &\geq -\phi(\Delta-1, \delta) - \phi(\delta+1, \delta) \\
&\quad -\phi(\Delta, \Delta).
\end{aligned} \tag{2.3}$$

By adding two sites of Equations (2.2) and (2.3), we deduce that the right side of (2.1) is not negative. This yields $p_\phi(G) > p_\phi(G^*)$, a contradiction.

□

We now apply Theorem 2.1 to derive the following corollaries.

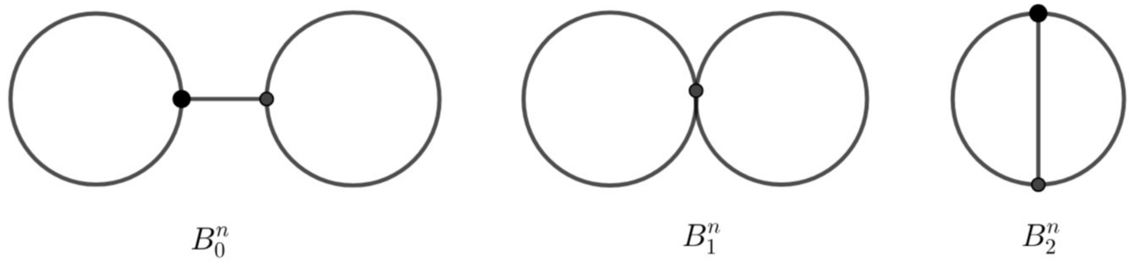

FIGURE 1. Types of bicyclic graphs with $\delta \neq 1$, in terms of their cycles

Corollary 2.2. *Under the hypotheses of Theorem 2.1, if T is a tree of order n with minimum p_ϕ index, then $T = P_n$.*

Proof. This result follows from the fact that every tree with $n \geq 2$ vertices has at least two vertices of degree one. □

Corollary 2.3. *Under the hypotheses of Theorem 2.1, among graphs of order n, path P_n has the minimum p_ϕ index.*

Proof. Suppose that G is a connected graph of order n, whose spanning tree is T . Since $\phi(x, y)$ is increasing in x and y, we have $p_\phi(G) \geq p_\phi(T)$. But, T is a tree of order n, and according to Lemma 2.2, $p_\phi(T) \geq p_\phi(P_n)$. Thus, $p_\phi(G) \geq p_\phi(P_n)$. □

Corollary 2.4. *Under the hypotheses of Theorem 2.1, if G is a unicyclic graph of order n with minimum p_ϕ index, then $G = C_n$.*

Proof. If G is a unicyclic graph and G is not a cycle, then $\delta(G) = 1$ and by Theorem 2.1, $\Delta(G) = 2$, a contradiction. □

Let G be a bicyclic graph of order n and $\delta(G) \neq 1$. Then, in terms of the number of vertices in the intersection of two cycles of G, we can distinguish three types of bicyclic graphs as follows (see, Figure 1):

- $G \in B_0^n$ if the two cycles of G are connected by a path in G.
- $G \in B_1^n$ if the two cycles of G have only one common vertex.
- $G \in B_2^n$ if the two cycles of G have a common path.

Corollary 2.5. *Suppose that G is a bicyclic graph of order n with minimum p_ϕ index, where ϕ satisfies the conditions of Theorem 2.1. Then $G \in B_0^n$ and its connecting path is of length at least two or $G \in B_2^n$ and its connecting path is of length at least two.*

Proof. It is easy to check that a bicyclic graph of type B_0^n, which does not have vertex on connecting path, and a bicyclic graph of B_2^n, which does not have vertex on common path, have the same value of p_ϕ index. Also, a bicyclic graph of type B_0^n, which has at least one vertex on the connecting path, and a bicyclic graph of type B_2^n, which has at least one vertex on the common path have, the same value of p_ϕ index. Now, suppose that G is a bicyclic graph and $G \notin B_0^n \cup B_1^n \cup B_2^n$. Then $\delta(G) = 1$ and by Theorem 2.1, $\Delta(G) = 2$, a contradiction. If $G \in B_1^n$, then $\Delta(G) = 4$ and $\delta(G) = 2$. But Theorem 2.1 implies $\Delta(G) - \delta(G) \leq 1$, which is impossible. Next, a straightforward computation shows that the deference between the p_ϕ indices of a bicyclic graph of type B_2^n with no vertex on common path and a bicyclic graph of type B_2^n with at least one vertex on common path is equal to $q := \phi(3,3) + \phi(2,2) - 2\phi(3,2)$. Substituting $a = b = 3$ and $c = d = 2$ into the condition 4 of theorem shows that $q \leq 0$, which completes the proof. □

The following lemma will be useful in the next section.

