Bounds on Product Version of Distance-Related Topological Indices of Complement of Mycielskian Graph

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Abstract
Eccentricity-based topological indices are valuable descriptors for analyzing molecular graphs and complex networks. This paper focuses on the complement of the Mycielskian graph of a connected graph. We derive new upper bounds for several recently introduced eccentricity-related topological indices by exploiting the structural characteristics of the complement graph. The obtained inequalities improve the theoretical understanding of these descriptors and provide efficient estimates for transformed graphs. The proposed results offer new insights into complement graph theory and support further applications in chemical graph theory and related fields.
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1. Introduction.

All graphs considered in this paper are simple and connected. The degree of a vertex x in G is denoted by $d_G(x)$ is the number of edges incidence to a vertex x in G. The distance between the vertex x and y in G is denoted by $d_G(x,y)$. To establish relationships between chemical structures and various physiochemical properties, including chemical reactivity, several graph invariants are employed. In chemical graph theory, these invariants are referred to as topological indices (TIs) of molecular graphs. Among them, distance-based topological indices (DBTIs) constitute a significant class and have been widely applied in chemical research. These indices play an important role in isomer discrimination, quantitative structure property relationship (QSPR) and quantitative structureactivity relationship (QSAR) studies, chemical documentation, structureproperty and structureacitivity correlations, as well as pharmaceuticals drug discovery and design across the disciplines of chemistry, biochemistry, and nanotechnology [26-30]. The first distance-based topological index, known as the Weiner index, was introduced by Harold Wiener in 1947 [1], [16]. Weiner originally developed this index to predict the boiling points of alkane compounds.

The Weiner index of a graph G is denoted by $W(G)$ and defined as the sum of distance between all pair of vertices in graph G, that is, $W(G)=\sum_{\{x,y\}\subseteq V(G)} d_G(x,y)$, similarly the Harary index of graph G is denoted by $H(G)$ and defined as $H(G)=\sum_{\{x,y\}\subseteq V(G)}\frac{1}{d_G(x,y)}$. The Zagreb indices are among the oldest TIs introduced by Gutman and Trinajstic in 1972. These indices have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. They are defined as $M_1(G)=\sum_{xy\in E(G)}\big(d_G(x)+d_G(y)\big)$ and $M_2(G)=\sum_{xy\in E(G)}\big(d_G(x)d_G(y)\big)$. The F-index of G is defined as $F(G)=\sum_{xy\in E(G)}(d_G(x)^2+d_G(y)^2)$.

The Harary-Gutman index and Harary-Futula indices of G are respectively defined for G as $RD^{+}_{HG}(G)=\sum_{x,y\subseteq V(G)}\frac{d_G(x)+d_G(y)}{d_G(x,y)}$ and $RD^{+}_{HF}(G)=\sum_{x,y\subseteq V(G)}\frac{d_G(x)^2+d_G(y)^2}{d_G(x,y)}$. Likwise the product version of these indices are respectively defined for G as $RD^{*}_{HG}(G)=\prod_{\{x,y\}\subseteq V(G)}\frac{d_G(x)+d_G(y)}{d_G(x,y)}$ and $RD^{*}_{HF}(G)=\prod_{\{x,y\}\subseteq V(G)}\frac{d_G(x)^2+d_G(y)^2}{d_G(x,y)}$.

Some distance-related TIs have been developed in recent years. These indices have been effectively used to mathematical models of a variety of biological processes [2-10]. Its been demonstrated that it offers a high level of predictability for medicinal characteristics and offers leads for the creation of secure and effective anti-HIV medicines [11-13, 16-25]. Alkane branching is also suggested to be measured using the eccentricity index (ICE) which is defined as $\xi^{-1}_{ce}(G)=\sum_{x\in V(G)}\frac{\epsilon_G(x)}{dg_G(x)}$. An innovative topological index known as the eccentric-distance sum index was presented by Gupta et al. [14]. Ilić et al. [15] given the various lower and upper bounds for the distance indices in terms of the other graph invariant. In this research, we derive good upper bounds for Mycielskian graph and its complement of a given graph.

2. RD^{*}_{HF} for $\overline{mg}(G)$

In this section, we establish the result for the value of RD_{HF}^{*} for the complement of Mycielskian of a given graph with diameter 2.

Observation 3: For each pair of vertices x and y in $\overline{mg}(G)$ of G, the distance from $x\ to\ y\ in\ \overline{mg}(G)\ is\ 1$.

