International Journal of Computer Information Systems and Industrial Management Applications
ISSN 2150-7988 Volume 18(15s) 2026 pp. 713-718
https://doi.org/10.70917/ijcisim-2026-4466
Article

Bounds on Product version of Distance Related Topological Indices of Construction Graphs

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Abstract: Topological indices are important graph invariants used to describe molecular structures and predict their physicochemical properties. Among them, eccentricity-based indices have received significant attention in chemical graph theory. In this paper, we investigate recent eccentricity-related topological indices of the Mycielskian graph associated with a connected graph. By utilizing the structural properties of the Mycielskian graph, we establish new upper bounds for these indices. The derived results extend existing bounds and provide useful theoretical estimates without requiring direct computation. These findings contribute to the study of graph transformations and their applications in mathematical chemistry.
MSC : 05C12, 05C76
Keywords: Distance, Topological index, Eccentricity, Mycielskian graph, Upper bounds.

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. 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}^{*} of Mycielskian graph

Let us denoted $\{v_1, v_2, v_3, \cdots, v_s\}$ by the vertex set of a connected graph G. The Mycielskian graph $mg(G)$ of G contains G itself as an isomorphic subgraph, together with $s+1$ extra vertices; a vertex u_i corresponding to v_i of G, and w a new vertex.

(i) Each vertex u_i is connected by an edge to w.

(ii) If $v_iv_j \in E(G)$, then v_iu_j and v_ju_i are edges in $mg(G)$.

From the construction of $mg(G)$ of G we have the following.

Observation 1. Let G be a connected graph. For $x, y \in V(mg(G))$, the distance from x to y in $mg(G)$ is 2. Whenever $x = u_i, y = u_j$ and $d_G(v_i, v_j)$ whenever $x = v_i, y = v_j, d_G(v_i, v_j) \leq 3$.

Similarly, if $x = v_i, y = u_j, i = j$, then the distance from x to y in $mg(G)$ is 2.

Moreover, if $x = v_i, y = u_j, i = j$, then the distance from x to y in $mg(G)$ is 2.

Let $x = v_i, y = u_j, i \neq j$, If $d_G(v_i, v_j \leq 2)$ and $d_G(v_i, v_j \geq 3)$ then the distance from x to y are respectively $d_G(v_i, v_j)$ and 3.

Finally, the distance from x to y in $mg(G)$ is 1 whenever $x = u_i, y = w$ and whenever $x = v_i, y = w$.

Observation 2. The degree of a vertex x in $mg(G)$ is s if $x = w$, $1 + d_G(v_i)$, if $x = u_i$, and $2d_G(v_i)$ if $x = v_i$.

By using observation ?? and observation ??, we obtain the following main theorem.

Theorem 2.1 Let $mg(G)$ be the Mycielskian graph of the $(s,t) -$ graph G. If G has $diamg(G) = 2$, then

$$RD_{HF}^{*}(mg(G)) \leq \left(\frac{\alpha}{2(2s+1)}\right)^{2s+1} \left(\frac{4RD_{HF}^{+}(G)}{2s+1}\right)^{2s+1} \left(\frac{5M_{1(G)} + 4t + s}{2(2s+1)}\right)^{2s+1}$$

$$\times \left(\frac{\beta}{2s+1}\right)^{2s+1} \left(\frac{\vartheta}{2s+1}\right)^{2s+1} \left(\frac{s^3 + 4M_1(G)}{2(2s+1)}\right)^{2s+1},$$

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

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

$$\vartheta = s(s^2+1) + M_1(G) + 4t.$$

Proof. To find the bound for RD_{HF}^{*} of mg(G), we consider the following six cases with respect to adjacent and non-adjacent vertices of mg(G), that is ,

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

$$\left(\prod_{\{x,y\} \subseteq V(G)} \frac{d_{mg(G)}^2(x) + d_{mg(G)}^2(y)}{d_{mg(G)}(x,y)}\right) \left(\prod_{i=1}^{s} \frac{d_{mg(G)}^2(x_i) + d_{mg(G)}^2(y_i)}{d_{mg(G)}(x_i, y_i)}\right)$$

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

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

Now we calculate the first product of the above equation.

