Research Article

On the Inverse Problem for Some Topological Indices

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The study of the inverse problem (IP) based on the topological indices (TIs) deals with the numerical relations to TIs. Mathematically, the IP can be expressed as follows: given a graph parameter/TI that assigns a non-negative integer value (g) to every graph within a given family ($\mathcal{G}$) of graphs, find some $G \in \mathcal{G}$ for which $TI(G) = g$. It was initiated by the Zefirov group in Moscow and later Gutman et al. proposed it. In this paper, we have established the IP only for the Y -index, Gourava indices, second hyper-Zagreb index, reformulated first Zagreb index, and reformulated F -index since they are closely related to each other. We have also studied the same which is true for the molecular, tree, unicyclic, and bicyclic graphs.

1. Introduction

Throughout the paper, we consider $\mathbb{L} = (V(\mathbb{L}), E(\mathbb{L}))$ as a simple (without loops and multiple edge loops) finite graph that contains $|V(\mathbb{L})| = n$ vertices and $|E(\mathbb{L})| = m$ edges, respectively. The notation $d(u/\mathbb{L})$ denotes the degree of a vertex $u \in V(\mathbb{L})$. All other notations and terminologies used but not clearly stated in this paper may be followed from [1].

In chemical graph theory, a TI, usually known as a molecular descriptor, can be expressed by a real number calculated from a chemical/molecular graph which is the representation of a chemical compound by replacing atoms with vertices and bonds with edges. The TI is calculated for evaluating the information about the atomic constitution and bond characteristics of a molecule/chemical compound. The TI of a molecular graph is a numerical number that enables us to collect information about the concerned chemical structure. It helps us to know its hidden properties without performing experiments [2–4]. The TIs also correlate and predict several physical, chemical, biological, pharmaceutical, pharmacological activities/properties from molecular structures of graphs corresponding to real-life situations. The IP is defined as the

feasibility of finding/modeling the chemical structure represented by a graph whose index value is equal to a given non-negative integer for the integer-valued problem. In the QSAR and QSPR studies [5], a method by which it is possible to predict the properties of a given molecular structure is called a forward problem. The inverse problem is concerned that, one can design the exact molecular structure that satisfies the given target properties by applying the forward problem solution.

The most popular as well as the oldest degree-based graph indices are the first and second Zagreb indices. Gutman et al. introduced the first Zagreb index $M_1(\mathbb{L})$ in [6] and second Zagreb index $M_2(\mathbb{L})$ in [7]. They are defined, respectively, as

$$M_1(\mathbb{L}) = \sum_{u \in V(\mathbb{L})} d^2\left(\frac{u}{\mathbb{L}}\right) = \sum_{uv \in E(\mathbb{L})} \left[d\left(\frac{u}{\mathbb{L}}\right) + d\left(\frac{v}{\mathbb{L}}\right) \right], \quad (1)$$

$$M_2(\mathbb{L}) = \sum_{uv \in E(\mathbb{L})} d\left(\frac{u}{\mathbb{L}}\right) d\left(\frac{v}{\mathbb{L}}\right).$$

In 2016, Farahani et al. [8] defined the second hyper-Zagreb index as follows:

$$HM_2(\mathbb{L}) = \sum_{uv \in E(\mathbb{L})} \left[d\left(\frac{u}{\mathbb{L}}\right) d\left(\frac{v}{\mathbb{L}}\right) \right]^2. \quad (2)$$

Kulli [9] introduced the first and second Gourava indices, defined, respectively, as

$$\begin{aligned} GO_1(\mathbb{L}) &= \sum_{uv \in E(\mathbb{L})} \left[d\left(\frac{u}{\mathbb{L}}\right) + d\left(\frac{v}{\mathbb{L}}\right) + d\left(\frac{u}{\mathbb{L}}\right) d\left(\frac{v}{\mathbb{L}}\right) \right], \\ GO_2(\mathbb{L}) &= \sum_{uv \in E(\mathbb{L})} \left[\left(d\left(\frac{u}{\mathbb{L}}\right) + d\left(\frac{v}{\mathbb{L}}\right) \right) d\left(\frac{u}{\mathbb{L}}\right) d\left(\frac{v}{\mathbb{L}}\right) \right]. \end{aligned} \quad (3)$$

