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Inverse Problem for The First Entire Zagreb Index

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Abstract

The inverse problem for topological graph indices is about the existence of a graph having its index value equal to a given non-negative integer. In this paper, we study the problem for the first entire Zagreb index. We will first show that the first entire Zagreb index must be even for any graph G, and can take all positive even integer values except 4, 6, 10, 12, 14, 18, 20, 22, 26, 28, 30, 36, 38 and 46.

1 Introduction

[1] [2] [3] Let $G = (V, E)$ be a simple graph with $\mid V(G) \mid = n$ vertices and $\mid E(G) \mid = m$ edges. That is, we do not allow loops or multiple edges. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v. A vertex with degree one is called a pendant vertex. Similarly, we shall use the term "pendant edge" for an edge having a pendant vertex. Generalizing this idea, with slight abuse of language, we define a "pendant path" as a path which is joined to the rest of the graph at a cut-vertex.

Topological graph indices are defined and used in many areas to study several properties of different objects such as atoms and molecules. Several topological graph indices have been defined and studied by many mathematicians and chemists as most graphs are generated from molecules by replacing atoms with vertices and bonds with edges. They are defined as topological graph invariants measuring several physical, chemical, pharmacological, pharmaceutical, biological, etc. properties of graphs which are modelling real life situations. They can be grouped into three classes according to the way they are defined: by vertex degrees, by matrices or by distances.

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Two of the most important topological graph indices are called the first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

They were first defined in 1972 by Gutman and Trinajstic, [15], and are referred to due to their uses in QSAR and QSPR studies. In [5], some results on the first Zagreb index together with some other indices are given. In [6], the multiplicative versions of these indices are studied. Some relations between Zagreb indices and some other indices such as ABC, GA and Randic indices are obtained in [18]. Zagreb indices of subdivision graphs were studied in [20] and these were calculated for the line graphs of the subdivision graphs in [19]. A more generalized version of subdivision graphs is called r-subdivision graphs and Zagreb indices of r-subdivision graphs are calculated in [22]. These indices are calculated for several important graph classes in [23].

There are thousands of results on calculation of these indices for several graphs, or sometimes for general graphs. There are inverse problems in many areas of science, and naturally mathematics, and the one for the graph theory is also an interesting one. The inverse problem for topological graph indices is the one which is about the existence of a graph having its index equal to a given non-negative integer. This problem which formed the beginning of what is now called the inverse problem for graph indices was proposed in [16]. In [21], the inverse problem for the first Zagreb index $M_1(G)$ was solved by showing that all positive even integers except for 4 and 8 are equal to the first Zagreb index of a caterpillar graph which is a special type of graph. In [24], Wagner showed that each integer greater than 469 is the Wiener index of a special graph class called starlike trees. In [25], all 49 positive integer values which are not the Wiener index of any graph are listed. Similar results for the Wiener index was obtained in [3] and [9]. In [13], Gutman et.al. compared the irregularity indices for chemical trees, and the inverse problem for four topological indices were studied in [17]. Recently, the authors completely solved the problem for the second Zagreb index $M_2(G)$, forgotten Zagreb index $F(G)$, hyper-Zagreb index $HM(G)$ in [26] and σ index in [?]. For the second Zagreb index $M_2(G)$, the authors found 10 values of positive integers which cannot be the second Zagreb index of any graph. Similarly, it was found that there are 10 values of positive even integers which cannot be the forgotten index of any graph. In the same paper, also the 50 values of positive even integers which cannot be the hyper-Zagreb index of any graph. For the σ index, the authors found that all positive even integers can be σ index of any graph.

In [2], the first entire Zagreb index was defined by

$$M_1^{\varepsilon}(G) = \sum_{x \in E(G) \cup V(G)} (d_x)^2$$

by considering the squares of the degrees of all edges and vertices entirely.

In this paper, we study the inverse problem for the first entire Zagreb index $M_1^{\varepsilon}(G)$. We shall show in Theorem 2 that $M_1^{\varepsilon}(G)$ must be even for any graph G and also $M_1^{\varepsilon}(G)$ covers all positive even integers except for 14 values between 4 and 46.

2 The First Entire Zagreb Index

First we have some important properties of the first entire Zagreb index which will be helpful in solving the inverse problem.

