Research Article

Note on the Reformulated Zagreb Indices of Two Classes of Graphs

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The reformulated Zagreb indices of a graph are obtained from the original Zagreb indices by replacing vertex degrees with edge degrees, where the degree of an edge is taken as the sum of degrees of its two end vertices minus 2. In this paper, we obtain two upper bounds of the first reformulated Zagreb index among all graphs with \( p \) pendant vertices and all graphs having key vertices for which they will become trees after deleting their one key vertex. Moreover, the corresponding extremal graphs which attained these bounds are characterized.

1. Introduction

Some constants are used to characterize some properties of the graph of a molecule, which are usually called topological indices. One of the most famous topological indices is the Randić index (Randić connectivity index), proposed by Randić [1] in 1975 (for details, see [2, 3]). Soon later, a lot of mathematicians focused on the structure and application of Randić connectivity index. In 1977, Kier and Kall [4] extended the concept of molecular connectivity index and defined the zeroth-order general Randić index. Note that the first Zagreb index is the zeroth-order general Randić index for \( \alpha = 2 \). For more results of the zeroth-order general Randić index and first Zagreb index, we refer to [5, 6, 7]. In addition, Zagreb indices have been explored as molecular descriptors in QSPR and QSAR (see [8, 9, 10, 11, 12, 13, 14, 15, 16, 17–20]). For a graph \( G \), the first Zagreb index \( M_1 \) and the second Zagreb index \( M_2 \) [21] are defined as

\[
M_1 = M_1(G) = \sum_{v \in V(G)} d(v)^2,
\]

\[
M_2 = M_2(G) = \sum_{uv \in E} d(u)d(v).
\]

For an edge \( e = uv \), the edge degree of \( e \) is referred as the sum of degrees of its two end vertices minus 2 and is denoted by \( d(e) = d(u) + d(v) - 2 \). \( e \sim f \) indicates the edges \( e \) and \( f \) are adjacent.

For a given \( G \), let \( L(G) \) be its line graph. Observe that two edges are adjacent in \( G \) if and only if the corresponding two vertices are adjacent in \( L(G) \). The edge version of the Zagreb indices [22], motivated by the above property, was proposed by Miličević et al. in 2004 through the edge degree instead of vertex degree, that is,

\[
EM_1(G) = \sum_{e \in E} d(e)^2,
\]

\[
EM_2(G) = \sum_{e \sim f} d(e) \cdot d(f).
\]

The reformulated Zagreb indices, particularly its bounds, have attracted recently the attention of many mathematicians (see, [12, 22–30]).

In order to describe this more clearly in the sequel, we now introduce some notations. Let \( G_p^p \) be the set of connected graphs with \( p (\geq 2) \) pendant vertices. Evidently, if \( G \in G_p^p \), then there will be a connected subgraph \( H_0 \) with order \( n - p \) for which \( G \) can be reconstructed by linking \( p \) vertices to some vertices \( H_0 \). For convenience, we call \( H_1 \) as the core of \( G \). Since \( H_0 \) is connected, it has two extremal cases, i.e., \( H_0 \cong K_{n-p} \) and \( H_0 \cong T_{n-p} \). Let \( A_n \subseteq G_p^p \) be the graph with core \( K_{n-p} \), and let all pendants of \( A_n \) have a common neighbor in \( K_{n-p} \). Let \( B_n \) be the set of all graphs for which each of its element will be changed to a tree by deleting some of its vertex. That is to say, if \( G \) belongs to \( B_n \), then there is a vertex \( v_0 \in V(G) \) such that \( G - v_0 \) is...
isomorphic to a tree. We call the vertex \( v_0 \) as the key of \( G \). Note that, for a given graph, its key may not be unique, e.g., \( G \) is a cycle, and every vertex is a key of \( G \). Let \( B_n \) be the graph with two vertices having degree \( n - 1 \) and other vertices owning degree 2. Obviously, \( B_n \in B_n \) and the two vertices possessing degree \( n - 1 \) are keys.

In this paper, we determined the two upper bounds of reformulated Zagreb indices of two kinds of graphs and characterized completely extremal graphs.

2. Main Results

In the section, we will research the maximal properties regarding the reformulated Zagreb index on \( G_n \) and \( B_n \), respectively. Meanwhile, the graphs attaining the bounds are obtained.

Based on the definition of \( EM_1 \), the following result holds obviously.

**Proposition 1.** Let \( G \) be a connected graph.

\[
EM_1(G') - EM_1(G) = r \sum_{i=1}^{r} (d_{G'}(v_i) + d_{G'}(u_i) - 2)^2 \\
+ \sum_{i=1}^{r} (d_{G'}(v_i) - 1)^2 + (d_{G'}(v_i) + d_{G'}(v_i) - 2)^2 \\
- \sum_{i=1}^{r} (d_{G'}(v_i) + d_{G'}(u_i) - 2)^2 - \sum_{i=1}^{r} (d_{G'}(u_i) + d_{G'}(u_i) - 2)^2 \\
- \sum_{i=1}^{k} (d_{G'}(v_i) - 1)^2 - \sum_{i=1}^{\ell} (d_{G'}(v_i) - 1)^2 - (d_{G'}(v_i) + d_{G'}(v_i) - 2)^2 \\
= r(2r)^2 + r(k + \ell + 2r)^2 + (k + \ell)(k + \ell + r)^2 \\
+ r(\ell + 2r)^2 + r(k + 2r)^2 + k(k + r)^2 + \ell(\ell + r)^2 \\
> 2rk\ell > 0.
\]

The proof hence is complete.

