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Maximum Zagreb Indices Among All $p-$Quasi $k-$Cyclic Graphs

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ABSTRACT

Suppose G is a simple and connected graph. The first and second Zagreb indices of G are two degree-based graph invariants defined as $M_1(G) = \sum_{v\in V(G)} deg(v)^2$ and $M_2(G) = \sum_{e=uv\in E(G)} deg(u)deg(v)$, respectively. The graph G is called $p-$quasi $k-$cyclic, if there exists a subset S of vertices such that $|S| = p$, $G \setminus S$ is $k-$cyclic and there is no a subset S' of $V(G)$ such that $|S'| < |S|$ and $G \setminus S'$ is $k-$cyclic. The aim of this paper is to characterize all graphs with maximum values of Zagreb indices among all $p-$quasi $k-$cyclic graphs with $k \leq 3$.

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1 Basic Definitions

Throughout this paper, all graphs are assumed to be finite, simple and connected. For such a graph G, the set of vertices and edges are denoted by $V(G)$ and $E(G)$, respectively. We use the notations P_n, C_n, S_n, K_n and $\emptyset_n$ to denote the $n-$vertex path, cycle, star, complete and empty graphs, respectively. The cyclomatic number of G is defined as

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$C(G) = |E(G)| - |V(G)| + 1$ and if $C(G) = k$ then we say that G is $k-$cyclic. If $C(G) = 0, 1, 2, 3$ then G is called a tree, unicyclic, bicyclic and tricyclic, respectively. The set of all $k-$cyclic graphs on a fixed vertex set of size n is denoted by $C^k(n)$.
The set of all vertices which are adjacent to v in G is denoted by $N_G(v)$. The degree of a vertex v, denoted by $d_G(v)$ ($d(v)$ for short), in a graph is the number of edges incident to it that clearly is the size of $N_G(v)$. A vertex of degree one is named a pendant vertex and an edge containing a pendant vertex is called a pendant edge. The maximum and minimum degrees of vertices in G are denoted by $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively.
A graph G is called a $p-$quasi $k-$cyclic, if there exists a subset S of vertices such that $|S| = p$, $G \setminus S$ is $k-$cyclic and there is no a subset S' of $V(G)$ such that $|S'| < |S|$ and $G \setminus S'$ is $k-$cyclic. The set of all such graphs is denoted by $Q_pC^k(n)$.
Suppose G and H are two graphs. The union $G \cup H$ is a graph with the vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. The join of G and H is a graph with the same vertex set as $G \cup H$ and $E(G + H) = E(G) \cup E(H) \cup \{xy \mid x \in V(G), y \in V(H)\}$. Our other notations are standard and can be taken from [5, 10].
The Zagreb indices are the most studied degree-based graph invariants were introduced by Gutman and Trinajstić [8], are among the most studied degree-based graph invariants. These graph invariants are defined as $M_1(G) = \sum_{v\in V(G)}(d_G(v))^2$ and $M_2(G) = \sum_{uv\in E(G)}(d_G(u)d_G(v))$.

2 Preliminary Results

In this section, we first give a review of the most important results on Zagreb group indices of graphs and then present some results which are crucial for proving the main results of this paper.
Nikolić et al. [11], reported applications of Zagreb indices for studying molecular complexity [12], chirality [6] and $ZE-$isomerism [7] in mathematical chemistry. They also illustrated the applications of this invariant in QSPR by modeling the structure boiling point relationship of C_3C_8 alkanes. Their theoretical results based on Zagreb group indices were compared with experimental data.
Das et al. [2], obtained lower and upper bounds for $M_1(G)$ in terms of $|V(G)|$, $|E(G)|$, $\Delta(G)$ and $\delta(G)$ by which it is possible to find lower and upper bounds on $M_2(G)$. They also gave a relation between the first and second Zagreb indices of G.
Let U_n^3 be the unicyclic graph obtained from the cycle C_3 by attaching $n-3$ pendent edges to a fixed vertex of C_3. Suppose e is an edge of the complete graph K_4 and $H = K_4 \setminus e$. Construct the graph $B_n^{3,3}$ by considering a copy of $K_4 \setminus e$, a copy of $\emptyset_{n-4}$ and contact all vertices of $\emptyset_{n-4}$ to a fixed vertex of degree 3 in $K_4 \setminus e$, see Figure 1.

