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GRAPH INVARIANTS BASED ON DISTANCE BETWEEN EDGES AND DOUBLE GRAPHS

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Abstract. Topological indices are numerical parameters of graph which characterize its topology and are invariant under graph isomorphism. They are applied in theoretical chemistry for the design of chemical compounds with certain physicochemical properties or biological activities. The Wiener index, hyper-Wiener index, degree distance, and Gutman index are among the best-known distance-based topological indices with known applications in chemistry. In this paper, we study the edge version of these graph invariants for a collection of graphs named double graphs.

Keywords: Distance between edges in graph, Topological index, Double graph.

AMS Subject Classification: 05C12, 05C76.

1. Introduction

All graphs considered in this paper are finite, simple and connected. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex $u \in V(G)$ is the number of edges incident to u. Two distinct edges $e = uv$ and $f = zt$ of G are said to be adjacent if they have a vertex in common. The line graph $L(G)$ is the graph whose vertices correspond to the edges of G with two vertices being adjacent if and only if the corresponding edges are adjacent in G. The degree $d_G(e)$ of an edge $e = uv \in E(G)$ is defined as the degree of the corresponding vertex e in the line graph of G which is equal to $d_G(e) = d_G(u) + d_G(v) - 2$. We denote by $N_G(e)$ the set of all edges adjacent to $e \in E(G)$ and by $\delta_G(e)$ the sum of degrees of all edges adjacent to e, i.e., $\delta_G(e) = \sum_{f \in N_G(e)} d_G(f)$.

The distance $d_G(u, v)$ between the vertices $u, v \in V(G)$ is defined as the length of any shortest path in G connecting u and v. The distance sum (also called status) $D_G(u)$ of a vertex $u \in V(G)$ is the sum of distances between u and all other vertices v of G, i.e., $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. We denote by $D_G^{(2)}(u)$, the sum of squares of distances between a vertex $u \in V(G)$ and all other vertices v of G, i.e., $D_G^{(2)}(u) = \sum_{v \in V(G)} d_G(u, v)^2$.

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The distance $d_G(e,f)$ between the edges $e = uv$ and $f = zt$ of G is defined as the distance between the corresponding vertices e and f in the line graph of G. This distance is equal [20] to

$$d_G(e,f) = \begin{cases} 0 & \text{if } e = f, \\ \min\{d_G(u,z), d_G(u,t), d_G(v,z), d_G(v,t)\} + 1 & \text{if } e \neq f. \end{cases}$$

We denote by $D_G(e)$, the sum of distances between an edge $e \in E(G)$ and all other edges f of G, i.e., $D_G(e) = \sum_{f \in E(G)} d_G(e,f)$, and by $D_G^{(2)}(e)$, the sum of squares of distances between an edge $e \in E(G)$ and all other edges f of G, i.e., $D_G^{(2)}(e) = \sum_{f \in E(G)} d_G(e,f)^2$.

A chemical graph or molecular graph of a chemical compound is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to the chemical bonds. In the context of π systems, a molecular graph is one that is connected and has a maximum degree at most 4 (see, for example, [16]). A topological index is a real number related to a graph which is invariant under graph isomorphism, that is it does not depend on the labeling or the pictorial representation of a graph. Topological indices help us to predict certain physicochemical, biological, and pharmacological properties of molecules like boiling point, enthalpy of vaporization, stability, energy, etc.

The *Wiener index*, introduced by Wiener [38] in 1947, is the first topological index recognized in chemical graph theory. The Wiener index of a graph G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) = \frac{1}{2} \sum_{u \in V(G)} D_G(u),$$

where the first summation runs over all unordered vertex pairs of G. This invariant is used for modeling the shape of organic molecules and for calculating several of their physicochemical properties [38].

The edge-Wiener index of a graph G was defined by Iranmanesh et al. [20] as

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d_G(e,f) = \frac{1}{2} \sum_{e \in E(G)} D_G(e),$$

where the first summation runs over all unordered pairs of edges of G. The edge-Wiener index of a graph can also be introduced as the Wiener index of its line graph. Further information on the edge versions of the Wiener index can be found in [19] and the references quoted therein.