**Theorem 1.** If \( G \in G_n \), then \( EM_1(G) \leq \left( \frac{n - p - 1}{2} \right)^2 (2n - 2p - 4)^2 + (n - p - 1)(2n - p - 4)^2 + p(n - 2)^2 \). Furthermore, the above equality is attained only if \( G \cong A_{n} \).

**Proof.** Let \( G \) be a graph with \( n \) vertices and \( p \) pendants and having the maximum with respect to \( EM_1 \). Let \( H_{0} \) denote the core of \( G \). Clearly, \( H_{0} \) is connected. On the contrary, suppose that \( H_{0} \) is not a complete subgraph of \( G \). That is to say, there are some nonadjacent vertex pairs in \( H_{0} \). After connecting these pairs of \( H_{0} \), we obtain a new graph \( G_{1} \). Evidently, \( G_{1} \in G_n \). From Proposition 1, \( EM_1(G_{1}) > EM_1(G) \), which is contradicted with the maximum of \( G \).

\( (i) \) If \( e \in E(G) \), then \( EM_1(G) > EM_1(G - e) \)

\( (ii) \) If \( e \notin E(G) \), then \( EM_1(G) < EM_1(G + e) \)

**Lemma 1.** \( G \) and \( G' \) denote the two graphs as shown in Figure 1, and \( G' \) is regarded as the graph from \( G \) by shifting all pendants of \( v_s \) to \( v_t \). If \( d_G(v_s) \geq \delta_G(v_s) \) and \( d_G(v_t) \geq n - p \), then \( EM_1(G') > EM_1(G) \).

**Proof.** Let \( G \) and \( G' \) be the two graphs as shown in Figure 1, and \( v_s \) and \( v_t \) be two vertices owning \( \ell \) pendants and \( k \) pendants, respectively. The common neighbors of \( v_s \) and \( v_t \) are labeled as \( u_1, u_2, \ldots, u_{n-p-2} \), and these \( n - p \) vertices induce a complete subgraph \( K_{p+1} \) of \( G \). We write \( r = n - p - 2 \) for short. Obviously, \( d_G(v_s) = k + r + 1 \), \( d_G(v_t) = k + \ell + r + 1 \), and \( d_{G'}(v_t) = r + 1 \). In order to show \( EM_1(G') > EM_1(G) \), we can confirm that \( EM_1(G') - EM_1(G) > 0 \). In fact, we arrive at

\[
EM_1(A_{n}) = \left( \frac{n - p - 1}{2} \right)^2 (2n - 2p - 4)^2 + (n - p - 1)(2n - p - 4)^2 + p(n - 2)^2.
\]

Therefore, we complete the proof.

**Lemma 2.** Let \( G \) be a graph with key \( v_0 \), and let \( T = G - v_0 \) be a tree having an edge \( e = vTv_1 \) with \( d_T(v_1) \geq d_T(v_t) \geq 2 \). If
Figure 1: G and G’ used in Lemma 1.

G’ is obtained by deleting the ℓ branches of v₂ and adding them to v₁, then EM₁(G’) > EM₁(G).

Proof. Let G and G’ are two graphs with n vertices as shown in Figure 2. Suppose that d₁(Tₙ) ≥ d₂(Tₙ) ≥ 2. It is clear that d₁(Tₙ) = ℓ + 1, d₂(Tₙ) = k + 1, d₁(Tₙ) = d₂(Tₙ) + ℓ, and d₁(Tₙ) = 1. We now consider the difference EM₁(G’) − EM₁(G) and deduce that

\[
\begin{align*}
\text{EM}_1(G') - \text{EM}_1(G) &= \sum_{i=1}^{k} (d_{G'}(v_i) + d_{G'}(u_i) - 2)^2 + \sum_{i=1}^{\ell} (d_{G'}(v_i) + d_{G'}(u_i) - 2)^2 \\
&\quad + (d_{G'}(v_i) + d_{G'}(v_0) - 2)^2 + (d_{G'}(v_0) + d_{G'}(v_i) - 2)^2 \\
&\quad + (d_{G'}(v_0) + d_{G'}(v_i) - 2)^2 - (d_{G}(v_i) + d_{G}(v_0) - 2)^2 \\
&\quad - (d_{G}(v_i) + d_{G}(v_0) - 2)^2 - (d_{G}(v_0) + d_{G}(v_i) - 2)^2 \\
&\quad - \sum_{i=1}^{k} (d_{G}(v_i) + d_{G}(u_i) - 2)^2 - \sum_{i=1}^{\ell} (d_{G}(v_i) + d_{G}(u_i) - 2)^2 \\
&\quad > (n - 1)^2 + (k + \ell + n - 1)^2 - (n - 1 + \ell)^2 - (k + n - 1)^2 \\
&\quad = 2k\ell > 0.
\end{align*}
\]

Therefore, the result holds.