Milicevic proposed the reformulated first Zagreb index $EM_1(\mathbb{L})$ in [10], defined as

$$EM_1(\mathbb{L}) = \sum_{e \in E(\mathbb{L})} d^2\left(\frac{e}{\mathbb{L}}\right); \quad d\left(\frac{e}{\mathbb{L}}\right) = d\left(\frac{u}{\mathbb{L}}\right) + d\left(\frac{v}{\mathbb{L}}\right) - 2. \quad (4)$$

Liu et al. [11] put forward the reformulated F -index, and it is defined as follows:

$$RF(\mathbb{L}) = \sum_{e \in E(\mathbb{L})} d^3\left(\frac{e}{\mathbb{L}}\right) = \sum_{e \sim f \in E(\mathbb{L})} \left[d^2\left(\frac{e}{\mathbb{L}}\right) + d^2\left(\frac{f}{\mathbb{L}}\right) \right]. \quad (5)$$

Alameri et al. [12] introduced Y -index, and it is defined by

$$Y(\mathbb{L}) = \sum_{u \in V(\mathbb{G})} d^4\left(\frac{u}{\mathbb{L}}\right) = \sum_{uv \in E(\mathbb{L})} \left[d^3\left(\frac{u}{\mathbb{L}}\right) + d^3\left(\frac{v}{\mathbb{L}}\right) \right]. \quad (6)$$

Graph theory, a branch of mathematics, provides the tools for solving problems of information theory, computer sciences, physics, and chemistry [13–15]. The study of the IP is encountered in various fields of science, especially in mathematics and chemistry. The IP for a TI is defined as follows: for a given TI and a non-negative integer value (x), find (chemical) graph ($\mathbb{L}$) for which $TI(\mathbb{L}) = x$. Also, the inverse existence problem [16] for the pair (G, Γ) can be asked as follows: given $(\mathcal{G})$ a class of graph and function $\Gamma: \mathcal{G} \rightarrow H$, for which $g \in H$ there is $G \in \mathcal{G}$ with $\Gamma(G) = g$? The idea of the IP based on TIs was initiated by the Zefirov group in Moscow [5, 17, 18] and was first proposed by Gutman et al. in [19]. The IP for Wiener index was solved in [20]. In [21], the IP was studied for sigma index as well as for acyclic, unicyclic, and bicyclic graphs. The same problem for the Steiner Wiener index was also solved in [22]. This type of problem for the Zagreb indices, forgotten Zagreb index, and the hyper-Zagreb index was studied in [23]. Tavakoli et al. [24] addressed the IP for first Zagreb index. Also, the IP for some graph indices was investigated in [25]. In [26], Czabarka et al. solved the IP for certain tree parameters. To study more about the inverse problems and the topological indices of graph operations, one can see these references [27–32].

There are so many benefits in the solution of IP. It helps to design of combinatorial libraries for drug discovery in combinatorial chemistry [33]. It may be helpful in speeding up the discovery of lead compounds with desired properties [34]. Also, the IP plays its significance in the application of trees [35]

such as the field of algorithms, chemical graph theory, signal processing, and electrical circuits.

2. Preliminaries

To study the IP for Y -index, we will use the following crucial observation.

Let $\mathbb{L}$ be a graph having u and v as vertices which are adjacent to each other. We subdivide each edge (uv) by introducing a new vertex (w) (of degree 2) to construct a new graph $\mathbb{L}^*$ (see Figure 1).

Here, the Y -index of the new graph $\mathbb{L}^*$ will be sixteen which is more than the graph $\mathbb{L}$.

