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General Multiplicative Zagreb Indices of Graphs With Bridges

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ABSTRACT Multiplicative Zagreb indices have been studied due to their extensive applications. They play a substantial role in chemistry, pharmaceutical sciences, materials science and engineering, because we can correlate them with numerous physico-chemical properties of molecules. We use graph theory to characterize these chemical structures. The vertices of graphs represent the atoms of a compound and edges of graphs represent the chemical bonds. We present upper and lower bounds on the general multiplicative Zagreb indices for graphs with given number of vertices and cut-edges called bridges. We give all the extremal graphs, which implies that our bounds are best possible.

INDEX TERMS Multiplicative Zagreb index, bridge, degree.

I. INTRODUCTION

We consider connected graphs without loops and multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The order of G is the number of vertices of G. A bridge (cut-edge) is an edge of G whose removal increases the number of components. The number of edges incident with a vertex $v \in V(G)$ is the degree $d_G(v)$ of v. A vertex of degree one is called a pendant vertex. A pendant path of G is a path having one terminal vertex of degree at least 3 in G, while the other terminal vertex is a pendant vertex and each internal vertex (if any exists) is of degree 2 in G.

The symbols K_n, P_n, S_n and C_n denote the complete graph, the path, the star and the cycle of order n, respectively. Let $C_r = c_1c_2 \dots c_r$ be the cycle with $V(C_r) = \{c_1, c_2, \dots, c_r\}$ and $E(C_r) = \{c_1c_2, c_2c_3, \dots, c_{r-1}c_r, c_rc_1\}$. A tree is a connected graph without cycles. We denote by $C_{n-k} \star S_k$ (by $K_{n-k} \star S_k$) the graph obtained by joining one vertex of C_{n-k} (of K_{n-k}) to k new vertices. The graph $C_{n-k} * P_k$ (the graph $K_{n-k} * P_k$) is obtained by attaching one vertex of C_{n-k} (of K_{n-k}) to a pendant vertex of P_{k+1}.

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Topological indices have been used for drug design, chemical documentation, isomer discrimination, quantitative structure versus property (or activity) relationships (QSPR/QSAR), toxicology hazard assessments and combinatorial library design. They have been applied in the process of correlating the chemical structures with various characteristics such as boiling points and molar heats of formation. These indices are a convenient method of translating chemical constitution into numerical values which are used for correlations with physical properties.

Multiplicative Zagreb indices have extensive applications. They have been investigated particularly in the past decade. They play a substantial role in chemistry, pharmaceutical sciences, materials science and engineering, because we can correlate them with numerous physico-chemical properties of molecules. We use graph theory to characterize these chemical structures. The vertices of graphs represent the atoms of a compound and edges of graphs represent the chemical bonds.

Tight lower and upper bounds on the multiplicative Zagreb indices for graphs with given number of vertices and bridges were given in [14], sharp upper bounds for graphs with given order and size were obtained in [9], bounds for graphs with respect to order and clique number wer given in [12], tight lower and upper bounds for trees, unicyclic graphs and

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bicyclic graphs of given order were presented in [15], upper bounds for graph products were obtained in [4], lower bounds for graph operations were investigated in [11], graphs of given order and chromatic number in [16], graphs with a small number of cycles in [1], derived graphs in [2], molecular graphs in [6] and upper bounds for bipartite graphs were studied in [13]. Classical Zagreb indices were investigated in [8] and [10], the augmented Zagreb index in [3] and [7], and weighted Harary indices for graphs with bridges in [5].

For any real number $a \neq 0$, the first and second general multiplicative Zagreb indices of a graph G are defined as

$$P_1^a(G) = \prod_{v \in V(G)} d_G(v)^a$$

and

$$P_2^a(G) = \prod_{v \in V(G)} d_G(v)^{a d_G(v)},$$

respectively. These indices generalize classical multiplicative Zagreb indices, since $P_1^1(G)$ is the Narumi-Katayama index, $P_1^2(G)$ is the first multiplicative Zagreb index and $P_2^1(G)$ is the second multiplicative Zagreb index.

We generalize results of Wang *et al.* [14] and present new methods and proofs. We obtain upper and lower bounds on the general multiplicative Zagreb indices for graphs with given number of vertices and bridges. We give all the extremal graphs which implies that our bounds are best possible.

II. PRELIMINARY RESULTS

First, we show that by adding an edge to a graph G, we get a graph with larger general multiplicative Zagreb indices.

Lemma 1: Let G be any connected graph with two nonadjacent vertices $v_1, v_2 \in V(G)$. Then for $a > 0$, $P_c^a(G) < P_c^a(G + v_1v_2)$, where $c = 1, 2$.