The hyper-Wiener index of acyclic graphs was introduced by Randić [33] in 1993. Then Klein et al. [25] generalized Randić's definition for all connected graphs in 1995. The hyper-Wiener index of a graph G is defined as

$$WW(G) = \frac{1}{2}\Big(W(G) + W^{(2)}(G)\Big),$$

where

$$W^{(2)}(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^2 = \frac{1}{2} \sum_{u \in V(G)} D_G^{(2)}(u).$$

The edge hyper-Wiener index of a graph G was defined by Iranmanesh et al. [22] as

$$WW_e(G) = \frac{1}{2}\Big(W_e(G) + W_e^{(2)}(G)\Big),$$

where

$$W_e^{(2)}(G) = \sum_{\{e,f\} \subseteq E(G)} d_G(e,f)^2 = \frac{1}{2} \sum_{e \in E(G)} D_G^{(2)}(e).$$

This invariant is used for the representation of computer networks and enhancing lattice hardware security.

The *degree distance* was introduced by Dobrynin and Kochetova [6] and at the same time by Gutman [12] as a weighted version of the Wiener index. The degree distance of a graph G is defined as

$$DD(G) = \sum_{u\in V(G)} d_G(u)D_G(u) = \sum_{\{u,v\}\subseteq V(G)} \big(d_G(u) + d_G(v)\big)d_G(u,v).$$

It was proved in [12] that, in the case of trees the Wiener index and degree distance are closely related.

The edge-degree distance of a graph G was put forward by Iranmanesh et al. [21] as

$$DD_e(G) = \sum_{e\in E(G)} d_G(e)D_G(e) = \sum_{\{e,f\}\subseteq E(G)} \big(d_G(e) + d_G(f)\big)d_G(e,f).$$

The Gutman index was introduced by Gutman [12] in 1994 as a kind of vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. The Gutman index of a graph G is defined as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)d_G(u,v) = \frac{1}{2}\sum_{u\in V(G)} d_G(u)S_G(u),$$

where

$$S_G(u) = \sum_{v\in V(G)} d_G(v)d_G(u,v).$$

This invariant reflects exactly the same structural properties of a molecular as the Wiener index does.

The edge-Gutman index of a graph G was defined by Iranmanesh et al. [21] as

$$Gut_e(G) = \sum_{\{e,f\}\subseteq E(G)} d_G(e)d_G(f)d_G(e,f) = \frac{1}{2}\sum_{e\in E(G)} d_G(e)S_G(e),$$

where

$$S_G(e) = \sum_{f\in E(G)} d_G(f)d_G(e,f).$$

See [3, 4, 5] for more informatation on the edge version of the hyper-Wiener index, degree-distance, and Gutman index.

The *first Zagreb index* of a graph G was introduced by Gutman and Trinajstić [13] in 1972 and the second Zagreb index was proposed by Gutman et al. [14] in 1975 as

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

The forgotten topological index (F-index) was first introduced by Gutman and Trinajstić [13] in 1972 as

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} \big(d_G(u)^2 + d_G(v)^2\big),$$

and revived by Furtula and Gutman [10] in 2015. It can be easily observed that,

$$\begin{aligned}\sum_{e\in E(G)} \delta_G(e) &= M_1(L(G)) = F(G) + 2M_2(G) - 4M_1(G) + 4|E(G)|,\\ \sum_{e\in E(G)} d_G(e)\delta_G(e) &= 2M_2(L(G)).\end{aligned} \tag{1}$$

