Degree Based Indices of Rhomtrees and Line Graph of Rhomtrees

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Abstract

Rhotrix theory deals with array of numbers in rhomboid mathematical form. The graphical representation of rhotrix of dimension n is known as rhomtree. In this paper the degree based indices of rhomtrees and line graph of rhomtrees are computed.

Keywords: first Zagreb index, forgotten index, hyper Zagreb index, irregularity index, Rhotrix, second Zagreb index.

1. Introduction

Let G (V, E)be a simple undirected graph. In the field of chemical graph theory and in mathematical chemistry, a topological index, also known as a connectivity index, is a type of a molecular descriptor that is calculated based on the distance between the atoms of molecular graph. Topological indices [3] are used for example in the development of quantitative structure-activity relationship (QSAR) and quantitative structure - property relationship (QSPR) in which the biological activity or other properties of molecules are correlated with their chemical structure. Among different topological indices, degree-based topological indices are most studied and have some important applications in chemical graph theory [8]. In [7] it was reported that the first and second Zagreb indices are useful in anti-inflammatory activities study of certain chemicals. In the same paper the F-index was introduced which is the sum of the cubes of the vertex degrees. In [4, 6], the authors reinvestigated the index and named it forgotten topological index or F-index. The F-index is defined as F(G)= $\sum_{uv\in E(G)}\left[d_G(u)^2+d_G(v)^2\right]$. In [4] this index is studied for different graph operations and in [5] the co-index version is introduced. Albetson in [2] defined another degree based topological index called irregularity of G as Irr (G) = $\sum_{uv\in E(G)}\left|d_G(u)-d_G(v)\right|$. The first and second Zagreb indices of a graph are denoted by $M_1(G)$ and $M_2(G)$ and are, respectively, defined as $M_1(G)= \sum_{uv\in E(G)}[d_G(u)+d_G(v)]$ and $M_2(G) = \sum_{uv\in E(G)}[d_G(u)d_G(v)]$. These indices are one of the oldest and extensively studied topological indices in both mathematical and chemical literature; for details interested readers are referred to [10]. Shirdel et al. [13] introduced a new version of Zagreb index and named as hyper-Zagreb index, which is defined as HM (G)= $\sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2$.

Construction of Rhomtree

The structure of n-dimensional rhotrix is as follows:

$$R_n = \left\langle \begin{array}{ccccccccc} & & & & a_{11} & & & & \\ & & & a_{21} & c_{11} & a_{12} & & & \\ & & a_{31} & c_{21} & a_{22} & c_{12} & a_{13} & & \\ & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ a_{t1} & c_{t-11} & & & h(R) & & & c_{1t-1} & a_{1t} \\ & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\ & & a_{tt-2} & c_{t-1t-2} & a_{t-1t-1} & c_{t-2t-1} & a_{t-2t} & & \\ & & & a_{tt-1} & c_{t-1t-1} & a_{t-1t} & & & \\ & & & & a_{tt} & & & & \end{array} \right\rangle$$

where a_{11}, a_{12}, … a_{tt} denote the major entries and c_{11}, c_{12}, … $c_{t-1}c_{t-1}$ in R_n denote the minor entries of the rhotrix by sani [11,12]. A Rhotrix would always have an odd dimension. Any n-dimensional Rhotrix R_n, will have $|R_n| = \frac{1}{2}(n^2+1)$ entries by Ajibade [1] and $n \in 2Z^+ + 1$. A heart of a Rhotrix denoted by h(R) is defined as the element at the perpendicular intersection of the two diagonals of a Rhotrix. Let $\hat{R}(n)$ be a set consisting all real rhotrices of dimension $n \in 2Z^+ + 1$ and let R(n) be any rhotrix in $\hat{R}(n)$. Then the graphical representation of rhotrix R(n) is a rhomtree T(m), with m $= \frac{1}{2}(n^2+1)$ number of vertices and $\frac{1}{2}(n^2-1)$ number of edges, having four components of binary branches and each component is bridged to the root vertex by one incident edge.