Lemma 1. *By applying the transformation $\mathbb{L} \rightarrow \mathbb{L}^*$, the Y -index value will be increased by 16. That is, $Y(\mathbb{L}^*) = Y(\mathbb{L}) + 16$.*

Proof. Let us consider the graph $\mathbb{L}$ with vertices u and v of degrees x and y , respectively. Since in the new constructed graph $\mathbb{L}^*$, a new vertex w is inserted between u and v ,

$$\begin{aligned} Y(\mathbb{L}^*) - Y(\mathbb{L}) &= d^4\left(\frac{u}{\mathbb{L}^*}\right) + d^4\left(\frac{w}{\mathbb{L}^*}\right) + d^4\left(\frac{v}{\mathbb{L}^*}\right) \\ &\quad - d^4\left(\frac{u}{\mathbb{L}}\right) - d^4\left(\frac{v}{\mathbb{L}}\right) \\ &= x^4 + 16 + y^4 - x^4 - y^4 \\ &= 16. \end{aligned} \quad (7)$$

□

Lemma 2. *If either $d(u/\mathbb{L}) = 2$ or $d(v/\mathbb{L}) = 2$ (or both), then by the means of the above transformation $\mathbb{L} \rightarrow \mathbb{L}^*$, the value of the first Gourava index increases by 8. That is,*

$$GO_1(\mathbb{L}^*) = GO_1(\mathbb{L}) + 8. \quad (8)$$

Similarly, the value of the second Gourava index increases by 16. Thus,

$$GO_2(\mathbb{L}^*) = GO_2(\mathbb{L}) + 16. \quad (9)$$

Lemma 3. *If either $d(u/\mathbb{L}) = 2$ or $d(v/\mathbb{L}) = 2$ (or both), then by means of the above transformation $\mathbb{L} \rightarrow \mathbb{L}^*$, the value of the second hyper-Zagreb index increases by 16. That is,*

$$HM_2(\mathbb{L}^*) = HM_2(\mathbb{L}) + 16. \quad (10)$$

Lemma 4. *If either $d(u/\mathbb{L}) = 2$ or $d(v/\mathbb{L}) = 2$ (or both), then by applying the transformation $\mathbb{L} \rightarrow \mathbb{L}^*$, the values of the reformulated first Zagreb index and reformulated F -index of the graph $\mathbb{L}$ increase by 4 and 8, respectively. Thus,*

$$\begin{aligned} EM_1(\mathbb{L}^*) &= EM_1(\mathbb{L}) + 4, \\ RF(\mathbb{L}^*) &= RF(\mathbb{L}) + 8. \end{aligned} \quad (11)$$

FIGURE 1: The graphs (a) L and (b) L^* used in auxiliary Lemmas 1–4.

3. Main Results and Discussion

In graph theory, the IP based on the TIs is an interesting one among the problems associated with the estimation of different graph invariants/TIs such as chromatic number, connectivity, girth, and number of independent sets. The IP plays a crucial role in many areas of science, especially in mathematics. In this section, we have investigated the IP for Y -index, Gourava indices, second hyper-Zagreb index, reformulated first Zagreb index, and reformulated F -index. Additionally, we have developed the same problem for molecular, tree, acyclic, unicyclic, and bicyclic graphs.

3.1. The IP for Y -Index. Here we will discuss the IP for Y -index.

Theorem 1. *The Y -index for connected graphs can take all positive even integers, except for 4, 6, 8, 10, 12, 14, 16, $2(8i + 2)$, $2(8j + 3)$, $2(8k + 4)$, $2(8m + 5)$, $2(8n + 6)$, $2(8p + 7)$ where $i = 1, 2, \dots, 4$; $j = 1, 2, \dots, 9$; $k = 1, 2, \dots, 14$; $m = 1, 2, \dots, 19$; $n = 1, 2, \dots, 24$; and $p = 1, 2, \dots, 29$.*

Proof. Proof. To prove the theorem, we establish a set of graphs $Y_0, Y_2, Y_4, Y_6, Y_8, Y_{10}, Y_{12}, Y_{14}$ whose Y -index values are 48, 2, 84, 166, 248, 330, 412, and 494, respectively. These numbers are congruent to 0, 2, 4, 6, 8, 10, 12, and 14 (mod 16), respectively.

