RELATIONSHIP BETWEEN MODIFIED ZAGREB INDICES AND REFORMULATED MODIFIED ZAGREB INDICES WITH RESPECT TO TREES

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Abstract: The Zagreb indices and the modified Zagreb indices are important topological indices in mathematical chemistry. In this paper we study the relationship between the modified Zagreb indices and the reformulated modified Zagreb indices with respect to trees.

INTRODUCTION

The Zagreb indices are introduced by Gutman and Trinajstić. The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are defined as follows [1—3]: for a simple connected graph G, let $M_1(G) = \sum_{v \in V(G)}(d(v))^2$, $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$, where $d(u)$ and $d(v)$ are the degrees of vertices u and v respectively.

In [4] A. Miličević, S. Nikolić and N. Trinajstić noted that the contributing elements to the Zagreb indices give greater weights to the inner (interior) vertices and edges and smaller weights to the outer (terminal) vertices and edges of a graph. This opposes intuitive reasoning that the outer atoms and bonds should have greater weights than inner vertices and bonds, because the outer vertices and bonds are associated with the larger part of the molecular surface and consequently are expected to make a greater contribution to physical, chemical and biological properties [4]. In [2] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić pointed that chemical intuition should not be disregarded even in theoretical research, as some tend to do, because many crucial discoveries in chemistry, such as the periodic law and the benzene structural formula, were achieved relying on intuitive rules. Reseacher's intuition is a very important guidance in many areas of modern chemistry and especially in drug design [2].

In [4] A. Miličević, S. Nikolić and N. Trinajstić pointed that one way to amend the Zagreb indices is to input in the definitions of the first Zagreb index and the second Zagreb index inverse values of the vetex-degrees. Hence, they are amended by A. Miličević, S. Nikolić and N. Trinajstić as follows [4]: for a simple connected graph G, let ${}^{m}M_1(G) = \sum_{v \in V(G)}(d(v))^{-2}$ which is called *the first modified Zagreb index*, ${}^{m}M_2(G) = \sum_{uv \in E(G)}(d(u)d(v))^{-1}$ which is called *the second modified Zagreb index*.

In [4] A. Miličević, S. Nikolić and N. Trinajstić pointed that there is an analogy between the idea of creating the modified Zagreb indices on the basis of the original Zagreb indices, and the idea of creating the Harary index on the basis of the Wiener index [4].

In [5] D. Vukičević and N. Trinajstić pointed that the discriminatory power of the second modified Zagreb index surpasses that of the Randić connectivity index for certain arbitrarily large classes of benzenoid systems. Their main results are as follows: (1). Let m be any natural number, there is a set of m benzenoid systems with the same number of vertices such that each of them has the same Randić connectivity index and no two of them have the same second modified Zagreb index. (2). Let m be any natural number, there is a set F' of m benzenoid systems such that for each pair of benzenoid systems S_1, $S_2 \in F'$ we have $n(S_1) = n(S_2)$, and $[{}^mM_2(S_1) < {}^mM_2(S_2)]$ if and only if $[\chi(S_1) > \chi(S_2)]$, where $n(S_i)$ is the number of vertices of S_i, i = 1, 2; $\chi(G)$ is the Randić connectivity index, which is defined as follows: $\chi(G) = \sum_{uv\in E(G)}(d(u)d(v))^{-0.5}$. These results shows that the second modified Zagreb index differs fundamentally from the Randić connectivity index [5].

In [4] A. Miličević, S. Nikolić and N. Trinajstić pointed that the Zagreb indices can be reformulated in terms of the edge — degrees: $EM_1(G) = \sum_{e\in E(G)}(d(e))^2$, $EM_2(G) = \sum_{e\wedge f}d(e)d(f)$, where d(e) denotes the degree of edge e in G, and d(e) is equal to the number of adjacent edges of edge e in G, $e\wedge f$ means that edges e and f share a common vertex in G [4].

