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Maximizing and Minimizing Multiplicative Zagreb Indices of Graphs Subject to Given Number of Cut Edges

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Abstract: Given a (molecular) graph, the first multiplicative Zagreb index Π_1 is considered to be the product of squares of the degree of its vertices, while the second multiplicative Zagreb index Π_2 is expressed as the product of endvertex degree of each edge over all edges. We consider a set of graphs $\mathbb{G}_{n,k}$ having n vertices and k cut edges, and explore the graphs subject to a number of cut edges. In addition, the maximum and minimum multiplicative Zagreb indices of graphs in $\mathbb{G}_{n,k}$ are provided. We also provide these graphs with the largest and smallest $\Pi_1(G)$ and $\Pi_2(G)$ in $\mathbb{G}_{n,k}$.

Keywords: cut edge; graph transformation; multiplicative zagreb indices; extremal values

1. Introduction

Within the areas of theoretical chemistry and mathematics, the structure invariant is an important tool to study the quantitative molecular properties [1]. One type of the most classical topological molecular expression is called as Zagreb indices M_1 and M_2 [2]. This information can be used as qualitative levels for integral π-electron energy of the conjugated molecules. In the view of successful considerations on the applications on Zagreb indices [3], Todeschini et al., (2010) [4–6] introduced the multiplicative Zagreb indices of molecular graphs, denoted by Π_1 and Π_2 the multiplicative Zagreb indices. (Multiplicative) Zagreb indices are employed as molecular expressions in quantitative structure–property relationships and quantitative structure–activity relationships [7,8].

Mathematicians have been interested in the information of Zagreb indices about the upper and lower bounds for special (chemical) graphs, as well as corresponding areas of determining their extremal graphs [9–23]. In addition to a plenty of applications for the usage of Zagreb indices in theoretical chemistry, there are many studies for multiplicative Zagreb indices, which attracted one of the focus of interests in physics and graph theory. Borovićanin et al. [24] investigated upper bounds on Zagreb indices of noncyclic graphs with given domination number. Wang and Wei [6] determined the maximal and minimal values of multiplicative Zagreb indices in the extended noncyclic graph, k-trees. In some graph classes, Liu and Zhang provided some upper bounds for Π_1-index and Π_2-index of graphs subject to structure parameters [25]. Xu and Hua [26] explored a common method to characterize the bounds of $0, 1, 2$-cyclic graphs. Iranmanesh et al. [27] gave these indices for a type of chemical molecules, specific dendrimers. Kazemi [28] found interesting extremal values for related moments and probability generating functions in random trees. The graphs subject to a given number of cut edges (or vertices) are intriguing in extremal mathematics [29–33]. It is a natural observation that trees having largest and smallest multiplicative Zagreb indices have been considered as interesting topics [27,34,35].

In view of mentioned outcomes, we continue this way and study multiplicative Zagreb indices of graphs subject to a given number of cut edges. In addition, the maximum and minimum of $\Pi_1(G)$ and $\Pi_2(G)$ of graphs in $\mathbb{G}_{n,k}$ subject to fixed number of cut edges are provided. Lastly, the corresponding graphs with the largest and smallest multiplicative Zagreb indices in $\mathbb{G}_{n,k}$ are determined.

2. Preliminaries

Denote by $G = (V(G), E(G))$ a simple undirected connected graph of vertex number n and edge number m with vertex set $V = V(G)$ and edge set $E = E(G)$. For $w \in V(G)$, $N(w)$ denotes the neighbors of w, that is, $N(w) = \{v| \ wv \in E(G)\}$, and $d(w) = |N(w)|$ is the degree of w. The Zagreb indices [3] of a connected graph are given by

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The first multiplicative Zagreb index $\Pi_1 = \Pi_1(G)$ and the second multiplicative Zagreb index $\Pi_2 = \Pi_2(G)$ [4,5] of any graph G are considered as

$$\Pi_1(G) = \prod_{u \in V(G)} d(u)^2 \text{ and } \Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v) = \prod_{u \in V(G)} d(u)^{d(u)}.$$

