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Relations between Zagreb Coindices and Some Distance–Based Topological Indices*

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Abstract

For a nontrivial graph G, its first Zagreb coindex is defined as the sum of degree sum over all non-adjacent vertex pairs in G and the second Zagreb coindex is defined as the sum of degree product over all non-adjacent vertex pairs in G. Till now, established results concerning Zagreb coindices are mainly related to composite graphs and extremal values of some special graphs. The existing literatures witnessed no results dealing with the relations between Zagreb coindices and distance-based topological indices so far. Aiming at filling in this gap, we reveal the relations between the first Zagreb coindex and some distance-based topological indices here. We establish sharp bounds on the first Zagreb coindex in terms of distance-based topological indices including Wiener index, eccentric connectivity index, eccentric distance sum, degree distance and reverse degree distance.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $V(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G and let $d_G(u, v)$ denote the distance between vertices u and v in G. Let $ec_G(u) = \max\{d_G(u, v) | v \in V(G)\}$ denote the eccentricity of G.

A graph invariant is a function defined on a graph which is independent of the labeling of its vertices. Till now, hundreds of different graphs invariants have been employed in QSAR/QSPR studies, some of which have been proved to be successful (see [22]). Among those successful invariants, there are two invariants called the *first Zagreb index* and the

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second Zagreb index (see [5,8,11,12,19,21,25–27]), defined as

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v),$$

respectively.

In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)). \tag{1}$$

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [7]), Ashrafi et al. [1,2] defined the *first Zagreb coindex* and *second Zagreb coindex* as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v)) \text{ and } \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v),$$

respectively.

It is well known that many graphs arise from simpler graphs via various graph operations. Hence, it is important to understand how certain invariants of such composite graphs are related to the corresponding invariants of the original graphs. Ashrafi et al. [1] explored basic mathematical properties of Zagreb coindices and in particular presented explicit formulae for these new graph invariants under several graph operations, such as, union, join, Cartesian product, disjunction product, and so on. Ashrafi et al. [2] determined the extremal values of Zagreb coindices over some special classes of graphs. However, among established results in the existing literature, we can hardly find a result dealing with the relations between Zagreb coindices and distance-based topological indices.

In this paper, we reveal the relations between the first Zagreb coindex and some distance-based topological indices. This paper is organized as follows. In Section 2, we give two general bounds on the first Zagreb coindex. In Section 3, we establish sharp bounds on the first Zagreb coindex in terms of distance-based topological indices including Wiener index, eccentric connectivity index, eccentric distance sum and degree distance. In Section 4, we establish sharp lower and upper bounds on the second Zagreb coindex in terms of modified degree distance.

2 General bounds on $\overline{M}_1$ index

In this section, we give two general bounds on the first Zagreb coindex in terms of order, size, maximum degree and minimum degree.

It is not difficult to see that the contribution of each vertex u in G to $\overline{M}_1(G)$ is exactly $(n - d_G(u) - 1)d_G(u)$. Thus, we can rewrite the first Zagreb coindex as

$$\overline{M}_1(G) = \sum_{u \in V(G)} (n - d_G(u) - 1)d_G(u). \tag{2}$$

Theorem 2.1 *Let G be a connected graph of order n. Then*

$$0 \leq \overline{M}_1(G) \leq \frac{n(n-1)^2}{4}$$

where the left-hand side equality holds if and only if $G \cong K_n$, and the right-hand side one holds if and only if n is odd and G is a $\frac{n-1}{2}$-regular graph.

Proof. Obviously, each vertex in K_n contributes 0 to $\overline{M}_1$ index. So $\overline{M}_1(K_n) = 0$. Any connected graph G not isomorphic to K_n has at least one non-adjacent vertex pair. Then $\overline{M}_1(G) > 0$.

Now, let us treat the right-hand side inequality. In view of the equation (2), we have $\overline{M}_1(G) \leq n \cdot \left(\frac{n-1}{2}\right)^2 = \frac{n(n-1)^2}{4}$ with equality if and only if for each vertex u, $d_G(u) = \frac{n-1}{2}$, i.e., n is odd and G is a $\frac{n-1}{2}$-regular graph. ∎

A graph G is said to be (a, b)-*biregular* if its vertex degrees assume exactly two different values: a and b.