In [4] the modified Zagreb indices can be reformulated in terms of edge— degrees similarly: ${}^mEM_1(G) = \sum_{e\in E(G)}(d(e))^{-2}$, ${}^mEM_2(G) = \sum_{e\wedge f}(d(e)d(f))^{-1}$. The original and the reformulated Zagreb indices are related as follows:
$EM_1(G) = M_1[L(G)]$, $EM_2(G) = M_2[L(G)]$, ${}^mEM_1(G) = {}^mM_1[L(G)]$, ${}^mEM_2(G) = {}^mM_2[L(G)]$,where L(G) denotes the line graph of G [4]. In [4] A. Miličević, S. Nikolić and N. Trinajstić pointed that these reformulated indices are useful in QSPR study.

Because the concept of line graph has found various applications in chemical research [6], the reformulated Zagreb indices and the reformulated modified Zagreb indices are useful in chemical research.

PRELIMINARIES

Definition 2.1[6]. The line graph, L(G), of a graph G has the vertex set V(L(G)) = E(G), and two distinct vertices of the graph L(G) are adjacent if and only if the corresponding edges of G have a common vertex.

Lemma 2.2[7]. A graph H is the line graph of some graph G if and only if H can be written as the union of complete subgraphs such that no point of H belongs to more than two of these complete subgraphs.

Definition 2.3. Let H = L(G). By Lemma 2.2 H can be written as the union of complete subgraphs $H_1, H_2, \ldots, H_s$. We define H^* as follows: we regard $H_1, H_2, \ldots, H_s$ as vertices of H^*, $H_iH_j \in E(H^*)$ if and only if H_i and H_j share a common vertex of H. That is, $V(H^*) = \{H_1, H_2, \ldots, H_s\}$, $E(H^*) = \{H_iH_j | H_i$ and H_j share a common vertex of H $\}$.

In fact, Lemma 2.4 is clear, Lemma 2.5 is well known.

Lemma 2.4. Let $n \geq 2$, ${}^mM_2(K_{1,n-1}) = 1$, ${}^mM_1(K_{1,n-1}) = n - 1 + (n-1)^{-2}$,

$^{m}M_2(K_n) = \frac{n}{2(n-1)}$, $^{m}M_1(K_n) = \frac{n}{(n-1)^2}$.

Lemma 2.5. If $f''(x) \geq 0$, we have $f(\frac{x_1+\ldots x_n}{n}) \leq \frac{f(x_1)+\ldots f(x_n)}{n}$. If $f''(x) > 0$, $f(\frac{x_1+\ldots x_n}{n}) = \frac{f(x_1)+\ldots f(x_n)}{n}$ if and only if $x_1 = \ldots = x_n$. $^{m}M_1(K_{1,n-1}) = n - 1 + (n-1)^{-2}$

MAIN RESULTS

Theorem 3.1. *Let G be a tree, $n = |V(G)| \geq 4$, we have $^{m}M_2(G) > {}^{m}EM_2(G)$.*

Proof. Claim 1: Let $H = L(G)$. If H_1 and H_2 belong to the union of complete subgraphs of H, then, H_1 and H_2 do not share a common edge.

Otherwise, let $V(H_1) = \{e_1, e_2, \ldots, e_k\}$, $V(H_2) = \{e_1, e_2, e_3', \ldots, e_t'\}$, $\{e_3, \ldots, e_k\} \neq \{e_3', \ldots, e_t'\}$, $e_1e_2 \in E(H_1) \cap E(H_2)$, $k \geq 3$, $t \geq 3$. Because H_1 is a complete subgraph of H, in G edges $e_1, e_2, \ldots, e_k$ share a common vertex $u \in V(G)$. Similarly, in G edges $e_1, e_2, e_3', \ldots, e_t'$ share $u \in V(G)$. Hence, in G edges $e_1, e_2, \ldots, e_k, e_3', \ldots, e_t'$ share a common vertex $u \in V(G)$. Thus, vertices $e_1, e_2, \ldots, e_k, e_3', \ldots, e_t'$ of H constitute a complete subgraph other than two different complete subgraphs, which is a contradiction.

Claim 2: Let $H = L(G)$. If G is a tree, $|V(G)| \geq 4$, H^* is a tree, where H^* is defined in Definition 2.3.