A vertex of degree one is called pendent vertex. The supporting vertex is a vertex in a graph which is incident to at least one pendent vertex. A pendent edge is an edge connecting a pendent vertex and a supporting vertex. If $G_1, G_2, \cdots, G_l$ with $l \geq 2$ share a common vertex v, then $G_1 v G_2 v \cdots v G_l$ denote the graph with edge set $E(G_1) \cup E(G_2) \cup \cdots \cup E(G_l)$ and $V(G_1) \cap V(G_2) \cap \cdots \cap V(G_l) = \{v\}$. For $u_1 \in V(G_1)$ and $u_s \in V(G_2)$, if $P = u_1 u_2 \cdots u_s$ is a path, then denote this graph by $G_1 P G_2$ or $G_1 u_1 u_2 \cdots u_s G_2$ in which P is called an internal path. By deleting a vertex or an edge, the resulting graph has at least two components, and this vertex or edge is called a cut. If G has no cut vertex, then G is 2-connected. A block is 2-connected, and an endblock has not more than two cut vertices. $G_1 \cong G_2$ means that G_1 is isomorphic to G_2. As usual, P_n, K_n, S_n and C_n are a path, a clique, a star and a cycle on n vertices, respectively. The cyclomatic number $c(G)$ of a graph G is defined as $m - n + 1$. In particular, if $c(G) = 0$, 1 and 2, then G will be trees, unicyclic graphs and bicyclic graphs, respectively. If $c(G) \geq 1$, then G has at most $n - 3$ cut edges. Thus, we suppose that G contains $1 \leq k \leq n - 3$ cut edges in our following discussion.

Let $\mathbb{G}_{n,k}$ be the set of the connected graphs with $k \in [1, n-3]$ cut edges, and $E_c = \{e_1, e_2, \cdots, e_k\}$ be a set of cut edges of the graph $G \in \mathbb{G}_{n,k}$. Then E_c can be considered as two categories, which are the pendent edges and nonpendent edges (or internal paths of length 1). $G - E_c$ contains some 2-connected graphs and isolated vertices. Denote by K_n^S (or K_n^P, respectively) a graph obtained by identifying (connecting to, respectively) the nonpendent vertex of a star S_{k+1} (or a pendent vertex of a path P_k, respectively) to a vertex of K_{n-k} (see Figure 1). In addition, let C_n^S (or C_n^P, respectively) be a graph obtained by identifying (connecting to, respectively) the nonpendent vertex of a star S_k (or a pendent vertex of a path P_k, respectively) to a vertex of C_{n-k}.

In our work, we may use some terminologies and notations of these textbooks of graph theory (see [36,37]). By elementary processes, the following results are not hard.

Proposition 1. *If $s(l) = \frac{l}{l+t}$ is a function for $t > 0$, then $s(l)$ is an increasing function in $\mathbb{R}$.*

Proposition 2. *If $k(l) = \frac{l^l}{(l+t)^{l+t}}$ is a function for $t > 0$, then $k(l)$ is a decreasing function in $\mathbb{R}$.*

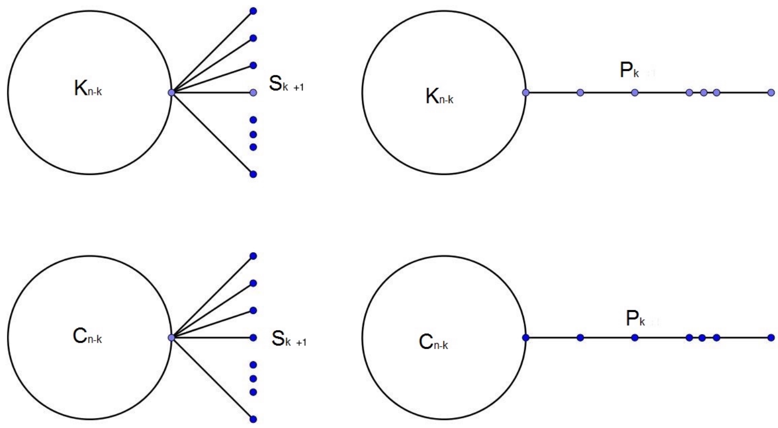

Figure 1. K_n^S, K_n^P, C_n^S and C_n^P.