Consider the cyclic graphs C_n for $n \geq 3$. Clearly, in Figure 2(a), $Y(Y_0 = C_3) = 48$, $Y(C_4) = 64$, $Y(C_5) = 80$, and $Y(C_n) = 16n$ for $n \geq 3$. Now we apply Lemma 1 for each graph in Figure 2. Thus, $Y(Y_0)$ takes all those even positive integer values which are divisible by 16, except 16 and 32.

In Figure 2(b), $Y(P_2) = 2$. By applying the transformation in Lemma 1, we arrive at graphs whose Y -index values are 18, 34, 50, 66, and so on. There are the path graphs. Thus, $Y(L)$ takes all positive even integer values which are congruent to 2 (mod 16).

Now consider the graph in Figure 2(c) with $Y(Y_4) = 84$. By applying Lemma 1, we can obtain graphs with Y -index values 100, 116, 132, 148, ... Here, $Y(Y_4)$ contains all positive even integer values $\equiv 4 \pmod{16}$, except the integers 20, 36, 52, and 68.

The graph is depicted in Figure 2(d) with $Y(Y_6) = 166$, and then by using Lemma 1, we can take the graphs with Y -index values 182, 198, 214, 230, ..., and so on. Therefore, $Y(Y_6)$ covers all positive even integer values $\equiv 6 \pmod{16}$ and ≥ 166 . Obviously, the integers 6, 22, ..., 134, 150 are not covered by the construction.

In Figure 2(e), we have $Y(Y_8) = 248$, and then by using Lemma 1, we can take the graphs with Y -index values 264, 280, 296, 314, ..., and so on. So, $Y(Y_8)$ takes all positive even integer values $\equiv 8 \pmod{16}$ and ≥ 248 . Obviously, the integers 24, 40, ..., 216, 232 are not covered by the construction.

The graph in Figure 2(f) contains $Y(Y_{10}) = 330$. Again by Lemma 1, $Y(Y_{10})$ goes to all those positive even integer values $\equiv 10 \pmod{16}$ and ≥ 330 giving 330, 348, 364, 380, ..., and so on.

From Figure 2(g), we have $Y(Y_{12}) = 412$. By applying Lemma 1, $Y(Y_{12})$ takes all positive even integer values $\equiv 12 \pmod{16}$ and also ≥ 412 having 412, 428, 444, 460, ..., and so on.

The graph in Figure 2(h) has $Y(Y_{14}) = 494$. By applying Lemma 1, $Y(Y_{14})$ takes all positive even integer values $\equiv 14 \pmod{16}$ and also ≥ 494 taking 494, 510, 526, 542, ..., and so on. There exist no connected graphs with the Y -indices mentioned in Table 1. $\square$

Corollary 1. *The Y -index of a tree (or molecular) graph can take all positive even integers, except for 4, 6, 8, 10, 12, 14, 16, $2(8r + 2)$, $2(8s + 3)$, $2(8t + 4)$, $2(8w + 5)$, $2(8x + 6)$, $2(8y + 7)$ where $r = 1, 2, 3, 4$; $s = 1, 2, \dots, 9$; $t = 1, 2, \dots, 14$; $w = 1, 2, \dots, 19$; $x = 1, 2, \dots, 24$; and $y = 1, 2, \dots, 29$.*

Corollary 2. *Let L be a connected unicyclic or bicyclic graph. Then, there exists the Y -index of the form $16h + 2k$ for all non-negative integers where $h \neq 0$ and $1 \leq k \leq 7$.*

Proof. Proof. Let L_1 be a unicyclic graph which is obtained by adding a path of length two to any vertex u of the cyclic graph C_n for $n = 5$. Thus, $Y(L_1) = 162 = 16 \times 10 + 2 \times 1$. Similarly, the unicyclic graph L_2 is obtained by adding another path of length two to one of the two adjacent vertices to u that lie on L_1 (see Figure 3). We get $Y(L_2) = 244$.