Lemma 1 *The degrees of the vertices of G which are forming an edge in G satisfy the following equality:*

$$\begin{aligned}\sum_{uv\in E(G)} ({d_u}^2 + {d_v}^2) &= \sum_{u\in V(G)} {d_u}^3 \\ &= \sum_{i=1}^{n} {d_i}^3.\end{aligned}$$

Proof. Let $e = uv \in E(G)$. For each vertex $u \in V(G)$, there are d_u edges incident to v. Therefore for each u, there are d_u times ${d_u}^2$ added to the sum on the left hand side. Therefore the result follows. ■

Theorem 2 *Let G be a graph with $n \geq 2$. Then $M_1^{\varepsilon}(G)$ is even.*

Proof. As $M_1^{\varepsilon}(G) = M_1(G) + \sum_{e\in E(G)} {d_e}^2$ and as $M_1(G)$ is even by Handshaking Lemma, it is only necessary to show that $\sum_{e\in E(G)} {d_e}^2$ is even. Now

$$\begin{aligned}\sum_{e\in E(G)} {d_e}^2 &= \sum_{e=uv\in E(G)} (d_u + d_v - 2)^2 \\ &= \sum_{e=uv\in E(G)} ({d_u}^2 + {d_v}^2 + 4 + 2(d_u d_v - 2d_u - 2d_v)) \\ &= \sum_{e=uv\in E(G)} ({d_u}^2 + {d_v}^2) + 2 \sum_{e=uv\in E(G)} (2 + d_u d_v - 2d_u - 2d_v).\end{aligned}$$

The first sum is even by Lemma 1 and by the Handshaking Lemma implying the result. ■

Corollary 3 *If all vertices in graph G have the degree 1 or 2, then $M_1^{\varepsilon}(G) = 2M_2(G)$.*

Proof.

$$\begin{aligned}
M_1^{\varepsilon}(G) &= \sum_{v\in V(G)} {d_v}^2 + \sum_{v\in V(G)} {d_v}^3 + 2\left[2m + \sum_{uv\in E(G)} d_u d_v - 4\sum_{uv\in E(G)} (d_u + d_v)\right]\\
&= -3\sum_{v\in V(G)} {d_v}^2 + \sum_{v\in V(G)} {d_v}^3 + 4m + 2M_2(G)\\
&= \sum_{v\in V(G)} ({d_v}^3 - 3{d_v}^2 + 2d_v) + 2M_2(G)\\
&= \sum_{v\in V(G)} d_v(d_v-1)(d_v-2) + 2M_2(G)
\end{aligned}$$

Hence the result follows. ∎

Corollary 3 is only valid when $G = P_n$ or C_n. In these cases, we have

Lemma 4 *$M_1^{\varepsilon}(P_n) = 8(n-2)$ and $M_1^{\varepsilon}(C_n) = 8n$.*

If $G \neq P_n,\ C_n$, then obviously $n \geq 4$. Recall that each vertex v with $d_v = 3$ contributes 6 to $M_1^{\varepsilon}(G)$. Similarly each vertex v of $d_v = 4$ contributes 24 to $M_1^{\varepsilon}(G)$ and each vertex v of $d_v = 5$ contributes 60 to $M_1^{\varepsilon}(G)$, etc. In general a vertex v of $d_v = k$ contributes $P(k,3)$ to $M_1^{\varepsilon}(G)$. Therefore if G has vertices of degree bigger than 2, then

$$6a + 24b + 60c + \cdots + 2M_2(G) = M_1^{\varepsilon}(G) \tag{1}$$

where a is the number of vertices of degree 3, b is the number of degree 4, c is the number of vertices of degree 5, etc.

Definition 5 *Let G be a graph possessing a vertex v of degree 2. Let the neighbours of v be u and w. The graph denoted by G^* is defined as a new graph obtained by attaching a new vertex to the vertex w of degree 1.*

Lemma 6 *$M_1^{\varepsilon}(G^*) = M_1^{\varepsilon}(G) + 8$.*

Proof. Let G be as in Figure 1.