Based on the concepts of $\Pi_1(G)$ and $\Pi_2(G)$ and the fact that adding edges increases the degrees, we have

Lemma 1. *Suppose that $G = (V, E)$ is a connected graph and $i = 1, 2$.*

(i) If u, v are not adjacent in G, then $\Pi_i(G + uv) > \Pi_i(G)$.

(ii) If $uv \in E(G)$, we have $\Pi_i(G - e) < \Pi_i(G)$.

Lemma 2 yields the following result.

Lemma 2. *Suppose that $G = (V, E)$ is a 2-connected graph with $i = 1, 2$.*

(i) If $\Pi_i(G)$ is maximal, then $G \cong K_n$.

(ii) If $\Pi_i(G)$ is minimal, then $G \cong C_n$.

Lemma 3. *Let C^1, C^2 be cycles, and $P_s = u_1u_2 \cdots u_s$ be an internal path of $G = C^1P_sC^2$ such that $u_1 \in V(C^1)$ and $u_s \in V(C^2)$. Assume that $u_1v_1, u_1v_2 \in E(C^1)$ and $u_sw_1, u_sw_2 \in E(C^2)$ such that $v_1 \neq v_2$ and $w_1 \neq w_2$. Let $G' = G - \{u_1v_2, u_sw_1, u_sw_2\} + \{v_2w_2, u_1w_1\}$. Then $\Pi_i(G) > \Pi_i(G')$ with $i = 1, 2$.*

Proof. By the graph operations from G to G', we have $d_{G'}(u_s) = 1 < d_G(u_s) = 3$. For $v \in V(G) - \{u_s\}$, $d_G(v) = d_{G'}(v)$. Then $\Pi_i(G) > \Pi_i(G')$ with $i = 1, 2$, and we complete the proof. □

Lemma 4. *Let $G_1P_mG_2$ and $G_1G_2P_m$ be graphs (see Figure 2), in which P_m is a path, and G_1, G_2 are connected. Then $\Pi_1(G_1P_mG_2) \geq \Pi_1(G_1G_2P_m)$ and $\Pi_2(G_1P_mG_2) \leq \Pi_2(G_1G_2P_m)$.*

Proof. Let $d_{G_1P_mG_2}(u) = x$ and $d_{G_1P_mG_2}(v) = y$. Then $d_{G_1G_2P_m}(u) = x + y - 1$. From the formulas of multiplicative Zagreb indices, we obtain

$$\frac{\Pi_1(G_1P_mG_2)}{\Pi_1(G_1G_2P_m)} = \frac{x^2y^2}{(x+y-1)^2 1^2} = \left(\frac{\frac{x}{x+y-1}}{\frac{1}{1+(y-1)}}\right)^2.$$

Since $x \geq 1, y \geq 1$, and by Proposition 1, we have $\Pi_1(G_1P_mG_2) \geq \Pi_1(G_1G_2P_m)$. Note that

$$\frac{\Pi_2(G_1P_mG_2)}{\Pi_2(G_1G_2P_m)} = \frac{x^x y^y}{(x+y-1)^{(x+y-1)}1^1} = \frac{\frac{x^x}{(x+y-1)^{(x+y-1)}}}{\frac{1^1}{(1+y-1)^{(1+y-1)}}}.$$

By $x \geq 1$ and Proposition 2, we have $\frac{\Pi_2(G_1P_mG_2)}{\Pi_2(G_1G_2P_m)} \leq 1$, that is, $\Pi_2(G_1P_mG_2) \leq \Pi_2(G_1G_2P_m)$. Thus, this completes the proof. □

From Lemma 4, if we have an internal path, then we can move out it. By keeping this process, we have the useful lemma below.

