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DEGREE BASED TOPOLOGICAL INVARIANTS OF SPLITTING GRAPH

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Abstract. Topological invariants are the graph theoretical tools to the theoretical chemists, that correlates the molecular structure with several chemical reactivity, physical properties or biological activity numerically. A function having a set of networks(graph, molecular structure) as its domain and a set of real numbers as its range is referred as a topological invariant(index). Topological invariants are numerical quantity of a network that are invariant under graph isomorphism. Topological invariants such as Zagreb index, Randić index and multiplicative Zagreb indices are used to predict the bioactiviy of chemical compounds in QSAR/QSPR study. In this paper, we compute the general expression of certain degree based topological invariants such as second Zagreb index, F-index, Hyper-Zagreb index, Symmetric division degree index, irregularity of Splitting graph. And also we obtain upper bound for first and second multiplicative Zagreb indices of Splitting graph of a graph H, $(S^{'}(H))$.

1. Introduction

Throughout this paper, We consider H as a simple, undirected, connected and finite graph(network) with with node set $V(H)$ and the link set $E(H)$, the order of $H = |V(H)| = m$ and the size of $H = |E(H)| = n$. A link $e \in E(H)$ with end nodes x and y, denoted by xy. The number of links having x as an end node is called the *degree* of x in H and represented by $deg_H(x)$ or $deg(x)$.

Topological invariants are numeric parameters which are mathematically derived from the molecular graph and it defines the topology of the molecular graph. The applicability of topological index in chemistry began in 1947 when Wiener, a chemist introduced a well-known distance based parameter called the Wiener index [16], used to determine the physical properties of alkanes. This index was originally defined as the sum of path distances between any two carbon in a hydrogen suppressed molecular structure.

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The study on degree based invariants are started in early $1970^{'}s$. Gutman and Trinajestic have introduced the first and second *Zagreb indices* in [4]. These invariants are entirely depend on the vertex degree as follows.

$$M_1(H) = \sum_{x\in V(H)} (d_H(x))^2 \tag{1}$$

and

$$M_2(H) = \sum_{xy\in E(H)} d_H(x)d_H(y) \tag{2}$$

Recently in [3], Furtula and Gutman defined *"forgotten topological index"* or *"F-index"* as

$$F(H) = \sum_{x\in V(H)} (d_H(x))^3 = \sum_{xy\in E(H)} [(d_H(x))^2 + (d_H(y))^2] \tag{3}$$

F-index is very much similar to first Zagreb index and shows a good predictive ability of physicochemical properties such as entropy and acentric factor. An another Zagreb index related invariant is *Hyper-Zagreb index* and is defined as

$$HM(H) = \sum_{xy\in E(H)} (d_H(x) + d_H(y))^2 \tag{4}$$

It was encountered in [12] by Shirrdel et al. Todeschini et al.[13, 14] introduced the multiplicative version of Zagreb additive graph invariant and named as *first and second multiplicative Zagreb indices* which are defined as

$$\prod_1(H) = \prod_{x\in V(H)} (d_H(x))^2 \tag{5}$$

and

$$\prod_2(H) = \prod_{xy\in E(H)} d_H(x)d_H(y) \tag{6}$$

The *Symmetric division degree index* of a graph is defined in [15] as

$$SDD(H) = \sum_{xy\in E(H)} \frac{d_H(x)^2 + d_H(y)^2}{d_H(x)d_H(y)} \tag{7}$$

The imbalance of a link $e = xy$ of H is defined as $|d_H(x) - d_H(y)|$. The sum of imbalance of all links of H is the *irregularity* of a graph H. This irregularity of a graph H was introduced by Alberson [1], given by

$$irr(H) = \sum_{xy\in E(H)} |d_H(x) - d_H(y)| \tag{8}$$

Now-a-days computing topological invariants for several graph operations has grabbed the attention of many researchers. For more on topological indices of graph operations one can refer [2, 5, 7, 9, 10, 11] . In this article, we compute the general expression of certain degree based topological invariants such as second Zagreb index, F-index, Hyper-Zagreb index, Symmetric division degree index, irregularity of Splitting graph and an upper bound for first and second multiplicative Zagreb indices of Splitting graph of graph H, $(S^{'}(H))$.

2. Preliminary

Graph operations are used to construct new graph from the parent graph. Here, we have studied certain degree based topological invariants of one such operation called *Splitting graph*. It was introduced by Sampathkumar et al. in [8].