Proof: Let $G' = G + v_1v_2$. For $j = 1, 2$, we have $1 \leq d_G(v_j) < d_{G'}(v_j)$, which implies that $1 \leq d_G(v_j)^a < d_{G'}(v_j)^a$, thus $P_1^a(G) < P_1^a(G')$. Similarly, $1 \leq d_G(v_j)^{a d_G(v_j)} < d_{G'}(v_j)^{a d_{G'}(v_j)}$, so $P_2^a(G) < P_2^a(G')$. □

The next lemmas are used in the proofs of our main results as well.

Lemma 2: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the smallest P_1^a index, where $a > 0$, then T is a star attached to H by its centre.

Proof: Let G be formed by a nonempty graph H with a tree T attached to one vertex of H. We show that if G has the smallest P_1^a index, where $a > 0$, then T is a star attached to H by its centre.

Suppose to the contrary that T is not a star attached to some vertex x by its centre. Thus T has a vertex y ($y \neq x$) of degree greater than 1 adjacent to some pendant vertices. Let y' be a vertex of T of degree greater than 1 that is farthest from x. Let $y_1, y_2, \ldots, y_t$ (with $t \geq 1$) be the pendant vertices adjacent to y'. We construct a new graph G'. Let $V(G') = V(G)$ and $E(G') = \{xy_1, xy_2, \ldots, xy_t\} \cup E(G) \setminus \{y'y_1, y'y_2, \ldots, y'y_t\}$. Then $d_G(y') = t + 1$, $d_{G'}(y') = 1$, $d_G(x) = s \geq 2$ and $d_{G'}(x) = s + t$. For the other vertices $w \in V(G) \setminus \{x, y'\}$, we obtain $d_G(w) = d_{G'}(w)$. Therefore,

$$\frac{P_1^a(G)}{P_1^a(G')} = \frac{(t+1)^a s^a}{(s+t)^a} = \left(\frac{ts+s}{t+s}\right)^a > 1,$$

since $\frac{ts+s}{t+s} > 1$. So $P_1^a(G) > P_1^a(G')$. Hence G does not have the smallest P_1^a index, which is a contradiction. Thus T is a star. □

Lemma 3: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the largest P_2^a index, where $a > 0$, then T is a star attached to H by its centre.

Proof: Let G be formed by a nonempty graph H with a tree T attached to one vertex of H. We show that if G has the largest P_2^a index, where $a > 0$, then T is a star.

Suppose to the contrary that T is not a star attached to some vertex x by its centre. Thus T has a vertex y ($y \neq x$) of degree greater than 1 adjacent to some pendant vertices. Let y' be a vertex of T of degree greater than 1 that is farthest from x. Let $y_1, y_2, \ldots, y_t$ (with $t \geq 1$) be the pendant vertices adjacent to y'. We construct graphs G' different from the graph constructed in the proof of Lemma 2, othewise it would be complicated to compare $P_2^a(G)$ and $P_2^a(G')$. Let $d_G(x) = s \geq 2$. We consider two cases.

Case 1. $s > t$.

Let $V(G') = V(G)$ and $E(G') = \{xy_1\} \cup E(G) \setminus \{y'y_1\}$. Then $d_G(y') = t + 1$, $d_{G'}(y') = t$, $d_G(x) = s$ and $d_{G'}(x) = s + 1$. For the other vertices $w \in V(G) \setminus \{x, y'\}$, we obtain $d_G(w) = d_{G'}(w)$. Therefore,

$$\frac{P_2^a(G)}{P_2^a(G')} = \frac{(t+1)^{a(t+1)} s^{as}}{t^{at}(s+1)^{a(s+1)}} = \left[\left(1+\frac{1}{t}\right)^t \left(1-\frac{1}{s+1}\right)^{s+1} \frac{t+1}{s}\right]^a < 1,$$

since $(1+\frac{1}{t})^t < e$, $(1-\frac{1}{s+1})^{s+1} < \frac{1}{e}$ and $\frac{t+1}{s} \leq 1$. So $P_2^a(G) < P_2^a(G')$ which is a contradiction.

Case 2. $s \leq t$.