Otherwise, without loss of generality, let H^* contain a cycle $H_1H_2\ldots H_tH_1$, H_i and H_{i+1} share a common vertex e_i, $i = 1, 2, \ldots, t$. Thus, in G, e_i is a common edge of K_{1,n_i} and $K_{1,n_{i+1}}$, where $n_i = |V(H_i)|$, $i = 1, 2, \ldots, t$. Hence, G contains a cycle, which is a contradiction. Since G is connected, L(G) is connected. Thus, H^* is connected. Claim 2 follows.

When $G = P_n$, the theorem follows clearly. In the following let $G \neq P_n$.

Claim 3: Let T_1 and T_2 be two trees, $|V(T_1)| \geq 2$, $|V(T_2)| \geq 2$, we obtain a new tree T from T_1 and T_2 by coinciding one vertex u_1 of T_1 with one vertex u_2 of T_2, let the coinciding vertex be u of T. Similarly, we obtain a new tree T^* from T_1 and T_2 as follows: connecting u_1 and u_2 with one edge. We have $^{m}M_2(T^*) > {}^{m}M_2(T)$.

In fact, we have $d_{T^*}(u_1) = d_{T_1}(u_1) + 1$, $d_{T^*}(u_2) = d_{T_2}(u_2) + 1$, $d_T(u) = d_{T_1}(u_1) + d_{T_2}(u_2)$. For $v \in V(T_1)$ and $v \neq u_1$, we have $d_{T_1}(v) = d_T(v) = d_{T^*}(v)$. Similarly, for $v \in V(T_2)$ and $v \neq u_2$, we have $d_{T_2}(v) = d_T(v) = d_{T^*}(v)$. Hence, we have $d_{T^*}(u_1) = d_T(u)$, $d_{T^*}(u_2) = d_T(u)$.

Thus, we have

$$ {}^{m}M_2(T)=\sum_{uv\in E(T'),v\in N_{T_1}(u)\cup N_{T_2}(u)}(d_T(u)d_T(v))^{-1}+\sum_{xy\in E(T'),x\neq u,y\neq u}(d_{T'}(x)d_{T'}(y))^{-1} $$

$$ <\sum_{u_1v\in E(T_1),v\in N_{T_1}(u_1)}(d_{T^*}(u_1)d_{T^*}(v))^{-1}+\sum_{u_2v\in E(T_2),v\in N_{T_2}(u_2)}(d_{T^*}(u_2)d_{T^*}(v))^{-1} $$

$$ +\sum_{xy\in E(T),x\neq u,y\neq u}(d_{T^*}(x)d_{T^*}(y))^{-1}+(d_{T^*}(u_1)d_{T^*}(u_2))^{-1}={}^{m}M_2(T^*). $$

Claim 3 follows.

By Lemma 2.2, let the union of complete subgraphs of L(G) be $H_1, H_2, \ldots, H_s$. By Claim 1 we have $|V(H_i)\cap V(H_j)|\leq 1$, where $i \neq j$. In the following let $n_i = |V(H_i)|$, $i = 1, 2, \ldots, s$. Clearly, we have $n_i\geq 2$.

Program 4: By Definition 2.3 and Claim 2, when G is a tree we obtain a new tree T from L(G) as follows: Step 1: when s = 1, let $T = K_{1,n_1-1}$. Step 2: when s = 2, let $T = K_{1,n_1+n_2-2}$, where $n_i = |V(H_i)|$, i = 1, 2. Step 3: when $s\geq 3$, without loss of generality, let $d_{H^*}(H_s) = 1$, and let H_{s-1} and H_s share a common vertex v_s in H. Define $H^{-1} = H-(V(H_s) -v_s)$. Let T^{-1} be a tree of H^{-1} constructed as Step 1, Step 2 and Step 3 (for $s-1$) recurrently. Let $W = K_{1,n_{s-1}-1}$. We adhere K_{1,n_s-1} to W with the centre of K_{1,n_s-1} at $v_s\in V(W)$, where $n_s = |V(H_s)|$, v_s is a pendant vertex of W. Denote the new tree T.

In the following let a, t and k be natural numbers, $a\geq t\geq 2$, $k\geq 2$. In fact, we can prove Claims 5, 6, 7 by mathematical induction for t, t, a respectively easily.

Claim 5: Let $h(t) = k^3-6k^2 + 8k-4 + 2k^2t-4kt + 4t$, we have $h(t) > 0$.