If $x = u_i, y = u_j\ (or)\ x = v_i,\ y = v_j,\ d_G(v_i, v_j) > 1\ (or)\ x = v_i, y = u_i$

Similarly, the distance from $x\ to\ y\ in\ \overline{mg}(G)\ is\ 2$

whenever $x = v_i,\ y = v_j,\ d_G(v_i, v_j) = 1$

Likewise, if $x = v_i,\ y = u_j,\ i \neq j,$ then the distance from $x\ to\ y\ in\ \overline{mg}(G)\ is\ 1$.(resp. 2)

Whenever $d_G(v_i, v_j) > 1$ (resp. $d_G(v_i, v_j) = 1$).

Finally, if $y = w$ then the distance from $x\ to\ y\ is\ 2\ if\ x = u_i,\ and\ 1\ if\ x = v_i$.

Observation 4: If G has s points, then the degree of a vertex $x\ in\ \overline{mg}(G)$ is $2s - 1 - d_G(v_i)$ whenever $x = u_i$ and $2s - 2d_G(v_i)$ whenever $x = v_i$. In addition, if $x = w, then\ d_{\overline{mg}(G)}(a) = s$.

Theorem 3.1. Let $\overline{mg}(G)$ be the complement of Mycielskian graph of G. Then

$$RD_{HF}^{*}(\overline{mg}(G)) \leq \left(\frac{\alpha}{h}\right)^{h}\left(\frac{\beta}{h}\right)^{h}\left(\frac{5M_1(G) + 6s^3 - 28s^2 + 6s}{h}\right)^{h} \times \left(\frac{\vartheta}{h}\right)^{h}\left(\frac{\alpha_1}{h}\right)^{h}\left(\frac{4M_1(G) + 5s^3 - 16st}{h}\right)^{h},$$

$$\alpha = (s-1)^2 M_1(G) + (s-1)(2s-1)(2s^2 - s - 4t),$$

$$\beta = 2F(G) + (4s^2 - 12s + 4)M_1(G) + (4s^3 - 4s^2 - 12s^2 t - 16st),$$

$$\vartheta = (2s-3)M_1(G) + 4s^3(s-1) + (2s-1)^2 t - 16s(s-1)t,$$

$$\alpha_1 = M_1(G) + s^3 + (2s-1)^2 s - 4(2s-1)t,$$

$$h = 2s + 1.$$

Proof: To prove this theorem we need to complete the following cases with respect to the adjacency and non-adjacency pairs of vertices of $\overline{mg}(G)$.

From the definition of RD_{HF}^{*} for the graph $\overline{mg}(G)$.

$$RD_{HF}^{*}(\overline{mg}(G)) = \prod_{\{x,y\}\subseteq V(\overline{mg}(G))} \frac{d_{\overline{mg}(G)}^2(x) + d_{\overline{mg}(G)}^2(y)}{d_{\overline{mg}(G)}(x,y)}$$

$$= \left(\prod_{\{x,y\}\subseteq V'} \frac{d_{\overline{mg}(G)}^2(x) + d_{\overline{mg}(G)}^2(y)}{d_{\overline{mg}(G)}(x,y)}\right)\left(\prod_{\{x,y\}\subseteq V(G)} \frac{d_{\overline{mg}(G)}^2(x) + d_{\overline{mg}(G)}^2(y)}{d_{\overline{mg}(G)}(x,y)}\right)$$

$$\times \left(\prod_{\substack{i=1\\x=v_i\\y=u_i}}^{s} \frac{d_{\overline{mg}(G)}^2(v_i) + d_{\overline{mg}(G)}^2(u_i)}{d_{\overline{mg}(G)}(v_i,u_i)}\right)\left(\prod_{\substack{\{v_i,u_j\}\subseteq V(\overline{mg}(G))\\i\neq j}}^{s} \frac{d_{\overline{mg}(G)}^2(v_i) + d_{\overline{mg}(G)}^2(u_j)}{d_{\overline{mg}(G)}(v_i,u_j)}\right)$$

$$\times \left(\prod_{\substack{i=1\\x=w\\y\in V'}}^{s} \frac{d_{\overline{mg}(G)}(w) + d_{\overline{mg}(G)}(u_i)}{d_{\overline{mg}(G)}(w,u_i)}\right)\left(\prod_{\substack{i=1\\x=w\\y\in V(G)}}^{s} \frac{d_{\overline{mg}(G)}^2(w) + d_{\overline{mg}(G)}^2(u_i)}{d_{\overline{mg}(G)}(w,u_i)}\right)$$

Let us find these products are separately.