If n=7, then $\hat{R}(7)$ is a set consisting of all real rhotrices of dimension three and let R(7) be any element in $\hat{R}(7)$ given by

$$R_7 = \left\langle \begin{array}{ccccccc} & & & a_{11} & & & \\ & & a_{21} & c_{11} & a_{12} & & \\ & a_{31} & c_{21} & a_{22} & c_{12} & a_{13} & \\ a_{14} & c_{31} & a_{32} & c_{22} & a_{23} & c_{13} & a_{14} \\ & a_{42} & c_{32} & a_{33} & c_{23} & a_{24} & \\ & & a_{43} & c_{33} & a_{34} & & \\ & & & a_{44} & & & \end{array} \right\rangle$$

with r_{13} = h(R) is the heart of the rhotrix. If we take each entry in R(7) as a node point and connecting all of the entries as network of twenty five vertices using a particular pattern or style for the construction, in such a way that the heart vertex will serve as the root of the tree while the non heart vertices will serve as branches, then a rhomtree T(25) corresponding to the rhotrix R(7) is obtained and shown in Fig.1.

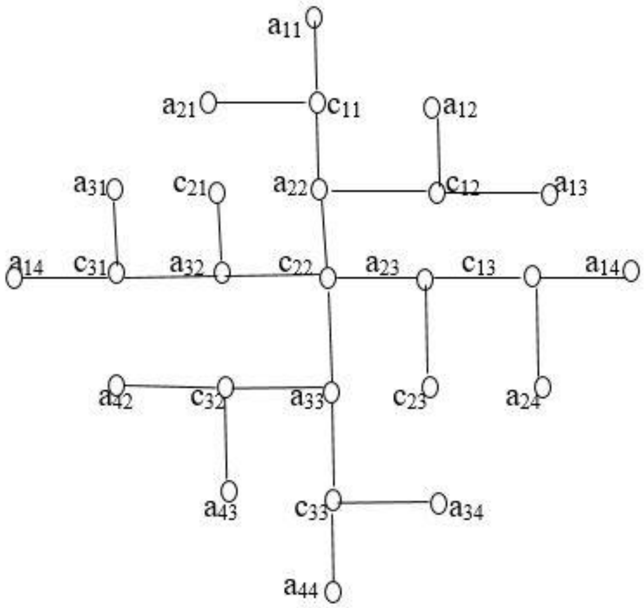

fig.1 Rhomtree T(25)

The line graph of [T (25)] is given in Fig.2

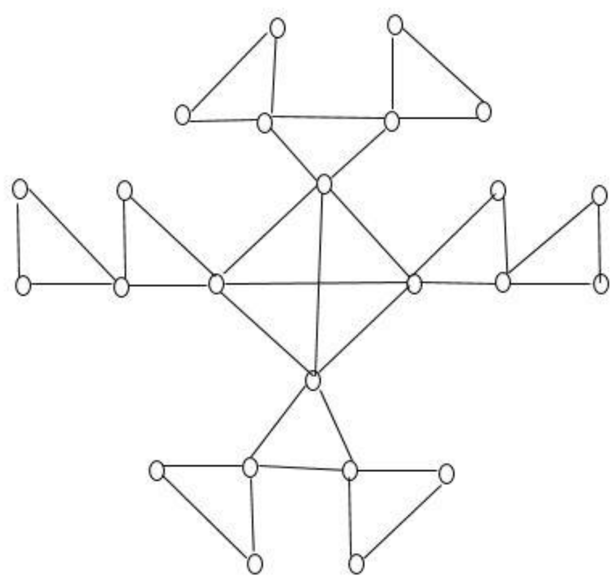

fig.2 L(T(25))

Let G=T(m) be the rhomtree of order m=$\frac{1}{2}(n^2+1)$. The partitions of the vertex set V (G) are denoted by V_i (G), where $v \in V_i(G)$ if d(v)= i. Thus the following partitions of the vertex set are obtained.

V_1= {v∈V(G): d(v)=1},V_3= {v∈V(G):d(v)=3} and V_4= {v∈V(G):d(v)=4}

From the structure of rhomtree, the cardinality of V_1, V_3 and V_4 are given below:
$|V_1| = \frac{1}{4}(n^2+7)$, $|V_3| = \frac{1}{4}(n^2-9)$ and $|V_4| = 1$

The edge set of G can also be divided into three partitions based on the sum of degrees of the end vertices and it is denoted by E_j so that if $e = uv \in E_j$ then $d(u) + d(v) = j$ for $\delta(G) \le j \le \Delta(G)$. Thus the edge set of G is the union of E_4, E_6 and E_7. The edge sets E_4, E_6 and E_7, which are subsets of E (G) are as follows:

$E_4=\{e=uv\in E(G):d(u)=1, d(v)=3\}$, $E_6=\{e=uv\in E(G):d(u)=3, d(v)=3\}$ and
$E_7= \{e=uv\in E(G): d(u)=3, d(v)=4\}$.

