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The modified first Zagreb connection index and the trees with given order and size of matchings

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Abstract: A subset of the edge set of a graph G is called a matching in G if its elements are not adjacent in G. A matching in G with the maximum cardinality among all the matchings in G is called a maximum matching. The matching number in the graph G is the number of elements in the maximum matching of G. This present paper is devoted to the investigation of the trees, which maximize the modified first Zagreb connection index among the trees with a given order and matching number.

Keywords: Topological indices, modified first Zagreb connection index, trees, matching number.

1 Introduction

All the considered graphs in this paper are simple, finite and undirected. Let G be a graph with vertex set denoted by $V(G)$ and edge set $E(G)$. The number of elements in $V(G)$ is called the order of G usually denoted by $\mid V(G) \mid$. As usual, uv denotes the edge connecting the vertices u and v, where $u, v \in V(G)$ and $d_v(G)$ the degree of vertex u. Let $N_G(u)$ denotes the set of all those vertices of a graph G that are adjacent to the vertex $u \in V(G)$. We denote by $\Delta = \Delta(G)$ the maximum degree of vertices of G. A graph with no cycles is called a tree, and S_n and P_n denote, respectively, the star and path on n vertices. A vertex of degree 1 is known as a pendent vertex. Let T be a tree with a path $P = v_1v_2...v_s$ such that $d_{v_2}(T) = d_{v_3}(T) = ...d_{v_{s-1}}(T) = 2$ (unless $s = 2$). If $d_{v_1}(T), d_{v_s}(T) \geq 3$, P is said to be an internal chain of length $s-1$ in T. If either of the vertices v_1 or v_s has degree 1 and other has degree greater than 2, P is called a pendent chain of length $s-1$. A matching M in a graph G is a set of pairwise non-adjacent edges from the graph G. A maximum matching in G is a matching that contains the largest possible number of edges. The matching number α in G, is the cardinality of a maximum matching of G. A vertex that is incident with an edge of a matching M, is an M-matched vertex, and a vertex is said to be an M-unmatched vertex

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if it is incident with no edges of M. A matching M in a graph G is called a perfect matching if every vertex of G is M-matched. Undefined notions and terminologies regarding graph theory can be found in the references [7, 22, 34].

Topological indices are numerical quantities of a graph, which remain invariant under graph isomorphism [17]. Among most studied topological indices are the Zagreb indices with noteworthy applications in chemistry. These indices were reported in 1972 by Gutman and Trinajstić [16]. The members of these indices the first Zagreb index denoted by M_1, and the second Zagreb index denoted by M_2. For a graph G, these Zagreb indices are defined as

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

Considerable work has been done by the researchers on these two indices, for detail see the surveys [12, 18, 29], particularly the recent ones [4, 5, 9, 10, 21] and the references cited therein. In recent years, many variants of these aforementioned indices have been proposed in the literature [3, 6, 19, 20, 29] etc. The modified first Zagreb connection index ZC_1^* is one of the variants of the first Zagreb index. For a graph G, ZC_1^* is defined [2] as

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

where τ_v is the connection number of the vertex v (that is, the number of vertices having distance 2 from v, see in [33]). This index was appeared for the first time within a certain formula, derived by Gutman et al. in the paper [16], and was introduced as the third leap Zagreb index by Naji et al. in [25]. Ali et al. in [2], tested the chemical applicability of ZC_1^* for the octane hydrocarbons, and reported that ZC_1^* correlates well with the entropy and acentric factor of these octane hydrocarbons.
Extremal graph theory is a branch of graph theory developed by Hungarians. It is based on the investigations that how graph properties depend on the value of various graph parameters. The investigation of extremal bounds on certain topological indices over different classes of graphs (trees, bipartite, unicyclic, etc.) and to characterize corresponding extremal structures, is one of the most popular research problems in the field of extremal graph theory. Ducoffe et al. [13] determined the extremal structures of the graphs with respect to the modified first Zagreb connection index for trees and unicyclic connected graphs. Zhu et al. [36] found a lower bound on ZC_1^* of tree graphs with given order and maximum degree. For further detail about this index, see the recent papers [1, 8, 11, 14, 15, 23, 24, 26–28, 30–32, 35] and the references cited therein.
In this paper, we contribute further in this direction by characterizing the graphs with maximum ZC_1^* values from the class of all trees having a fixed order and matching number. Denote $\mathscr{T}_{n,\alpha}$ by the class of trees with n vertices and α-matching (or matching number α), where n and α are positive integers.