The bicyclic graph L_3 is obtained by gluing two cyclic graphs with one side of both, and we have $Y(L_3) = 306$ which also can be expressed in the said form. Similarly, another bicyclic graph L_4 is obtained by adding a path of length two to any vertex u of L_3 . Thus, $Y(L_4) = 388$ is of the form $16h + 2k$ for $h = 24, k = 2$. $\square$

3.2. The IP for Gourava Indices. Here we study the IP for Gourava indices.

Theorem 2. *The first Gourava index of a connected graph can take any positive integer except for 1, 2, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 19, 20, 22, 23, 25, 27, 28, 29, 31, 33, 35, 41, 44, 49, 57, and 73.*

Proof. By applying Lemma 2, we construct eight series of graphs $(G_j, j = 0, 1, 2, \dots, 7)$ containing at least one vertex of degree 2, whose GO_1 -values are of the form $8s + t$ for $t = 0, 1, 2, \dots, 7$. These graphs are drawn in Figures 4(a)–4(h).

FIGURE 2: The graphs Y_i , for $i=0, 2, 4, 6, 8, 10, 12$, and 14 : (a) Y_0 , (b) Y_2 , (c) Y_4 , (d) Y_6 , (e) Y_8 , (f) Y_{10} , (g) Y_{12} , and (i) Y_{14} .

TABLE 1: Y -index values which do not exist.

Y_0	Y_4	Y_6	Y_8	Y_{10}	Y_{12}	Y_{14}
	4	6	8, 24	10, 26	12, 28, 44	14, 30, 46
16	20	22	40, 56	42, 58	60, 76, 92	62, 78, 94
32	36	38	72, 88	74, 90	108, 124, 140	110, 126, 142
	52	54	104, 120	106, 122	156, 172, 188	158, 174, 190
	68	70	136, 152	138, 154	204, 220, 236	206, 222, 238
		86	168, 184	170, 186	252, 268, 284	254, 270, 286
		102	200, 216	202, 218	300, 316, 332	302, 318, 334
		118	232	234, 250	348, 364, 380	350, 366, 382
		134		266, 282	396	398, 414, 430
		150		298, 314		446, 462, 478

FIGURE 3: The graphs L_1, L_2, L_3 , and L_4 with Y -index values: (a) let L_1 be a unicyclic graph with $Y(L_1) = 162$, (b) let L_2 be a unicycle graph with $Y(L_3) = 244$, (c) let L_3 be a bicyclic graph with $Y(L_3) = 306$, and (d) let L_4 be a bicyclic graph with $Y(L_4) = 388$.

Consider a cycle graph C_n with $n \geq 3$. Clearly, $GO_1(C_n) = 8n$. Therefore, $GO_1(L)$ can take all those positive integer values which are divisible by 8. From the graph G_0 (Figure 4) and Lemma 2, we obtain the graphs with $GO_1(L)$ -values $32, 40, 48, 56, 64, \dots$. Thus, $GO_1(L)$ takes all positive integers $\equiv 0 \pmod{8}$ and ≥ 24 .

Consider the graph G_1 in Figure 4 with $GO_1(L) = 81$, i.e., $GO_1(L)$ implies all positive integer values $\equiv 1 \pmod{8}$. Then, by Lemma 2, we obtain graphs with $GO_1(L) = 89, 97, 105, 113, 121, \dots$. Again for the graph G_2 , $GO_1(L) = 10$. Thus, we can arrive at graphs whose GO_1 values are $18, 26, 34, 42, 50, 58, 66, 74, 82, \dots$. Similarly, by applying Lemma 2 to the graphs G_3, G_4, G_5, G_6 , and G_7 , we get the graphs with $GO_1 = 59, 67, 75, 83, 91, 99, 107, 115, \dots, 60, 68, 76, 84, 92,$

$100, 108, \dots, 45, 53, 61, 69, 77, 85, \dots, 38, 46, 54, 62, 70, 78, \dots$, and $47, 55, 63, 71, 79, 87, \dots$, respectively. The star graphs S_4, S_5 and examples depicted in Figures 2(d) and 5(b) show that there exist graphs with $GO_1(L)$ as $21, 36, 43$, and 65 , respectively. There exist no connected graphs with first Gourava index as listed in Table 2. $\square$

Corollary 3. *The first Gourava index of a tree (or molecular) graph can take any positive integer, except for $1, 2, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 19, 20, 22, 23, 25, 27, 28, 29, 31, 33, 35, 41, 44, 49, 57$, and 73 .*

Now we study to settle the IP for the second Gourava index.