Claim 6: Let $g(t) = k^3t-k^3 + k^2t^2-7k^2t + 6k^2-2kt^2 + 10kt-8k + 2t^2-6t + 4$, we have $g(t) \geq 0$.

Claim 7: Let $f(a) = ak^3t-ak^3 + ak^2t^2-7ak^2t + 6ak^2-2akt^2 + 10akt-8ak + 2at^2 -6at + 4a-2k^3t + 4k^3-2k^2t^2 + 10k^2t-12k^2 + 4kt^2-14kt + 12k-2t^2 + 6t-4$, we have $f(a) \geq 0$.

Claim 8: $-a^{-1} + (ka)^{-1} + (k-1)k^{-1} \geqslant -[a(t-1)]^{-1} + [a(t + k-2)]^{-1} + (t + k-2)^{-1} + 0.5(k-2)(k-1)^{-1}$.

In fact, by Claim 7 we have $(-2k^2 + 4k-2 + k^2a-2ka + 2a)(t-1)(t + k-2)\geq (at-k-a + 1)(2k^2-2k)$.

Thus, we have $\dfrac{-2k^2 + 4k-2 + k^2a-2ka + 2a}{2k(k-1)a} \geq \dfrac{at-k-a+1}{(t-1)(t+k-2)a}$.

Hence, $\dfrac{1-k}{ka} + 0.5 + \dfrac{2-k}{2k(k-1)} \geq -\dfrac{1}{(t-1)a} + \dfrac{a+1}{(t+k-2)a}$. Thus, $-a^{-1} + (ka)^{-1} + 0.5 + 0.5(k-1)^{-1} -k^{-1} \geqslant -[a(t-1)]^{-1} + [a(t + k-2)]^{-1} + (t + k-2)^{-1}$. Hence, $-a^{-1} + (ka)^{-1} + 1 -k^{-1} \geqslant -[a(t-1)]^{-1} + [a(t + k-2)]^{-1} + (t + k-2)^{-1} + 0.5-0.5(k-1)^{-1}$. Claim 8 follows.

Claim 9: ${}^{m}M_2(L(G))\leq {}^{m}M_2(T)$, where $|V(L(G))|\geq 3$, T is obtained by Program 4.

Let H = L(G), where H is the union of complete subgraphs $H_1, H_2, \ldots, H_s$. We prove Claim 9 by mathematical induction for s.

When s = 1, by Lemma 2.4 Claim 9 follows. When s = 2, let $|V(H_1)| = r$, $|V(H_2)| = t$, we have ${}^{m}M_2(L(G)) = \frac{r-1}{(r+t-2)(r-1)} + \frac{t-1}{(r+t-2)(t-1)} + \frac{(r-1)(r-2)}{2(r-1)^2} + \frac{(t-1)(t-2)}{2(t-1)^2} = \frac{r+t}{r+t-2} - \frac{1}{2(r-1)} - \frac{1}{2(t-1)}$. By Lemma 2.4, we have ${}^{m}M_2(T) = 1$. Let $f(x) = x^{-1}$, where $x > 0$. Thus, $f''(x) = 2x^{-3} > 0$. By Lemma 2.5 we have $2(r+t-2)^{-1} \leqslant 0.5(r-1)^{-1} + 0.5(t-1)^{-1}$. Thus, when s = 2 Claim 9 follows. When s≥3, suppose Claim 9 holds for s−1. In Program 4, let $|V(H_s)| = k$, $|V(H_{s-1})| = t$, $a_1, a_2, \dots, a_{t-1}$ are the degrees of vertices of $V(H_{s-1}) - v_s$ with respect to H^{-1}. Thus, we have ${}^{m}M_2(H) = {}^{m}M_2(H^{-1}) - \frac{1}{(t-1)a_1} - \dots - \frac{1}{(t-1)a_{t-1}} + \frac{1}{(t+k-2)a_1} + \dots + \frac{1}{(t+k-2)a_{t-1}} + \frac{k-1}{(t+k-2)(k-1)} + \frac{(k-1)(k-2)}{2(k-1)^2}$, ${}^{m}M_2(T) = {}^{m}M_2(T^{-1}) - \frac{1}{a_1} + \frac{1}{ka_1} + \frac{k-1}{k}$.

