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Research Article

Inverse Problem for the Forgotten and the Hyper Zagreb Indices of Trees

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Abstract: Let $G = (E(G), V(G))$ be a (molecular) graph with vertex set $V(G)$ and edge set $E(G)$. The forgotten Zagreb index and the hyper Zagreb index of G are defined by $F(G) = \sum_{u \in V(G)} d(u)^3$ and $HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2$ where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in G, respectively. A recent problem called the inverse problem deals with the numerical realizations of topological indices. We see that there exist trees for all even positive integers with $F(G) > 88$ and with $HM(G) > 158$. Along with the result, we show that there exist no trees with $F(G) < 90$ and $HM(G) < 160$ with some exceptional even positive integers and hence characterize the forgotten Zagreb index and the hyper Zagreb index for trees.

Keywords: Topological Index, The Forgotten Zagreb Index, The hyper Zagreb Index

AMS Subject classification: 05C05, 05C09, 05C10, 05C92

1. Introduction

A topological index is a molecular descriptor that forms a relation from the set of chemical compounds to the set of positive real numbers enumerated from the molecular graphs. A molecular graph is the topological representation of a chemical compound with atoms as the vertices and the chemical bonds between the two atoms as the edges between the vertices, respectively. Here, we consider undirected and connected molecular graphs with no loops and cycles. The significance of the topological indices is increasing abundantly [1–3, 7, 8]. Most of the topological indices

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show close correlation with some of the physicochemical properties of the chemical compounds, thus enhancing the importance of more research on various topological indices, thereby reducing the number of experiments to be conducted which is time consuming and expensive.

In the field of combinatorial chemistry, inverse problem plays an important role in the discovery of new drugs [5, 6]. The inverse problem promises the feasibility of finding a graph whose invariant value equals to a given integer for the integer-valued problems. There are a few degree-based indices acquainted in testing the properties of compounds and drugs which have been generally utilized in chemical and pharmaceutical engineering [4]. We investigate two of them, viz., the forgotten Zagreb index denoted by $F(G)$ and the hyper Zagreb index denoted by $HM(G)$, defined as

$$F(G) = \sum_{u \in V(G)} d(u)^3 \tag{1}$$

and

$$HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2 \tag{2}$$

where $d(u)$ and $d(v)$ are the degrees of the vertices u and v in graph G, respectively. Yurtas et al.[9] have solved the inverse problem for the first and second Zagreb indices for trees and unicyclic graphs. They have characterized the indices for molecular graphs. They have presented that characterizing the possible values of the F-index of trees and unicyclic graphs as open problems [9].

In this paper, we investigate the idea of the inverse problem for trees with respect to the forgotten and hyper Zagreb indices and hence characterize the F-Index and HM-Index for trees. To achieve this, we use various equations and constructions stated in the preliminaries (Section 2). In Section 3, we settle the inverse problem of the forgotten Zagreb index of trees. The inverse problem of the hyper Zagreb index of trees is solved in Section 4.

2. Preliminaries

The forgotten and hyper Zagreb indices can take only even positive integers [9]. Let G be a graph with vertices u and v where uv forms an edge of the graph G. We subdivide each edge uv by introducing a new vertex to obtain a new graph say G^*. Then we can see that the forgotten Zagreb index of the new graph G^* will be eight more than that of the graph G [9]. This is given by the expression,

$$F(G^*) = F(G) + 8. \tag{3}$$

Similarly, if we introduce a new vertex by the subdivision of an edge, say, uv of graph G with at least one of the vertices of degree 2, the hyper Zagreb index will be increased by 16. The expression for the hyper Zagreb index of the new graph G^* found in [9], is,

$$HM(G^*) = HM(G) + 16. \tag{4}$$

3. The Forgotten Zagreb Index of Trees

In this section, we characterize the forgotten Zagreb index of trees.

Theorem 1. *The forgotten Zagreb index of trees can be any even positive integer except 4, 6, 8, 12, 14, 16, 20, 22, 24, 28, 32, 36, 40, 44, 48, 52, 56, 60, 64, 72, 80 and 88.*

Proof. The proof of the theorem is presented in two parts. To prove the first part of the theorem, say, the establishment of existence of a tree G with $F(G) > 88$ for all even positive integers, we establish a set of trees F_0, F_2, F_4 and F_6 with F-indices 96, 2, 68 and 30, respectively. These numbers are congruent to 0, 2, 4 and 6 (mod 8). The trees F_0, F_2, F_4 and F_6 are given in Figure 1 (a), (b), (c) and (d).
Let us begin with the tree F_0. The subdivision of an edge uv in F_0 constructs a new tree with F-index 108 using Equation (3). The repeated subdivision of an edge uv in F_0 generates trees with F-indices 108, 116, 124, ... These numbers are integers of the form $96 + 8k$ where k is the number of subdivisions. Now, the same construction method in F_2, F_4 and F_6 enables us to generate trees with F-indices of the form $2+8k$ giving the integers $2, 10, 18, \ldots, 90, \ldots$; $68 + 8k$ giving $68, 76, 84, 92, \ldots$ and $30 + 8k$ giving $30, 38, 46, \ldots, 94, \ldots$, respectively, where k is again the number of subdivisions in the corresponding graph. We can easily see that all even positive integers greater than 88 are covered by the subdivisions of F_0, F_2, F_4 and F_6. Precisely, all the even positive integers mod 2, 4, 6 greater than 88 are covered by the subdivisions of F_2, F_4 and F_6, respectively. In the second part of the proof, we show that there exist