Theorem 2.2 *Let G be a connected graph of order n, size m, maximum degree $\triangle(G)$ and minimum degree $\delta(G)$. Then*

$$(n^2 - n - 2m)\delta(G) \leq \overline{M}_1(G) \leq (n^2 - n - 2m)\triangle(G)$$

where the left-hand side equality holds if and only if G is a $\frac{2m}{n}$-regular graph or a $(n-1, \delta(G))$-biregular graph with $\frac{2m-n\delta(G)}{n-1-\delta(G)}$ vertices having degree $n-1$ and $\frac{n^2-n-2m}{n-1-\delta(G)}$ vertices having degree $\delta(G)$, and the right-hand side equality holds if and only if G is a $\frac{2m}{n}$-regular graph or a $(n-1, \triangle(G))$-biregular graph with $\frac{2m-n\triangle(G)}{n-1-\triangle(G)}$ vertices having degree $n-1$ and $\frac{n^2-n-2m}{n-1-\triangle(G)}$ vertices having degree $\triangle(G)$.

Proof. If $G \cong K_n$, then $\overline{M}_1(G) = 0$ and the result follows readily. Suppose that $G \ncong K_n$ and that there are $t\,(0 \leq t \leq n-2)$ vertices of degree $n-1$. It is obvious that the number of vertex pairs $\{u, v\}$ in G at distance greater than or equal to 2 is exactly $\binom{n}{2} - m = \frac{n(n-1)}{2} - m$. Thus

$$2\delta(G)\left[\frac{n(n-1)}{2} - m\right] \leq \overline{M}_1(G) \leq 2\triangle(G)\left[\frac{n(n-1)}{2} - m\right],$$

that is,

$$(n^2 - n - 2m)\delta(G) \leq \overline{M}_1(G) \leq (n^2 - n - 2m)\triangle(G).$$

The above left (resp., right) equality holds if and only if for each vertex x in G, if $d_G(x) \neq n-1$, then $d_G(x) = \delta(G)$ (resp., $\triangle(G)$). Then $t(n-1)+(n-t)\delta(G) = 2m$ (resp., $t(n-1)+(n-t)\delta(G) = 2m$). So we have $t = \frac{2m-n\delta(G)}{n-1-\delta(G)}$ (resp., $t = \frac{2m-n\triangle(G)}{n-1-\triangle(G)}$).

If $t = 0$, then each of above two equalities holds if and only if G is a $\frac{2m}{n}$-regular graph. Otherwise, we have the left-hand side equality holds if and only if G is a $(n-1, \delta(G))$-biregular graph with $\frac{2m-n\delta(G)}{n-1-\delta(G)}$ vertices having degree $n-1$ and $\frac{n^2-n-2m}{n-1-\delta(G)}$ vertices having degree $\delta(G)$, and the right-hand side equality holds if and only if G is a $(n-1, \triangle(G))$-biregular graph with $\frac{2m-n\triangle(G)}{n-1-\triangle(G)}$ vertices having degree $n-1$ and $\frac{n^2-n-2m}{n-1-\triangle(G)}$ vertices having degree $\triangle(G)$. This proves theorem. ∎

3 Sharp bounds on $\overline{M}_1$ index involving distance-based topological indices

In this section, we present sharp bounds on the first Zagreb coindex in terms of some distance-based topological indices including Wiener index, eccentric connectivity index, eccentric distance sum, and degree distance.

The *eccentric connectivity index* (see [3, 16, 17]) of a connected graph G, denoted by $\xi^c(G)$, is defined as

$$\xi^c(G) = \sum_{u \in V(G)} ec_G(u) d_G(u). \tag{3}$$

As introduced in [4], we call $\xi(G) = \sum\limits_{u \in V(G)} ec_G(u)$ the *total eccentricity* of a connected graph G.

Theorem 3.1 *Let G be a connected graph of order n and size m. Then*

$$\xi^c(G) - 2m \leq \overline{M}_1(G) \leq (n-1)n^2 - 2mn - (n-1)\xi(G) + \xi^c(G)$$

with either equality if and only if $G \cong P_4$ or $K_n - iK_2$ $(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$.

