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Research Article

On a linear combination of Zagreb indices

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Abstract

The modified first Zagreb connection index of a triangle-free and quadrangle-free graph G is equal to $2M_2(G) - M_1(G)$, where $M_2(G)$ and $M_1(G)$ are the well-known second and first Zagreb indices of G, respectively. This paper involves the study of the linear combination $2M_2(G) - M_1(G)$ of $M_2(G)$ and $M_1(G)$ when G is a connected graph of a given order and cyclomatic number. More precisely, graphs having the minimum value of the graph invariant $2M_2 - M_1$ are determined from the class of all connected graphs of order n and cyclomatic number c_y, when $c_y \geq 1$ and $n \geq 2(c_y - 1)$.

Keywords: graph invariant; Zagreb connection indices; topological index; modified first Zagreb connection index; Zagreb indices; cyclomatic number.

2020 Mathematics Subject Classification: 05C07, 05C09.

1. Introduction

Throughout this study, only finite and connected graphs are exclusively considered. For the undefined notations and concepts from graph theory, the readers are suggested to consult books [4, 7, 12].

A topological index associated with a graph is a number that does not change under graph isomorphism. In [2], a topological index appeared in [11] was thoroughly studied first time after its appearance. This index is the modified first Zagreb connection index [2], which is defined for a graph G as

$$ZC_1^*(G) = \sum_{v \in V(G)} d_v \tau_v$$

where $V(G)$ represents the set of vertices of G, τ_v is the number of those vertices of G that are at distance 2 from v, and d_v denotes the degree of v. Zagreb connection indices have gained a considerable attention from mathematical community; for example see [6, 8, 15–17].

The sum of squares of vertex degrees of a graph is often denoted by M_1 and is recognized as the first Zagreb index; for example, see [3, 13]. The sum of the products of degrees of adjacent vertices of a graph is usually denoted by M_2 and is generally known as the second Zagreb index (see for example [18]). Thus, for a graph G, one has

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

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where $E(G)$ represents the set of edges of G. Additional information on Zagreb indices may be found in the review papers [5, 10, 14] and references cited therein.

If a graph G is quadrangle-free and triangle-free, then

$$ZC_1^*(G) = 2M_2(G) - M_1(G) \quad \text{(see [2])}. \tag{1}$$

Motivated from Equation (1), the linear combination $2M_2 - M_1$ of M_2 and M_1 is studied in this paper for connected graphs of fixed order and cyclomatic number, where the cyclomatic number of a graph is the least number of edges whose removal

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gives cycle-free graph. Since Equation (1) does not hold for infinitely many graphs containing triangle(s) or/and quadrangle(s), so when removing the conditions of being triangle-free and quadrangle-free from G, the right-hand side of Equation (1) is denoted by a modified notation: $ZC_1^{\dagger}$. Thus, for any graph G, one has

$$ZC_1^{\dagger}(G) = \sum_{uv\in E(G)} (2d_u d_v - d_u - d_v).$$

In the present study, graphs having the minimum value of the graph invariant $ZC_1^{\dagger}$ are determined from the class of all connected graphs of order n and cyclomatic number c_y, when $c_y \geq 1$ and $n \geq 2(c_y - 1)$. The case $c_y = 0$ corresponds to trees, which has already been resolved in [2, 9].

2. Main results

Before stating and proving the main results of this paper, some notations and definitions are recalled in the following. For a vertex $v \in V(G)$, define $N_G(v) = \{w \in V(G) : vw \in E(G)\}$. If $w \in N_G(v)$ then w is called a neighbor of v. A vertex in a graph is said to be a pendent vertex (branching vertex, respectively) if it has degree one (at least three, respectively). A non-trivial path $P : u_1u_2\cdots u_t$ of a graph is called pendent path whenever $\min\{d_{v_1}, d_{v_t}\} = 1$ and $\max\{d_{v_1}, d_{v_t}\} \geq 3$, and every remaining vertex of P (if it exists) has degree two. A graph with n vertices is also known as an n-vertex graph. Denote by G' a graph deduced from some other graph G after utilizing a transformation provided that $V(G') = V(G)$. In the remaining part of this paper, wherever such types of graphs are considered simultaneously, the notion d_v represents the degree of $v \in V(G') = V(G)$ in G.