(a) F_0 (b) F_2 (c) F_4 (d) F_6

Figure 1. **The graphs** F_0, F_2, F_4, F_6

no trees with the F-indices mentioned in the Table 1. For this, we consider three different cases.

Case 1. $F(G) < 30$.
The smallest non-trivial tree is a path P_2 (F_2) with F-index 2. All paths, P_n, have the F-index of the form $2 + 8(n - 1)$. This covers all the integers 10, 18, 26, ...

F_0	F_2	F_4	F_6
	2	4	6
8		12	14
16		20	22
24		28	
32		36	
40		44	
48		52	
56		60	
64			
72			
80			
88			

Table 1. **F-indices for which trees do not exist**

The graph F_6 given in Figure 1(d) is the only tree with four vertices other than P_4. As the F-index of F_6 is 30, trees with the F-index $30+8k$ exist, where k is the number of subdivisions of F_6. Thus there exists no tree with $F(G)$ as 4, 6, 8, 12, 14, 16, 20, 22, 24, or 28.

Case 2. $30 < F(G) < 68$.
The graph F_4 given in Figure 1(c) is a tree with F-index 68. Hence, by a similar analysis given in Case 1, we can see that there are no trees with $30 < F(G) < 68$, other than those with indices 34, 38, 42, 46, 50, 54, 58, 62 and 66.

Case 3. $68 < F(G) < 88$.
As we had seen in the above discussions, graphs F_2, F_4 and F_6 cannot generate graphs with the $F(G)$ (mod 8) by the edge subdivision alone. By inspection, it is found out that the graph F_0 has the smallest $F(G)$, i. e., 96. Hence, there are no trees with $F(G)$ as 64, 72, 80 or 88.
Thus, Theorem 1 has been proved. □

The following result is immediate.

Corollary 1. *If G is a path P_n of order n, then the forgotten Zagreb index of P_n is 0 if $n = 1$, 2 if $n = 2$ and $8n - 14$ if $n > 2$.*

4. The Hyper Zagreb Index of Trees

In this section, we settle the inverse problem of the hyper Zagreb index of trees.

Theorem 2. *The hyper Zagreb index of trees can be any even positive integer except 2, 6, 8, 10, 12, 14, 16, 20, 22, 24, 26, 28, 30, 32, 36, 38, 40, 42, 44, 46, 52, 54, 56, 58, 60, 62, 64, 68, 70, 72, 74, 76, 78, 80, 86, 88, 90, 92, 94, 96, 104, 106, 108, 110, 112, 122, 124, 126, 128, 138, 142, 144 and 158.*