Definition 2.1. The *Splitting graph* $S^{'}(H)$ *of a graph* H is obtained by adding to each node x a new node $x^{'}$ such that $x^{'}$ is adjacent to every node that is adjacent to $x \in H$. Thus by the definition of $S^{'}(H)$, we have the following $\left|V(S^{'}(H))\right| = 2m$, $H = \left|E(S^{'}(H))\right| = 3n$, $deg_{S^{'}(H)}(x) = 2deg_H(x)$ and $deg_{S^{'}(H)}(x^{'}) = deg_H(x)$.

Lemma 2.1. (AM-GM inequality [6]). Let $m_1, m_2, ..., m_t$ be nonnegative numbers then

$$\frac{m_1 + m_2 + ... + m_t}{t} \geq \sqrt[t]{m_1 m_2 ... m_t}$$

equality holds if and only if all $m_t^{'}s$ are equal.

Lemma 2.2. (Weighted AM-GM inequality [6]). Let $m_1, m_2, ..., m_t$ be nonnegative numbers and also let $s_1, s_2, ..., s_t$ be nonnegative weights. Set $s = s_1 + s_2 + ... + s_t$. Then the inequality

$$\frac{s_1 m_1 + s_2 m_2 + ... + s_t m_t}{s} \geq \sqrt[s]{m_1^{s_1} m_2^{s_2} ... m_t^{s_t}}$$

equality holds if and only if all $m_t^{'}s$ with $s_1 > 0$ are equal.

Result 2.1. [17]. $M_1(S^{'}(H)) = 5M_1(H)$

3. Main Results

3.1. Degree Based Topological Invariants of Splitting Graph.

In this section, we compute the general expression of certain degree based topological invariants such as second Zagreb index, F-index, Hyper-Zagreb index, Symmetric division degree index, irregularity of a Splitting graph and an upper bound for first and second multiplicative Zagreb indices of Splitting graph of a graph H, $(S^{'}(H))$.

Theorem 1. *Let H be any graph. Then the second Zagreb index of splitting graph of H denoted by $M_2(S^{'}(H))$ is*

$$M_2(S^{'}(H)) = 8M_2(H)$$

Proof. From the definition of the second Zagreb index we have

$$M_2(H) = \sum_{xy \in E(H)} d_H(x) d_H(y)$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x') = deg_H(x)$. Therefore,

$$M_2(S^{'}(H)) = \sum_{xx^{'} \in E(S^{'}(H))} (d_{S'(H)}(x) d_{S'(H)}(x'))$$

$$
\begin{aligned}
&= \sum_{xx' \in E(H)} (2d_H(x)2d_H(x')) + \sum_{xx' \in E(H)} (2d_H(x)d_H(x'))(d_H(x)2d_H(x')) \\
&= \sum_{xx' \in E(H)} 4(d_H(x)d_H(x')) + \sum_{xx' \in E(H)} 4(d_H(x)d_H(x')) \\
&= 8M_2(H).
\end{aligned}
$$

□

Theorem 2. *Let H be any graph. Then the F-index of splitting graph of H denoted by $F(S^{'}(H))$ is*

$$F(S^{'}(H)) = 9F(H)$$

Proof. From the definition of the F-index we have

$$F(H) = \sum_{x \in V(H)} (d_H(x))^3 = \sum_{xy \in E(H)} [(d_H(x))^2 + (d_H(y))^2]$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$
\begin{aligned}
F(S^{'}(H)) &= \sum_{xx' \in E(S'(H))} [(d_{S'(H)}(x))^2 + (d_{S'(H)}(x^{'}))^2] \\
&= \sum_{xx' \in E(H)} [(2d_H(x))^2 + (2d_H(x^{'}))^2] \\
&+ \sum_{xx' \in E(H)} [(2d_H(x))^2 + (d_H(x^{'}))^2] + [(d_H(x))^2 + (2d_H(x^{'}))^2] \\
&= \sum_{xx' \in E(H)} [4(d_H(x))^2 + 4(d_H(x^{'}))^2] \\
&+ \sum_{xx' \in E(H)} [4(d_H(x))^2 + (d_H(x^{'}))^2] + [(d_H(x))^2 + 4(d_H(x^{'}))^2] \\
&= 4F(H) + 5F(H) \\
&= 9F(H).
\end{aligned}
$$