Some molecular graphs can be obtained from simpler molecular graphs by using operations on graphs. Certainly, computing topological indices of the constructive structures is much easier than the main structure. Hence, studying topological indices of graph operations specially those can generate molecular graphs is one of the important subjects in chemical graph theory. One of such operations is the double operation whose definition was first appeared in a paper by Indulal and Vijayakumary [18], where this operation was used to construct non-cospectral but equienergetic graphs. A few years later, motivated by completely different reasons, Munarini et al. [28] proposed the concept of double graphs, and studied elementary properties of these graphs, extensively. After the paper by Munarini et al., double graphs attracted a great interest and various properties of this structure studied in the literature. See, for example, [17, 27, 31, 39] for some nice results on double graphs from pure mathematics perspective. The double operation has also received attention in the context of chemical graphs and topological indices. Dehghan-Zadeh et al. [8] used double graphs to construct infinite classes of connected graphs, with cyclomatic number greater than 4, for which a conjecture of Fajtlowicz [9] regarding the comparison between Randić index (see [32]) and radius of graphs holds. After that, with the purpose of investigation of Alveoli in Human lungs by using topological indices, Lukesha et al. [26] applied double graphs by considering the alveoli as a connected graph and determined topological indices for healthy and ruptured alveoli by using double operation. Ganie et al. [11] investigated the energy and Laplacian energy of double graphs. Huang et al. [15] studied resistance distances and Kirchhoff index (see [24]) of double graphs. Sardar et al. [35, 36], used double graphs to compute closed formulas for some degree-based topological indices of silicon carbide Si_2C_3-$I[p,q]$ and circumcoronene series of benzenoids H_m. Besides, double graphs were used in various papers to ease some calculations especially in computing topological indices of chemical graphs (see, for example, [1]). In this paper, we propose a formula for the distance between two edges in double graphs and apply our results to compute the edge version of the Wiener, hyper-Wiener, degree distance, and Gutman indices of double graphs in terms of the respective indices of the parent graph. Our paper continues the line of research of some recent papers [2, 7, 23, 29, 30, 34, 37] studying topological indices of double graphs.

2. Main results

We start this section with definition of double graph.

Definition 2.1. *Let G be a graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$. The double graph $\mathcal{D}[G]$ of G is obtained by taking two distinct copies $X = \{x_1, x_2, ..., x_n\}$ and $Y = \{y_1, y_2, ..., y_n\}$ of G by preserving the primary edge set of each copy and adding the edges x_iy_j and x_jy_i for every edge $v_iv_j \in E(G)$ (see Figure 1).*

It is worth noting that, the double graph of the complete graph K_n is just the graph obtained by deleting a perfect matching from the complete graph K_{2n}, which is just the well-known cocktail party graph.

From the definition 2.1, $\mathcal{D}[G]$ has $2n$ vertices and $4m$ edges, where m is the number of edges of G.

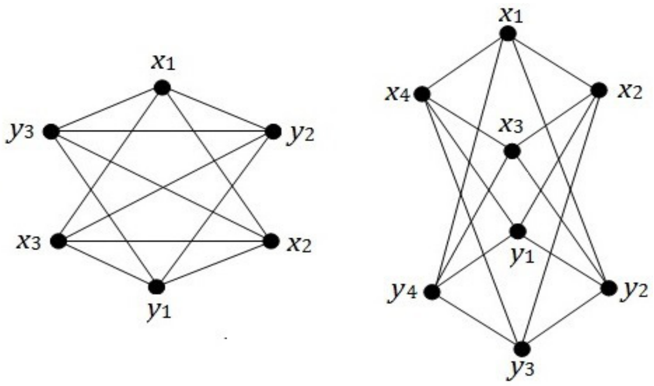

FIGURE 1. The double graphs of 3-cycle and 4-cycle.

Lemma 2.1. [28] *The degree of each vertex in $\mathcal{D}[G]$ is given by*

$$d_{\mathcal{D}[G]}(x_i) = d_{\mathcal{D}[G]}(y_i) = 2d_G(v_i).$$

Lemma 2.2. [23] *The distance between each pair of vertices in $\mathcal{D}[G]$ is given by*

$$d_{\mathcal{D}[G]}(x_i, x_j) = d_{\mathcal{D}[G]}(y_i, y_j) = d_G(v_i, v_j),\ d_{\mathcal{D}[G]}(x_i, y_j) = \begin{cases} d_G(v_i, v_j) & \text{if } i \neq j, \\ 2 & \text{if } i = j. \end{cases}$$

In the following lemma, we compute the degree of an edge and the distance between two edges in double graph. The results follow from Lemmas 2.1 and 2.2 and the proofs are therefore omitted.