2 Characterization of trees with order n and matching number α having maximum Modified first Zagreb connection index

In this section, the characterization of the extremal tree(s) having maximum modified first Zagreb connection index ZC_1^* among all members of the class $\mathscr{T}_{n,\alpha}$ is addressed. It can be noted that $\mathscr{T}_{n,1}$ consists of only star graph S_n and $\mathscr{T}_{4,2}$ contains only path graph P_4. In the rest of the section, we will proceed with the consideration that $\alpha > 1$ and $n > 4$. Let MT_{max} be the tree with maximum modified first connection index among the class $\mathscr{T}_{n,\alpha}$ and M_{max} be a fixed maximum matching of MT_{max}, that is, for any $T \in \mathscr{T}_{n,\alpha}$, $ZC_1^*(MT_{max}) \geq ZC_1^*(T)$. It is obvious that for $\alpha = 1$, MT_{max} is a star S_n and for $\alpha = 2$ along with $n \leq 4$, MT_{max} is a path P_4. Hence in the rest of the section, we will proceed with the consideration that $\alpha > 1$ and $n > 4$. Let B be the set of all vertices of degree greater than 2 in the tree MT_{max}, then we have the following observations:

Lemma 2.1. *For $n > 4$ and $m > 1$, if $MT_{max} \in \mathscr{T}_{n,\alpha}$, $B \neq \emptyset$.*

Proof. Contrarily, we assume that $B = \emptyset$ that is $MT_{max} := v_1 v_2 \cdots v_n$ is a path with $d_{v_1}(MT_{max}) = 1 = d_{v_n}(MT_{max})$ and $d_{v_i}(MT_{max}) = 2$ for all $2 \leq i \leq n-1$. Let T' be the tree obtained from MT_{max} such as $T' = MT_{max} - \{v_2 v_3\} + \{v_2 v_4\}$, then we observe that $T' \in \mathscr{T}_{n,\alpha}$. We consider the following possible cases:
Case 1. If $n = 5$, it holds

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(MT_{max}) &= 2(2(3)-3-1) + (2(6)-2-3) + (2(2)-2-1) \\ &\quad -2(2(2)-2-1) - 2(4) = 2 > 0, \end{aligned}$$

which is a contradiction.
Case 2. For $n \geq 6$, we have

$$ZC_1^*(T') - ZC_1^*(MT_{max}) = 4 > 0.$$

In both cases, we get $ZC_1^*(T') > ZC_1^*(MT_{max})$, a contradiction. □

Lemma 2.2. *Every pendent chain (if exists) in the tree $MT_{max} \in \mathscr{T}_{n,\alpha}$ contains maximum one vertex with degree 2.*

Proof. Assume, on the contrary, that MT_{max} contains a pendent chain $P = v_1 v_2 \cdots v_l$ $(l \geq 4)$ with $d_{v_1}(MT_{max}) = t \geq 3$, $d_{v_l}(MT_{max}) = 1$ and $d_{v_i}(MT_{max}) = 2$ for all $2 \leq i \leq l-1$. Let us denote $N_1 = N_{MT_{max}}(v_1) \setminus \{v_2\}$ and T' be a tree obtained from MT_{max} such as $T' = MT_{max} - \{v_{l-1} v_{l-2}\} + \{v_1 v_{l-1}\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and if $l \geq 5$, then we get

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) \\ &\quad +2(2(2)(t+1) - 2 - t - 1) + (2(2) - 2 - 1) \\ &\quad -(2(2t) - 2 - t) - 2(2(4) - 2 - 2) \\ &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + 3t - 3 > 0, \end{aligned}$$

a contradiction. Now if $l = 4$, then we get

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + (2(2)(t+1) - 2 - t - 1) \\ &\quad + (2(t+1) - 1 - t - 1) - (2(2t) - 2 - t) \\ &\quad - (2(4) - 2 - 2) \\ &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + t - 1 > 0, \end{aligned}$$

which is again a contradiction. □

Lemma 2.3. *Any internal chain (if exists) in the tree $MT_{max} \in \mathscr{T}_{n,\alpha}$ is of length at most 1.*