Lemma 5. *Let GT be a graph by identifying a vertex of a tree T (not S_n) to a vertex u of G, and GS be a graph by attaching $|E(T)|$ pendent edges to u (see Figure 3). Then $\Pi_1(GT) > \Pi_1(GS)$ and $\Pi_2(GT) < \Pi_2(GS)$.*

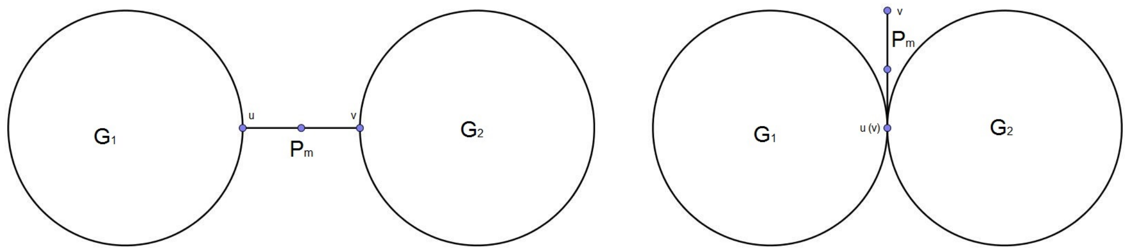

Figure 2. $G_1P_mG_2$ and $G_1G_2P_m$.

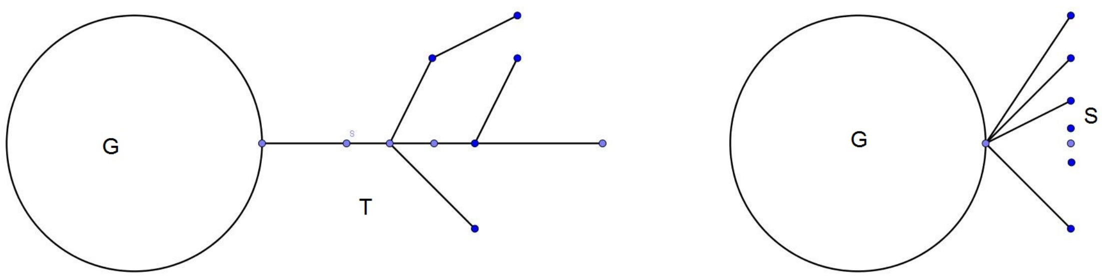

Figure 3. GT and GS.

Lemma 6. *Let u (v, respectively) be a vertex in G, and $u_1, u_2, \ldots, u_s$ be the endvertices of pendent path $P_1, P_2, \cdots, P_s$ ($v_1, v_2, \ldots, v_t$ be the endvertices of $P'_1, P'_2, \cdots, P'_t$, respectively). Set $uu'_i \in E(P_i)$ with $1 \leq i \leq s$, and $vv'_j \in E(P'_j)$ with $1 \leq j \leq t$. Let $G' = G - \{uu'_i\} + \{vu'_i\}$ with $1 \leq i \leq s$, $G'' = G - \{vv'_j\} + \{uv'_j\}$ with $1 \leq j \leq t$ and $|V(G_0)| \geq 3$ (see Figure 4). Then either $\Pi_1(G) \geq \Pi_1(G')$ and $\Pi_2(G) \leq \Pi_2(G')$, or $\Pi_1(G) > \Pi_1(G'')$ and $\Pi_2(G) < \Pi_2(G'')$.*

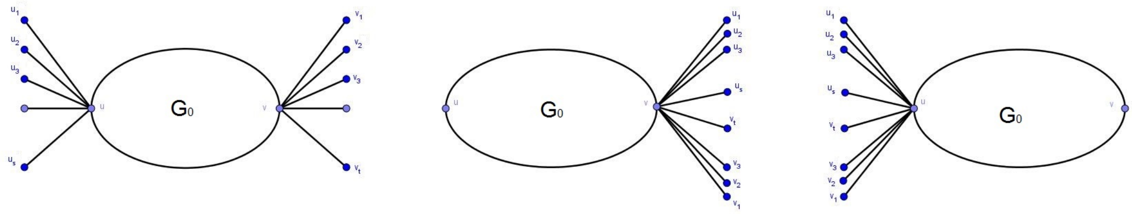

Figure 4. G, G' and G''.