$$P_1 = \left(\prod_{\{x_i,x_j\} \subseteq V'} \frac{d_{mg(G)}^2(x_i) + d_{mg(G)}^2(x_j)}{d_{mg(G)}(x_i, x_j)} \right),$$

Since $\{x, y\} \subseteq V'$

$$= \prod_{\{x_i,x_j\} \subseteq V'} \frac{\left(1 + d_G(x_i)\right)^2 + \left(1 + d_G(x_j)\right)^2}{2},$$

$$= \prod_{\{x_i,x_j\} \subseteq V'} \frac{\left(d_G^2(x_i) + d_G^2(x_j)\right) + 2\left(d_G(x_i) + d_G(x_j)\right) + 2}{2}$$

We can easily write

$$P_1 \leq \left(\frac{1}{2(2s+1)_{\{x_i,x_j\} \subseteq V'}} \ \left(d_G^2(x_i) + d_G^2(x_j)\right) + 2\left(d_G(x_i) + d_G(x_j)\right) + 2 \right)^{2s+1}$$

One can easily count that for each $x_k \in V'$, we have $\left|\{\{x_k, x_j\}: k \neq j\}\right| = s - 1$.

Hence, $P_1 \leq \left(\frac{s_{k=1}(s-1)d^2(x_k) + 2_{k=1}^{s}(s-1)d(x_k) + x_i, x_j \subseteq V' 2}{2(2s+1)} \right)^{2s+1}$

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

Similarly, we compute

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

In this case, both $v_i \; and \; v_j$ are in $V(G)$, and $d_{mg(G)}(v_i, v_j) = d_G(v_i, v_j)$. Thus, by the definition of RD_{HF}^{+}, we have

$$P_2 = \prod_{v_i,v_j \subseteq V(G)} \frac{4d_{(G)}^2(v_i) + 4d_{(G)}^2(v_j)}{d_{(G)}(v_i, v_j)}$$

$$\leq \left(\frac{4RD_{HF}^{+}(G)}{2s+1} \right)^{2s+1}$$

Likewise, we calculate

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

In this case, normally we consider $x = v_i \; and \; y = u_i, 1 \leq i \leq s$. Thus,

$$P_3 = \prod_{i=1}^{s} \frac{4d_G^2(v_i) + \left(1 + d_G(v_i)\right)^2}{2}$$

$$\leq \left(\frac{s_{i=1}(4d_G^2(v_i) + d_G^2(v_i) + 2d_G(v_i) + 1)}{2(2s+1)} \right)^{2s+1}$$

$$= \left(\frac{5M_1(G) + 4t + s}{2(2s+1)} \right)^{2s+1}$$

Next we find the product

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

In this case, $x = v_i$ *and* $y = u_j$ *with* $i \neq j$. *Thus*

$$P_4 = \prod_{\substack{\{v_i,u_j\}\subseteq V(mg(G))\\ i\neq j}} \frac{4d^2_G(v_i) + \big(1 + d_G(v_i)\big)^2}{d_{mg(G)}(v_i,u_i)}$$

$$= \prod_{\substack{\{v_i,u_j\}\subseteq V(mg(G))\\ i\neq j}} \frac{d^2_G(v_i) + d^2_G(u_j) + 3d^2_G(v_i) + 2d_G(u_j) + 1}{d_{mg(G)}(v_i,u_j)}$$

$$\leq \left[\frac{\{v_i,u_j\}\subseteq V(mg(G))\dfrac{d^2_G(v_i) + d^2_G(v_j)}{ud_{mg(G)}(v_i,u_j)} + \{v_i,u_j\}\subseteq V(mg(G))\dfrac{3d^2_G(v_i) + 2d_G(u_j) + 1}{d_{mg(G)}(v_i,u_j)}}{2s+1}\right]^{2s+1}$$

Let $T_1 = \{v_i,u_j\}\subseteq V(mg(G))\frac{d^2_G(v_i)+d^2_G(u_j)}{d_{mg(G)}(v_i,u_j)}$

