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 \( \mathcal{L} = (V(\mathcal{L}), E(\mathcal{L})) \) as a simple (without loops and multiple edge loops) finite graph that contains \( |V(\mathcal{L})| = n \) vertices and \( |E(\mathcal{L})| = m \) edges, respectively. The notation \( d(u/\mathcal{L}) \) denotes the degree of a vertex \( u \in V(\mathcal{L}) \). 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 \( M_1(\mathcal{L}) \) in [6] and second Zagreb index \( M_2(\mathcal{L}) \) in [7]. They are defined, respectively, as

\[
M_1(\mathcal{L}) = \sum_{u \in V(\mathcal{L})} d^2(u/\mathcal{E}) = \sum_{u \in E(\mathcal{L})} d(u/\mathcal{L})d(v/\mathcal{L}),
\]

\[
M_2(\mathcal{L}) = \sum_{u \in V(\mathcal{L})} d(u/\mathcal{E}) = \sum_{u \in E(\mathcal{L})} d(u/\mathcal{L})d(v/\mathcal{L}).
\]

In 2016, Farahani et al. [8] defined the second hyper-Zagreb index as follows:
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 $L$ 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 $L^*$ (see Figure 1).

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

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

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

$$Y(L^*) - Y(L) = d^4 \frac{u}{L} + d^4 \frac{v}{L} \quad \text{or} \quad d^4 \frac{w}{L} + d^4 \frac{y}{L}$$

$$= x^4 + 16 y^4 - x^4 - y^4 = 16.$$  \[ \Box \]

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

$$G_0(L^*) = G_0(L) + 8.$$  \[ (8) \]

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

$$G_0(L^*) = G_0(L) + 16.$$  \[ (9) \]

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

$$H_{M_2}(L^*) = H_{M_2}(L) + 16.$$  \[ (10) \]

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

$$EM_1(L^*) = EM_1(L) + 4,$$

$$RF(L^*) = RF(L) + 8.$$  \[ (11) \]
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 $i = 1, 2, \ldots, 4; j = 1, 2, \ldots, 9; k = 1, 2, \ldots, 14; m = 1, 2, \ldots, 19; n = 1, 2, \ldots, 24$; and $p = 1, 2, \ldots, 29$.

Proof. To prove the theorem, we establish a set of graphs $Y_1, Y_2, Y_4, Y_6, Y_8, Y_{10}, Y_{12}, Y_{14}$ 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), $Y(Y_n) = C_4 = 48$, $Y(C_6) = 64$, $Y(C_8) = 80$, and $Y(C_n) = 16n$ for $n \geq 3$. Now we apply Lemma 1 for each graph in Figure 2. Thus, $Y(C_n)$ 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, \ldots. Here, $Y(Y_4)$ contains all positive even integer values $\equiv 4$ (mod 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, \ldots, and so on. Therefore, $Y(Y_6)$ covers all positive even integer values $\equiv 6$ (mod 16) and $\geq 166$. Obviously, the integers 6, 22, \ldots, 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, \ldots, and so on. So, $Y(Y_8)$ takes all positive even integer values $\equiv 8$ (mod 16) and $\geq 248$. Obviously, the integers 24, 40, \ldots, 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 $\equiv 10$ (mod 16) and $\geq 330$ giving 330, 348, 364, 380, \ldots, 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 $\equiv 12$ (mod 16) and also $\geq 412$ having 412, 428, 444, 460, \ldots, 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 $\equiv 14$ (mod 16) and also $\geq 494$ taking 494, 510, 526, 542, \ldots, and so on. There exist no connected graphs with the $Y$-indices mentioned in Table 1.

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(8i + 2), 2(8j + 3), 2(8k + 4), 2(8m + 5), 2(8n + 6), 2(8p + 7) where $r = 1, 2, \ldots, 4; s = 1, 2, \ldots, 9; t = 1, 2, \ldots, 14; w = 1, 2, \ldots, 19; x = 1, 2, \ldots, 24$; and $y = 1, 2, \ldots, 29$.

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. 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 $Y(L_3) = 360$ which also can be expressed in the said form. Similarly, another bicyclic graph $L_4$ is obtained by adding a path with length two to any vertex $u$ of $L_3$. Thus, $Y(L_4) = 388$ is of the form $16h + 2k$ for $h = 24, k = 2$.