In this case we need to introduce a more complicated transformation. Let $V(G') = V(G)$ and $E(G') = \{xy_1, xy_2, \ldots, xy_{t+2-s}\} \cup E(G) \setminus \{y'y_1, y'y_2, \ldots, y'y_{t+2-s}\}$. Then $d_G(y') = t + 1$, $d_{G'}(y') = t + 1 - (t + 2 - s) = s - 1$, $d_G(x) = s \geq 2$ and $d_{G'}(x) = s + (t + 2 - s) = t + 2$. For the other vertices $w \in V(G) \setminus \{x, y'\}$, we have $d_G(w) = d_{G'}(w)$. Therefore,

$$\frac{P_2^a(G)}{P_2^a(G')} = \frac{(t+1)^{a(t+1)} s^{as}}{(t+2)^{a(t+2)}(s-1)^{a(s-1)}} = \left[\left(1-\frac{1}{t+2}\right)^{t+2}\left(1+\frac{1}{s-1}\right)^{s-1} \frac{s}{t+1}\right]^a < 1,$$

since $(1-\frac{1}{t+2})^{t+2} < \frac{1}{e}$, $(1+\frac{1}{s-1})^{s-1} < e$ and $\frac{s}{t+1} < 1$. So $P_2^a(G) < P_2^a(G')$, Hence G does not have the largest P_2^a index, which is a contradiction. Thus T is a star. □

Lemma 4: Let G be formed by a cycle H (by a complete graph H), where any vertex of H can be adjacent to pendant vertices. If G has the smallest P_1^a index (the largest P_2^a index), where $a > 0$, then G contains at most one vertex adjacent to pendant vertices.

Proof: We show that if G has the smallest P_1^a index (the largest P_2^a index), where $a > 0$, then G contains at most one vertex adjacent to pendant vertices.

Suppose to the contrary that G has at least two vertices v, w adjacent to pendant vertices. Without loss of generality, assume that $s = d_G(v) \geq d_G(w) = t$. Let w' be any pendant vertex adjacent to w in G.

Let G' be the graph with $V(G') = V(G)$ and $E(G') = \{vw'\} \cup E(G) \setminus \{ww'\}$. Then $d_G(v) = s$, $d_{G'}(v) = s+1$, $d_G(w) = t$ and $d_{G'}(w) = t-1$. Thus

$$\frac{P_1^a(G)}{P_1^a(G')} = \frac{t^a s^a}{(t-1)^a(s+1)^a} = \left(\frac{ts}{ts+t-s-1}\right)^a > 1,$$

since $t-s \leq 0$. So $P_1^a(G) > P_1^a(G')$, which means that G does not have the smallest P_1^a index.

For the P_2^a index,

$$\frac{P_2^a(G)}{P_2^a(G')} = \frac{t^{at}s^{as}}{(t-1)^{a(t-1)}(s+1)^{a(s+1)}} = \left[\left(1+\frac{1}{t-1}\right)^{t-1}\left(1-\frac{1}{s+1}\right)^{s+1}\frac{t}{s}\right]^a < 1,$$

since $(1+\frac{1}{t-1})^{t-1} < e$, $(1-\frac{1}{s+1})^{s+1} < \frac{1}{e}$ and $\frac{t}{s} \leq 1$. Thus $P_2^a(G) < P_2^a(G')$, so G does not have the largest P_2^a index, which is a contradiction. □

Lemma 5: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the largest P_1^a index (the smallest P_2^a index), where $a > 0$, then T is a path attached to H by its pendant vertex.

Proof: Let G be formed by a nonempty graph H with a tree T attached to one vertex, say x, of H. We show that if G has the largest P_1^a index (the smallest P_2^a index), where $a > 0$, then T is a path attached to H by its pendant vertex.

We prove it by contradiction. Assume that T is not a path. Let y be a vertex of T of degree at least 3 farthest from x (possibly $y = x$). Thus T has two pendant paths, say $yy_1y_2\ldots y_s$ and $yy'_1y'_2\ldots y'_r$, where $s, r \geq 1$. Define the graph G' with $V(G') = V(G)$ and $E(G') = \{y_sy'_1\} \cup E(G) \setminus \{yy'_1\}$. Then $d_G(y) = t \geq 3$, $d_{G'}(y) = t-1$, $d_G(y_s) = 1$, $d_{G'}(y_s) = 2$ and $d_G(w) = d_{G'}(w)$ for the other vertices $w \in V(G) \setminus \{yy_s\}$. Then

$$\frac{P_1^a(G')}{P_1^a(G)} = \frac{2^a(t-1)^a}{t^a} = \left(\frac{2t-2}{t}\right)^a > 1$$

and

$$\frac{P_2^a(G')}{P_2^a(G)} = \frac{2^{2a}(t-1)^{a(t-1)}}{t^{at}} = \left[\left(1-\frac{1}{t}\right)^t\frac{4}{t-1}\right]^a < 1,$$

since $(1-\frac{1}{t})^t < \frac{1}{e}$ and $\frac{4}{t-1} \leq 2 < e$. Thus $P_1^a(G') > P_1^a(G)$ and $P_2^a(G') < P_2^a(G)$. Hence G does not have the largest P_1^a index (the smallest P_2^a index), a contradiction. So T is a path. □

Lemma 6: Let G be formed by a complete graph H (by a cycle H), where any vertex of H can be adjacent to a pendant path. If G has the largest P_1^a index (the smallest P_2^a index), where $a > 0$, then G contains at most one pendant path.