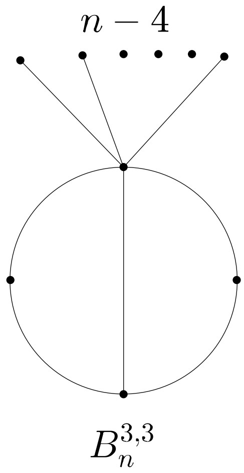

Figure 1: The bicyclic graph $B_n^{3,3}$ in Theorem 3.5.

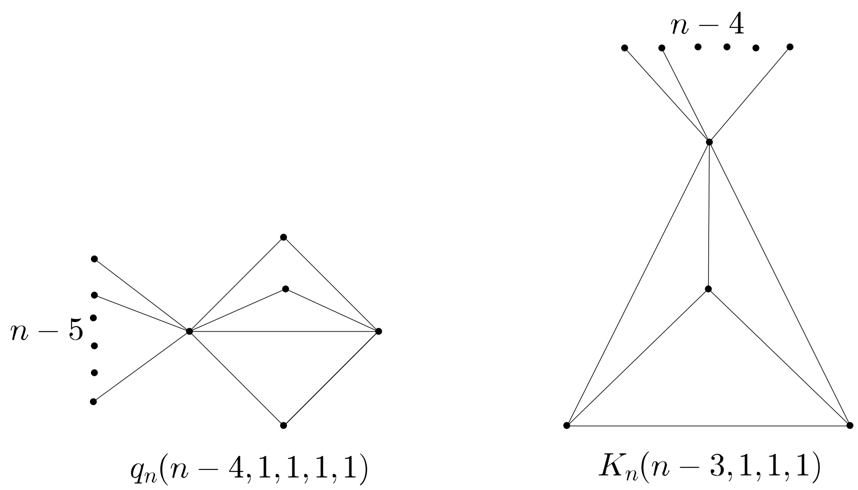

Figure 2: The tricyclic graphs $q_n(n-4,1,1,1,1)$ and $K_n(n-3,1,1,1)$ in Theorem 3.6.

3 Main Results

The aim of this paper is to characterize graphs with maximum values of Zagreb indices among all $p-$quasi $k-$cyclic graphs with $k \leq 3$.

Theorem 3.1. *Let G be a $p-$quasi $k-$cyclic graph. If $S \subset V(G)$, $|S| = p$ and $G - S \in C^k(n-p)$, then*

1. $M_1(G) \leq M_1(G-S) + p(4k + n^2 + 2n + p(n-4) - p^2 - 3)$,
2. $M_2(G) \leq M_2(G-S) + pM_1(G-S) + (k+n-p-1)(p^2+2p(n-1)) + \frac{p(p-1)(n-1)}{2} + p^2(n-p)(n-1)$,

with equality in each if and only if $G \cong (G-S) + K_p$.

Proof. To prove (1), we assume that $u \in V(G-S)$ and define l_u to be the number of vertices in S adjacent to u. By definition of M_1,

$$M_1(G) = \sum_{u \in V(G-S)} d_G^2(u) + \sum_{u \in S} d_G^2(u) = \sum_{u \in V(G-S)} (d_{G-S}(u) + l_u)^2 + \sum_{u \in S} d_G^2(u).$$

By simplifying this equality,

$$\begin{aligned} M_1(G) &= \sum_{u \in V(G-S)} (d_{G-S}^2(u) + l_u^2 + 2d_{G-S}(u)l_u) + \sum_{u \in S} d_G^2(u) \\ &= M_1(G-S) + \sum_{u \in V(G-S)} l_u^2 + \sum_{u \in V(G-S)} 2d_{G-S}(u)l_u + \sum_{u \in S} d_G^2(u) \\ &\leq M_1(G-S) + \sum_{u \in V(G-S)} p^2 + \sum_{u \in V(G-S)} 2d_{G-S}(u)p + \sum_{u \in S}(n-1)^2 \\ &= M_1(G-S) + (n-p)p^2 + 4p(k+n-p-1) + p(n-1)^2 \\ &= M_1(G-S) + p(4k + n^2 + 2n + p(n-4) - p^2 - 3). \end{aligned}$$