□

Theorem 3. *Let H be any graph. Then the Hyper-Zagreb index of splitting graph of H denoted by $HM(S^{'}(H))$ is*

$$HM(S^{'}(H)) = 4HM(H) + 5F(H) + 8M_2(H).$$

Proof. From the definition of the Hyper-Zagreb index we have

$$HM(H) = \sum_{xy \in E(H)} (d_H(x) + d_H(y))^2$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$\begin{aligned}
HM(H) &= \sum_{xx^{'} \in E(H)} (d_H(x) + d_H(x^{'}))^2 \\
&= \sum_{xx^{'} \in E(H)} [(2d_H(x)) + (2d_H(x^{'}))]^2 \\
&+ \sum_{xx^{'} \in E(H)} [(2d_H(x)) + (d_H(x^{'}))]^2 + [(d_H(x)) + (2d_H(x^{'}))]^2 \\
&= \sum_{xx^{'} \in E(H)} 4[(d_H(x)) + (d_H(x^{'}))]^2 \\
&+ \sum_{xx^{'} \in E(H)} [(2d_H(x)) + (d_H(x^{'}))]^2 + [(d_H(x)) + (2d_H(x^{'}))]^2 \\
&= \sum_{xx^{'} \in E(H)} 4[(d_H(x)) + (d_H(x^{'}))]^2 \\
&+ \sum_{xx^{'} \in E(H)} 5[(d_H(x))^2 + (d_H(x^{'}))^2] + \sum_{xx^{'} \in E(H)} 8[d_H(x) d_H x^{'}] \\
&= 4HM(H) + 5F(H) + 8M_2(H).
\end{aligned}$$

□

Theorem 4. *Let H be any graph. Then the Symmetric Division Degree index of splitting graph of H denoted by $SDD(S^{'}(H))$ is*

$$SDD(S^{'}(H)) = \frac{7}{2} SDD(H)$$

Proof. From the definition of the Symmetric Division Degree index we have

$$SDD(H) = \sum_{xy \in E(H)} \frac{d_H(x)^2 + d_H(y)^2}{d_H(x) d_H(y)}$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$\begin{aligned}
SDD(S^{'}(H)) &= \sum_{xx^{'} \in E(S'(H))} \frac{d_{S'(H)}(x)^2 + d_{S'(H)}(x^{'})^2}{d_{S'(H)}(x) d_{S'(H)}(x')} \\
&= \sum_{xx^{'} \in E(H)} \frac{(2d_H(x))^2 + (2d_H(x^{'}))^2}{2d_H(x) 2d_H(x')} \\
&+ \sum_{xx^{'} \in E(H)} \frac{(2d_H(x))^2 + d_H(x^{'})^2}{2d_H(x) d_H(x')} + \sum_{xx^{'} \in E(H)} \frac{d_H(x)^2 + (2d_H(x^{'}))^2}{d_H(x) 2d_H(x')} \\
&= \sum_{xx^{'} \in E(H)} \frac{4d_H(x)^2 + 4d_H(x^{'})^2}{4d_H(x) d_H(x')} + \sum_{xx^{'} \in E(H)} \frac{5d_H(x)^2 + 5d_H(x^{'})^2}{2d_H(x) d_H(x')}
\end{aligned}$$

$$= SDD(H) + \frac{5}{2}SDD(H)$$
$$= \frac{7}{2}SDD(H).$$

□

Theorem 5. *Let H be any graph. Then the irregularity of splitting graph of H denoted by $irr(S^{'}(H))$ is*

$$irr(S^{'}(H)) = 5(irr(H))$$

Proof. From the definition of the irregularity of a graph we have

$$irr(H) = \sum_{xy \in E(H)} |d_H(x) - d_H(y)|$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$\begin{aligned} irr(H) &= \sum_{xx^{'} \in E(S^{'}(H))} \left| d_{S'(H)}(x) - d_{S'(H)}(x^{'}) \right| \\ &= \sum_{xx^{'} \in E(H)} \left| 2d_{(H)}(x) - 2d_{(H)}(x^{'}) \right| + \sum_{xx^{'} \in E(H)} \left| 2d_{(H)}(x) - d_{(H)}(x^{'}) \right| \\ &+ \sum_{xx^{'} \in E(H)} \left| d_{(H)}(x) - 2d_{(H)}(x^{'}) \right| \\ &\geq \sum_{xx^{'} \in E(H)} 2\left| d_{(H)}(x) - d_{(H)}(x^{'}) \right| + \sum_{xx^{'} \in E(H)} 3\left| d_{(H)}(x) - d_{(H)}(x^{'}) \right| \\ &= 5(irr(H)). \end{aligned}$$

□

Theorem 6. *Let H be any graph. Then the first multiplicative Zagreb index of splitting graph of H denoted by $\prod_1(S^{'}(H))$ is*

$$\prod_1(S^{'}(H)) \leq 4^m \left(\frac{M_1(H)}{m}\right)^{2m}$$

Equality holds if and only if H is a regular graph.