Proof: We show that if G has the largest P_1^a index (the smallest P_2^a index), where $a > 0$, then G contains at most one pendant path.

Assume to the contrary that G has at least 2 pendant paths, say say $vy_1y_2\ldots y_s$ and $v'y'_1y'_2\ldots y'_r$, where $v, v' \in H$ and $s, r \geq 1$. Define the graph G' with $V(G') = V(G)$ and $E(G') = \{y_sy'_1\} \cup E(G) \setminus \{v'y'_1\}$. Then $d_G(v') = t \geq 3$, $d_{G'}(v') = t-1$, $d_G(y_s) = 1$, $d_{G'}(y_s) = 2$ and $d_G(w) = d_{G'}(w)$ for the other vertices $w \in V(G) \setminus \{v', y_s\}$. Then, similarly as in the proof of Lemma 5,

$$\frac{P_1^a(G')}{P_1^a(G)} = \frac{2^a(t-1)^a}{t^a} > 1$$

and

$$\frac{P_2^a(G')}{P_2^a(G)} = \frac{2^{2a}(t-1)^{a(t-1)}}{t^{at}} < 1,$$

so $P_1^a(G') > P_1^a(G)$ and $P_2^a(G') < P_2^a(G)$. Hence G does not have the largest P_1^a index (the smallest P_2^a index), a contradiction. □

III. MAIN RESULTS

We study graphs with n vertices and k bridges. Note that there is no graph with $n-2$ bridges, since every tree has $n-1$ bridges and every graph with a cycle has at most $n-3$ bridges. It is easy to show that the extremal graphs for the general multiplicative Zagren indices with n vertices and 0 bridges are the cycles C_n or the complete graphs K_n, therefore we investigate graphs with k bridges, where $1 \leq k \leq n-3$ which means that $n \geq 4$.

Theorem 1: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a > 0$,

$$P_1^a(G) \geq (k+2)^a 2^{(n-k-1)a}$$

with equality if and only if G is $C_{n-k} \star S_{k+1}$, and

$$P_2^a(G) \geq 3^{3a}2^{2a(n-2)}$$

with equality if and only if G is $C_{n-k} * P_{k+1}$.

Proof: Let G' be a graph with the smallest P_1^a index (with the smallest P_2^a index) among graphs with n vertices and k bridges. Let E_b be the set of bridges of G'. Since G' has k bridges, $G' - E_b$ contains $k+1$ components, say $G_1, G_2, \ldots, G_{k+1}$.

Since for each $i = 1, 2, \ldots, k+1$, G_i does not have bridges, it follows that G_i must be an isolated vertex or a 2-edge connected graph. Since every pendant edge is a bridge, G_i does not have vertices of degree one. To get $d_{G_i}(v)^a$ and $d_{G_i}(v)^{ad_{G_i}(v)}$ as small as possible, we need the degree of any vertex $v \in V(G_i)$ as small as possible, thus if G_i is not an isolated graph, the degree of every vertex in G_i is 2, which implies that G_i is a cycle. So each component G_i for $i = 1, 2, \ldots, k+1$, is an isolated vertex or a cycle C_p for some $p \geq 3$.

Claim 1. At most one component G_i, where $1 \leq i \leq k+1$, is a cycle.

Assume to the contrary that there are two components G_i and G_j, where $1 \leq i < j \leq k+1$, which are cycles. Let $G_i = c_1c_2 \ldots c_r$ and $G_j = c'_1c'_2 \ldots c'_s$, where $r, s \geq 3$. Since G' is connected, there is some path P in G' connecting G_i and G_j. We can assume that the path P has the terminal vertices c_1 and c'_1.

Define the graph G'' with $V(G'') = V(G')$ and $E(G'') = \{c_1c'_s, c_2c'_2\} \cup E(G') \setminus \{c_1c_2, c'_1c'_2, c'_1c'_s\}$. Then $d_{G'}(c'_1) = z$ and $d_{G''}(c'_1) = z-2$ for some $z \geq 3$ (since c'_1 can be incident with many bridges in G') and $d_{G'}(y) = d_{G''}(y)$ for all the other vertices $y \in V(G')$. We obtain

$$\frac{P_1^a(G')}{P_1^a(G'')} = \frac{z^a}{(z-2)^a} = \left(\frac{z}{z-2}\right)^a > 1$$

and

$$\frac{P_2^a(G')}{P_2^a(G'')} = \frac{z^{az}}{(z-2)^{a(z-2)}} = \left[\frac{z^z}{(z-2)^{z-2}}\right]^a > 1,$$

thus $P_c^a(G') > P_c^a(G'')$ for $c = 1, 2$, so G' is not a graph with the smallest P_c^a index. A contradiction. Hence, Claim 1 is proved.