Proof. Let $d_G(u) = x$, $d_G(v) = y$. By the constructions of G' and G'' , we have $d_{G'}(u) = d_G(u) - s = x - s$, $d_{G'}(v) = d_G(v) + s = y + s$, $d_{G''}(u) = d_G(u) + t = x + t$ and $d_{G''}(v) = d_G(v) - t = y - t$. Combining with the concepts of multiplicative Zagreb indices, we have

$$\frac{\Pi_1(G)}{\Pi_1(G')} = \frac{x^2y^2}{(x-s)^2(y+s)^2} = \frac{(\frac{y}{y+s})^2}{(\frac{x-s}{(x-s)+s})^2},$$

$$\frac{\Pi_2(G)}{\Pi_2(G')} = \frac{x^xy^y}{(x-s)^{x-s}(y+s)^{y+s}} = \frac{\frac{y^y}{(y+s)^{y+s}}}{\frac{(x-s)^{x-s}}{x^x}} = \frac{\frac{y^y}{(y+s)^{y+s}}}{\frac{(x-s)^{x-s}}{[(x-s)+s]^{(x-s)+s}}},$$

$$\frac{\Pi_1(G)}{\Pi_1(G'')} = \frac{x^2y^2}{(x+t)^2(y-t)^2} = \frac{(\frac{x}{x+t})^2}{(\frac{y-t}{(y-t)+t})^2},$$

$$\frac{\Pi_2(G)}{\Pi_2(G'')} = \frac{x^xy^y}{(x+t)^{x+t}(y-t)^{y-t}} = \frac{\frac{x^x}{(x+t)^{x+t}}}{\frac{(y-t)^{y-t}}{y^y}} = \frac{\frac{x^x}{(x+t)^{x+t}}}{\frac{(y-t)^{y-t}}{[(y-t)+t]^{(y-t)+t}}}.$$

If $x - s \leq y$, by Propositions 1 and 2, we can obtain that $\Pi_1(G) \geq \Pi_1(G')$ and $\Pi_2(G) \leq \Pi_2(G')$. If $x - s - 1 \geq y$, then $x \geq y + s + 1 > y - t$. Propositions 1 and 2 yield that $\Pi_1(G) > \Pi_1(G'')$ and $\Pi_2(G) < \Pi_2(G'')$. Thus, the lemma is proved. □

Lemma 7. *Let $P_1 = u_1u_2 \cdots u_s$ and $P_2 = v_1v_2 \cdots v_t$ be two pendent paths of G with $s, t \geq 2$ and $d(u_s) = d(v_t) = 1$ (see Figure 5). Let $G' = G - v_1v_2 + u_sv_2$. Then $\Pi_1(G) < \Pi_1(G')$ and $\Pi_2(G) > \Pi_2(G')$.*

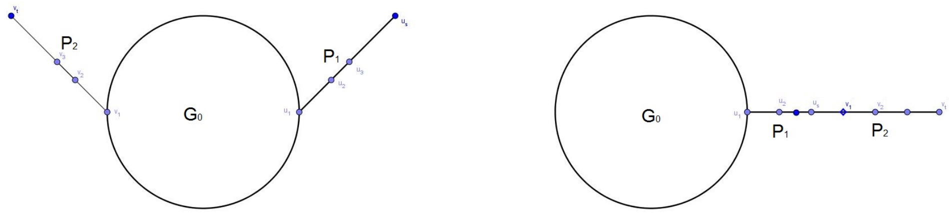

Figure 5. G and G'.

Proof. Note that $d(u_1) \geq 3, d(v_1) \geq 3$. From the expressions of multiplicative Zagreb indices, we have

$$\frac{\Pi_1(G)}{\Pi_1(G')} = \frac{d(u_s)^2d(v_1)^2}{d_{G'}(u_s)^2d_{G'}(v_1)^2} = \left(\frac{\frac{1}{2}}{\frac{d(v_1)-1}{d(v_1)}}\right)^2.$$

By Proposition 1, we have $\frac{\Pi_1(G)}{\Pi_1(G')} < 1$, that is, $\Pi_1(G) < \Pi_1(G')$.