Lemma 2.6. *Let x be a positive real number. Then $\frac{\ln(1+x)}{x} > \frac{2}{2+x}$.*

Proof. Let $g(x) = \ln(x+1) - \frac{2x}{x+2}$. Since $x > 0$, we get

$$g'(x) = \frac{x^2}{(x+1)(x+2)^2} > 0.$$

Thus, $g(x)$ is a monotonically increasing function, and hence $g(x) > g(0) = 0$. □

3. Minimal (n, m)-graphs

In this section, we apply Theorem 2.1 and its corollaries to the characterization of the graphs with minimal VDB indices among (n, m)-graphs. First, we consider the general sum-connectivity index χ_β, for $0 < \beta < 1$.

Theorem 3.1. *Let $0 < \beta < 1$. If G has the minimal χ_β value among (n, m)-graphs, then $\Delta(G) - \delta(G) \leq 1$.*

Proof. Suppose that $\beta = \frac{1}{\alpha}$, where $\alpha > 1$ is a constant real number. We define $\phi(x, y) = (x+y)^{\frac{1}{\alpha}}$ and show that assumptions $(1) - (4)$ of Theorem 2.1 hold. Since $\frac{\partial \phi}{\partial x}(x, y) = \frac{1}{\alpha(x+y)^{1-\frac{1}{\alpha}}}$, $\frac{\partial^2 \phi}{\partial x \partial y}(x, y) = -\frac{(\alpha-1)(x+y)^{\frac{1}{\alpha}}}{\alpha^2 (x+y)^2}$ and $\alpha > 1$, we conclude that $\frac{\partial \phi}{\partial x}(x, y)$ is positive and decreasing in y. In the same manner we can see that $\frac{\partial \phi}{\partial y}(x, y)$ is positive and decreasing in x. Now, suppose that positive integers t, s are so chosen that $t > s + 1$. Then, by Lagrange's Mean Value Theorem, there exist numbers $t > \xi > t - 1$ and $s + 1 > \eta > s$, such that

$$\phi(t, t) - \phi(t-1, t) = \frac{\partial \phi}{\partial x}(\xi, t) = \frac{1}{\alpha(\xi + t)^{1-\frac{1}{\alpha}}}, \tag{3.1}$$

$$\phi(s+1, s) - \phi(s, s) = \frac{\partial \phi}{\partial x}(\eta, s) = \frac{1}{\alpha(\eta + s)^{1-\frac{1}{\alpha}}}. \tag{3.2}$$

From Equations (3.1) and (3.2) we obtain:

$t[\phi(t,t)-\phi(t-1,t)]-s[\phi(s+1,s)-\phi(s,s)]$

$$\begin{aligned} &= \frac{t}{\alpha(\xi+t)^{1-\frac{1}{\alpha}}}-\frac{s}{\alpha(\eta+s)^{1-\frac{1}{\alpha}}} \\ &> \frac{t}{\alpha(t+t)^{1-\frac{1}{\alpha}}}-\frac{s}{\alpha(s+s)^{1-\frac{1}{\alpha}}} \\ &= \frac{t^{\frac{1}{\alpha}}-s^{\frac{1}{\alpha}}}{\alpha 2^{1-\frac{1}{\alpha}}}>0. \end{aligned}$$

Now, suppose that $a\geq b>c\geq d\geq 0$. Define $g(x)=(x+c)^{\frac{1}{\alpha}}-(x+b)^{\frac{1}{\alpha}}$. Then

$$g'(x) = \frac{(b+x)\,(c+x)^{\frac{1}{\alpha}}-(b+x)^{\frac{1}{\alpha}}\,(c+x)}{\alpha\,(b+x)\,(c+x)} \tag{3.3}$$

$$= \frac{(b+x)^{1-\frac{1}{\alpha}}-(c+x)^{1-\frac{1}{\alpha}}}{\alpha(b+x)^{1-\frac{1}{\alpha}}(c+x)^{1-\frac{1}{\alpha}}}>0, \tag{3.4}$$

and hence $g(x)$ is increasing for $x>0$. Thus $g(a)\geq g(d)$ or, equivalently,

$$(a+c)^{\frac{1}{\alpha}}+(d+b)^{\frac{1}{\alpha}}\geq(a+b)^{\frac{1}{\alpha}}+(d+c)^{\frac{1}{\alpha}}.$$