Therefore, at most one component of $G' - E_b$ is a cycle. Not all the edges of G' are bridges, thus G' must contain one cycle. Since G' contains exactly k bridges, G' consists of the cycle C_{n-k} of length $n-k$ and trees which might be attached to some vertices of the cycle.

For the P_1^a index, from Lemma 2 it follows that a tree attached to a vertex of the cycle must be a star and from Lemma 4 it follows that all the bridges are attached to one vertex of the cycle, hence G' is $C_{n-k} \star S_{k+1}$; see Figure 1.

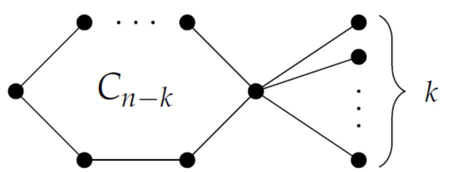

FIGURE 1. Graph $C_{n-k} \star S_{k+1}$.

The graph $C_{n-k} \star S_{k+1}$ contains k vertices having degree 1, one vertex having degree $k+2$ and $n-k-1$ vertices of degree 2, thus

$$P_1^a(C_{n-k} \star S_{k+1}) = (k+2)^a 2^{(n-k-1)a} 1^{ka} = (k+2)^a 2^{(n-k-1)a}.$$

For the P_2^a index, from Lemma 5 it follows that a tree attached to a vertex of the cycle must be a path and from Lemma 6 it follows that G' contains at most one pendant path. Thus G' is $C_{n-k} * P_{k+1}$; see Figure 2.

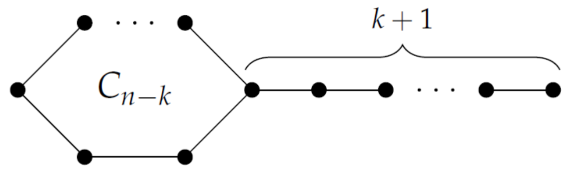

FIGURE 2. Graph $C_{n-k} * P_{k+1}$.

The graph $C_{n-k} * P_{k+1}$ contains one vertex having degree 1, one vertex having degree 3 and $n-2$ vertices having degree 2, thus

$$P_2^a(C_{n-k} * P_{k+1}) = 3^{3a} 2^{2a(n-2)} 1^a = 3^{3a} 2^{2a(n-2)}.$$

□

Now we present upper bounds on the general multiplicative Zagreb indices for graphs with given number of vertices and bridges.

Theorem 2: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a > 0$,

$$P_1^a(G) \leq (n-k)^a (n-k-1)^{a(n-k-1)} 2^{a(k-1)}$$

with equality if and only if G is $K_{n-k} \star P_{k+1}$.

Proof: Let G' be any graph having the largest P_1^a index among graphs with n vertices and k bridges. Let E_b be the set of bridges of G'. The removal of a bridge inscreases the number of components by one. Since G' has k bridges, $G' - E_b$ contains $k+1$ components, say $G_1, G_2, \ldots, G_{k+1}$.

Since the P_1^a index increases by adding edges and G' is maximal, by Lemma 1, each component G_i for $i = 1, 2, \ldots, k+1$, is a complete graph. Note that G_i cannot be K_2, otherwise it would be a bridge. So G_i is either K_1 or K_p for some $p \geq 3$.

Claim 1. At most one component G_i, where $1 \leq i \leq k+1$, is K_p for some $p \geq 3$.

Assume to the contrary that we have at least two components which are complete graphs with at least 3 vertices. Let G_i and G_j be the farthest components in G'. So G_i is K_r with $V(K_r) = \{u_1, u_2, \ldots, u_r\}$ and G_j is K_s with $V(K_s) = \{v_1, v_2, \ldots, v_s\}$, where $r, s \geq 3$. Since G' is connected, there is some path P in G' connecting K_r and K_s. We can assume that the path P has the terminal vertices u_1 and v_1. Without loss of generality, assume that $r \leq s$. By Lemma 5, every vertex u_i can be adjacent (except for the vertices of K_r and P) to at most one vertex which is a vertex of a pendant path; $i = 1, 2, \ldots, r$. By the proof of Lemma 6, a pendant path can be attached only to one vertex of K_r and we can assume that u_r is that vertex. Thus $d_{G'}(u_r) = r - 1 + \epsilon$, where $\epsilon = 0$ or 1, $d_{G'}(u_1) = r$ and $d_{G'}(u_i) = r-1$ for $i = 2, 3, \ldots, r-1$.