$$\frac{\Pi_2(G)}{\Pi_2(G')} = \frac{d(u_s)^{d(u_s)} d(v_1)^{d(v_1)}}{d_{G'}(u_s)^{d_{G'}(u_s)} d_{G'}(v_1)^{d_{G'}(v_1)}} = \left(\frac{\frac{1^1}{2^2}}{\frac{(d(v_1)-1)^{d(v_1)-1}}{d(v_1)^{d(v_1)}}} \right)^2.$$

By Proposition 2, we have $\frac{\Pi_2(G)}{\Pi_2(G')} > 1$, that is, $\Pi_2(G) > \Pi_2(G')$.
Thus, this completes the proof. □

3. Graphs with Smallest Multiplicative Zagreb Indices in $\mathbb{G}_{n,k}$

We begin to determine the graphs having the smallest $\Pi_1(G)$ and $\Pi_2(G)$ in $\mathbb{G}_{n,k}$.

Theorem 1. *Let G be a graph in $\mathbb{G}_{n,k}$ with $1 \le k \le n-3$. Then*

$$\Pi_1(G) \ge 4^{n-k-1}(k+2)^2,$$

where the equality holds if and only $G \cong C_n^S$, respectively.

Proof. Choose a graph $G \in \mathbb{G}_{n,k}$ such that the value of $\Pi_1(G)$ is as small as possible. Let E_c be a cut edge set of G and $B_1, B_2, \cdots, B_{k+1}$ be the components of $G - E_c$. We first do some graph operations by previous lemmas. By Lemma 2, we have B_i is a cycle or an isolated vertex. Lemma 3 implies that G has a unique cycle. By Lemma 5, all cut edges in G are pendent edge. By Lemma 6, all pendent edges share a common supporting vertex, that is, $G \cong C_n^S$. Thus, this completes the proof. □

Theorem 2. *Assume that G is a graph in $\mathbb{G}_{n,k}$ for $1 \le k \le n-3$. We have*

$$\Pi_2(G) \ge 27 * 4^{n-2},$$

where the equality holds if and only $G \cong C_n^P$.

Proof. Let $G \in \mathbb{G}_{n,k}$ be a graph such that $\Pi_2(G)$ is minimal. Let E_c be a cut edge set of G and $B_1, B_2, \cdots, B_{k+1}$ be the components of $G - E_c$. By Lemma 2, we have B_i is a cycle or an isolated vertex. Lemma 3 implies that G has a unique cycle. By Lemma 7, there is only one pendent path in G. Thus $G \cong C_n^P$, and we prove this theorem. □

4. Graphs with Largest Multiplicative Zagreb Indices in $\mathbb{G}_{n,k}$

We proceed to consider graphs with the largest $\Pi_1(G)$ and $\Pi_2(G)$ in $\mathbb{G}_{n,k}$ in this section.

Theorem 3. *If G is a graph in $\mathbb{G}_{n,k}$ for $1 \le k \le n-3$, we have*

$$\Pi_1(G) \le 4^{k-1}(n-k-1)^{2(n-k-1)}(n-k)^2,$$

where the equality holds if and only $G \cong K_n^P$.

Proof. Denote by a graph $G \in \mathbb{G}_{n,k}$ such that $\Pi_1(G)$ is maximal. Set E_c to be a cut edge set of G and $B_1, B_2, \cdots, B_{k+1}$ the components of $G - E_c$. By Lemma 2, we have B_i is a clique of size at least 3 or an isolated vertex. Next we start with the following claims.

Claim 1. *Every two cliques of size at least 3 do not share a common vertex.*

Proof of Claim 1. We prove it by a contradiction. Assume there are at least two blocks B_1, B_2 sharing a common vertex v_0 in G such that $|B_1|, |B_2| \ge 3$. Choose $v_1 \in V(B_1)$, $v_2 \in V(B_2)$ and $v_1, v_2 \ne v_0$.

Let $G' = G + v_1v_2$. By Lemma 1, $\Pi_2(G') > \Pi_2(G)$, that is a contradiction to the assumption of G. The claim is proved. □

We introduce a graph transformation that is used in the rest of our proof.