Let $a_1 = a$, by Claim 8 we have $-\frac{1}{a_1} + \frac{1}{ka_1} + \frac{k-1}{k} \geq -\frac{1}{(t-1)a_1} - \dots - \frac{1}{(t-1)a_{t-1}} + \frac{1}{(t+k-2)a_1} + \dots + \frac{1}{(t+k-2)a_{t-1}} + \frac{1}{t+k-2} + \frac{k-2}{2(k-1)}$. Since ${}^{m}M_2(H^{-1}) \leq {}^{m}M_2(T^{-1})$, Claim 9 follows.

Program 10: When s≥2, we change Step 2 of Program 4 as follows: when s = 2, we use one edge connects the centers of K_{1,n_1-1} and K_{1,n_2-1}, we denote the new tree G^*. The remaining steps are the same as those in Program 4 except that we change T to G^*.

By Claim 3 the following claim is obvious.

Claim 11: ${}^{m}M_2(G^*) > {}^{m}M_2(T)$, where T is constructed by Program 4, G^* is constructed by Program 10.

By Claim 9 and Claim 11 we have

Claim 12: ${}^{m}M_2(G^*) > {}^{m}M_2(L(G))$, where $|V(L(G))| \geq 3$.

Let G be a tree, $n = |V(G)| \geq 4$, from G we obtain L(G) which is the union of complete subgraphs $H_1, H_2, \dots, H_s$. By Program 10 we obtain G^*. By Definition 2.1 $L(G^*)$ is isomorphism to L(G).

Claim 13: Let G and G^* be trees, if L(G) is isomorphism to $L(G^*)$, G is isomorphism to G^*.

In fact, since $L(G^*)$ is isomorphism to $L(G)$, without loss of generality, let them be the union of complete subgraphs $H_1, H_2, \ldots, H_s$. By Claim 2, when $s \geq 2$, without loss of generality, let $d_{H^*}(H_s) = 1$, H_{s-1} and H_s share a common vertex v_s. Let $n_i = |V(H_i)|$, $i = 1, 2, \ldots, s$. We prove Claim 13 by mathematical induction with respect to s.

(1). When $s = 1$, since $L(G)$ is isomorphism to $L(G^*)$, we have $|V(L(G))| = |V(L(G^*))|$. Thus, we have $|E(G)| = |E(G^*)|$. Since $|E(G)| = |V(G)| - 1$, $|E(G^*)| = |V(G^*)| - 1$, we have $|V(G)| = |V(G^*)| = n$. Thus, G is isomorphism to $K_{1,n}$, G^* is isomorphism to $K_{1,n}$. Otherwise, H_1 is not a complete graph with n vertices, which is a contradiction. Hence, G is isomorphism to G^*.

Suppose Claim 13 holds for $s = k$. In the following, let $s = k + 1$. Since H_{s-1} and H_s share a common vertex v_s uniquely, K_{1,n_k} and $K_{1,n_{k+1}}$ must share a common edge uniquely. Let $L(G_1) = L(G) - (V(H_s) - v_s)$, $L(G_2) = L(G^*) - (V(H_s) - v_s)$. By hypothesis G_1 is isomorphism to G_2. Thus, G is isomorphism to G^*. Claim 13 follows. Theorem 3.1 follows.

Theorem 3.2. *Let G be a tree, $n = |V(G)| \geq 3$, we have ${}^mM_1(G) > {}^mEM_1(G)$.*

Proof. When $G = K_{1,n-1}$, by Lemma 2.4 the theorem follows. When $G \neq K_{1,n-1}$, by the definition of the first modified Zagreb index we have ${}^mM_1(L(G)) \leq {}^mM_1(T) < {}^mM_1(G^*) = {}^mM_1(G)$, where T is constructed by Program 4 contained in the proof of Theorem 3.1, G^* is constructed by Program 10 contained in the proof of Theorem 3.1. Theorem 3.2 follows.

Remark: There exist some graphs such that ${}^mM_2(G) < {}^mEM_2(G)$, such as $G = K_4$.

Acknowledgements: The project supported by National Nature Science Foundation of China (No. 11271334, No. 11271335).

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