Let $V(G'') = V(G')$ and $E(G'') = \{u_iv_j | i = 2, 3 \ldots, r; j = 1, 2, \ldots, s\} \cup E(G') \setminus \{u_1\, u_i | \, i = 2, 3 \ldots, r\}$. Then $d_{G''}(u_1) = 1$, $d_{G''}(u_r) = (r-2+\epsilon)+s$ and $d_{G''}(u_i) = (r-2)+s$, therefore $d_{G''}(u_i) \geq 2d_{G'}(u_i)$ for $i = 2, 3, \ldots, r-1$. We also know that $d_{G'}(v_j) < d_{G''}(v_j)$ for $j = 1, 2, \ldots, s$, and $d_{G'}(y) = d_{G''}(y)$

for all the other vertices. Thus

$$\begin{aligned}\frac{P_1^a(G'')}{P_1^a(G')} &> \frac{d_{G''}(u_1)^a d_{G''}(u_2)^a \dots d_{G''}(u_r)^a}{d_{G'}(u_1)^a d_{G'}(u_2)^a \dots d_{G'}(u_r)^a}\\ &= \left(\frac{1(r-2+s)^{r-2}(r-2+\epsilon+s)}{r(r-1)^{r-2}(r-1+\epsilon)}\right)^a\\ &\geq \left(\frac{2^{r-2}(r-2+\epsilon+s)}{r(r-1+\epsilon)}\right)^a.\end{aligned}$$

For $r \geq 4$, we have $2^{r-2} \geq r$, thus $\frac{P_1^a(G'')}{P_1^a(G')} > 1$.

If $r = 3$, we obtain $\frac{P_1^a(G'')}{P_1^a(G')} > \left(\frac{2^1(s+1+\epsilon)}{3(2+\epsilon)}\right)^a > 1$, since $s \geq 3$ and $\epsilon = 0$ or 1. Thus $P_1^a(G'') > P_1^a(G')$ which means that G' does not have the largest P_1^a index, a contradiction. Hence, Claim 1 is proved.

Therefore, at most one component of $G' - E_b$ is K_p for some $p \geq 3$. Since not all the edges of G' are bridges, G' must contain exactly one complete graph with at least 3 vertices. We know that G' has k bridges, therefore G' consists of the complete graph K_{n-k} of order $n-k$ and trees which might be attached to some vertices of that K_{n-k}.

From Lemma 5 it follows that a tree attached to a vertex of K_{n-k} must be a path and from Lemma 6 it follows that G' contains at most one pendant path. Thus G' is $K_{n-k} \star P_{k+1}$; see Figure 3.

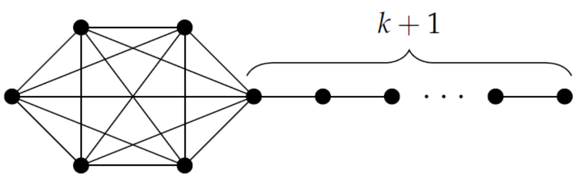

FIGURE 3. Graph $K_{n-k} * P_{k+1}$.

The graph $K_{n-k} \star P_{k+1}$ contains one vertex having degree 1, $k-1$ vertices having degree 2, one vertex having degree $n-k$ and $n-k-1$ vertices having degree $n-k-1$, thus

$$P_2^a(K_{n-k} \star P_{k+1}) = (n-k)^a (n-k-1)^{a(n-k-1)} 2^{a(k-1)}.$$

□

Theorem 3: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a > 0$,

$$P_2^a(G) \leq (n-1)^{a(n-1)}(n-k-1)^{a(n-k-1)^2}$$

with equality if and only if G is $K_{n-k} * S_{k+1}$.

Proof: Let G' be any graph with the largest P_2^a index among graphs with n vertices and k bridges. Let E_b be the set of bridges of G'. The removal of a bridge inscreases the number of components by one. Since G' has k bridges, $G' - E_b$ contains $k+1$ components, say $G_1, G_2, \dots, G_{k+1}$.

Since the P_2^a index increases by adding edges and G' is maximal, by Lemma 1, each component G_i for $i = 1, 2, \dots, k+1$, is a complete graph. Note that G_i cannot be K_2, otherwise it would be a bridge. So G_i is either K_1 or K_p for some $p \geq 3$.

Claim 1. At most one component G_i, where $1 \leq i \leq k+1$, is K_p for some $p \geq 3$.