In this case from direct calculations, the cardinality of E_4, E_6 and E_7 are respectively $\frac{1}{4}(n^2+7)$, $\frac{1}{4}(n^2-25)$ and 4. The partitions of the vertex set V (G) and edge set E (G) are given in Table 1 and Table 2 respectively.

Vertex partition	V_1	V_3	V_4
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-9)$	1

Table1: The vertex partition of Rhomtree T (m)

Edge partition	E_4	E_6	E_7
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-25)$	4

Table 2: The edge partition of Rhomtree T (m)

Similarly the vertex set and edge set of line graph of rhomtree can be partitioned. The partitions of the vertex set of L (G) are given by
$V_2^*= \{v\in V(L(G)): d(v)=2\}$, $V_4^*= \{v\in V(L(G)):d(v)=4\}$ and $V_5^*= \{v\in V(L(G)):d(v)=5\}$.

Vertex Partition of L(G)	V_2^*	V_4^*	V_5^*
Cardinality	$\frac{1}{4}(n^2+7)$	$\frac{1}{4}(n^2-25)$	4

Table 3: The Vertex partition of L (T (m))

The partitions of the edge set of L(G) are given by
$E_4^*=\{e=uv\in E(L(G)): d(u)=2 , d(v)=2\}$, $E_6^*=\{e=uv\in E(L(G)) :d(u)=2, d(v)=4\}$ and
$E_7^*=\{e=uv\in E(G): d(u)=2, d(v)=5\}$, $E_8^*=\{e=uv\in E(G): d(u)=4, d(v)=4\}$
$E_9^*=\{e=uv\in E(G): d(u)=4, d(v)=5\}$, $E_{10}^*=\{e=uv\in E(G): d(u)=5, d(v)=5\}$

Edge partition of L(G)	E_4^*	E_6^*	E_7^*	E_8^*	E_9^*	E_{10}^*
Cardinality	n-1	$\frac{1}{2}(n^2-4n+7)$	2	$\frac{1}{4}(n^2+4n-69)$	6	6

Table 4: The Edge partition of L (T (m))

2. F-index, irregularity index of T(m) and L(T(m))

Theorem 2.1 The F- index of Rhomtree T (m) is given by F (G)= $\frac{1}{2}\left(7n^2+5\right)$

Proof F index of rhomtree T (m) is

$$F(G)=\sum_{uv\in E(G)}\left[d_G(u)^2+d_G(v)^2\right]$$

$$=\sum_{uv\in E_4}\left[d_G(u)^2+d_G(v)^2\right]+\sum_{uv\in E_6}\left[d_G(u)^2+d_G(v)^2\right]+\sum_{uv\in E_7}\left[d_G(u)^2+d_G(v)^2\right]$$

$$=\left|E_4^*\right|(10)+\left|E_6^*\right|(18)+\left|E_7^*\right|(25)=\frac{1}{4}\left(n^2+7\right)(10)+\frac{1}{4}\left(n^2-25\right)(18)+4(25)=\frac{1}{2}\left(7n^2+5\right)$$

Theorem 2.2 The F index of Line graph of Rhomtree L (T (m)) is given by

F (L (T(m))) = $18n^2+114$

Proof The F-index of Line graph of T (m) is

$$F(L(G))=\sum_{uv\in E(G)}[d_G(u)^2+d_G(v)^2]$$

$$=\sum_{uv\in E_4^*}[d_G(u)^2+d_G(v)^2]+\sum_{uv\in E_6^*}[d_G(u)^2+d_G(v)^2]+\sum_{uv\in E_7^*}[d_G(u)^2+d_G(v)^2]+$$

$$\sum_{uv\in E_8^*}[d_G(u)^2+d_G(v)^2]+\sum_{uv\in E_9^*}[d_G(u)^2+d_G(v)^2]+\sum_{uv\in E_{10}^*}[d_G(u)^2+d_G(v)^2]$$

$$=\left|E_4^*\right|(8)+\left|E_6^*\right|(20)+\left|E_7^*\right|(29)+\left|E_8^*\right|(32)+\left|E_9^*\right|(41)+\left|E_{10}^*\right|(50)$$

$$=(n-1)(8)+\frac{1}{2}\left(n^2-4n+7\right)(20)+2(29)+\frac{1}{4}\left(n^2+4n-69\right)(32)+6(41)+6(50)=18n^2+114.$$