Proof. Contrarily, suppose that MT_{max} has an internal chain $P = v_1 v_2 \cdots v_k$ of length at least 2 with $d_{v_1}(MT_{max}) = t \geq 3$, $d_{v_k}(MT_{max}) = s \geq 3$ and $d_{v_i}(MT_{max}) = 2$ for all $2 \leq i \leq k-1$. Let $N_1 = N_{MT_{max}}(v_1) \setminus \{v_2\}$ and $N_k = N_{MT_{max}}(v_k) \setminus \{v_{k-1}\}$. We consider the following possible cases:

Case 1. For $k \geq 6$, if $T' = MT_{max} - \{v_2v_3, v_4v_5\} + \{v_1v_3, v_2v_5\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and we have

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(MT_{max}) &= 2(2(2)(t+1) - 2 - t - 1) + (2(2) - 1 - 2) \\ &\quad + \sum_{u \in N_1} (2d_u(MT_{max}) - 1) - (2(2t) - 2 - t) - 2(4) \\ &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + 3t - 3 > 0, \end{aligned}$$

a contradiction.

Case 2. For $k = 5$, we have the following subcases:

Subcase 2.1. v_3 is not M_{max}-matched.
In this case, v_2 and v_4 are M_{max}-matched. Let $T' = MT_{max} - \{v_2v_3, v_3v_4\} + \{v_1v_3, v_2v_4\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and $ZC_1^*(T') - ZC_1^*(MT_{max}) = \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + t - 1 > 0$, a contradiction.

Subcase 2.2. v_3 is M_{max}-matched and without loss of generality, it can be assumed that $v_2v_3 \in M_{max}$.
Now, at least one vertex from $\{v_1, v_4\}$ is M_{max}-matched. If $T' = MT_{max} - \{v_3v_4\} + \{v_1v_4\}$, $T' \in \mathscr{T}_{n,\alpha}$ and $ZC_1^*(T') - ZC_1^*(MT_{max}) = \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + 3t - 3 > 0$, which is again a contradiction.

Case 3. For $k = 4$, we consider the following possible subcases:

Subcase 3.1. $v_2v_3 \in M_{max}$.

Let $T' = MT_{max} - \{v_3v_4\} + \{v_1v_4\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and

$$\begin{aligned}
ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) \\
&\quad + (2(2)(t+1) - 2 - t - 1) + 1 \\
&\quad + (2s(t+1) - s - t - 1) - (2(2t) - 2 - t) - 4 \\
&\quad - (2(2s) - 2 - s) \\
&= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + (2s-1)(t-1) > 0,
\end{aligned}$$

a contradiction.

Subcase 3.2. $v_2v_3 \notin M_{max}$.
Let $T' = MT_{max} - \{v_2v_3\} + \{v_1v_4\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and

$$\begin{aligned}
ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) \\
&\quad + (2(t+1) - 1 - t - 1) \\
&\quad + (2(s+1)(t+1) - s - 1 - t - 1) \\
&\quad + (2(s+1) - 1 - s - 1) + \sum_{v \in N_k} (2d_v(MT_{max}) - 1) \\
&\quad - (2(2t) - 2 - t) - 4 - (2(2s) - 2 - s) \\
&= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) \\
&\quad + \sum_{v \in N_k} (2d_v(MT_{max}) - 1) + 2st - s - t,
\end{aligned}$$

which is positive due to the fact that the function $f(s,t) = 2st - s - t$ is strictly increasing for $s \geq 3$ and $t \geq 3$. Therefore $ZC_1^*(T') > ZC_1^*(MT_{max})$, which leads to a contradiction.

Case 4. For $k = 3$, we have the following subcases:

Subcase 4.1. v_2 is not M_{max}-matched.
In this case, v_1 and v_3 are M_{max}-matched. Let $T' = MT_{max} - \{v_2v_3\} + \{v_1v_3\}$, then $T' \in \mathscr{T}_{n,\alpha}$ and

$$\begin{aligned}
ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + (2(t+1) - 1 - t - 1) \\
&\quad + (2s(t+1) - s - t - 1) - (2(2t) - 2 - t) \\
&\quad - (2(2s) - 2 - s) \\
&= \sum_{u \in N_1} (2d_u(MT_{max}) - 1) + (2s-3)(t-1) > 0,
\end{aligned}$$

a contradiction.