Theorem 2.1 and Corollaries 2.2, 2.3, 2.4 and 2.5 complete the proof. □

Theorem 3.2. *Suppose that G has the minimal multiplicative first Zagreb index among (n,m)-graphs. Then $\Delta(G)-\delta(G)\leq 1$.*

Proof. By definition $\Pi_1^*(G)=\prod_{uv\in E(G)}\ln(d(u)+d(v))$. Thus $\ln\Pi_1^*(G)=\sum_{uv\in E(G)}\ln(d(u)+d(v))$. Let $\phi(x,y)=\ln(x+y)$. We show that ϕ meets the assumptions $(1)-(4)$ of Theorem 2.1. Note that $\frac{\partial\phi}{\partial x}(x,y)=\frac{1}{x+y}>0$ and $\frac{\partial\phi}{\partial y}(x,y)=\frac{1}{x+y}>0$. Also, $\frac{\partial^2\phi}{\partial x\partial y}(x,y)=-\frac{1}{(x+y)^2}$. Hence, $\frac{\partial\phi}{\partial x}(x,y)$ is decreasing in y. Similarly, we can see that $\frac{\partial\phi}{\partial y}(x,y)$ is decreasing in x. Now, suppose that $t>s+1$. Then, by Lagrange's Mean Value Theorem, there exist numbers $t>\xi>t-1$ and $s+1>\eta>s$, such that:

$$\begin{aligned} \phi(t,t)-\phi(t-1,t) &= \frac{\partial\phi}{\partial x}(\xi,t)=\frac{1}{\xi+t}, \\ \phi(s+1,s)-\phi(s,s) &= \frac{\partial\phi}{\partial x}(\eta,s)=\frac{1}{\eta+s}. \end{aligned}$$

Therefore, we get

$$\begin{aligned} t[\phi(t,t)-\phi(t-1,t)]-s[\phi(s+1,s)-\phi(s,s)] &= \frac{t}{\xi+t}-\frac{s}{\eta+s} \\ &> \frac{t}{t+t}-\frac{s}{s+s}=0. \end{aligned}$$

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Eventually, suppose that $0 \leq d < c \leq a$. Then we obtain:

$$\begin{aligned} & \phi(a,c)+\phi(b,d) \geq \phi(a,b)+\phi(c,d) \\ \Leftrightarrow\ & \ln(a+c)+\ln(b+d) \geq \ln(a+b)+\ln(c+d) \\ \Leftrightarrow\ & (a+c)(b+d) \geq (a+b)(c+d) \\ \Leftrightarrow\ & ab+ad+cb+cd \geq ac+ad+bc+bd \\ \Leftrightarrow\ & ab+cd \geq ac+bd \\ \Leftrightarrow\ & ab-ac \geq bd-cd \\ \Leftrightarrow\ & a(b-c) \geq d(b-c) \\ \Leftrightarrow\ & a \geq d. \end{aligned}$$

Now, Theorem 2.1 and Corollaries 2.2, 2.3, 2.4 and 2.5 complete the proof. □

Theorem 3.3. *Suppose that G has the minimal multiplicative second Zagreb index among (n, m)-graphs. Then $\Delta(G) - \delta(G) \leq 1$.*

Proof. By definition $\Pi_2(G) = \prod_{uv\in E(G)} (d(u)d(v))$. Thus, $\ln \Pi_2(G) = \sum_{uv\in E(G)} \ln d(u) + \ln d(v)$. Let $\phi(x, y) = \ln x + \ln y$. The task is now to show that ϕ meets the assumptions $(1)-(4)$ of Theorem 2.1. We first observe that $\frac{\partial\phi}{\partial x}(x, y) = \frac{1}{x} > 0$ and $\frac{\partial\phi}{\partial y} = \frac{1}{y} > 0$. Next, if $t > s + 1$, then by Lagrange's Mean Value Theorem, there exist numbers $t > \xi > t - 1$ and $s + 1 > \eta > s$, such that

$$\begin{aligned} \phi(t,t)-\phi(t-1,t) &= \ln t - \ln(t-1) = \frac{1}{\xi}, \\ \phi(s+1,s)-\phi(s,s) &= \ln(s+1) - \ln s = \frac{1}{\eta}. \end{aligned}$$