Lemma 2.1. *Every graph having the least value of $ZC_1^{\dagger}$ over the class of all n-vertex graphs with $c_y \geq 1$ cyclomatic number has the minimum degree at least 2.*

Proof. Let G be a graph having the least value of $ZC_1^{\dagger}$ over the class of all n-vertex graphs with $c_y \geq 1$ cyclomatic number. Contrarily, suppose that the minimum degree of G is 1. Suppose that $P : vv_1v_2\ldots v_r$ is a pendent path of G, provided that $d_v \geq 3$. Since $c_y \geq 1$, at least one of the neighbors of v is non-pendent. Let $u \notin \{v_1\}$ be a non-pendent neighbor of v. Denote by G' the graph formed by dropping the edge uv from G and inserting there the edge v_ru. It is obvious that the cyclomatic numbers of G and G' are the same. When $r = 1$, one has

$$\begin{aligned} ZC_1^{\dagger}(G) - ZC_1^{\dagger}(G') &= 2\left(d_u(d_v - 2) - 2d_v + 4 + \sum_{w\in N_G(v)\setminus\{v_1,u\}} d_w\right) \\ &\geq 2\Big(d_u(d_v - 2) - 2d_v + 4 + (d_v - 2)\Big) \\ &= 2(d_u - 1)(d_v - 2) \geq 2(d_v - 2) > 0, \end{aligned}$$

which contradicts the definition of G. When $r \geq 2$, one has

$$ZC_1^{\dagger}(G) - ZC_1^{\dagger}(G') = 2\left((d_u - 1)(d_v - 2) + \sum_{w\in N_G(v)\setminus\{v_1,u\}} d_w\right) > 0,$$

a contradiction again. □

Lemma 2.1 gives the following result.

Corollary 2.1. *The cycle graph C_n is the unique graph having the minimum $ZC_1^{\dagger}$ value among all n-vertex unicyclic graphs.*

Denote by $\Delta(G)$ and $\delta(G)$ (or simply by Δ and δ) the maximum and minimum vertex degree, respectively, in a graph G. Define

$$n_i = n_i(G) = \big|\{w \in V(G) : d_w = i\}\big|.$$

Lemma 2.2. *For $c_y \geq 2$ and $n \geq 2(c_y - 1)$, if G is a graph achieving the least value of $ZC_1^{\dagger}$ over the class of all n-vertex graphs with c_y cyclomatic number, then $\Delta(G) = 3$.*

Proof. Take $\Delta = \Delta(G)$. Since only connected graphs are being considered and $c_y \geq 2$, one has $\Delta \geq 3$. Suppose to the contrary that $\Delta > 3$. From Lemma 2.1, it follows that $\delta(G) \geq 2$. Since $c_y = |E(G)| - n + 1$ and

$$\sum_{i=1}^{\Delta} i\, n_i = 2|E(G)|,$$

the constraint $n \geq 2(c_y - 1)$ yields

$$\sum_{i=1}^{\Delta} n_i \geq 2\big(|E(G)| - n\big) = 2\left(\sum_{i=1}^{\Delta} \frac{in_i}{2} - \sum_{i=1}^{\Delta} n_i\right) = 2\left(\sum_{i=3}^{\Delta} \frac{in_i}{2} - \sum_{i=3}^{\Delta} n_i\right),$$

which implies that

$$n_2 \geq \sum_{i=4}^{\Delta} n_i(i-3). \tag{2}$$

Equation (2) guaranties that G posses some vertex having degree 2. In the following, the vertex $v \in V(G)$ is assumed to be a vertex of maximum degree, that is, $d_v = \Delta$.