Subcase 4.2. v_2 is M_{max}-matched, and we may assume that $v_1v_2 \in M_{max}$.
Using the same transformation $T' = MT_{max} - \{v_2v_3\} + \{v_1v_3\}$ described in the Subcase 4.1, we have a contradiction to the choice of MT_{max}, which completes the proof. □

Lemma 2.4. *For $n > 4$ and $\alpha > 1$, if $MT_{max} \in \mathscr{T}_{n,\alpha}$, then $| B |< 3$.*

Proof. Contrarily, suppose that $| B |> 2$, then by Lemma 2.3, there exist $v_1, v_2, v_2 \in B$, such that $v_1v_2, v_2v_3 \in E(MT_{max})$. Let $d_{v_1}(MT_{max}) = r \geq 3$, $d_{v_2}(MT_{max}) = s \geq 3$ and $d_{v_3}(MT_{max}) = t \geq 3$. We consider the following possible cases:

Case 1. If exactly one element from $\{v_1, v_2, v_3\}$ is M_{max}-matched, v_2 must be M_{max}-matched. Define $N_1 = N_{MT_{max}}(v_1) \setminus \{v_2\}$, $N_2 = N_{MT_{max}}(v_2) \setminus \{v_1, v_3\}$ and $N_3 = N_{MT_{max}}(v_3) \setminus \{v_2\}$. Then every vertex in N_1 and N_3 is M_{max}-matched. If $T' = MT_{max} - \bigcup_{v\in N_3}\{v_3v\} + \bigcup_{v\in N_3}\{v_1v\}$, it can be observed that M_{max} is the maximum matching of T' and $T' \in \mathscr{T}_{n,\alpha}$, also

$$\begin{aligned}
ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u\in N_1}(d_u(MT_{max})(2(r+t-1)-1)-r-t+1) \\
&\quad + \sum_{v\in N_3}(d_v(MT_{max})(2(r+t-1)-1)-r-t+1) \\
&\quad +(2(s)-s-1)+(2s(r+t-1)-s-r-t+1) \\
&\quad - \sum_{u\in N_1}(d_u(MT_{max})(2r-1)-r) \\
&\quad -(2rs-r-s)-(2st-s-t) \\
&\quad - \sum_{v\in N_3}(2td_v(MT_{max})-d_v(MT_{max})-t) \\
&= (t-1)\sum_{u\in N_1}(2d_u(MT_{max})-1) \\
&\quad +(r-1)\sum_{v\in N_3}(2d_v(MT_{max})-1) > 0,
\end{aligned}$$

which is a contradiction.

Case 2. If only two elements from $\{v_1, v_2, v_3\}$ are M_{max}-matched, here are the following possibilities:

Subcase 2.1. If v_1, v_3 are M_{max}-matched, it can be assumed that $v_3x \in M_{max}$.
If $T' = MT_{max} - \bigcup_{v\in N_3}\{v_3v\} + \bigcup_{v\in N_3}\{v_1v\}$, the maximum matching of T' is $M_{max} - \{v_3x\} + \{v_3v_2\}$, and $T' \in \mathscr{T}_{n,\alpha}$. The calculation is analogous to Case 1, which gives a contradiction.

Subcase 2.2. If v_1 and v_2 are M_{max}-matched, using the transformation used in the Subcase 2.1, one can easily observe that M_{max} is the maximum matching of the tree T', a contradiction.

Subcase 2.3. If v_2 and v_3 are M_{max}-matched, we assume that $v_3x \in M_{max}$.
If $T' = MT_{max} - \bigcup_{v\in N_1}\{v_1v\} + \bigcup_{v\in N_1}\{v_3v\}$, M_{max} is the maximum matching of T', that is $T' \in \mathscr{T}_{n,\alpha}$. Using the results deduced in Case 1, we get $ZC_1^*(T') > ZC_1^*(MT_{max})$, a contradiction.

Case 3. If every element in $\{v_1, v_2, v_3\}$ is M_{max}-matched, we have the following possibilities:

Subcase 3.1. If $v_2v_3 \in M_{max}$ or $v_1v_2 \in M_{max}$, without loss of generality, it can be assumed that $v_1v_2 \in M_{max}$. Let there exists $w \in V(MT_{max}) \setminus \{v_1, v_2\}$ such that $v_3w \in M_{max}$. If $T' = MT_{max} - \bigcup_{v \in N_3}\{v_3v\} + \bigcup_{v \in N_3}\{v_1v\}$, $M_{max} - \{v_1v_2, v_3w\} + \{v_1w, v_2v_3\}$ is the maximum matching of T', which leads to a contradiction.