Hence,

$$t[\phi(t,t)-\phi(t-1,t)] - s[\phi(s+1,s)-\phi(s,s)] = \frac{t}{\xi} - \frac{s}{\eta} > \frac{t}{t} - \frac{s}{s} = 0.$$

Finally, suppose that $a \geq b > c \geq d \geq 0$. Then we have:

$$\begin{aligned} & \phi(a,c)+\phi(b,d) \geq \phi(a,b)+\phi(c,d) \\ \Leftrightarrow\ & \ln ac + \ln bd \geq \ln ab + \ln cd \\ \Leftrightarrow\ & \ln(acbd) \geq \ln(abcd) \\ \Leftrightarrow\ & (acbd) \geq (abcd) \end{aligned}$$

□

Theorem 3.4. *If G has the minimal multiplicative versions of the Sombor index among (n, m)-graphs, then $\Delta(G) - \delta(G) \leq 1$.*

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Proof. Our aim is to show that $\phi(x,y) = \ln(x^2+y^2)$ meets the assumptions $(1)-(4)$ of Theorem 2.1. First, we have $\frac{\partial\phi}{\partial x}(x,y) = \frac{2x}{x^2+y^2} > 0$ and $\frac{\partial\phi}{\partial y}(x,y) = \frac{2y}{x^2+y^2} >$. Also, $\frac{\partial^2\phi}{\partial x\partial y}(x,y) = -\frac{4xy}{(x^2+y^2)^2}$. Thus, $\frac{\partial\phi}{\partial x}(x,y)$ is decreasing in y. Likewise, $\frac{\partial\phi}{\partial y}(x,y)$ is decreasing in x. Now, suppose that $\alpha > s+1$. We prove that

$$\alpha[\phi(\alpha,\alpha) - \phi(\alpha-1,\alpha)] - s[\phi(s+1,s) - \phi(s,s)] > 0.$$

For this purpose, we define $g(\alpha) = \alpha[\phi(\alpha,\alpha) - \phi(\alpha-1,\alpha)] = \alpha\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)$ and show that g is an increasing function on $[2,\infty)$. Note that

$$g'(\alpha) = \frac{2-2\alpha+(\alpha^2+(\alpha-1)^2)\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)}{\alpha^2+(\alpha-1)^2}.$$

But,

$$\begin{aligned}
&(\alpha^2+(\alpha-1)^2)\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)\\
&= (\alpha^2+(\alpha-1)^2)\ln\left(1+[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]\right)\\
&= (\alpha^2+(\alpha-1)^2)[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]\frac{\ln\left(1+[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]\right)}{[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]}\\
&= [\alpha^2-(\alpha-1)^2]\frac{\ln\left(1+[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]\right)}{[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]}\\
&\geq [\alpha^2-(\alpha-1)^2]\frac{2}{2+[\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}-1]} \text{ By Lemma 2.6}\\
&= [\alpha^2-(\alpha-1)^2]\frac{2(\alpha^2+(\alpha-1)^2)}{3\alpha^2+(\alpha-1)^2}.
\end{aligned}$$

Thus we get

$$\begin{aligned}
g'(\alpha) &\geq \frac{-2\alpha+2+[\alpha^2-(\alpha-1)^2]\frac{2(\alpha^2+(\alpha-1)^2)}{3\alpha^2+(\alpha-1)^2}}{\alpha^2+(\alpha-1)^2}\\
&= \frac{2\alpha}{(\alpha^2+(\alpha-1)^2)(3\alpha^2+(\alpha-1)^2)} > 0.
\end{aligned}$$

Consequently, $g(\alpha)$ is an increasing function on $[2,\infty)$.