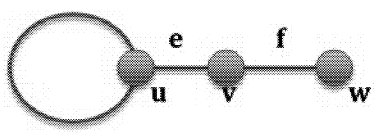

Figure 1: A graph G with a pendant path P

Then $d_v = 2$ and $d_w = 1$. Now

$$\begin{aligned}
M_1^\varepsilon(G) &= \sum_{\substack{i \neq u,v,w \\ v \in V(G)}} {d_i}^2 + {d_u}^2 + {d_v}^2 + {d_w}^2 + \sum_{\substack{i \neq e,f \\ v \in E(G)}} {d_i}^2 + {d_e}^2 + {d_f}^2 \\
&= \sum_{\substack{i \neq u,v,w \\ v \in V(G)}} {d_i}^2 + {d_u}^2 + 4 + 1 + \sum_{\substack{i \neq e,f \\ v \in E(G)}} {d_i}^2 + (d_u + 2 - 2)^2 + (2 + 1 - 2)^2 \\
&= \sum_{\substack{i \neq u,v,w \\ v \in V(G)}} {d_i}^2 + \sum_{\substack{i \neq e,f \\ v \in E(G)}} {d_i}^2 + 2d_u^2 + 6.
\end{aligned}$$

Let us add a new edge g to the pendant vertex w, see Figure 2. That is we apply the transformation in 5 to obtain $G^* = G + g$. As

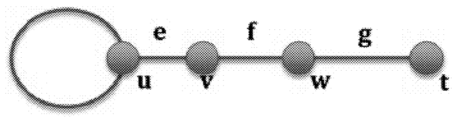

Figure 2: The transformed graph $G^* = G + g$

$$\begin{aligned}
M_1^\varepsilon(G^*) &= \sum_{\substack{i \neq u,v,w,t \\ v \in V(G+g)}} {d_i}^2 + {d_u}^2 + {d_v}^2 + {d_w}^2 + {d_t}^2 + \sum_{\substack{i \neq e,f,g \\ v \in E(G)}} {d_i}^2 + {d_e}^2 + {d_f}^2 + {d_g}^2 \\
&= \sum_{\substack{i \neq u,v,w,t \\ v \in V(G+g)}} {d_i}^2 + {d_u}^2 + 4 + 4 + 1 + \sum_{\substack{i \neq e,f,g \\ v \in E(G)}} {d_i}^2 + (d_u + 2 - 2)^2 + 4 + 1 \\
&= \sum_{\substack{i \neq u,v,w,t \\ v \in V(G+g)}} {d_i}^2 + \sum_{\substack{i \neq e,f,g \\ v \in E(G)}} {d_i}^2 + 2{d_u}^2 + 14,
\end{aligned}$$

we have $M_1^\varepsilon(G^*) - M_1^\varepsilon(G) = 8$. ■

We now want to give the main theorem of this paper to settle the inverse problem for $M_1^\varepsilon(G)$. We should first observe the first few smallest values of $M_2(G)$ to eliminate possibilities in the main result:

Remark 7 *Note that the first few values of* $M_2(G)$ *are* 9, 14, 18, 19, 23 *and* 24 *when there is at least one vertex of degree* 3 *(that is,* $a \geq 1$*) and* 16, 22, 26, 28, 30, 34, 37, $\cdots$ *when there is at least one vertex of degree* 4 *(that is,* $b \geq 1$*).*

Now we are ready to give the main result:

Theorem 8 *If* G *is a connected simple graph, then* $M_1^\varepsilon(G)$ *can take all positive integer values except for* 4, 6, 10, 12, 14, 18, 20, 22, 26, 28, 30, 36, 38 *and* 46.

Proof. Consider first path graphs P_n for $n \geq 2$. Clearly $M_1^{\varepsilon}(P_2) = 2$, $M_1^{\varepsilon}(P_3) = 8$, $M_1^{\varepsilon}(P_4) = 16$. By Lemma 4, since $M_1^{\varepsilon}(P_n) = 8(n-2)$ for $n \geq 3$, then $M_1^{\varepsilon}(G)$ takes all positive even integer values divisible by 8.

Secondly consider the caterpillar graph in Figure 3 which has $M_1^{\varepsilon}(G) = 34$. If we continue to add other edges to the branch on the right in Figure 3, $M_1^{\varepsilon}(G)$ will increase by 8 each time by Lemma 6. That is $M_1^{\varepsilon}(G)$ takes all even integer values $\equiv 2 \pmod 8$ and ≥ 34.

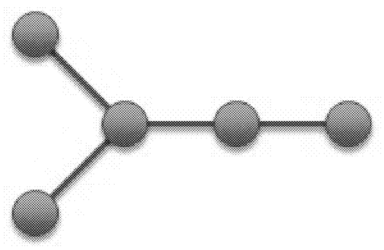

Figure 3:

The graph in Figure 4 has $M_1^{\varepsilon}(G) = 44$. Similarly by Lemma 6, $M_1^{\varepsilon}(G)$ takes all even integer values $\equiv 4 \pmod 8$ and ≥ 44.