Theorem 2. Let G ∈ Bₙ. Then, EM₁(G) ≤ 2n³ - 4n² - 10n + 12 with equality if and only if G ≅ Bₙ.

Proof. Let G be a graph in Bₙ. Hence, there is a vertex v₀ ∈ V(G) such that T = G - v₀ is a tree with n - 1 vertices. Assume that G is the maximal graph with respect to EM₁. We firstly claim that d₁(G(v₀)) = n - 1. Otherwise, if G - v₀ is a tree for v₀ ∈ V(G), we have d₁(G(v₀)) < n - 1. Let the new graph G₁ is obtained from G by connecting v₀ to all of its nonadjacent vertices in G. Hence, by Proposition 1, EM₁(G₁) > EM₁(G), which is contradicted with the choice of G.

We next claim that the tree T is isomorphic to a star with n - 1 vertices. If not, we find an edge e = v₁v₂ in E(T) such that d₁(T(v₁), T(v₂)) ≥ 2. Suppose now that d₁(T(v₁), T(v₂)) ≥ 2. From Lemma 2, we will obtain a new graph G₂ ∈ Bₙ and EM₁(G₂) > EM₁(G), a contradiction. Based on the above discussion, we deduce that G ≅ Bₙ. Furthermore, by direct calculation, EM₁(Bₙ) = 2n³ - 4n² - 10n + 12.

Consequently, the proof is complete.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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References

[1] M. Randic, “Characterization of molecular branching,” Journal of the American Chemical Society, vol. 97, no. 23, pp. 6609–6615, 1975.
[2] I. Gutman, B. Furtula, and C. Elphick, "Three new/old vertex-degree-based topological indices," MATCH Communications
in Mathematical and in Computer Chemistry, vol. 72, pp. 617–632, 2014.

[3] J. Rada and R. Cruz, “Vertex-degree-based topological indices over graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 603–616, 2014.

[4] L. B. Kier and L. H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, NY, USA, 1976.

[5] X. Li and Y. Shi, “A survey on the Randić index,” MATCH Communications in Mathematical and Computer Chemistry, vol. 59, no. 1, pp. 127–156, 2008.

[6] X. Li and Y. Shi, “On a relation between the Randić index and the chromatic number,” Discrete Mathematics, vol. 310, no. 17-18, pp. 2448–2451, 2010.

[7] Y. Shi, “Note on two generalizations of the Randić index,” Applied Mathematics and Computation, vol. 265, pp. 1019–1025, 2015.

[8] H. Abdo, D. Dimitrov, T. Reti, and D. Stevanović, “Estimating the spectral radius of a graph by the second Zagreb index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, no. 3, pp. 741–751, 2014.

[9] D. de Caen, “An upper bound on the sum of squares of degrees in a graph,” Discrete Mathematics, vol. 185, no. 1–3, pp. 245–248, 1998.

[10] I. Gutman, “An exceptional property of first Zagreb index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 733–740, 2014.

[11] A. Hamzeh and T. Reti, “An analogue of Zagreb index inequality obtained from graph irregularity measures,” MATCH Communications in Mathematical and Computer Chemistry, vol. 72, no. 3, pp. 669–683, 2014.

[12] S. Ji and S. Wang, “On the sharp lower bounds of Zagreb indices of graphs with given number of cut vertices,” Journal of Mathematical Analysis and Applications, vol. 458, no. 1, pp. 21–29, 2018.

[13] R. Kazemi, “The second Zagreb index of molecular graphs with tree structure,” MATCH Communications in Mathematical and Computer Chemistry, vol. 72, no. 3, pp. 733–760, 2014.

[14] H. Lin, “Vertices of degree two and the first Zagreb index of trees,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 825–834, 2014.

[15] A. Vasilyev, R. Darda, and D. Stevanović, “Trees of given order and independence number with minimal first Zagreb index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 775–782, 2014.

[16] K. Xu, K. C. Das, and S. Balachandran, “Maximizing the Zagreb indices of (n,m)-graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 641–654, 2014.

[17] C. S. Edwards, “The largest vertex degree sum for a triangle in a graph,” Bulletin of the London Mathematical Society, vol. 9, no. 2, pp. 203–208, 1977.

[18] A. Ilić and D. Stevanović, “On comparing Zagreb indices,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 62, pp. 681–687, 2009.

[19] J. B. Liu, J. Zhao, and Z. X. Zhu, “On the number of spanning trees and normalized Laplacian of linear octagonal-quadrilateral networks,” International Journal of Quantum Chemistry, vol. 119, no. 17, Article ID e25971, 2019.

[20] J.-B. Liu, J. Zhao, and Z.-Q. Cai, “On the generalized adjacency, Laplacian and signless Laplacian spectra of the weighted edge corona networks,” Physica A: Statistical Mechanics and Its Applications, vol. 540, Article ID 123073, 2020.