Subcase 3.2. If $v_1v_2, v_2v_3 \notin M_{max}$, then there exist vertices $x \in N_1$, $y \in N_2$ and $z \in N_3$, such that $xv_1, yv_2, zv_3 \in M_{max}$.
Therefore each vertex of B is M_{max}-matched. Now, we show that if $v \in B$ and $uv \in M_{max}$, then $d_u(MT_{max}) = 1$. Since $xv_1 \in M_{max}$, if $d_x(MT_{max}) \geq 3$, we may choose x, v_1, v_2 instead of v_1, v_2, v_3 for consideration, which gives a contradiction by using the same calculation given in the Subcase 3.1.
If $d_x(MT_{max}) = 2$, then by Lemmas 2.2 and 2.3, the degree of an adjacent vertex $u(\neq v_1)$ of x is 1. Therefore, $M_{max} - \{xv_1\} + \{xu\}$ is the maximum matching of T'. So, there are exactly two vertices of $\{v_1, v_2, v_3\}$ that are $M_{max} - \{xv_1\} + \{xu\}$-matched, same as Case 2, a contradiction is obtained.
Hence, $d_x(MT_{max}) = 1$, similarly $d_y(MT_{max}) = 1 = d_z(MT_{max})$. Without loss of generality we assume that $3 \leq t \leq r$. If $T' = MT_{max} - \bigcup_{w \in N_3 \setminus \{z\}}\{wv_3\} + \bigcup_{w \in N_3 \setminus \{z\}}\{wv_1\}$, we have

$$\begin{aligned}
ZC_1^*(T') - ZC_1^*(MT_{max}) &= \sum_{u \in N_1 \setminus \{x\}} (d_u(MT_{max})(2(r+t-2)-1) - r - t + 2) \\
&\quad + \sum_{w \in N_3 \setminus \{z\}} (d_w(MT_{max})(2(r+t-2)-1) - r - t + 2) \\
&\quad +(2(r+t-2) - 1 - r - t + 2) + (2(2) - 1 - 2) \\
&\quad +(2s(r+t-2) - s - r - t + 2) + (2(2s) - 2 - s) \\
&\quad -(2r - 1 - r) - (2rs - r - s) \\
&\quad - \sum_{u \in N_1 \setminus \{x\}} (2rd_u(MT_{max}) - d_u(MT_{max}) - r) \\
&\quad -(2st - s - t) - (2t - t - 1) \\
&\quad - \sum_{w \in N_3 \setminus \{z\}} (2td_w(MT_{max}) - d_w(MT_{max}) - t) \\
&= (t-2) \sum_{u \in N_1 \setminus \{x\}} (2d_u(MT_{max}) - 1) \\
&\quad +(r-2) \sum_{w \in N_3 \setminus \{z\}} (2d_w(MT_{max}) - 1) \\
&> 0,
\end{aligned}$$

a contradiction, which completes the proof. □

Consequently, by using Lemmas 2.1-2.4, the following result can be concluded:

Corollary 2.1. *In the tree $MT_{max} \in \mathscr{T}_{n,\alpha}$, where $\alpha > 1$ and $n > 4$.*

(1) If $|B| = 2$, then both elements say v_1 and v_2 of B are adjacent to each other and rest of the attached parts of these elements are the pendent chains of length at most 2 (see

Figure 1).

(2) *If* $| B |= 1$*, then the attached parts of the unique element say v of B are the pendent chains of length at most 2 (see Figure 1).*

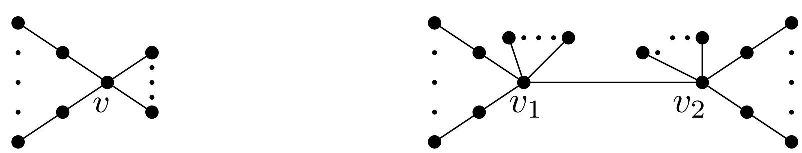

Fig. 1. Maximal graph among the class $\mathscr{T}_{n,\alpha}$

3 Concluding remarks

In this paper, we prove some properties of the extremal tree(s) having maximum modified first Zagreb connection index ZC_1^* among the elements from $\mathscr{T}_{n,\alpha}$. Complete characterization and the investigation of the upper bound is left as an open problem.

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