Claim 2. *Let K_{n_1} and K_{n_2} be two farthest endblocks of $K_{n_1}G_0K_{n_2}$ such that $v_{11} \in V(K_{n1}) \cap V(G_0)$ and $v_{l1} \in V(K_{n2}) \cap V(G_0)$ (see Figure 6). If $d(v_{11}) = n_1 \geq 3$ and $d(v_{l1}) = n_2 \geq 3$, then $\Pi_1(K_{n_1}G_0K_{n_2}) < \Pi_1(K_{n_1+n_2-1}G_0)$.*

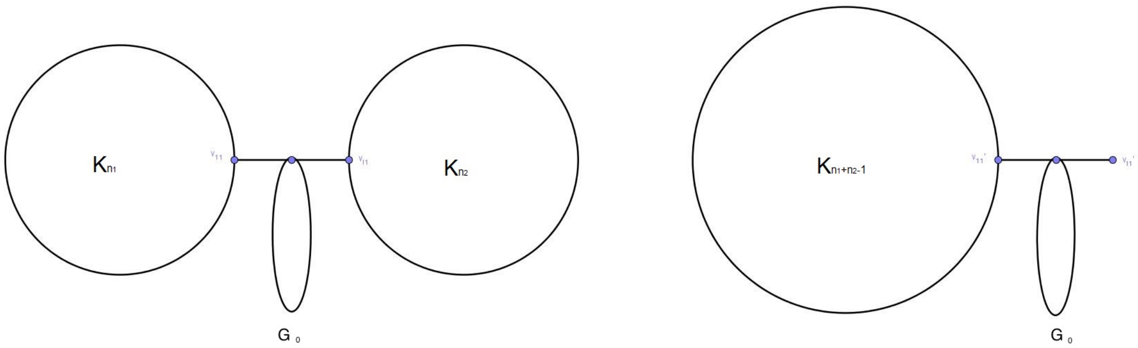

Figure 6. G and G'.

Proof of Claim 2. Let $V(K_{n_1}) = \{v_{11}, v_{12}, \cdots, v_{1n_1}\}$ and $V(K_{n_2}) = \{v_{l1}, v_{l2}, \cdots, v_{ln_2}\}$. Denote by $G = K_{n_1}G_0K_{n_2}$ and $G' = G - \{v_{l1}v_{li}, i \geq 2\} + \{v_{li}v_{1j}, i \geq 2, j \geq 1\} = K_{n_1+n_2-1}G_0$. From concepts of multiplicative Zagreb indices, one may obtain that

$$\begin{aligned}
\frac{\Pi_1(G)}{\Pi_1(G')} &= \left(\frac{d(v_{11})d(v_{12})d(v_{13})\cdots d(v_{1n_1})d(v_{l1})d(v_{l2})d(v_{l3})\cdots d(v_{ln_2})}{d'(v_{11})d'(v_{12})d'(v_{13})\cdots d'(v_{1n_1})d'(v_{l1})d'(v_{l2})d'(v_{l3})\cdots d'(v_{ln_2})}\right)^2 \\
&= \left(\frac{n_1n_2(n_1-1)^{n_1-1}(n_2-1)^{n_2-1}}{(n_1+n_2-1)(n_1+n_2-2)^{n_1+n_2-2}}\right)^2 \\
&\leq \left(\frac{n_1n_2(n_1-1)^{n_1-1}(n_2-1)^{n_2-1}}{(n_1+n_2-2)^{n_1+n_2-1}}\right)^2.
\end{aligned}$$

Let $f(x) = \frac{xn_2(x-1)^{x-1}(n_2-1)^{n_2-1}}{(x+n_2-2)^{x+n_2-1}}$. Then we take a derivative of $ln(f(x))$ as $\frac{1}{x} + ln(x-1) + 1 - ln(x+n_2-2) - \frac{x+n_2-1}{x+n_2-2} < \frac{1}{x} + ln(x-1) - ln(x+n_2-2) \leq \frac{1}{x} + ln(x-1) - ln(x+1)$, by $n_2 \geq 3$.