Lemma 2.3. *The following hold:*

(1) *For each edge $v_iv_j \in E(G)$,*
$d_{\mathcal{D}[G]}(x_ix_j) = d_{\mathcal{D}[G]}(y_iy_j) = d_{\mathcal{D}[G]}(x_iy_j) = d_{\mathcal{D}[G]}(x_jy_i) = 2d_G(v_iv_j) + 2;$

(2) *For each pair of edges $v_iv_j, v_rv_s \in E(G)$,*
$d_{\mathcal{D}[G]}(x_ix_j, x_rx_s) = d_{\mathcal{D}[G]}(y_iy_j, y_ry_s) = d_G(v_iv_j, v_rv_s),$

$$d_{\mathcal{D}[G]}(x_ix_j, y_ry_s) = \begin{cases} d_G(v_iv_j, v_rv_s) + 2 & \text{if } \{r, s\} = \{i, j\}, \\ d_G(v_iv_j, v_rv_s) + 1 & \text{if } r \in \{i, j\} \text{ or } s \in \{i, j\},\ \{r, s\} \neq \{i, j\}, \\ d_G(v_iv_j, v_rv_s) & \text{if } r, s \notin \{i, j\}; \end{cases}$$

$$d_{\mathcal{D}[G]}(x_iy_j, x_ry_s) = \begin{cases} d_G(v_iv_j, v_rv_s) + 2 & \text{if } r = j,\ s = i, \\ d_G(v_iv_j, v_rv_s) + 1 & \text{if } r = j, s \neq i \text{ or } s = i, r \neq j, \\ d_G(v_iv_j, v_rv_s) & \text{if } r = i, s = j \text{ or } r, s \notin \{i, j\}; \end{cases}$$

$$d_{\mathcal{D}[G]}(x_ix_j, x_ry_s) = d_{\mathcal{D}[G]}(y_iy_j, y_rx_s) = \begin{cases} d_G(v_iv_j, v_rv_s) + 1 & \text{if } s \in \{i, j\}, \\ d_G(v_iv_j, v_rv_s) & \text{if } s \notin \{i, j\}. \end{cases}$$

Theorem 2.1. *The edge-Wiener index of $\mathcal{D}[G]$ is given by*

$$W_e(\mathcal{D}[G]) = 16W_e(G) + 4M_1(G). \tag{2}$$

Proof. Corresponding to each edge $v_iv_j \in E(G)$, there exist four edges $x_ix_j, y_iy_j, x_iy_j, x_jy_i \in E(\mathcal{D}[G])$. Then

$$\begin{aligned}
D_{\mathcal{D}[G]}(x_ix_j) = & \sum_{x_rx_s \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_rx_s) + \Big[d_{\mathcal{D}[G]}(x_ix_j, y_iy_j) \\
& + \sum_{\substack{y_iy_s \in E(\mathcal{D}[G]): \\ s \neq j}} d_{\mathcal{D}[G]}(x_ix_j, y_iy_s) + \sum_{\substack{y_ry_j \in E(\mathcal{D}[G]): \\ r \neq i}} d_{\mathcal{D}[G]}(x_ix_j, y_ry_j) \\
& + \sum_{\substack{y_ry_s \in E(\mathcal{D}[G]): \\ r,s \neq i,j}} d_{\mathcal{D}[G]}(x_ix_j, y_ry_s) \Big] + \Big[\sum_{x_ry_i \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_ry_i) \\
& + \sum_{x_ry_j \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_ry_j) + \sum_{\substack{x_ry_s \in E(\mathcal{D}[G]): \\ s \neq i,j}} d_{\mathcal{D}[G]}(x_ix_j, x_ry_s) \Big].
\end{aligned}$$