The equality holds if and only if for each $u \in V(G-S)$, $l_u = p$ and for every vertex $u \in S$, we have $d_G(u) = n-1$. This condition is satisfied if and only if $G \cong (G-S) + K_p$, proving the first part of the theorem.
To prove (2), we assume that u^*v^* is an edge of G such that $u^* \in V(G-S)$ and $v^* \in S$. By definition of M_2,

$$\begin{aligned} M_2(G) &= \sum_{uv\in E(G-S)} d_G(u)d_G(v) + \sum_{uv\in E(G-(V(G)\setminus S))} d_G(u)d_G(v) \\ &+ \sum_{u^*v^*\in E(G)} d_G(u^*)d_G(v^*) \\ &= \sum_{uv\in E(G-S)} (d_{G-S}(u)+l_u)(d_{G-S}(v)+l_v) + \sum_{uv\in E(G-(V(G)\setminus S))} d_G(u)d_G(v) \\ &+ \sum_{u^*v^*\in E(G)} (d_{G-S}(u^*)+l_{u^*})d_G(v^*). \end{aligned}$$

By simplifying the last equality,

$$\begin{aligned} M_2(G) &= \sum_{uv\in E(G-S)} (d_{G-S}(u)d_{G-S}(v) + d_{G-S}(u)l_v + d_{G-S}(v)l_u + l_ul_v) \\ &+ \sum_{uv\in E(G-(V(G)\setminus S))} d_G(u)d_G(v) + \sum_{u^*v^*\in E(G)} (d_{G-S}(u^*)d_G(v^*) + d_G(v^*)l_{u^*}). \end{aligned}$$

Therefore,

$$\begin{aligned} M_2(G) &= M_2(G-S) + \sum_{uv\in E(G-S)} (d_{G-S}(u)l_v + d_{G-S}(v)l_u + l_ul_v) \\ &+ \sum_{uv\in E(G-(V(G)\setminus S))} d_G(u)d_G(v) + \sum_{u^*v^*\in E(G)} (d_{G-S}(u^*)d_G(v^*) + d_G(v^*)l_{u^*}) \\ &\leq M_2(G-S) + p\sum_{uv\in E(G-S)} (d_{G-S}(u) + d_{G-S}(v) + p) \\ &+ \sum_{uv\in E(G-(V(G)\setminus S))} (n-1)^2 + \sum_{u^*v^*\in E(G)} (d_{G-S}(u^*)(n-1) + (n-1)p) \\ &= M_2(G-S) + pM_1(G-S) + (k+n-p-1)p^2 + \frac{p(p-1)(n-1)^2}{2} \\ &+ 2p(n-1)(k+n-p-1) + p^2(n-p)(n-1) \\ &= M_2(G-S) + pM_1(G-S) + (k+n-p-1)(p^2+2p(n-1)) \\ &+ \frac{p(p-1)(n-1)}{2} + p^2(n-p)(n-1). \end{aligned}$$

The equality is satisfied if and only if for each $u \in V(G-S)$, $l_u = p$ and for every vertex $u \in S$, $d_G(u) = n-1$. This condition is also equivalent to the fact that $G \cong (G-S)+K_p$ which completes the proof. □

Theorem 3.2. *Suppose* $A = \{H_1, H_2, ..., H_r\} \subset C^k(n-p)$, $H \in C^k(n-p) \setminus A$, $B = \{H_i + K_p | i = 1, 2, ..., r\}$ *and* $G \in Q_pC^k(n) \setminus B$. *If* $M_1(H) < M_1(H_1) = ... = M_1(H_r)$ *and* $M_2(H) < M_2(H_1) = ... = M_2(H_r)$, *then*

1. $M_1(G) < M_1(H_1 + K_p) = \cdots = M_1(H_r + K_p)$,

2. $M_2(G) < M_2(H_1 + K_p) = \cdots = M_2(H_r + K_p)$.