Likewise, we define $h(s) = s[f(s+1,s) - f(s,s) = s\ln\left(\frac{s^2+(s+1)^2}{2s^2}\right)$ and prove that h is an increasing function on $[1,\infty)$. We see at once that

$$h'(s) = \frac{-2-2s+(s^2+(s+1)^2)\ln\left(\frac{s^2+(s+1)^2}{2s^2}\right)}{s^2+(s+1)^2}.$$

Indeed,
$(s^2+(s+1)^2)\ln\left(\frac{s^2+(s+1)^2}{2s^2}\right)$

$$\begin{aligned}
&= (s^2+(s+1)^2)\ln\left(1+[\frac{s^2+(s+1)^2}{2s^2}-1]\right)\\
&= (s^2+(s+1)^2)[\frac{s^2+(s+1)^2}{2s^2}-1]\frac{\ln\left(1+[\frac{s^2+(s+1)^2}{2s^2}-1]\right)}{[\frac{s^2+(s+1)^2}{2s^2}-1]}\\
&\geq [\frac{(s+1)^4-s^4}{2s^2}]\frac{2}{2+[\frac{s^2+(s+1)^2}{2s^2}-1]} \text{ By Lemma 2.6}\\
&= [\frac{(s+1)^4-s^4}{2s^2}]\frac{4s^2}{3s^2+(s+1)^2}\\
&= 2\frac{(s+1)^4-s^4}{3s^2+(s+1)^2}
\end{aligned}$$

This yields:

$$h'(s) \geq \frac{-2-2s+2\frac{(s+1)^4-s^4}{3s^2+(s+1)^2}}{s^2+(s+1)^2} = \frac{2s}{(3s^2+(s+1)^2)(s^2+(s+1)^2)} > 0,$$

which implies that $h(s)$ is an increasing function on $[1,\infty)$.

Since $\alpha > s+1$, it follows that $g(\alpha) \geq g(s+1)$. We show that $g(\alpha) \geq h(\alpha-1)$. First, note that $g(\alpha) - h(\alpha-1)$

$$\begin{aligned}
&= \alpha\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right) - (\alpha-1)\ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right)\\
&= \alpha\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right) + \ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right)\\
&\quad -\alpha\ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right).
\end{aligned}$$

Analysis similar to the above implies that $\alpha\ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right)$ is an increasing function. Therefore,

$$\alpha\ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right) \geq \lim_{\alpha\to\infty}\alpha\ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right) = 1.$$

Next, let $k(\alpha) = \alpha \ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right) + \ln\left(\frac{\alpha^2+(\alpha-1)^2}{2(\alpha-1)^2}\right)$. Then

$$\begin{aligned} k'(\alpha) &= \frac{-2\alpha^2+2\alpha-2+(\alpha-1)\left(\alpha^2+(\alpha-1)^2\right)\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)}{(\alpha-1)\left(\alpha^2+(\alpha-1)^2\right)} \\ &< \frac{-2\alpha^2+2\alpha-1+(\alpha-1)\left(\alpha^2+(\alpha-1)^2\right)\ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)}{(\alpha-1)\left(\alpha^2+(\alpha-1)^2\right)} \\ &= \frac{-1}{\alpha-1} + \ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right). \end{aligned}$$

The derivation of $\frac{-1}{\alpha-1} + \ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right)$ is equal to $\frac{4\alpha^2-5\alpha+2}{\alpha(\alpha-1)^2(2\alpha^2-2\alpha+1)}$, which is positive for $\alpha \geq 2$. Hence,

$$\frac{-1}{\alpha-1} + \ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right) < \lim_{\alpha\to\infty} \frac{-1}{\alpha-1} + \ln\left(\frac{2\alpha^2}{\alpha^2+(\alpha-1)^2}\right) = 0.$$

Consequently, $k(\alpha)$ is a decreasing function. Finally, we have

$$g(\alpha) - h(\alpha-1) \geq k(\alpha) - 1 > \lim_{\alpha\to\infty} k(\alpha) - 1 = 1 - 1 = 0.$$

This means that $g(\alpha) \geq h(\alpha-1)$, and since h is increasing and $\alpha-1 \geq s$, we conclude that $g(\alpha) \geq h(s)$, or equivalently; $\alpha[\phi(\alpha,\alpha) - \phi(\alpha,\alpha-1)] - s[\phi(s+1,s) - \phi(s,s)] > 0$.