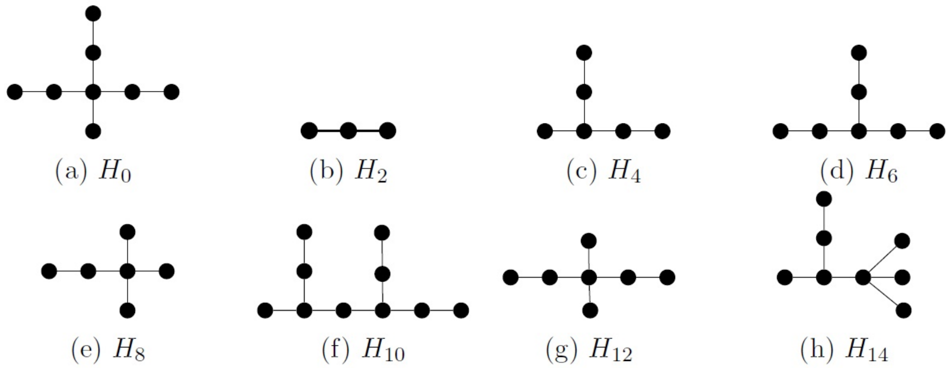

Figure 2. **The graphs H_0, H_2, H_4, ..., H_{14}**

Proof. We consider a set 8 of trees namely H_0, H_1, H_2, H_4, H_6, H_8, H_{10}, H_{12} and H_{14} with hyper Zagreb indices 160, 18, 84, 102, 120, 154, 140 and 174, respectively. In turn, these indices are congruent to 0, 2, 4, 6, 8, 10, 12 and 14 (mod 16), respectively. We can see that the set of 8 trees of our consideration contain the subgraph P_3. Now applying Equation (4) to each of the trees mentioned above, we arrive at graphs with hyper Zagreb indices of the form $160+16m$ giving $160, 176, 192, \dots,$ $18+16m$ giving $18, 34, 50, \dots,$ $84+16m$ giving $84, 100, 116, \dots,$ $102+16m$ giving $102, 118, 134, \dots,$ $120+16m$ giving $120, 236, 252, \dots,$ $154+16m$ giving $154, 170, 186, \dots,$ $140+16m$ giving $140, 156, 172, \dots$ and $174+16m$ giving $174, 190, 206, \cdots$, respectively, where m is the number of subdivisions made in the subgraphs P_3 in the corresponding trees. It is observed that the transformation of graph G to G^* as explained in the preliminaries enables us to generate trees of order 4 at most with $HM(G) > 158$. Also, all even positive integers mod 2, 4, 6, 8, 10, 12 greater than 18, 68, 86, 104, 138, 124 and less than 158 are covered by H_2, H_4, H_6, H_8, H_{10} and H_{12}, respectively. The integers not covered by the above transformations are 2 and those mentioned in Table 2.

H_0	H_2	H_4	H_6	H_8	H_{10}	H_{12}	H_{14}
	2		6	8	10	12	14
16		20	22	24	26	28	30
32		36	38	40	42	44	46
		52	54	56	58	60	62
64		68	70	72	74	76	78
80			86	88	90	92	94
96				104	106	108	110
112					122	124	126
128					138		142
144							158

Table 2. **Hyper Zagreb indices for which trees do not exist**

Now, we need to show that there exist no trees with hyper Zagreb index as listed in

Table 2.

Case 1. $0 < HM(G) < 20$.
Path P_2 is with $HM(G)$ 4. There is only one tree of order 3, i. e., P_3 (H_2). It is of $HM(G)$ 18. Hence, there are no trees with $HM(G)$ 2, 6, 8, 10, 12, 14 or 16.

Case 2. $18 < HM(G) < 52$.
There two trees of order 4, viz., P_4 and $K_{1,3}$, with $HM(G)$ 34 and 48, respectively. Hence, there are no trees with $HM(G)$ 20, 22, 24, 26, 28, 30, 32, 36, 38, 40, 42, 44 or 46. Moreover, $HM(P_5)$ is 50.

Case 3. $50 < HM(G) < 82$.
As any subdivision of a path or $K_{1,3}$ increases the $HM(G)$ by 16 or 18, respectively, there are no trees whose hyper Zagreb index is 52 to 64 or 68 to 80. Path P_6 has the hyper Zagreb index 66.

Case 4. $84 < HM(G) < 146$.
We see that H_0, H_1, H_2, H_4, H_6, H_8, H_{10} and H_{12} have the smallest value for the hyper Zagreb index among all trees of order n from 2 to 10 with hyper Zagreb indices 160, 18, 84, 102, 120, 154, 140 and 174 which are equivalent to 0, 2, 4, 6, 8, 10, 12 and 14 (mod 16), respectively, and contain a P_3. All the above mentioned graphs are of order at most 10. Let us now consider the path P_{11} with order 11 having $HM(P_{11}) = 146$. Since the hyper Zagreb index of a path P_n has the smallest value than any other trees for a given n, we conclude that no trees with $n \geq 11$ can have $HM(G) < 146$ except P_{11}. Hence we are justified that there exist no trees with the hyper Zagreb indices 86, 88, 90, 92, 94, 96, 104, 106, 108, 110, 112, 122, 124, 126, 128, 138, 142 or 144.

Case 5. $HM(G) = 158$.
The tree with the smallest hyper Zagreb index 14 (mod 16) is H_{14} as easily understandable from the subdivision process explained earlier in this Theorem. The hyper Zagreb index of H_{14} is 174. This implies that there exists no tree with $HM(G)$ 158. Hence, the proof is complete. □

The following result is immediate.

Corollary 2. *Let P_n be a path of order $n > 1$. The hyper Zagreb index of P_n is 4 if $n = 2$, 18 if $n = 3$ and $16n - 30$ if $n > 3$.*

5. Conclusion

In this paper, we have characterized all trees with the Forgotten Zagreb Index and the Hyper Zagreb Index. Trees are very important in the field of algorithms, chemical graph theory, signal processing, and electronics. In the enumeration of saturated hydrocarbons and in the study of electrical circuits, the applications of trees are very important. Hence, the inverse problem finds its significance. Inverse problems associated with other topological indices and other graph structures are worth studying.

As monocyclic and polycyclic molecular structures have very important applications in Chemistry, the study could be extended to those classes of graphs.

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