Proof. First, let us prove the left-hand side inequality. For each vertex v, we clearly have $ec_G(v) \leq n - d_G(v)$. According to the equations (2) and (3), we have

$$\begin{aligned}\overline{M}_1(G) &\geq \sum_{v \in V(G)} (ec_G(v) - 1) d_G(v) \\ &= \xi^c(G) - 2m.\end{aligned}$$

Suppose now that $\overline{M}_1(G) = \xi^c(G) - 2m$. Then we must have $ec_G(v) = n - d_G(v)$ for each vertex v in $V(G)$. We first prove the following claim.

Claim 1 *Suppose that $ec_G(v) = n - d_G(v)$ for each vertex v in $V(G)$. If $G \ncong P_4$, then $ec_G(v) \leq 2$ for each v.*

Proof. Suppose to the contrary that $ec_G(v) \geq 3$ for some v. Let $ec_G(v) = d_G(v, u)$ for some vertex u. Then $d_G(v, u) \geq 3$. Set $N_G(v) = \{v_1, \ldots, v_{d_G(v)}\}$ and assume that the vertex $v_{d_G(v)}$ lies within the $u - v$ path. Clearly, $uv_i \notin E(G)$ $(i = 1, \ldots, v_{d_G(v)})$, for otherwise, $d_G(v, u) = 2$, a contradiction. Thus, $d_G(u) = 1$. Note that $ec_G(u) \leq 1 + ec_G(v)$ with equality only if each v_i is not adjacent to any vertex in the set $V(G) \setminus \{v_1, \ldots, v_{d_G(v)-1}, u, v\}$. So we have $d_G(u) + ec_G(u) = 1 + ec_G(u) \leq 2 + ec_G(v) = 2 + [n - d_G(v)]$. Note that $ec_G(u) + d_G(u) = n$, thus, we have $d_G(v) \leq 2$ with equality only if $d_G(v_1) = 1$. By above analysis, G is just the path P_n when $d_G(v) = 1$ or 2.

By our assumption that $G \ncong P_4$ and $ec_G(v) \geq 3$, we must have G is a path P_n of order at least 5. However, for such a path P_n, the equality $ec_G(v) = n - d_G(v)$ cannot hold for each vertex v in P_n, a contradiction. This proves the claim. ∎

By Claim 1, if $G \ncong P_4$, then $ec_G(v) = 1$ or 2 for each v in G. Since $ec_G(v) + d_G(v) = n$ for each vertex v, we must have $d_G(v) = n - 1$ or $n - 2$ for each v in G, that is, $G \cong K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$. So we have $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$.

Conversely, if $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$, then we clearly have $ec_G(v) = n - d_G(v)$ for each vertex v in $V(G)$. Thus, $\overline{M}_1(G) = \xi^c(G) - 2m$, as desired.

Now, we turn to the right-hand side inequality.

Again, by the equation (2), we have

$$\begin{aligned}\overline{M}_1(G) &\leq \sum_{v \in V(G)} (n - d_G(v) - 1)(n - ec_G(v)) \\ &= (n-1)n^2 - 2mn - (n-1)\xi(G) + \xi^c(G).\end{aligned}$$

The equality holds if and only if for any vertex v, $d_G(v) = n - ec_G(v)$. By previous analysis, we must have $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$. This completes the proof. ∎

For a connected graph G, we let $W(G) = \sum\limits_{\{u,v\} \subseteq V(G)} d_G(u, v)$ denote the *Wiener index* (see [6] for a survey).

Theorem 3.2 *Let G be a connected graph of order n and size m. Then*

$$\overline{M}_1(G) \geq 2W(G) - 2M_1(G) + 6m(n-1) - n^3 + n^2$$

with equality if and only if $G \cong K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$.

Proof. Let $D_G(x) = \sum\limits_{y \in V(G)} d_G(x, y)$. Then $W(G) = \frac{1}{2} \sum\limits_{x \in V(G)} D_G(x)$. We have

$$\begin{aligned}D_G(x) &= \sum_{y \in V(G)} d_G(x, y) \\ &= d_G(x) + \sum_{y \in V(G) \setminus N_G[v]} d_G(x, y)\end{aligned}$$

$$\begin{aligned}
&\le d_G(x) + \sum_{y\in V(G)\setminus N_G[v]} ec_G(x)\\
&= d_G(x) + (n - d_G(x) - 1)ec_G(x)\\
&\le d_G(x) + (n - d_G(x) - 1)(n - d_G(x))\\
&= (d_G(x))^2 - 2(n-1)d_G(x) + n^2 - n.
\end{aligned}$$