Theorem 2.3 The third Zagreb index or irregularity index of Rhomtree T (m) is given by

iir (T(m))= $\frac{1}{2}\left(n^2+15\right)$

Proof The irr-index of T (m) is

$$irr(G) = \sum_{uv\in E(G)} \left|d_G(u) - d_G(v)\right|$$

$$= \sum_{uv\in E_4^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_6^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_7^*} \left|d_G(u) - d_G(v)\right|$$

$$= \left|E_4^*\right|(2) + \left|E_6^*\right|(0) + \left|E_7^*\right|(1) = \frac{1}{4}(n^2+7)(2) + \frac{1}{4}(n^2-25)(0) + 4(1) = \frac{1}{2}(n^2+15)$$

Theorem 2.4 The third Zagreb index or irregularity index of Line graph of Rhomtree L (T (m)) is given by iir (L (T(m)))= n^2-4n+19

Proof The irr-index of Line graph of T (m) is

$$irr(L(G)) = \sum_{uv\in E_4^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_6^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_7^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_8^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_9^*} \left|d_G(u) - d_G(v)\right| + \sum_{uv\in E_{10}^*} \left|d_G(u) - d_G(v)\right|$$

$$= \left|E_4^*\right|(0) + \left|E_6^*\right|(2) + \left|E_7^*\right|(3) + +\left|E_8^*\right|(0) + \left|E_9^*\right|(1) + \left|E_{10}^*\right|(0)$$

$$= (n-1)(0) + \frac{1}{2}(n^2-4n+7)(2) + 2(3) + \frac{1}{4}(n^2+4n-69)(0) + 6(1) + 6(0) = n^2-4n+19$$

3. First, Second Zagreb index and hyper Zagreb index of Rhomtree and Line graph of Rhomtree

Theorem 3.1 The First Zagreb index of Rhomtree T (m) is given by M_1 (T (m)) = $\frac{5}{2}(n^2-1)$

Proof The M_1-index of T (m) is

$$M_1(G) = \sum_{uv\in E(G)} \left[d_G(u) + d_G(v)\right]$$

$$= \sum_{uv\in E_4^*} \left[d_G(u) + d_G(v)\right] + \sum_{uv\in E_6^*} \left[d_G(u) + d_G(v)\right] + \sum_{uv\in E_7^*} \left[d_G(u) + d_G(v)\right]$$

$$= \left|E_4^*\right|(4) + \left|E_6^*\right|(6) + \left|E_7^*\right|(7) = \frac{1}{4}(n^2+7)(4) + \frac{1}{4}(n^2-25)(6) + 4(7) = \frac{5}{2}(n^2-1)$$

Theorem 3.2 The First Zagreb index of Line graph of Rhomtree L (T (m)) is given by

M_1 (L (T(m)))= $5n^2+7$

Proof The M_1-index of Line graph of T (m) is

$$M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$

$$= \sum_{uv\in E_4^*}\left[d_G(u)+d_G(v)\right]+\sum_{uv\in E_6^*}\left[d_G(u)+d_G(v)\right]+\sum_{uv\in E_7^*}\left[d_G(u)+d_G(v)\right]$$

$$+\sum_{uv\in E_8^*}[d_G(u)+d_G(v)]+\sum_{uv\in E_9^*}\left[d_G(u)+d_G(v)\right]+\sum_{uv\in E_{10}^*}\left[d_G(u)+d_G(v)\right]$$

$$=\left|E_4^*\right|(4)+\left|E_6^*\right|(6)+\left|E_7^*\right|(7)+\left|E_8^*\right|(8)+\left|E_9^*\right|(9)+\left|E_{10}^*\right|(10)$$

$$=(n-1)(4)+\frac{1}{2}\left(n^2-4n+7\right)(6)+2(7)+\frac{1}{4}\left(n^2+4n-69\right)(8)+6(9)+6(10)=5n^2+7$$

Theorem 3.3 The Second Zagreb index of Rhomtree T (m) is given by M_2 (T(m)) = $3\left(n^2-1\right)$

Proof The M_2-index of T (m) is

M_2 (G) = $\sum_{uv\in E(G)}\left[d_G(u)d_G(v)\right]$.