Proof. By Theorem 3.1(1), for each i, $1 \le i \le r$, $M_1(H_i + K_p) = M_1(H_i) + p(4k + n^2 + 2n + p(n-4) - p^2 - 3)$. Since $G \notin B$, for every subset S of $V(G)$ with this property that $G - S \in C^k(n-p)$, we have $G - S \notin A$ or $G - S \in A$ and $G \neq (G - S) + K_p$. Thus, by Theorem 3.1(1), $M_1(G) < M_1(H_1 + K_p) = ... = M_1(H_r + K_p)$. To prove the second part, we apply Theorem 3.1(2) and a similar argument as above. □

The following theorems are crucial in our next result:

Theorem 3.3. (*See [1, 9]*). *Let T be a tree of order n. If T is different from S_n, then $M_1(T) < M_1(S_n)$ and $M_2(T) < M_2(S_n)$.*

Theorem 3.4. (*See [13, 14]*). *U_n^3 is the unique graph with the largest Zagreb indices M_1 and M_2 among all unicyclic graphs with n vertices.*

Theorem 3.5. (*See [4]*). *$B_n^{3,3}$ is the unique graph with the largest Zagreb indices M_1 and M_2 among all bicyclic graphs with n vertices, see Figure 1.*

Suppose $q_n(n-4, 1, 1, 1, 1)$ and $K_n(n-3, 1, 1, 1)$ are tricyclic graphs depicted in Figure 2.

Theorem 3.6. (*See [3]*). *Among all tricyclic graphs with $n(\ge 5)$ vertices,*

1. *$K_n(n-3, 1, 1, 1)$ and $q_n(n-4, 1, 1, 1, 1)$ have the maximum values of first Zagreb index.*

2. *The graph $K_n(n-3, 1, 1, 1)$ has maximum value of the second Zagreb index.*

From Theorems 3.2, 3.3, 3.4, 3.5 and 3.6, we have the following corollary.

Corollary 3.7. Suppose n is a given positive integer and $G \in Q_pC^k(n)$. Then,

1. If $k = 0$ and $n \ge p+2$ then $M_1(G) \le M_1(S_{n-p} + K_p)$ and $M_2(G) \le M_2(S_{n-p} + K_p)$. Hence $S_{n-p} + K_p$ has the maximum first and second Zagreb indices in the class $Q_pC^0(n)$ with $n \ge p + 2$.

2. If $k = 1$ and $n \ge p+3$ then $M_1(G) \le M_1(U_{n-p}^3 + K_p)$ and $M_2(G) \le M_2(U_{n-p}^3 + K_p)$. Hence $U_{n-p}^3 + K_p$ has the maximum first and second Zagreb indices in the class $Q_pC^1(n)$ with $n \ge p + 3$.

3. If $k = 2$ and $n \ge p+4$ then $M_1(G) \le M_1(B_{n-p}^{3,3} + K_p)$ and $M_2(G) \le M_2(B_{n-p}^{3,3} + K_p)$. Hence $B_{n-p}^{3,3} + K_p$ has the maximum first and second Zagreb indices in the class $Q_pC^2(n)$ with $n \ge p + 4$.

4. If $k = 3$ and $n \ge p+5$ then $M_1(G) \le M_1(K_{n-p}(n-p-3, 1, 1, 1) + K_p) = M_1(q_{n-p}(n-p-4, 1, 1, 1, 1) + K_p)$. Hence $K_{n-p}(n-p-3, 1, 1, 1) + K_p$ and $q_{n-p}(n-p-4, 1, 1, 1, 1) + K_p$ have the maximum first Zagreb index in the class $Q_pC^3(n)$ with $n \ge p + 5$.

5. If $k = 3$ and $n \geq p + 5$ then $M_2(G) \leq M_2(K_{n-p}(n - p - 3, 1, 1, 1) + K_p)$. Hence $K_{n-p}(n - p - 3, 1, 1, 1) + K_p$ has the maximum second Zagreb index in the class $Q_pC^3(n)$ with $n \geq p + 5$.

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