Now from Lemma 2.3, we get

$$\begin{aligned}
D_{\mathcal{D}[G]}(x_ix_j) = & \sum_{v_rv_s \in E(G)} d_G(v_iv_j, v_rv_s) + \Big[\big(d_G(v_iv_j, v_iv_j) + 2 \big) \\
& + \sum_{\substack{v_iv_s \in E(G): \\ s \neq j}} \big(d_G(v_iv_j, v_iv_s) + 1 \big) + \sum_{\substack{v_rv_j \in E(G): \\ r \neq i}} \big(d_G(v_iv_j, v_rv_j) + 1 \big) \\
& + \sum_{\substack{v_rv_s \in E(G): \\ r,s \neq i,j}} d_G(v_iv_j, v_rv_s) \Big] + \Big[\sum_{v_rv_i \in E(G)} \big(d_G(v_iv_j, v_rv_i) + 1 \big) \\
& + \sum_{v_rv_j \in E(G)} \big(d_G(v_iv_j, v_rv_j) + 1 \big) + \sum_{\substack{v_rv_s \in E(G): \\ s \neq i,j}} d_G(v_iv_j, v_rv_s) \Big] \\
= & D_G(v_iv_j) + \big(2 + D_G(v_iv_j) + d_G(v_i) - 1 + d_G(v_j) - 1 \big) \\
& + \big(2D_G(v_iv_j) + d_G(v_i) + d_G(v_j) \big) \\
= & 4D_G(v_iv_j) + 2\big(d_G(v_i) + d_G(v_j) \big).
\end{aligned}$$

By symmetry, for each edge $v_iv_j \in E(G)$, we have

$$\begin{aligned}
D_{\mathcal{D}[G]}(y_iy_j) = & D_{\mathcal{D}[G]}(x_iy_j) = D_{\mathcal{D}[G]}(x_jy_i) = D_{\mathcal{D}[G]}(x_ix_j) \\
= & 4D_G(v_iv_j) + 2\big(d_G(v_i) + d_G(v_j) \big).
\end{aligned} \tag{3}$$

Now from the definition of the edge-Wiener index and Eq. (3), we obtain

$$\begin{aligned}
W_e(\mathcal{D}[G]) = & 4 \times \frac{1}{2} \sum_{x_ix_j \in E(\mathcal{D}[G])} D_{\mathcal{D}[G]}(x_ix_j) \\
= & 2 \sum_{v_iv_j \in E(G)} \Big(4D_G(v_iv_j) + 2\big(d_G(v_i) + d_G(v_j) \big) \Big) \\
= & 16W_e(G) + 4M_1(G).
\end{aligned}$$

from which Eq. (2) follows. □

Theorem 2.2. *Let G be a graph on m edges. The edge-hyper Wiener of $\mathcal{D}[G]$ is given by*

$$WW_e(\mathcal{D}[G]) = 16WW_e(G) + 8M_1(G) - 6m. \tag{4}$$

Proof. Let $v_iv_j \in E(G)$. Then

$$\begin{aligned} D^{(2)}_{\mathcal{D}[G]}(x_ix_j) = & \sum_{x_rx_s\in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_rx_s)^2 + \Big[d_{\mathcal{D}[G]}(x_ix_j, y_iy_j)^2 \\ & + \sum_{\substack{y_iy_s\in E(\mathcal{D}[G]):\\ s\neq j}} d_{\mathcal{D}[G]}(x_ix_j, y_iy_s)^2 + \sum_{\substack{y_ry_j\in E(\mathcal{D}[G]):\\ r\neq i}} d_{\mathcal{D}[G]}(x_ix_j, y_ry_j)^2 \\ & + \sum_{\substack{y_ry_s\in E(\mathcal{D}[G]):\\ r,s\neq i,j}} d_{\mathcal{D}[G]}(x_ix_j, y_ry_s)^2\Big] + \Big[\sum_{x_ry_i\in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_ry_i)^2 \\ & + \sum_{x_ry_j\in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j, x_ry_j)^2 + \sum_{\substack{x_ry_s\in E(\mathcal{D}[G]):\\ s\neq i,j}} d_{\mathcal{D}[G]}(x_ix_j, x_ry_s)^2\Big]. \end{aligned}$$