Set $g(x) = \frac{1}{x} + ln(x-1) - ln(x+1)$. Note that $g'(x) = \frac{x^2+1}{x^2(x^2-1)} > 0$ and $lim_{x\to\infty}g(x) = lim_{x\to\infty}ln(\frac{(x-1)e^{\frac{1}{x}}}{x+1}) = 0$, by L' Hospital's Rule. Thus, $g(x) < 0$, that is, the function $f(x)$ is decreasing. We have

$$\frac{\Pi_1(G_1)}{\Pi_1(G_2)} \leq \frac{3n_2(3-1)^{3-1}(n_2-1)^{n_2-1}}{(3+n_2-2)^{3+n_2-1}} = \frac{12 * n_2 * (n_2-1)^{n_2-1}}{(n_2+1)^2(n_2+1)(n_2+1)^{n_2-1}}.$$

Since $12 \leq (n_2+1)^2$ and $n_2 < n_2+1$, then $\frac{\Pi_1(G_1)}{\Pi_1(G_2)} < 1$. This completes the proof of Claim 2. □

Claim 3. *If $\Pi_1(G)$ is maximal, then there exists exactly one path in G.*

Proof of Claim 3. We prove it by contradictions. Assume that there are at least two paths $P_1 = u_1u_2\cdots u_s, P_2 = v_1v_2\cdots v_l$ with $d(u_1), d(v_1) \geq 3$. We consider three cases that P_i is either a pendent path or an internal path with $i = 1, 2$. □

Case 1. $d(u_s) = d(v_l) = 1$.

Proof of Case 1. By Lemma 7, there is another graph $G' \in \mathbb{G}_n^k$ such that $\Pi_1(G) < \Pi_1(G')$, which is a contradiction to the choice of G. $\square$

Case 2. $d(u_s) = 1, d(v_l) \geq 3$.

Proof of Case 2. Let $G'' = G - \{v_1v_2, u_1u_2\} + \{v_1u_2, v_2u_s\}$. Note that

$$\frac{\Pi_1(G)}{\Pi_1(G'')} = \frac{d(u_1)^2 d(u_s)^2}{d_{G''}(u_1)^2 d_{G''}(u_s)^2} = \left(\frac{\frac{1}{2}}{\frac{d(u_1)-1}{d(u_1)}}\right)^2.$$

Since $d(u_1) \geq 3$, by Proposition 1, we have $\Pi_1(G) < \Pi_1(G'')$, that is a contradiction to the choice of G. $\square$

Case 3. $d(u_s) \geq 3, d(v_l) \geq 3$.

Proof of Case 3. By Case 2, there does not exist any pendent paths in G. Then every cut edge is in an internal path. By choosing two farthest endblocks and Claim 2, there is another graph G''' such that $\Pi_1(G''') > \Pi_1(G)$, which contradicts that $\Pi_1(G)$ is maximal. This completes the proof of Case 3. $\square$

Therefore, G contains a unique clique of size at least 3 and the unique path is a pendent path. Thus $G \cong K_n^P$, and this completes the proof. $\square$

Theorem 4. *Let G be a graph in $\mathbb{G}_{n,k}$ with $1 \leq k \leq n-3$. Then*

$$\Pi_2(G) \leq (n-1)^{n-1}(n-k-1)^{(n-k-1)^2},$$

where the equality holds if and only $G \cong K_n^S$.

Proof. Pick a graph $G \in \mathbb{G}_{n,k}$ such that $\Pi_2(G)$ is as large as possible. Denote by E_c a cut edge set of G and $B_1, B_2, \cdots, B_{k+1}$ be the components of $G - E_c$. By Lemma 2, we have B_i is a clique of size at least 3 or an isolated vertex. By Lemma 4, if two blocks are connected by a path, then they share a common vertex.

Claim 4. *There is a unique block B such that $|B| \geq 3$.*

Proof of Claim 4. We prove it by a contradiction. Assume that there are at least two blocks B_1, B_2 sharing a common vertex v_0 in G such that $|B_1|, |B_2| \geq 3$. Choose $v_1 \in V(B_1)$ and $v_2 \in V(B_2)$ and $v_1, v_2 \neq v_0$. Let $G' = G + v_1v_2$. By Lemma 1, $\Pi_2(G') > \Pi_2(G)$ and this claim is proved. $\square$

By Lemmas 5 and 6, we have $G \cong K_n^S$, and this completes the proof. $\square$

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