Assume to the contrary that there are two components which are complete graphs with at least 3 vertices, say $K_{r'}$ with $V(K_{r'}) = \{u_1, u_2, \dots, u_{r'}\}$ and $K_{s'}$ with $V(K_{s'}) = \{v_1, v_2, \dots, v_{s'}\}$, where $r', s' \geq 3$. Since G' is connected, there is some path P in G' connecting $K_{r'}$ and $K_{s'}$. We can assume that the path P has the terminal vertices u_1 and v_1. Without loss of generality, suppose that $r = d_{G'}(u_1) \leq d_{G'}(v_1) = s$. Clearly, $r \geq r'$ and $s \geq s'$. Let us note that any verrtex of $K_{r'}$ or $K_{s'}$ can be incident with many bridges in G'.

Let $V(G'') = V(G')$ and $E(G'') = \{u_i v_j | i = 2, 3 \dots, r'; j = 1, 2, \dots, s'\} \cup E(G') \setminus \{u_1 u_i | \ i = 2, 3 \dots, r'\}$. Then $d_{G''}(u_1) = r - (r'-1)$ and $d_{G''}(v_1) = s + (r'-1)$. Obviously, $d_{G'}(y) \leq d_{G''}(y)$ for the other vertices $y \in V(G') \setminus \{u_1, v_1\}$. Thus $d_{G'}(y)^{ad_{G'}(y)} \leq d_{G''}(y)^{ad_{G''}(y)}$ and $\frac{P_2^a(G')}{P_2^a(G'')}$

$$\begin{aligned}&\leq \frac{d_{G'}(u_1)^{ad_{G'}(u_1)} d_{G'}(v_1)^{ad_{G'}(v_1)}}{d_{G''}(u_1)^{ad_{G''}(u_1)} d_{G''}(v_1)^{ad_{G''}(v_1)}}\\ &= \frac{r^{ar}s^{as}}{[r-(r'-1)]^{a[r-(r'-1)]}[s+(r'-1)]^{a[s+(r'-1)]}}\\ &= \left[\left(1+\frac{r'-1}{r-(r'-1)}\right)^{r-(r'-1)}\right.\\ &\quad \left.\left(1-\frac{r'-1}{s+(r'-1)}\right)^{s+(r'-1)} \frac{r^{r'-1}}{s^{r'-1}}\right]^a\\ &< 1,\end{aligned}$$

since $(1+\frac{r'-1}{r-(r'-1)})^{r-(r'-1)} < e^{r'-1}$, $(1-\frac{r'-1}{s+(r'-1)})^{s+(r'-1)} < \frac{1}{e^{r'-1}}$ and $\frac{r^{r'-1}}{s^{r'-1}} \leq 1$. Therefore, $P_2^a(G') < P_2^a(G'')$, which means that G' does not have the largest P_2^a index, a contradiction. Thus Claim 1 is proved.

Therefore, at most one component of $G' - E_b$ is K_p for some $p \geq 3$. Since not all the edges of G' are bridges, G' must contain exactly one complete graph with at least 3 vertices. We know that G' has k bridges, therefore G' consists of the complete graph K_{n-k} of order $n-k$ and trees which might be attached to some vertices of that K_{n-k}.

From Lemma 3 it follows that a tree attached to a vertex of K_{n-k} must be a star and from Lemma 4 it follows that all the bridges are attached to one vertex of that complete graph, hence G' is $K_{n-k} \star S_{k+1}$; see Figure 4.

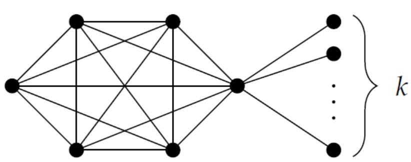

FIGURE 4. Graph $K_{n-k} \star S_{k+1}$.

The graph $K_{n-k} \star S_{k+1}$ contains k vertices having degree 1, one vertex having degree $n-1$ and $n-k-1$ vertices having degree $n-k-1$, thus $P_2^a(C_{n-k} \star S_{k+1})$

$$= (n-1)^{a(n-1)}(n-k-1)^{a(n-k-1)(n-k-1)}1^{ka}$$
$$= (n-1)^{a(n-1)}(n-k-1)^{a(n-k-1)^2}.$$

□

IV. BOUNDS FOR $a < 0$

In the proofs of our results for $a > 0$ we often used that if $f > 1$, then $f^a > 1$; or more generally, if $f_1 > f_2 \geq 1$, then $f_1^a > f_2^a \geq 1$, Similarly, if $0 < f < 1$ and $a > 0$, we obtain $0 < f^a < 1$.

Note that if $f > 1$ and $a < 0$, we get $0 < f^a < 1$; or more generally, if $f_1 > f_2 \geq 1$, then $0 < f_1^a < f_2^a \leq 1$, Similarly, if $0 < f < 1$ and $a < 0$, we obtain $f^a > 1$.

Using these inequalities and the proofs of the results given in Sections II and III we obtain results for $a < 0$.