$$= \sum_{uv\in E_4^*} d_G(u)d_G(v)+\sum_{uv\in E_6^*} d_G(u)d_G(v)+\sum_{uv\in E_7^*} d_G(u)d_G(v)$$

$$=\left|E_4^*\right|(3)+\left|E_6^*\right|(9)+\left|E_7^*\right|(12)$$

$$=\frac{1}{4}\left(n^2+7\right)(3)+\frac{1}{4}\left(n^2-25\right)(9)+4(12)$$

$$=3\left(n^2-1\right)$$

Theorem 3.4 The Second Zagreb index of Line graph of Rhomtree L(T(m)) is given by

M_2 (L(T(m)))= $8n^2+4n+38$

Proof The M_2-index of line graph of T(m) is

M_2 (G) = $\sum_{uv\in E(G)} d_G(u)d_G(v)$.

$$= \sum_{uv\in eE_4^*} d_G(u)d_G(v)+\sum_{uv\in E_6^*} d_G(u)d_G(v)+\sum_{uv\in E_7^*} d_G(u)d_G(v)+\sum_{uv\in E_8^*} d_G(u)d_G(v)$$

$$+\sum_{uv\in E_9^*} d_G(u)d_G(v)+\sum_{uv\in E_{10}^*} d_G(u)d_G(v)$$

$$=\left|E_4^*\right|(4)+\left|E_6^*\right|(8)+\left|E_7^*\right|(10)+\left|E_8^*\right|(16)+\left|E_9^*\right|(20)+\left|E_{10}^*\right|(25)$$

$$=(n-1)(4)+\frac{1}{2}\left(n^2-4n+7\right)(8)+2(10)+\frac{1}{4}\left(n^2+4n-69\right)(16)+6(20)+6(25)=8n^2+4n+38$$

Theorem 3.5 The HM index of Rhomtree T(m) is given by HM(T(m))= $13n^2-1$

Proof The HM-index of T(m) is

HM (G) = $\sum_{uv\in E(G)}[d_G(u)+d_G(u)]^2$

$$= \sum_{uv\in E_4^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_6^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_7^*}\left[d_G(u)+d_G(v)\right]^2$$

$$=\left|E_4^*\right|(16)+\left|E_6^*\right|(36)+\left|E_7^*\right|(49)=\frac{1}{4}\left(n^2+7\right)(16)+\frac{1}{4}\left(n^2-25\right)(36)+4(49)\ =13n^2-1$$

Theorem 3.6 The HM index of Line graph of Rhomtree L (T(m)) is given by
HM (L(T(m)))= $34n^2+8n+190$

Proof The HM-index of line graph of T (m) is

HM (L (G)) = $\sum_{uv\in E(G)}[d_G(u)+d_G(u)]^2$

$$= \sum_{uv\in E_4^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_6^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_7^*}\left[d_G(u)+d_G(v)\right]^2$$

$$+ \sum_{uv\in E_8^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_9^*}\left[d_G(u)+d_G(v)\right]^2 + \sum_{uv\in E_{10}^*}\left[d_G(u)+d_G(v)\right]^2$$

$$=\left|E_4^*\right|(16)+\left|E_6^*\right|(36)+\left|E_7^*\right|(49)+\left|E_8^*\right|(64)+\left|E_9^*\right|(81)+\left|E_{10}^*\right|(100)$$

$$=(n-1)(16)+\frac{1}{2}\left(n^2-4n+7\right)(36)+2(49)+\frac{1}{4}\left(n^2+4n-69\right)(64)+6(81)+6(100)\ =\ 34n^2+8n+190$$

Conclusion

The molecular name for T(25) is 4,4- Bis-(1-isopropyl-2-methyl-propyl)-2,3,5,6-tetramethyl-heptane and that of T(41) is 4-(1-Isopropyl-2-methyl-propyl)-5-[1-(1-isopropyl-2-methyl-propyl)-2,3-dimethyl-butyl]-2,3,6,7,8-pentamethyl-5-(1,2,3-trimethyl-butyl)-nonane. In chemical graph theory, topological indices provide an important tool to quantify the molecular structure and it is found that there is a strong correlation between the properties of chemical compounds and their molecular structure. Among different topological indices, degree-based topological indices are most studied and have some important applications. In this study, degree-based topological indices are calculated for rhomtrees and line graph of rhomtrees.

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