FIGURE 4: The graphs G_j , for $j = 0, 1, 2, \dots, 7$ with first Gourava index values: (a) G_0 $GO_1(G_0) = 24$, (b) G_1 $GO_1(G_1) = 81$, (c) G_2 $GO_1(G_2) = 10$, (d) G_3 $GO_1(G_3) = 51$, (e) G_4 $GO_1(G_4) = 52$, (f) G_5 $GO_1(G_5) = 37$, (g) G_6 $GO_1(G_6) = 30$, and (h) G_7 $GO_1(G_7) = 39$.

FIGURE 5: The star graph (a) S_6 and tree (b) T with second hyper-Zagreb index values.

TABLE 2: The first Gourava index values which do not exist.

G_0	G_1	G_2	G_3	G_4	G_5	G_6	G_7
	1	2		4	5	6	7
8	9		11	12	13	14	15
16	17, 25		19	20		22	23
	33, 41		27	28	29		31
	49, 57		35				
	73			44			

Theorem 3. The second Gourava index of a connected graph can take any positive even integer except for 4, 6, 8, 10, 14, 16, 20, 22, 24, 26, 30, 32, 34, 38, 40, 42, 46, 50, 52, 54, 56, 58, 62, 66, 68, 70, 72, 74, 78, 82, 86, 90, 94, 98, 102, 106, 110, 118, 122, and 134.

Proof. Consider first path graphs P_n for $n \geq 2$. It is clear that $GO_2(P_2) = 2$ and $GO_2(P_3) = 12$. By Lemma 2, since $GO_2(P_n) = 16n - 36$ for $n \geq 3$, we obtain the graphs whose GO_2 -values are 28, 44, 60, 76, 92, 108, ... which are congruent to 12 (mod 16). If we consider a cyclic graph C_n with n vertices, then $GO_2(C_n) = 16n$ for $(n \geq 3)$. Clearly, we get the graphs with GO_2 -values 48, 64, 80, 96, 112, ... Now the graph G_7 drawn in Figure 4 has $GO_2(G_7) = 84$. Therefore, by applying Lemma 2, we obtain the graphs with second Gourava index values 100, 116, 132, 148, 164, ... The graphs G_4 and G_5 in Figure 4 contain $GO_2(G_4) = 126$ and $GO_2(G_5) = 88$,

respectively. Therefore, by Lemma 2, $GO_2(G)$ obtains all those even integer values 126, 142, 158, 174, 190, 206, 222, ... and 104, 120, 136, 152, ..., respectively. In same procedure, from Figure 4, we get the graph G_3 with $GO_2(G_3) = 138$. So, it follows the GO_2 -values 154, 170, 186, 202, 218, ...

In Figure 6, by Lemma 2, we have $GO_2(G_8) = 150$ and $GO_2(G_9) = 114$ with. Then by using the Lemma 2, we can take the graphs with 166, 182, 198, 214, ... and 130, 146, 162, 178, 194, ..., respectively. The integers not covered by the above transformation for the second Gourava index are listed in Table 3. $\square$

Corollary 4. The second Gourava index of a tree (or molecular) graph can take any positive even integer, except for 4, 6, 8, 10, 14, 16, 20, 22, 24, 26, 30, 32, 34, 38, 40, 42, 46, 50, 52, 54, 56, 58, 62, 66, 68, 70, 72, 74, 78, 82, 86, 90, 94, 98, 102, 106, 110, 118, 122, and 134.

FIGURE 6: The graphs (a) G_8 and (b) G_9 with second Gourava index values.

TABLE 3: The second Gourava index values which do not exist.