Case 1. At least one of the neighbors of v, say w, has degree 2.
Since $\Delta > 3$, there exists $u \in N_G(v)$ such that $uw \notin E(G)$. Let $z \notin \{v\}$ be the other neighbor of w. Denote by G' the graph deduced from G after dropping vu and adding uw. Since $\delta \geq 2$ and $d_v = \Delta \geq 4$, one has

$$\begin{aligned}
ZC_1^{\dagger}(G) - ZC_1^{\dagger}(G') &= 2\left(d_u(d_v - 3) - d_z - 2d_v + 8 + \sum_{y \in N_G(v)\setminus\{u,w\}} d_y\right) \\
&\geq 2\big(d_u(d_v-3) - d_z - 2d_v + 8 + 2(d_v - 2)\big) = 2\big(d_u(d_v-3) - d_z + 4\big) \\
&\geq 2\big(2(d_v - 3) - d_z + 4\big) \geq 2(d_v - 2) > 0,
\end{aligned}$$

a contradiction to the definition of G.

Case 2. None of the neighbors of v has degree 2.
Since $\delta \geq 2$, every neighbor of v has degree at least 3. Recall that Equation (2) implies that G posses some vertex having degree 2. Since $\Delta \geq 4$, there are vertices $w' \in V(G) \setminus N_G(v)$ and $v' \in N_G(v)$ such that $d_{w'} = 2$ and $w'v' \notin E(G)$. Denote by G'' the graph deduced from G after dropping vv' and adding $v'w'$. Because every neighbor of v has degree at least 3 and $d_v = \Delta \geq 4$, one has

$$\begin{aligned}
ZC_1^{\dagger}(G) - ZC_1^{\dagger}(G'') &= 2\left((d_{v'} - 1)(d_v - 3) + \sum_{x \in N_G(v)\setminus\{v'\}} d_x - \sum_{y \in N_G(w')} d_y\right) \\
&\geq 2\left(2(d_v - 3) + \sum_{x \in N_G(v)\setminus\{v'\}} d_x - \sum_{y \in N_G(w')} d_y\right) \\
&\geq 2\big(2(d_v-3) + 3(d_v - 1) - 2d_v\big) = 6(d_v - 3) > 0,
\end{aligned}$$

a contradiction again. □

For a graph G, define

$$m_{i,j} = m_{i,j}(G) = \big|\{vw \in E(G) : d_v = i \text{ and } d_w = j\}\big|.$$

Lemma 2.3. [1] *Let G be an n-vertex graph with cyclomatic number $c_y \geq 2$, minimum degree 2, and maximum degree 3.*

(i). *If the inequality $2(c_y - 1) \leq n < 5(c_y - 1)$ holds then $m_{3,3} \geq 1$.*

(ii). *If the inequality $n > 5(c_y - 1)$ holds then $m_{2,2} \geq 1$.*

(iii). *If the equations $n = 5(c_y - 1)$ and $\min\{m_{2,2}, m_{3,3}\} = 0$ hold then $\max\{m_{2,2}, m_{3,3}\} = 0$.*

Lemma 2.4. *For $n > 5(c_y - 1)$ with $c_y \geq 2$, if G is a graph achieving the least value of $ZC_1^{\dagger}$ among all n-vertex graphs with c_y cyclomatic number and if $ab \in E(G)$, then $\min\{d_a, d_b\} = 2$.*

Proof. By Lemmas 2.1, 2.2, and 2.3, one has $\delta(G)=2$, $\Delta(G)=3$, and $m_{2,2}\geq 1$. Take $v,w\in V(G)$ such that $d_v=d_w=2$ and $vw\in E(G)$. Contrarily, assume that $s,t\in V(G)$ are adjacent vertices of degree 3. Let $x\notin\{v\}$ be the neighbor of w. It is possible that $x\in\{s,t\}$; if it happens, then one takes $x=t$, without loss of generality.

Case 1. The sets $N_G(v)$ and $N_G(w)$ are disjoint.
Denote by G' the graph deduced from G after dropping vw, wx, st and inserting vx, sw, tw. In either of the cases $x\neq t$ and $x=t$, one has $ZC_1^\dagger(G)-ZC_1^\dagger(G')=2$, which contradicts the definition of G.

Case 2. The sets $N_G(v)$ and $N_G(w)$ are not disjoint.
Since G is connected and $c_y\geq 2$, it holds that $d_x=3$.

When $x\neq t$, then for the graph G'' obtained by dropping "wx, st" from G and inserting "wt, sx" there, one has

$$ZC_1^\dagger(G)=ZC_1^\dagger(G'').$$

Note that the sets $N_{G''}(v)$ and $N_{G''}(w)$ are disjoint and thus by Case 1, one gets a contradiction.