Lemma 7: Let G be a connected graph with two nonadjacent vertices $v_1, v_2 \in V(G)$. Then for $a < 0$, $P_c^a(G) > P_c^a(G + v_1v_2)$, where $c = 1, 2$.

Proof: Let $G' = G + v_1 v_2$. For $j = 1, 2$, we have $1 \leq d_G(v_j) < d_{G'}(v_j)$, which implies that $1 \geq d_G(v_j)^a > d_{G'}(v_j)^a > 0$, thus $P_1^a(G) > P_1^a(G')$. Similarly, since $1 \leq d_G(v_j)^{d_G(v_j)} < d_{G'}(v_j)^{d_{G'}(v_j)}$, we obtain

$$\begin{aligned} 1 &\geq d_G(v_j)^{ad_G(v_j)} \\ &= [d_G(v_j)^{d_G(v_j)}]^a \\ &> [d_{G'}(v_j)^{d_{G'}(v_j)}]^a \\ &= d_{G'}(v_j)^{ad_{G'}(v_j)} > 0, \end{aligned}$$

so $P_2^a(G) > P_2^a(G')$. □

Lemma 8: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the largest P_1^a index, where $a < 0$, then T is a star attached to H by its centre.

The main difference between the proofs of Lemmas 2 and 8 is that in the proof of Lemma 8 we would use

$$\frac{P_1^a(G)}{P_1^a(G')} = \left(\frac{ts+s}{t+s}\right)^a < 1,$$

since $\frac{ts+s}{t+s} > 1$.

Lemma 9: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the smallest P_2^a index, where $a < 0$, then T is a star attached to H by its centre.

Lemma 10: Let G be formed by a cycle H (by a complete graph H), where any vertex of H can be adjacent to pendant vertices. If G has the largest P_1^a index (the smallest P_2^a index), where $a < 0$, then G contains at most one vertex adjacent to pendant vertices.

Lemma 11: Let G be formed by any connected nonempty graph H with a tree T attached to one vertex of H. If G has the smallest P_1^a index (the largest P_2^a index), where $a < 0$, then T is a path attached to H by its pendant vertex.

Lemma 12: Let G be formed by a complete graph H (by a cycle H), where any vertex of H can be adjacent to a pendant path. If G has the smallest P_1^a index (the largest P_2^a index), where $a < 0$, then G contains at most one pendant path.

The main difference between the proofs of Lemmas 5, 6 and proofs of Lemmas 11, 12 is that in the proofs of Lemmas 11, 12 we would use

$$\frac{P_1^a(G')}{P_1^a(G)} = \left(\frac{2t-2}{t}\right)^a < 1,$$

since $\frac{2t-2}{t} > 1$, and

$$\frac{P_2^a(G')}{P_2^a(G)} = \left[\left(1-\frac{1}{t}\right)^t \frac{4}{t-1}\right]^a > 1,$$

since $(1-\frac{1}{t})^t \frac{4}{t-1} < 1$.

We can use Lemmas 7 – 12 to obtain the following bounds for $a < 0$.

Theorem 4: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a < 0$,

$$P_1^a(G) \leq (k+2)^a 2^{(n-k-1)a}$$

with equality if and only if G is $C_{n-k} \star S_{k+1}$, and

$$P_2^a(G) \leq 3^{3a} 2^{2a(n-2)}$$

with equality if and only if G is $C_{n-k} * P_{k+1}$.

The main difference between the proofs of Theorems 1 and 4 is that in the proof of Theorem 4 we would use

$$\frac{P_1^a(G')}{P_1^a(G'')} = \left(\frac{z}{z-2}\right)^a < 1$$

and

$$\frac{P_2^a(G')}{P_2^a(G'')} = \left[\frac{z^z}{(z-2)^{z-2}}\right]^a < 1,$$

since $\frac{z}{z-2} > 1$ and $\frac{z^z}{(z-2)^{z-2}} > 1$.

Upper bounds on the P_1^a and P_2^a indices are given in Theorems 5 and 6.

Theorem 5: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a < 0$,

$$P_1^a(G) \geq (n-k)^a (n-k-1)^{a(n-k-1)} 2^{a(k-1)}$$

with equality if and only if G is $K_{n-k} \star P_{k+1}$.

Theorem 6: Let G be a graph having n vertices and k bridges, where $1 \leq k \leq n-3$. Then for $a < 0$,

$$P_2^a(G) \geq (n-1)^{a(n-1)}(n-k-1)^{a(n-k-1)^2}$$

with equality if and only if G is $K_{n-k} * S_{k+1}$.

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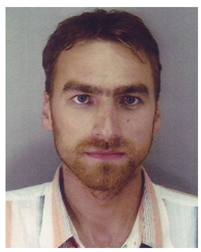

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