G_0	G_2	G_4	G_6	G_8	G_{10}	G_{14}
		4	6	8	10	14
16		20	22	24	26	30
32	34		38	40	42	46
	50	52	54	56	58	62
	66	68	70	72	74	78
	82		86		90	94
	98		102		106	110
			118		122	
			134			

3.3. The IP for Second Hyper-Zagreb Index

Theorem 4. *The second hyper-Zagreb index of a connected graph can be any positive integer, except 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 41, 42, 43, 44, 45, 46, 47, 49, 50, 51, 52, 53, 54, 55, 57, 59, 60, 61, 62, 63, 65, 66, 67, 68, 69, 70, 71, 73, 75, 76, 77, 78, 79, 81, 82, 83, 84, 85, 86, 87, 91, 92, 93, 94, 95, 98, 99, 100, 101, 102, 103, 107, 109, 110, 111, 114, 115, 118, 119, 123, 126, 127, 130, 131, 133, 134, 135, 141, 142, 143, 146, 147, 149, 150, 151, 157, 158, 159, 163, 165, 167, 173, 174, 175, 181, 183, 190, 191, 199, 206, 215, 222, 223, 231, 239, 255, and 271.*

Proof. We construct a series of sixteen graphs such as $H_0, H_1, H_2, \dots, H_{15}$. The HM_2 values of these graphs can be expressed in the form $16h + i$ for $i = 0, 1, 2, \dots, 15$. In Figure 7, we construct the graphs H_k for $k = 2, 3, 4, 5, 6, 7$ and 11, 12, 13, 14, 15. Note that the graphs $H_0, H_1, H_8, H_9, H_{10}$ are similar to Figures 4(a), 4(f), 4(c), 4(h), and 4(g) respectively. We have $HM_2(H_0) = 48$. Then by using Lemma 3, we can take the graphs with HM_2 values 64, 80, 96, 112, ... which are congruent to 0 (mod 16). Secondly, consider the graph H_1 which generates the HM_2 -values 97, 113, 129, 145, 161, ..., and all these are congruent to 1 (mod 16).

Since $HM_2(H_2) = 162$, by mean of the construction method upon the graph H_2 from the Lemma 3, we get the graphs with HM_2 values 178, 194, 210, 226, ... which are congruent to 2 (mod 16). For H_3 , the HM_2 -values cover the integers 179, 195, 211, 227, ... which are $\equiv 3$ (mod 16). Analogously, the HM_2 values for the graph H_4 cover all the integers 116, 132, 148, ..., and all these numbers are congruent to 4 (mod 16). For H_5 , it provides the HM_2 values 197, 213, 229, ... which are $\equiv 5$ (mod 16). For H_6 there exist HM_2 values 166, 182, 198, ... which are $\equiv 6$ (mod 16). It follows 247, 263, 379, ... for the graph H_7 , and these integers

are congruent to 7 (mod 16). Similarly by Lemma 3, we get for the graphs $H_8, H_9, H_{10}, H_{11}, H_{12}, H_{13}, H_{14}, H_{15}$ with Now, using the construction method in Lemma 3 to $H_8, H_9, H_{10}, H_{11}, H_{12}, H_{13}, H_{14}$, and H_{15} , we can generate the graphs with HM_2 values 8, 24, 40, ... congruent to 8 (mod 16); 89, 105, 121, ... congruent to 9 (mod 16); 58, 74, 90, ... congruent to 10 (mod 16); 139, 155, 171, ... congruent to 11 (mod 16); 108, 124, 140, ... congruent to 12 (mod 16); 189, 205, 221, ... congruent to 13 (mod 16); 238, 254, 270, ... congruent to 14 (mod 16); and 257, 303, 319, ... congruent to 15 (mod 16), respectively.