When $x=t$, then let $s_1\notin t$ be a neighbor of s. Denote by G''' the graph formed by dropping the edges wt, s_1s and inserting the edges sw, s_1t. Then, $ZC_1^\dagger(G)=ZC_1^\dagger(G''')$. Again, the sets $N_{G'''}(v)$ and $N_{G'''}(w)$ are disjoint, and thus by Case 1, one has a contradiction. □

Lemma 2.5. *For $n=5(c_y-1)$ with $c_y\geq 2$, if G is a graph achieving the least value of $ZC_1^\dagger$ among all n-vertex graphs with c_y cyclomatic number and if $ab\in E(G)$, then $\min\{d_a,d_b\}=2$ and $\max\{d_a,d_b\}=3$.*

Proof. By Lemmas 2.1 and 2.2, one has $\delta(G)=2$ and $\Delta(G)=3$. It is claimed that $\max\{m_{2,2},m_{3,3}\}=0$. Suppose to the contrary that $\max\{m_{2,2},m_{3,3}\}>0$.

If $\min\{m_{2,2},m_{3,3}\}=0$ then by Lemma 2.3, it holds that $\max\{m_{2,2},m_{3,3}\}=0$, which is a contradiction.

If $\min\{m_{2,2},m_{3,3}\}>0$ then by the proof of Lemma 2.4 one deduce that there is an n-vertex graph G^* with cyclomatic number c_y such that $ZC_1^\dagger(G)>ZC_1^\dagger(G^*)$, which contradicts the definition of G. □

Lemma 2.6. *For $2(c_y-1)\leq n<5(c_y-1)$ with $c_y\geq 2$, if G is a graph achieving the least value of $ZC_1^\dagger$ among all n-vertex graphs with c_y cyclomatic number, then $m_{2,2}=0$.*

Proof. Suppose to the contrary that $m_{2,2}>0$. By Lemmas 2.1, 2.2, and 2.3, one has $\delta(G)=2$, $\Delta(G)=3$, and $m_{3,3}\geq 1$. By the proof of Lemma 2.4 one deduces that there is an n-vertex graph G^* with cyclomatic number c_y such that $ZC_1^\dagger(G)>ZC_1^\dagger(G^*)$, which contradicts the definition of G.

□

Theorem 2.1. *For $c_y\geq 2$, in the class of all n-vertex graphs with c_y cyclomatic number,*

(i) *the cubic graphs are the only graphs having the minimum $ZC_1^\dagger$ value whenever $n=2(c_y-1)$;*

(ii) *the graphs of maximum degree 3 and minimum degree 2 with the constraint $m_{2,2}=0$, are the only graphs having the minimum $ZC_1^\dagger$ value whenever $2(c_y-1)<n<5(c_y-1)$;*

(iii) *the graphs of maximum degree 3 and minimum degree 2 with the constraint $m_{2,2}=m_{3,3}=0$, are the only graphs having the minimum $ZC_1^\dagger$ value whenever $n=5(c_y-1)$;*

(iv) *the graphs of maximum degree 3 and minimum degree 2 with the constraint $m_{3,3}=0$, are the only graphs having the minimum $ZC_1^\dagger$ value whenever $n>5(c_y-1)$.*

Proof. Let G be a graph having the least value of $ZC_1^\dagger$ among all n-vertex graphs with c_y cyclomatic number. By Lemmas 2.1 and 2.2, one has $\delta(G)=2$ and $\Delta(G)=3$. Thus, the following system of equations holds

$$n_2+n_3=n, \tag{3}$$

$$2n_2+3n_3=2(n+c_y-1). \tag{4}$$

i). If $n=2(c_y-1)$ then from (3) and (4) it follows that $n_2=0$ and thus G consists of the vertices of degree 3 only.
ii). If $2(c_y-1)<n<5(c_y-1)$ then Lemma 2.6 confirms that $m_{2,2}=0$.
iii). This part follows directly from Lemma 2.5.
iv). It follows from Lemma 2.4.

□

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