Now by Lemma 2.3, we get

$$\begin{aligned} D^{(2)}_{\mathcal{D}[G]}(x_ix_j) = & \sum_{v_rv_s\in E(G)} d_G(v_iv_j, v_rv_s)^2 + \Big[\big(d_G(v_iv_j, v_iv_j) + 2\big)^2 \\ & + \sum_{\substack{v_iv_s\in E(G):\\ s\neq j}} \big(d_G(v_iv_j, v_iv_s) + 1\big)^2 + \sum_{\substack{v_rv_j\in E(G):\\ r\neq i}} \big(d_G(v_iv_j, v_rv_j) + 1\big)^2 \\ & + \sum_{\substack{v_rv_s\in E(G):\\ r,s\neq i,j}} d_G(v_iv_j, v_rv_s)^2\Big] + \Big[\sum_{v_rv_i\in E(G)} \big(d_G(v_iv_j, v_rv_i) + 1\big)^2 \\ & + \sum_{v_rv_j\in E(G)} \big(d_G(v_iv_j, v_rv_j) + 1\big)^2 + \sum_{\substack{v_rv_s\in E(G):\\ s\neq i,j}} d_G(v_iv_j, v_rv_s)^2\Big] \\ = & D^{(2)}_G(v_iv_j) + \big(4 + D^{(2)}_G(v_iv_j) + 3(d_G(v_i) - 1) + 3(d_G(v_j) - 1)\big) \\ & + \big(2D^{(2)}_G(v_iv_j) + 2(d_G(v_i) - 1) + d_G(v_i) + 2(d_G(v_j) - 1) + d_G(v_j)\big) \\ = & 4D^{(2)}_G(v_iv_j) + 6\big(d_G(v_i) + d_G(v_j)\big) - 6. \end{aligned}$$

By symmetry, for each edge $v_iv_j \in E(G)$, we have

$$\begin{aligned} D^{(2)}_{\mathcal{D}[G]}(y_iy_j) = & D^{(2)}_{\mathcal{D}[G]}(x_iy_j) = D^{(2)}_{\mathcal{D}[G]}(x_jy_i) = D^{(2)}_{\mathcal{D}[G]}(x_ix_j) \\ = & 4D^{(2)}_G(v_iv_j) + 6\big(d_G(v_i) + d_G(v_j)\big) - 6. \end{aligned}$$

Hence

$$\begin{aligned} W^{(2)}_e(\mathcal{D}[G]) = & 4 \times \frac{1}{2} \sum_{x_ix_j\in E(\mathcal{D}[G])} D^{(2)}_{\mathcal{D}[G]}(x_ix_j) \\ = & 2 \sum_{v_iv_j\in E(G)} \Big(4D^{(2)}_G(v_iv_j) + 6\big(d_G(v_i) + d_G(v_j)\big) - 6\Big) \\ = & 16W^{(2)}_e(G) + 12M_1(G) - 12m. \end{aligned}$$

Now from the definition of the edge-hyper Wiener index and Eq. (2), we obtain

$$\begin{aligned}
WW_e(\mathcal{D}[G]) =& \frac{1}{2}\Big(W_e(\mathcal{D}[G]) + W_e^{(2)}(\mathcal{D}[G])\Big) \\
=& \frac{1}{2}\big(16W_e(G) + 4M_1(G) + 16W_e^{(2)}(G) + 12M_1(G) - 12m\big) \\
=& 16WW_e(G) + 8M_1(G) - 6m.
\end{aligned}$$

from which Eq. (4) follows. □

Theorem 2.3. *The edge-degree distance of* $\mathcal{D}[G]$ *is given by*

$$DD_e(\mathcal{D}[G]) = 16\big(2DD_e(G) + 4W_e(G) + F(G) - M_1(G) + 2M_2(G)\big). \tag{5}$$

Proof. From the definition of the edge-degree distance and definition 2.1, we obtain

$$DD_e(\mathcal{D}[G]) = 4 \sum_{x_i x_j \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_i x_j) D_{\mathcal{D}[G]}(x_i x_j).$$