But the distance from v_i *and* u_j in the graph $mg(G)$ is equal to the distance from v_j *and* u_i *in* $mg(G)$. Thus

$$T_1 = RD^+_{HF}(G).$$

Let

$$T_2 = \{v_i,u_j\}\subseteq V(mg(G))\frac{3d^2_G(v_i) + 2d_G(u_j) + 1}{d_{mg(G)}(v_i,u_j)}$$

$$= \{v_i,u_j\}\subseteq V(mg(G)), d_G(v_i,u_j = 1)\big(3d^2_G(v_i) + 2d_G(u_j) + 1\big)$$

$$+ \frac{1}{2}_{\substack{\{v_i,u_j\}\subseteq V(mg(G))\\ d_G(v_i,u_j=2)}} \big(3d^2_G(v_i) + 2d_G(u_j) + 1\big)$$

$$= 3_{v_i,v_j\in E(G)}\left(d^2_G(v_i) + d^2_G(v_j)\right) + 2_{v_i,v_j\in E(G)}\left(d_{G(v_i)} + d_{G(v_j)}\right) + 2t$$

$$+ \frac{3}{2}_{\substack{\{v_i,u_j\}\subseteq V(mg(G))\\ d_G(v_i,u_j=2)}}\left(d^2_G(v_i) + d^2_G(v_j)\right) + \frac{\{v_i,u_j\}\subseteq V(mg(G))}{d_G(v_i,u_j=2)}\left(d_{G(v_i)} + d_{G(v_j)}\right) + \frac{s(s-1-2t)}{2}$$

$T_2 = (3F(G) + 2M_1(G) + 2t) + \frac{3}{2}\big(2(s-1)^2t - F(G)\big) + \big(2(s-1)t - M_1(G)\big) + \frac{s(s-1)-2t}{2}$

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

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

Hence $P_4 \leq \left[\frac{RD^+_{HF}(G)+\frac{3F(G)}{2}+M_1(G)+3(s-1)^2t+\frac{(s-1)(s+4t)}{2}+t}{2s+1}\right]^{2s+1}$

Now we establish the value of the product

$$P_5 = \prod_{i=1}^{s} \frac{d^2_{mg(G)}(w) + d^2_{mg(G)}(u_i)}{d_{mg(G)}(w,u_i)}$$

In this case, we consider $x = w$ *and* $y = V_i$. Then

$$P_5 = \prod_{i=1}^{s} (s^2 + d_G^2(v_i) + 2d_G(v_i) + 1)$$
$$\leq \left(\frac{s(s^2+1) + M_1(G) + 4t}{2s+1}\right)^{2s+1}$$

Finally, we count the value of the product

$$P_6 = \prod_{i=1}^{s} \frac{d_{mg(G)}^2(w) + d_{mg(G)}^2(v_i)}{d_{mg(G)}(w, v_i)}$$

In this case, we take $x = w \ and \ y \in V(G)$. Thus

$$P_6 = \prod_{i=1}^{s} \frac{s^2 + 4d_G^2(v_i)}{2}$$
$$\leq \left(\frac{s^3 + 4M_1(G)}{2(2s+1)}\right)^{2s+1}$$

Summarizing the total contributions of all cases of adjacent and non-adjacent pairs of vertices of $mg(G)$, we obtain

$$RD_{HF}^{*}(mg(G)) \leq \left(\frac{\alpha}{2(2s+1)}\right)^{2s+1} \left(\frac{4RD_{HF}^{+}(G)}{2s+1}\right)^{2s+1} \left(\frac{5M_{1(G)} + 4t + s}{2(2s+1)}\right)^{2s+1}$$
$$\times \left(\frac{\beta}{2s+1}\right)^{2s+1} \left(\frac{\vartheta}{2s+1}\right)^{2s+1} \left(\frac{s^3 + 4M_1(G)}{2(2s+1)}\right)^{2s+1},$$

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

$$\beta = RD_{HF}^{+}(G) + \frac{3}{2}F(G) + M_1(G) + 3(s-1)^2 t + \left(\frac{s-1}{2}\right)(s+4t) + t,$$
$$\vartheta = s(s^2+1) + M_1(G) + 4t.$$

3. Conclusion

In this paper, we investigated the product versions of distance-related topological indices for the Mycielskian graph of a connected graph. By exploiting the structural properties of the Mycielskian graph, we established new upper bounds for these indices. The obtained results extend the existing theory of eccentricity-based topological descriptors and provide efficient estimates without direct computation. We expect that these bounds will be useful in further studies of graph transformations, chemical graph theory, and related mathematical applications.

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