Note that $\overline{M}_1(G) = \sum_{x\in V(G)} [(n-1)d_G(x) - (d_G(x))^2]$. Thus,

$$\begin{aligned}
W(G) &= \frac{1}{2}\sum_{x\in V(G)} D_G(x)\\
&\le \frac{1}{2}\sum_{x\in V(G)} [(d_G(x))^2 - 2(n-1)d_G(x) + n^2 - n]\\
&= \frac{1}{2}\overline{M}_1(G) + \frac{1}{2}\sum_{x\in V(G)} [2(d_G(x))^2 - 3(n-1)d_G(x) + n^2 - n]\\
&= \frac{1}{2}\overline{M}_1(G) + M_1(G) - 3m(n-1) + \frac{n^3 - n^2}{2}.
\end{aligned}$$

Suppose now that $W(G) = \frac{1}{2}\overline{M}_1(G) + M_1(G) - 3m(n-1) + \frac{n^3-n^2}{2}$. Then we must guarantee that for each x in $V(G)$ and any $y \in V(G) \setminus N_G[v]$, $d_G(x, y) = ec_G(x)$, that is, $ec_G(x) \le 2$. Also, we must guarantee that for each $x \in V(G)$, $d_G(x) + ec_G(x) = n$. By the previous analysis in Theorem 3.1, we must have $G \cong P_4$ or $K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$.

Since P_4 has diameter 3, we must have $G \cong K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$.

Conversely, if $G \cong K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$, then $W(G) = \frac{1}{2}\overline{M}_1(G) + M_1(G) - 3m(n-1) + \frac{n^3-n^2}{2}$, that is, $\overline{M}_1(G) = 2W(G) - 2M_1(G) + 6m(n-1) - n^3 + n^2$.

This completes the proof. ∎

The *degree distance or schultz index* of a connected graph G is defined [10] as

$$D'(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))d_G(u, v). \tag{4}$$

For recent results on degree distance, see [14, 15, 23, 24].

Note that K_n has diameter one and $\overline{M}_1(K_n) = 0$. So, we will always assume that the underlying graphs have diameter greater than or equal to two in the subsequent part of this paper.

Theorem 3.3 *Let G be a nontrivial connected graph of diameter $d \ge 2$. Then*

$$\frac{D'(G) - M_1(G)}{d} \le \overline{M}_1(G) \le \frac{D'(G) - M_1(G)}{2}$$

with either equality if and only if $d = 2$.

Proof. By means of the equations (1) and (4),

$$\begin{aligned} D^{'}(G) &= \sum_{uv\in E(G)} (d_G(u)+d_G(v))d_G(u,\,v) + \sum_{uv\notin E(G)} (d_G(u)+d_G(v))d_G(u,\,v) \\ &= M_1(G) + \sum_{uv\notin E(G)} (d_G(u)+d_G(v))d_G(u,\,v) \\ &\geq M_1(G) + 2\sum_{uv\notin E(G)} (d_G(u)+d_G(v)) \\ &= M_1(G) + 2\overline{M}_1(G). \end{aligned}$$

Therefore, $\overline{M}_1(G) \leq \frac{D^{'}(G)-M_1(G)}{2}$ with equality if and only if for any non-adjacent vertex pairs $\{u,\,v\}$, $d_G(u,\,v)=2$, that is, $d=2$.

Similarly, we have

$$\begin{aligned} D^{'}(G) &= \sum_{uv\in E(G)} (d_G(u)+d_G(v))d_G(u,\,v) + \sum_{uv\notin E(G)} (d_G(u)+d_G(v))d_G(u,\,v) \\ &= M_1(G) + \sum_{uv\notin E(G)} (d_G(u)+d_G(v))d_G(u,\,v) \\ &\leq M_1(G) + d\sum_{uv\notin E(G)} (d_G(u)+d_G(v)) \\ &= M_1(G) + d\overline{M}_1(G). \end{aligned}$$

Therefore, $\overline{M}_1(G) \geq \frac{D^{'}(G)-M_1(G)}{d}$ with equality if and only if for any non-adjacent vertex pairs $\{u,\,v\}$, $d_G(u,\,v)=d$, that is, $d=2$. This completes the proof. ∎

The *reverse degree distance* of a connected graph G of order n, size m and diameter d is defined [28] as ${}^{r}D^{'}(G) = 2(n-1)md - D^{'}(G)$.