Now by Lemma 2.3 and Eq. (3), we obtain

$$\begin{aligned}
DD_e(\mathcal{D}[G]) =& 4 \sum_{v_i v_j \in E(G)} \big(2d_G(v_i v_j) + 2\big)\Big(4D_G(v_i v_j) + 2\big(d_G(v_i) + d_G(v_j)\big)\Big) \\
=& 4 \sum_{v_i v_j \in E(G)} \Big(8d_G(v_i v_j) D_G(v_i v_j) + 4d_G(v_i v_j)\big(d_G(v_i) + d_G(v_j)\big) \\
&+ 8D_G(v_i v_j) + 4(d_G(v_i) + d_G(v_j))\Big).
\end{aligned}$$

Using the fact that $d_G(v_i v_j) = d_G(v_i) + d_G(v_j) - 2$, we obtain

$$DD_e(\mathcal{D}[G]) = 4\Big(8DD_e(G) + 4\big(F(G) + 2M_2(G) - 2M_1(G)\big) + 16W_e(G) + 4M_1(G)\Big).$$

from which Eq. (5) follows. □

Theorem 2.4. *Let* G *be a graph with* m *edges. The edge-Gutman index of* $\mathcal{D}[G]$ *is given by*

$$\begin{aligned}
Gut_e(\mathcal{D}[G]) =& 64Gut_e(G) + 64DD_e(G) + 64W_e(G) + 32M_2(L(G)) \\
&+ 64F(G) + 128M_2(G) - 176M_1(G) + 128m.
\end{aligned} \tag{6}$$

Proof. Let $v_iv_j \in E(G)$. Then

$$\begin{aligned}
S_{\mathcal{D}[G]}(x_ix_j) = &\sum_{x_rx_s \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_rx_s) d_{\mathcal{D}[G]}(x_ix_j, x_rx_s) + \Big[d_{\mathcal{D}[G]}(y_iy_j) d_{\mathcal{D}[G]}(x_ix_j, y_iy_j) \\
&+ \sum_{\substack{y_iy_s \in E(\mathcal{D}[G]):\\ s \neq j}} d_{\mathcal{D}[G]}(y_iy_s) d_{\mathcal{D}[G]}(x_ix_j, y_iy_s) \\
&+ \sum_{\substack{y_ry_j \in E(\mathcal{D}[G]):\\ r \neq i}} d_{\mathcal{D}[G]}(y_ry_j) d_{\mathcal{D}[G]}(x_ix_j, y_ry_j) \\
&+ \sum_{\substack{y_ry_s \in E(\mathcal{D}[G]):\\ r,s \neq i,j}} d_{\mathcal{D}[G]}(y_ry_s) d_{\mathcal{D}[G]}(x_ix_j, y_ry_s) \Big] \\
&+ \Big[\sum_{x_ry_i \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ry_i) d_{\mathcal{D}[G]}(x_ix_j, x_ry_i) \\
&+ \sum_{x_ry_j \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ry_j) d_{\mathcal{D}[G]}(x_ix_j, x_ry_j) \\
&+ \sum_{\substack{x_ry_s \in E(\mathcal{D}[G]):\\ s \neq i,j}} d_{\mathcal{D}[G]}(x_ry_s) d_{\mathcal{D}[G]}(x_ix_j, x_ry_s) \Big].
\end{aligned}$$