First we consider

$$P_1 = \prod_{\{u_i,u_j\}\subseteq V'} \frac{d_{\overline{mg}(G)}^2(u_i) + d_{\overline{mg}(G)}^2(u_j)}{d_{\overline{mg}(G)}(u_i,u_j)}$$

In this case, $x = u_i, y = u_j$ and both in v'. Then

$$P_1 = \prod_{\{u_i,u_j\}\subseteq V'} \frac{\left(2s - 1 - d_G(v_i)^2 + \left(2s - 1 - d_G(v_j)\right)^2\right)}{d_G(v_i, v_j) = 1}$$

$$\leq \left(\frac{1}{2s+1}_{\{u_i,u_j\}\subseteq V'}\left[\left(2s - 1 - d_G(v_i)^2 + \left(2s - 1 - d_G(v_j)\right)^2\right)\right]\right)^{2s+1}$$

Since

$$\left(2s - 1 - d_G(v_i)^2 + \left(2s - 1 - d_G(v_j)\right)^2\right) = 2(2s-1)^2 + \left(d_G^2(v_i) + d_G^2(v_j)\right) - 2(2s-1)\left(d_G(v_i) + d_G(v_j)\right)$$

Thus,

$$P_1 = \left(\frac{1}{2s+1}(s(s-1)(2s-1)^2 + (s-1)^2 M_1(G) - 4(2s-1)(s-1)t)\right)^{2s+1}$$

Next we shall see the product

$$P_2 = \prod_{\{v_i,v_j\}\subseteq V(G)} \frac{d_{\overline{mg}(G)}^2(v_i) + d_{\overline{mg}(G)}^2(v_j)}{d_{\overline{mg}(G)}(v_i,v_j)}$$

$$= \prod_{\{v_i,v_j\}\subseteq V(G)} \frac{\left(2s - 2d_G(v_i)\right)^2 + \left(2s - 2d_G(v_j)\right)^2}{d_{(G)}(v_i, v_j)}$$

$$\leq \left(\frac{1}{2s+1}_{\{v_i,v_j\}\subseteq V(G)} \frac{\left(2s-2d_G(v_i)\right)^2 + \left(2s-2d_G(v_j)\right)^2}{d_{(G)}(v_i,v_j)} \right)^{2s+1}$$

Since

$$\left(2s-2d_G(v_i)\right)^2 + \left(2s-2d_G(v_j)\right)^2 = 8s^2 + 4(d_{(G)}^2(v_i) + d_{(G)}^2(v_j)) - 8s(d_G(v_i) + d_G(v_j))$$

Thus

$$P_2 \leq \left(\frac{1}{2s+1}_{\{v_i,v_j\}\subseteq V(G)} \frac{8s^2 + 4(d_{(G)}^2(v_i) + d_{(G)}^2(v_j)) - 8s(d_G(v_i) + d_G(v_j))}{d_{(G)}(v_i,v_j)} \right)^{2s+1}$$

In this case, if $v_i, v_j \in E(G)$, then $d_{(G)}(v_i,v_j) = 1$ and if $v_i, v_j \notin E(G)$, then $d_{(G)}(v_i,v_j) = 2$.

Thus,

$$P_2 \leq \left[\frac{1}{2s+1} \left(4s^2(s-1) + 4(s-1)M_1(G) - 16s(s-1)t + \frac{8s^2t + 4F(G) - 8sM_1(G)}{2} \right) \right]^{2s+1}$$

$$= [\frac{1}{2s+1}(4s^2(s-1) + 4s^2t + (4(s-1) - 4s)M_1(G) + 2F(G) - 16s(s-1)t]^{2s+1}$$

$$= \left[\frac{1}{2s+1} \left((4s^3 - 4s^2 - 12s^2t - 16st) + 2F(G) + (4s^2 - 12s + 4)M_1(G) \right) \right]^{2s+1}$$

Now we obtain

$$P_3 = \prod_{i=1}^{s} \frac{d_{\overline{mg}(G)}^2(v_i) + d_{\overline{mg}(G)}^2(u_i)}{d_{\overline{mg}(G)}(v_i,u_i)}$$