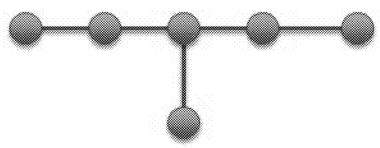

Figure 4:

Now consider the graph in Figure 5 with $M_1^{\varepsilon}(G) = 70$. Again by Lemma6, $M_1^{\varepsilon}(G)$ can take all positive even integer values $\equiv 6 \pmod 8$ and ≥ 70.

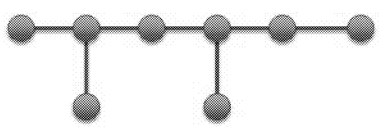

Figure 5:

We shall eliminate the remaining cases by considering the Equation 1. We know that at least one of the $a,\ b,\ c, \cdots$ is positive as otherwise Corollary 3 would be achieved. We now consider all the possibilities:

Let $M_1^{\varepsilon}(G) = 54$. In case of $a = 1$, there is a vertex of degree 3. Hence there are at least three more vertices of degree ≥ 1. If they all have $deg = 1$, then $M_2(G) = 3 \cdot 1 + 3 \cdot 1 + 3 \cdot 1 = 9 \neq 24$. If one has $deg = 2$ and the others have $deg = 1$, then $M_2(G) = 3 \cdot 2 + 3 \cdot 1 + 3 \cdot 1 + 2 \cdot 1 = 14 \neq 24$. If two have $deg = 2$ and the others have $deg = 1$, then $M_2(G) = 19$. If finally all three vertices have $deg = 2$, then $M_2(G) = 24$, see Figure 6. This graph is the required graph with $M_1^{\varepsilon}(G) = 54$.

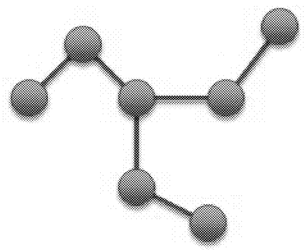

Figure 6:

Let $M_1^{\varepsilon}(G) = 62$. Acting similarly to the above, we conclude that the graph in Figure 7 is the graph with $M_1^{\varepsilon}(G) = 62$.

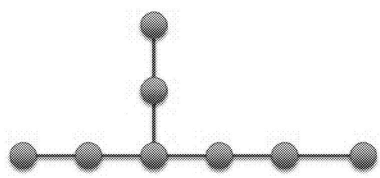

Figure 7:

We finally show that when there is at least one vertex in G having degree at least 3, by Equation 1, the other remaining values can not be attained by $M_1^{\varepsilon}(G)$.

$M_1^{\varepsilon}(G)$ can clearly not be 4. If $M_1^{\varepsilon}(G) = 6$, then $a = 1$ and $M_2(G) = 0$, which is a contradiction. If $M_1^{\varepsilon}(G) = 10$, then $a = 1$ and $M_2(G) = 2$, which is a contradiction again. The remaining cases where $M_1^{\varepsilon}(G) = 12$, implying $a = 2$ and $M_2(G) = 0$, or $a = 1$ and $M_2(G) = 3$; $M_1^{\varepsilon}(G) = 14$, implying $a = 2$ and $M_2(G) = 1$, or $a = 1$ and $M_2(G) = 4$; $M_1^{\varepsilon}(G) = 18$, implying $a = 3$ and $M_2(G) = 0$, or $a = 2$ and $M_2(G) = 3$, or $a = 1$ and $M_2(G) = 6$; $M_1^{\varepsilon}(G) = 20$, implying $a = 3$ and $M_2(G) = 1$, or $a = 2$ and $M_2(G) = 4$, or $a = 1$ and $M_2(G) = 7$; $M_1^{\varepsilon}(G) = 22$, implying $a = 3$ and $M_2(G) = 2$, or $a = 2$ and $M_2(G) = 5$, or $a = 1$ and $M_2(G) = 8$; $M_1^{\varepsilon}(G) = 26$, implying $a = 0$, $b = 1$ and $M_2(G) = 1$, or $a = 1$ and $M_2(G) = 10$, or $a = 2$ and $M_2(G) = 7$, or $a = 3$ and $M_2(G) = 4$, or $a = 4$ and $M_2(G) = 1$, all give a contradiction, and therefore should be omitted. If one continues this analysis, one can see that $M_1^{\varepsilon}(G) \neq 28,\ 30,\ 36,\ 38$ and 46. ■

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