Proof. From the definition of the first multiplicative Zagreb index we have

$$\prod_1(H) = \prod_{x \in V(H)} (d_H(x))^2$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$\begin{aligned} \prod_1(S^{'}(H)) &= \prod_{x \in V(S'(H))} (d_{S'(H)}(x))^2 \prod_{x' \in V(S'(H))} (d_{S'(H)}(x^{'}))^2 \\ &= \prod_{x \in V(H)} (2d_H(x))^2 \prod_{x \in V(H)} (d_H(x))^2 \end{aligned}$$

$$= \prod_{x\in V(H)} 4d_H(x)^2 \prod_{x\in V(H)} d_H(x)^2$$

Thus by using the Lemma 2.1, we have

$$\begin{aligned}\prod_1(S^{'}(H)) &\leq \left(4\frac{\sum_{x\in V(H)}(d_H(x))^2}{m}\right)^m \left(\frac{\sum_{x\in V(H)}(d_H(x))^2}{m}\right)^m\\ &= \left(4\frac{M_1(H)}{m}\right)^m \left(\frac{M_1(H)}{m}\right)^m\\ &\leq 4^m \left(\frac{M_1(H)}{m}\right)^{2m}\\ &= 4^m \left(\frac{M_1(H)}{m}\right)^{2m}\end{aligned}$$

Therefore, the equality holds good if H is a regular graph. □

Theorem 7. *Let H be any graph. Then the second multiplicative Zagreb index of splitting graph of H denoted by $\prod_1(S^{'}(H))$ is*

$$\prod_2(S^{'}(H)) \leq 2^{4m}\left(\frac{M_2(H)}{m}\right)^{3m}$$

Equality holds if and only if H is a regular graph.

Proof. From the definition of the second multiplicative Zagreb index we have

$$\prod_2(S^{'}(H)) = \prod_{xy\in E(H)} d_H(x)d_H(y)$$

By the definition of Splitting graph of H, we have $deg_{S'(H)}(x) = 2deg_H(x)$ and $deg_{S'(H)}(x^{'}) = deg_H(x)$. Therefore,

$$\begin{aligned}\prod_2(S^{'}(H)) &= \prod_{xx^{'}\in E(S^{'}(H))} (d_{S^{'}(H)}(x)) \prod_{xx^{'}\in E(S^{'}(H))} (d_{S^{'}(H)}(x^{'}))\\ &= \prod_{xx^{'}\in E(H)} (2d_H(x))(2d_H(x^{'})) \prod_{xx^{'}\in E(H)} (2d_H(x))(d_H(x^{'})) \prod_{xx^{'}\in E(H)} (d_H(x))(2d_H(x^{'}))\\ &= \prod_{xx^{'}\in E(H)} 4d_H(x)d_H(x^{'}) \prod_{xx^{'}\in E(H)} 2d_H(x)d_H(x^{'}) \prod_{xx^{'}\in E(H)} 2d_H(x)d_H(x^{'})\end{aligned}$$

Thus by using the Lemma 2.1, we have

$$\begin{aligned}\prod_2(S^{'}(H)) &\leq \left(4\frac{\sum_{xx^{'}\in E(H)}(d_H(x))(d_H(x^{'}))}{m}\right)^m \left(2\frac{\sum_{xx^{'}\in E(H)}(d_H(x))(d_H(x^{'}))}{m}\right)^m\\ &\quad \left(2\frac{\sum_{xx^{'}\in E(H)}(d_H(x))(d_H(x^{'}))}{m}\right)^m\\ &= \left(4\frac{M_2(H)}{m}\right)^m \left(2\frac{M_2(H)}{m}\right)^m \left(2\frac{M_2(H)}{m}\right)^m\end{aligned}$$

$$\leq 2^{4m}\left(\frac{M_2(H)}{m}\right)^{3m}$$
$$= 2^{4m}\left(\frac{M_2(H)}{m}\right)^{3m}$$

Therefore, the equality holds good if H is a regular graph. □

4. Conclusion

In this article, we compute the general expression of certain degree based topological invariants such as second Zagreb index, F-index, Hyper-Zagreb index, Symmetric division degree index, irregularity of Splitting graph and an upper bound for first and second multiplicative Zagreb indices of Splitting graph of a graph H, $(S^{'}(H))$.

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