Since $x = v_i and y = u_i, 1 \leq i \leq n$

$$= \prod_{i=1}^{s} \left(\left(2s-2d_G(v_i)\right)^2 + \left(2s-1-d_G(v_i)\right)^2 \right)$$

$$\leq \left(\frac{(6s^2-4s+2)s + 5M_1(G) - (12s-s)(2s)}{2s+1} \right)^{2s+1}$$

Similarly, we concentrate

$$P_4 = \prod_{\substack{\{v_i,u_j\}\subseteq V(\overline{mg}(G)) \\ i\neq j}} \frac{d_{\overline{mg}(G)}^2(v_i) + d_{\overline{mg}(G)}^2(u_j)}{d_{\overline{mg}(G)}(v_i,u_j)}$$

$$\leq \left[\frac{1}{2s+1} [_{\{v_i,v_j\}\notin E(G)} \left(\left(2s-2d_G(v_i)\right)^2 + \left(2s-1-d_G(v_i)\right)^2 \right) + \{v_i,v_j\} \notin E(G) \frac{\left(2s-2d_G(v_i)\right)^2 + \left(2s-1-d_G(v_i)\right)^2}{2}] \right]^{2s+1}$$

$$\leq \left[\frac{1}{2s+1} \left[4s^3(s-1) + 4(s-1)M_1(G) - (8s)\left(2t(s-1)\right) + \frac{2(2s-1)^2t + M_1(G) - 2(2s-1)M_1(G)}{2} \right] \right]^{2s+1}$$

$$= \left[\frac{1}{2s+1} \left(4s^3(s-1) + (2s-1)^2t - 16s(s-1)t + (2s-3)M_1(G) \right) \right]^{2s+1}$$

Likewise, we focus on

$$P_5 = \prod_{i=1}^{s} \frac{d_{\overline{mg}(G)}(w) + d_{\overline{mg}(G)}(u_i)}{d_{\overline{mg}(G)}(w,u_i)}$$

When $x = w, y \in V'$.

$$= \prod_{i=1}^{s} \frac{s^2 + \left(2s-1-d_G(v_i)\right)^2}{2}$$

$$\leq \left(\frac{s^3 + (2s-1)^2s + M_1(G) - 2(2s-1)(2t)}{2(2s+1)} \right)^{2s+1}$$

$$= \left(\frac{M_1(G) + s^3 + (2s-1)^2s - 4(2s-1)t}{2(2s+1)} \right)^{2s+1}$$

Finally, we obtain

$$P_6 = \prod_{i=1}^{s} \frac{d_{\overline{mg}(G)}(w) + d_{\overline{mg}(G)}(v_i)}{d_{\overline{mg}(G)}(w,v_i)}$$

Where $x = w \ and \ y \in V(G)$.

Thus

$$P_6 = \prod_{i=1}^{s} \left(s^2 + 4s^2 + 4d_G^2(v_i) - 8sd_G(v_i) \right)$$

$$\leq \left(\frac{s^3 + 4s^3 + 4M_1(G) - (8s)(2t)}{2s+1} \right)^{2s+1}$$

$$= \left(\frac{5s^3 - 16st + 4M_1(G)}{2s+1} \right)^{2s+1}$$

Combining all the cases, we get the total contributions of RD_{HF}^* for the complement of Mycielskian graph, that is,

$$RD_{HF}^{*}\left(\overline{mg}(G)\right) \le \left(\frac{\alpha}{h}\right)^{h}\left(\frac{\beta}{h}\right)^{h}\left(\frac{5M_1(G)+6s^3-28s^2+6s}{h}\right)^{h} \times \left(\frac{\vartheta}{h}\right)^{h}\left(\frac{\alpha_1}{h}\right)^{h}\left(\frac{4M_1(G)+5s^3-16st}{h}\right)^{h},$$

$$\alpha = (s-1)^2M_1(G) + (s-1)(2s-1)(2s^2-s-4t),$$

$$\beta = 2F(G) + (4s^2-12s+4)M_1(G) + (4s^3-4s^2-12s^2t-16st),$$

$$\vartheta = (2s-3)M_1(G) + 4s^3(s-1) + (2s-1)^2t - 16s(s-1)t,$$

$$\alpha_1 = M_1(G) + s^3 + (2s-1)^2s - 4(2s-1)t,$$

$$h = 2s+1.$$

3 Conclusion

This paper focused on the complement of the Mycielskian graph and presented new upper bounds for the corresponding product versions of distance-related topological indices. The derived inequalities were obtained using the structural characteristics of the complement graph and provide theoretical estimates for these descriptors. The results enrich the study of transformed graphs and contribute to the development of eccentricity-based topological indices. Future work may consider analogous bounds for other graph transformations and additional classes of topological descriptors.

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