To complete the proof, we show that if $0 \leq d \leq c < b \leq a$, then $\phi(a,b) + \phi(c,d) \leq \phi(a,c) + \phi(b,d)$. This is true because

$$\begin{aligned} & \phi(a,c) + \phi(b,d) \geq \phi(a,b) + \phi(c,d) \\ \Leftrightarrow\ & \ln(a^2+c^2) + \ln(b^2+d^2) \geq ln(a^2+b^2) + \ln(c^2+d^2) \\ \Leftrightarrow\ & (a^2+c^2)(b^2+d^2) \geq (a^2+b^2)(c^2+d^2) \\ \Leftrightarrow\ & a^2b^2 + a^2d^2 + c^2b^2 + c^2d^2 \geq a^2c^2 + a^2d^2 + b^2c^2 + b^2d^2 \\ \Leftrightarrow\ & a^2b^2 + c^2d^2 \geq a^2c^2 + b^2d^2 \\ \Leftrightarrow\ & a^2b^2 - a^2c^2 \geq b^2d^2 - c^2d^2 \\ \Leftrightarrow\ & a^2(b-c) \geq d^2(b-c) \\ \Leftrightarrow\ & a \geq d. \end{aligned}$$

□

Theorem 3.5. *Suppose that G has the minimal multiplicative versions of the forgotten index (Π_F^*) among (n,m)-graphs. Then, $\Delta(G) - \delta(G) \leq 1$. In particular,*

- *P_n has the minimal multiplicative versions of the forgotten index among graphs of order n.*

- P_n *has the minimal multiplicative versions of the forgotten index among trees with* n *vertices.*
- C_n *has the minimal multiplicative versions of the forgotten index among unicyclic graphs with* n *vertices.*
- *In bicyclic graphs of order* n*, we have* $G \in B_0^n$ *and there is at least one vertex on the connecting path or* $G \in B_2^n$ *and there is at least one vertex on the common path.*

Proof. Analysis similar to that in the proof of Theorem 3.4 gives the result. □

Let us conclude the paper with some final remarks.

Remark 3.6. *The conditions of Theorem 2.1 are not perfect. Therefore, improving these conditions, especially for functions like* $\frac{1}{x+y}, \frac{1}{\sqrt{xy}}$ *or* $\frac{1}{\sqrt{x+y}}$ *, could be the subject of future studies.*

Remark 3.7. *Obviously, the complete graph* K_n *has the maximum value of* Π_F^* *index among all connected simple graphs of order* n*. We guest the star graph* S_n *has the maximum value of this index among* n *vertices trees. The maximum graphs among* n *vertices unicyclic and bicyclic graphs remain as open problems.*

Remark 3.8. *The first and second Zagreb indices are defined by*

$$M_1(G) = \sum_{u \in V(G)} d(v)^2 = \sum_{uv \in E(G)} (d(u) + d(v))$$

and $M_2(G) = \sum_{uv \in E(G)} (d(u)d(v))$*, respectively. Caporossi and Hansen [6] proposed the conjecture* $\frac{M_1}{n} \leq \frac{M_2}{m}$ *(the bound is tight for complete graphs). This conjuncture has been proven for trees [29], unicyclic graphs [24] and chemical graphs [17], while counterexamples were found for both connected and disconnected graphs [19]. In [10], Eliasi and Vukicević compared the multiplicative versions of these indices. They proved that if* $\Pi_1(G) = \prod_{u \in V(G)} d(u)$*,* $\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v))$ *and* $\Pi_2(G) = \prod_{uv \in E(G)} (d(u)d(v))$*, then for a simple connected graph* G *of order* n *;* $\Pi_1(G) \leq \Pi_1^*(G)$ *and the equality holds if and only if* $G = C_n$*. Also, for a simple connected graph* G *with* n *vertices and* m *edges,* $\sqrt[n]{\Pi_1(G)} \leq \sqrt[m]{\Pi_2(G)}$ *and equality holds only for regular graphs. Hence, it is natural that we compare the multiplicative versions of the forgotten index.*

Our computations lead us to the following conjectures:

Conjecture 3.9. *Let* G *be a simple connected graph of order* n*. Then* $\Pi_F(G) \leq \Pi_F^*(G)$ *and the equality holds if and only if* $G = C_n$*.*

Conjecture 3.10. *For a simple connected graph* G *with* n *vertices and* m *edges,* $\sqrt[n]{\Pi_F(G)} \leq \sqrt[m]{\Pi_F^*(G)}$*.*

Acknowledgments The author is very grateful to the anonymous referees for their valuable suggestions and corrections, which have improved the presentation of the paper.

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