By means of Theorem 3.3, we immediately get the following consequence.

Corollary 3.1 *Let G be a nontrivial connected graph of order n, size m and diameter $d \geq 2$. Then*

$$\frac{2(n-1)md - {}^{r}D^{'}(G) - M_1(G)}{d} \leq \overline{M}_1(G) \leq \frac{2(n-1)md - {}^{r}D^{'}(G) - M_1(G)}{2}$$

with either equality if and only if $d=2$.

Let $\xi^d(G) = \sum_{u\in V(G)} ec_G(u)D_G(u)$ denote the *eccentric distance sum* (see [13,18]), where $D_G(u)$ is the sum of distances between u and all other vertices in G.

Lemma 3.1 *([18]) Let G be a nontrivial connected graph on $n \geq 3$ vertices. Then*

$$\xi^d(G) \leq 2nW(G) - D^{'}(G)$$

with equality if and only if $G \cong P_4$ or $K_n - ie$, where $i = 0,\,1,\,\ldots,\,\lfloor \frac{n}{2} \rfloor$.

Corollary 3.2 *Let G be a nontrivial connected graph. Then*

$$\overline{M}_1(G) \leq \frac{2nW(G) - \xi^d(G) - M_1(G)}{2}$$

with equality if and only if $G \cong K_n - ie$, where $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$.

Proof. Note that K_n has diameter 1, P_n has diameter 3 and $K_n - ie$, $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$, has diameter 2.

According to Theorem 3.3 and Lemma 3.1, we have

$$\overline{M}_1(G) \leq \frac{2nW(G) - \xi^d(G) - M_1(G)}{2}$$

with equality if and only if $G \cong K_n - ie$, where $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. ∎

4 Concluding remarks

In this paper, we have established sharp bounds for the first Zagreb coindex in terms of distance-based topological indices including Wiener index, eccentric connectivity index, eccentric distance sum, degree distance and reverse degree distance. It seems to be natural to consider the relations between the second Zagreb coindex and these distance-based topological indices. As expected, the properties of second Zagreb coindex are less elegant than those of first Zagreb coindex. We present here a result revealing the relation between second Zagreb coindex and the modified schultz index.

The *modified degree distance* or *modified schultz index* of a connected graph G is defined [20] as

$$S^*(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u) d_G(v) d_G(u, v). \tag{5}$$

Theorem 4.1 *Let G be a nontrivial connected graph of diameter $d \geq 2$. Then*

$$\frac{S^*(G) - M_2(G)}{d} \leq \overline{M}_2(G) \leq \frac{S^*(G) - M_2(G)}{2}$$

with either equality if and only if $d = 2$.

Proof. According to the equation (5),

$$\begin{aligned} S^*(G) &= \sum_{uv \in E(G)} d_G(u) d_G(v) d_G(u, v) + \sum_{uv \notin E(G)} d_G(u) d_G(v) d_G(u, v) \\ &= M_2(G) + \sum_{uv \notin E(G)} d_G(u) d_G(v) d_G(u, v) \\ &\geq M_2(G) + 2 \sum_{uv \notin E(G)} d_G(u) d_G(v) \end{aligned}$$

$$= \quad M_2(G) + 2\overline{M}_2(G).$$

Therefore, $\overline{M}_2(G) \leq \frac{S^*(G) - M_2(G)}{2}$ with equality if and only if $d = 2$. Similarly, we have

$$\begin{aligned}
S^*(G) &= \sum_{uv \in E(G)} d_G(u) d_G(v) d_G(u, v) + \sum_{uv \notin E(G)} d_G(u) d_G(v) d_G(u, v) \\
&= M_2(G) + \sum_{uv \notin E(G)} d_G(u) d_G(v) d_G(u, v) \\
&\leq M_2(G) + d \sum_{uv \notin E(G)} d_G(u) d_G(v) \\
&= M_2(G) + d\overline{M}_2(G).
\end{aligned}$$

Therefore, $\overline{M}_2(G) \geq \frac{S^*(G) - M_2(G)}{d}$ with equality if and only if $d = 2$. ■

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