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 $(G_j, j = 0, 1, 2, \ldots, 7)$ containing at least one vertex of degree 2, whose $G_{O_j}$-values are of the form $8s + t$ for $t = 0, 1, 2, \ldots, 7$. These graphs are drawn in Figures 4(a)–4(h).
Consider a cycle graph $C_n$ with $n \geq 3$. Clearly, $GO_1(C_n) \equiv 8n$. 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, . . . Thus, $GO_1(L)$ takes all positive integers $\equiv 0 \pmod{8}$ and $\geq 24$.

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 $GO_1(L) = 89, 97, 105, 113, 121, \ldots$ 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, . . . Similarly, by applying Lemma 2 to the graphs $G_3, G_4, G_5, G_6$, and $G_7$, we get the graphs with $GO_1 = 59, 67, 75, 83, 91, 99, 107, 115, \ldots, 60, 68, 76, 84, 92, 100, 108, \ldots, 45, 53, 61, 69, 77, 85, \ldots, 38, 46, 54, 62, 70, 78, \ldots, and 47, 55, 63, 71, 79, 87, \ldots$, 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.

**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.

### 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| 138, 154| 204, 220, 236 | 206, 222, 238 |
| 68    | 70    | 136, 152| 170, 186| 202, 218| 300, 316, 332 | 302, 318, 334 |
| 86    | 86    | 168, 184| 170, 186| 202, 218| 300, 316, 332 | 302, 318, 334 |
| 102   | 102   | 200, 216| 202, 218| 300, 316, 332 | 302, 318, 334 |
| 118   | 118   | 232    | 234, 250| 348, 364, 380 | 350, 366, 382 |
| 134   | 134   | 266, 282| 296    | 396      | 398, 414, 430 |
| 150   | 150   | 298, 314| 396    | 398, 414, 430 | 446, 462, 478 |

Consider a cycle graph $C_n$ with $n \geq 3$. Clearly, $GO_2(C_n) = 8n$. Therefore, $GO_2(L)$ 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 $GO_2(L)$-values 32, 40, 48, 56, 64, . . . Thus, $GO_2(L)$ takes all positive integers $\equiv 0 \pmod{8}$ and $\geq 24$.

Consider the graph $G_1$ in Figure 4 with $GO_2(L) = 81$, i.e., $GO_2(L)$ implies all positive integer values $\equiv 1 \pmod{8}$. Then, by Lemma 2, we obtain graphs with $GO_2(L) = 89, 97, 105, 113, 121, \ldots$. Again for the graph $G_2$, $GO_2(L) = 10$. Thus, we can arrive at graphs whose $GO_2$ values are 18, 26, 34, 42, 50, 58, 66, 74, 82, . . . Similarly, by applying Lemma 2 to the graphs $G_3, G_4, G_5, G_6$, and $G_7$, we get the graphs with $GO_2 = 59, 67, 75, 83, 91, 99, 107, 115, \ldots, 60, 68, 76, 84, 92, 100, 108, \ldots, 45, 53, 61, 69, 77, 85, \ldots, 38, 46, 54, 62, 70, 78, \ldots, and 47, 55, 63, 71, 79, 87, \ldots$, respectively. The star graphs $S_4, S_5$ and examples depicted in Figures 2(d) and 5(b) show that there exist graphs with $GO_2(L)$ as 21, 36, 43, and 65, respectively. There exist no connected graphs with first Gourava index as listed in Table 2.

**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.

![Graphs](image-url)
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 $GO_2(L) = 84$. 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 $GO_2(L) = 126$ and $GO_2(L) = 88$, respectively. Therefore, by Lemma 2, $GO_2(L)$ 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 $GO_2(L) = 138$. So, it follows the $GO_2$-values 154, 170, 186, 202, 218, . . .

In Figure 6, by Lemma 2, we have $GO_2(G_4) = 150$ and $GO_2(G_5) = 114$ 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.

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.
We construct a series of sixteen graphs such as 

$$H_{239, 255, 271}. \quad 142, 143, 146, 147, 149, 150, 151, 153, 154, 155, 157, 158, 159, 163, 165, 167, 173, 174, 175, 181, 183, 190, 191, 199, 206, 215, 222, 223, 231, 239, 255, 271. \quad \Box$$

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 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, Rez($L$) covers all positive even integers except 4 and 8. \hfill $\Box$

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 $P_n$, we get $RF(P_n) = 2$. Thus, by applying Lemma 4, we obtain graphs with $RF(L)$-values equal to 10, 18, 26, 34, ... . Similarly, for the cyclic graph $C_n$, we have $RF(C_n) = 24$ and next obtained graphs having $RF(L)$-values 32, 40, 48, 56, ... . In an analogous manner,
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.

**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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