Now by Lemma 2.3, we get

$$\begin{aligned}
S_{\mathcal{D}[G]}(x_ix_j) = &\sum_{v_rv_s \in E(G)} \big(2d_G(v_rv_s) + 2\big) d_G(v_iv_j, v_rv_s) + \Big[\big(2d_G(v_iv_j) + 2\big) \big(d_G(v_iv_j, v_iv_j) + 2\big) \\
&+ \sum_{\substack{v_iv_s \in E(G):\\ s \neq j}} \big(2d_G(v_iv_s) + 2\big) \big(d_G(v_iv_j, v_iv_s) + 1\big) \\
&+ \sum_{\substack{v_rv_j \in E(G):\\ r \neq i}} \big(2d_G(v_rv_j) + 2\big) \big(d_G(v_iv_j, v_rv_j) + 1\big) \\
&+ \sum_{\substack{v_rv_s \in E(G):\\ r,s \neq i,j}} \big(2d_G(v_rv_s) + 2\big) d_G(v_iv_j, v_rv_s) \Big] \\
&+ \Big[\sum_{v_rv_i \in E(G)} \big(2d_G(v_rv_i) + 2\big) \big(d_G(v_iv_j, v_rv_i) + 1\big) \\
&+ \sum_{v_rv_j \in E(G)} \big(2d_G(v_rv_j) + 2\big) \big(d_G(v_iv_j, v_rv_j) + 1\big) \\
&+ \sum_{\substack{v_rv_s \in E(G):\\ s \neq i,j}} \big(2d_G(v_rv_s) + 2\big) d_G(v_iv_j, v_rv_s) \Big] \\
= &\big(2S_G(v_iv_j) + 2D_G(v_iv_j)\big) + \big[4(d_G(v_iv_j) + 1) + 2S_G(v_iv_j) \\
&+ 2D_G(v_iv_j) + 2\delta_G(v_iv_j) + 2(d_G(v_i) - 1) + 2(d_G(v_j) - 1)\big] \\
&+ \big[4S_G(v_iv_j) + 4D_G(v_iv_j) + 2\delta_G(v_iv_j) + 4d_G(v_iv_j) + 2(d_G(v_i) + d_G(v_j))\big] \\
= &8S_G(v_iv_j) + 8D_G(v_iv_j) + 12\big(d_G(v_i) + d_G(v_j)\big) + 4\delta_G(v_iv_j) - 16.
\end{aligned}$$

By symmetry, for each edge $v_iv_j \in E(G)$, we have

$$\begin{aligned} S_{\mathcal{D}[G]}(y_iy_j) =& S_{\mathcal{D}[G]}(x_iy_j) = S_{\mathcal{D}[G]}(x_jy_i) = S_{\mathcal{D}[G]}(x_ix_j) \\ =& 8S_G(v_iv_j) + 8D_G(v_iv_j) + 12\big(d_G(v_i) + d_G(v_j)\big) + 4\delta_G(v_iv_j) - 16. \end{aligned}$$

Now from the definition of the edge-Gutman index and Lemma 2.3, we obtain

$$\begin{aligned} Gut_e(\mathcal{D}[G]) =& 4 \times \frac{1}{2} \sum_{x_ix_j \in E(\mathcal{D}[G])} d_{\mathcal{D}[G]}(x_ix_j) S_{\mathcal{D}[G]}(x_ix_j) \\ =& 2 \sum_{v_iv_j \in E(G)} \big(2d_G(v_iv_j) + 2\big)\Big(8S_G(v_iv_j) + 8D_G(v_iv_j) \\ &+ 12\big(d_G(v_i) + d_G(v_j)\big) + 4\delta_G(v_iv_j) - 16\Big). \end{aligned}$$

Using the fact that $d_G(v_iv_j) = d_G(v_i) + d_G(v_j) - 2$ and by Eq. (1), we obtain

$$\begin{aligned} Gut_e(\mathcal{D}[G]) =& 2 \sum_{v_iv_j \in E(G)} \Big(16d_G(v_iv_j)S_G(v_iv_j) + 16d_G(v_iv_j)D_G(v_iv_j) \\ &+ 24d_G(v_iv_j)\big(d_G(v_i) + d_G(v_j)\big) + 8d_G(v_iv_j)\delta_G(v_iv_j) - 32d_G(v_iv_j) \\ &+ 16S_G(v_iv_j) + 16D_G(v_iv_j) + 24\big(d_G(v_i) + d_G(v_j)\big) + 8\delta_G(v_iv_j) - 32\Big) \\ =& 64Gut_e(G) + 32DD_e(G) + 48(F(G) + 2M_2(G) - 2M_1(G)) \\ &+ 32M_2(L(G)) - 64(M_1(G) - 2m) + 32DD_e(G) + 64W_e(G) \\ &+ 48M_1(G) + 16(F(G) + 2M_2(G) - 4M_1(G) + 4m) - 64m \\ =& 64Gut_e(G) + 64DD_e(G) + 64W_e(G) + 32M_2(L(G)) + 64F(G) \\ &+ 128M_2(G) - 176M_1(G) + 128m, \end{aligned}$$

from which Eq. (6) follows. □

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