The examples drawn in the Figures 2(c), 2(d), 5(a), and 5(b) have HM_2 values 117, 27, 125, and 207, respectively. These numbers are congruent to 5, 11, 13, and 15 (mod 16), chronologically. There exist no connected graphs with the HM_2 -indices mentioned in Table 4. $\square$

Corollary 5. *The second hyper-Zagreb index of a tree (or molecular) graph can be any positive integer, except 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 41, 42, 43, 44, 45, 46, 47, 49, 50, 51, 52, 53, 54, 55, 57, 59, 60, 61, 62, 63, 65, 66, 67, 68, 69, 70, 71, 73, 75, 76, 77, 78, 79, 81, 82, 83, 84, 85, 86, 87, 91, 92, 93, 94, 95, 98, 99, 100, 101, 102, 103, 107, 109, 110, 111, 114, 115, 118, 119, 123, 126, 127, 130, 131, 133, 134, 135, 141, 142, 143, 146, 147, 149, 150, 151, 157, 158, 159, 163, 165, 167, 173, 174, 175, 181, 183, 190, 191, 199, 206, 215, 222, 223, 231, 239, 255, and 271.*

3.4. The IP for Reformulated First Zagreb Index

Theorem 5. *The first reformulated Zagreb index of a connected graph can take all positive even integer values except for 4 and 8.*

Proof. At first, we consider the path P_n with $n \geq 3$. The Rez-value for P_3 is equal to 2. By Lemma 4, we obtain graphs with Rez-values 6, 10, 14, 18, ..., and so on. Also, since $\text{Rez}(S_3) = 12$, by means of the construction described in Lemma 4, we have the graphs whose Rez-values are 16, 20, 24, 28, 32, 36, 40, ... Hence, $\text{Rez}(\mathbb{L})$ covers all positive even integers except 4 and 8. $\square$

Corollary 6. *The first reformulated Zagreb index of a tree (or molecular) graph can take all positive even integer values, except for 4 and 8.*

3.5. The IP for Reformulated F-Index

Theorem 6. *The reformulated F-index of a connected graph can be any positive even integer, except for 4, 6, 8, 12, 14, 16, 20, 22, 28, 30, 36, 38, 46, 54, and 62.*

Proof. For the path graphs P_3 , we get $\text{RF}(P_3) = 2$. Thus, by applying Lemma 4, we obtain graphs with $\text{RF}(\mathbb{L})$ -values equal to 10, 18, 26, 34, ... Similarly, for the cyclic graph C_3 , we have $\text{RF}(C_3) = 24$ and next obtained graphs having $\text{RF}(\mathbb{L})$ -values 32, 40, 48, 56, ... In an analogous manner,

FIGURE 7: The graphs H_k , for $k=2, 3, 4, 5, 6, 7$ and $11, 12, 13, 14, 15$.

TABLE 4: HM_2 values which do not exist.

H_0	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_9	H_{10}	H_{11}	H_{12}	H_{13}	H_{14}	H_{15}
		2	3	4	5	6	7	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23	25	26		28	29	30	31
32	33	34	35	36	37	38	39	41	42	43	44	45	46	47
	49	50	51	52	53	54	55	57		59	60	61	62	63
	65	66	67	68	69	70	71	73		75	76	77	78	79
	81	82	83	84	85	86	87			91	92	93	94	95
		98	99	100	101	102	103			107		109	110	111
		114	115			118	119			123			126	127
		130	131		133	134	135					141	142	143
		146	147		149	150	151					157	158	159
			163		165		167					173	174	175
					181		183						190	191
							199						206	223, 239
							215, 231						222	255, 271

starting with G_5 and G_6 in Figure 4, we obtain the graphs with RF-values 78, 86, 94, 102, ... and 52, 60, 68, 76, ..., respectively. $\square$

Corollary 7. *The reformulated F -index of a tree (or molecular) graph can be any positive even integer, except for 4, 6, 8, 12, 14, 16, 20, 22, 28, 30, 36, 38, 46, 54, and 62.*

4. Conclusion

The inverse problem is one of the recent problems of graph theory related to the applicative area. Here, we have studied the IP based on some topological graph indices such as Y -index, Gourava indices, second hyper-Zagreb index, reformulated first Zagreb index, and reformulated F -index. We have studied the inverse problems for the aforesaid indices since they are closely related to each other. We have also investigated the results for tree, molecular, unicyclic, and bicyclic graphs. The inverse problem is still open for other graph indices and other molecular structures.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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