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Inverse Problem for Sigma Index*

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Abstract

If G is a (molecular) graph and d_v the degree of its vertex u, then its sigma index is defined as $\sigma(G) = \sum(d_u - d_v)^2$, with summation going over all pairs of adjacent vertices. Some basic properties of $\sigma(G)$ are established. The inverse problem for topological indices is about the existence of a graph having its index value equal to a given non-negative integer. We study the problem for the sigma index and first show that $\sigma(G)$ is an even integer. Then we construct graph classes in which $\sigma(G)$ covers all positive even integers. We also study the inverse problem for acyclic, unicyclic, and bicyclic graphs.

1 Introduction

Let $G = (V, E)$ be a graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. For a vertex $v \in V(G)$, we denote the degree of v by d_v. A vertex with degree one is called a pendent vertex. With slight abuse of language, we shall use the term "pendent edge" for an edge having a pendent vertex. If u and v are adjacent vertices of G, then the edge connected them will be denoted by uv.

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Topological indices are defined and used in many areas to study several properties of different objects such as atoms and molecules. Several topological indices have been defined and studied by mathematicians and chemists [26, 27]. They are defined as graph invariants corresponding to and reflecting several physical, chemical, pharmacological, pharmaceutical, biological, etc. properties of the underlying chemical species.

Two of the most important degree–based topological graph indices are the first and second Zagreb indices:

$$M_1(G) = \sum_{u\in V(G)} (d_u)^2 = \sum_{uv\in E(G)} \left[d_u + d_v\right] \tag{1}$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_u\, d_v\,. \tag{2}$$

respectively. These were introduced in the 1970s [15,16]. For details of their mathematical theory and chemical applications see [5, 7, 13, 21] and the references cited therein.

Two additional Zagreb–type indices are the forgotten index [11]

$$F(G) = \sum_{u\in V(G)} (d_u)^3 = \sum_{uv\in E(G)} \left[(d_u)^2 + (d_v)^2\right] \tag{3}$$

and the hyper–Zagreb index [24]

$$Hyp(G) = \sum_{uv\in E(G)} (d_u + d_v)^2\,. \tag{4}$$

Also the present Turkish authors contributed recently to the research of Zagreb–type indices. In [6], some results on the first Zagreb index together with some other indices are given. In [8], the multiplicative versions of these indices are studied. Some relations between Zagreb indices and some other indices, such as ABC, GA and Randić, are obtained in [20]. Zagreb indices of the line graphs of subdivision graphs were studied in [22]. A more generalized version of subdivision graphs is called r-subdivision graphs and their Zagreb indices are calculated in [28]. These indices were calculated for several important graph classes in [30].

If all vertices of a graph have the same degree, then the graph is said to be regular. Regularity makes calculations easier in many occasions. A graph which is not regular, that is which has at least two different vertex degrees, is said to be irregular. Irregularity may occur slightly or strongly. As a result of this, several measures for irregularity have been defined and used by some authors [14, 18, 23]. Some of these measures are in terms of vertex degrees. The most thoroughly investigated ones are the Albertson index [2]

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|$$

see also [10], and the Bell index [4]

$$B(G) = \sum_{v \in V(G)} \left(d_v - \frac{2m}{n} \right)^2 .$$

Another irregularity index was briefly mentioned in [1, 12], but seems that has not been investigated in any detail. Motivated by this fact, we studied this index and its properties, especially the inverse problem for it. We propose that this graph invariant be called *sigma index* and be denoted by σ in resemblance with the standard deviation in statistics. It is defined as

$$\sigma = \sigma(G) = \sum_{uv \in E(G)} (d_u - d_v)^2 . \tag{5}$$

In this paper, we mainly study the inverse problem for the sigma index. We show in Theorem 2.1 that $\sigma(G)$ must be even for any graph G, and then we construct some graph classes such that their sigma indices cover all positive even integers.

2 Sigma index

We first establish some simple properties of the sigma index that will be helpful in solving the inverse problem. First of all, we point out the identity

$$\sigma(G) = F(G) - 2M_2(G) \tag{6}$$

which is directly obtained by combining Eqs. (2), (3), and (5).

Theorem 2.1. *For every simple graph G, $\sigma(G)$ is an even integer.*

Proof. The well known relation $\sum_{u \in V(G)} d_u = 2m$ implies that in the graph G there must be an even number (or zero) vertices of odd degree. Therefore, on the right–hand side of Eq. (3), an even number of terms $(d_u)^3$ are odd, implying that $F(G)$ is an even integer. Theorem 2.1 follows then from the identity (6). ∎

Note that by the same argument, also $M_1(G)$, $Hyp(G)$, and $Alb(G)$ are even integers.

In addition to the above simple proof, we demonstrate the validity of Theorem 2.1 in a less straightforward manner. By this we will be able to arrive at some relations that are needed in the subsequent considerations.

Proof. By induction. The smallest graph for which σ can be calculated is N_2, the edgeless graph with two vertices. Obviously $\sigma(N_2) = 0$, which is even. Now we move to the induction step. Let G be a simple graph with n vertices. We can assume that G is connected as otherwise we can sum up the sigma indices of all components to get $\sigma(G)$.

We now prove the statement by means of a simple and accurate idea of demonstrating that by adding a new edge e to a graph G, the parity of σ remains the same. There are two cases to consider:

i) e connects two non-adjacent vertices u and v;

ii) e joins a vertex u of G to a new vertex $v \notin V(G)$.

Case *i)* Let u and v be two non-adjacent vertices of G. Let the degrees of u and v in G be denoted by $d_u = k$ and $d_v = t$. Let also $N_G(u) = \{v_1, v_2, \ldots, v_k\}$ and $N_G(v) = \{v'_1, v'_2, \ldots, v'_t\}$. Finally let the degrees of v_i for $1 \le i \le k$ be d_i and the degrees of v'_i for $1 \le i \le t$ be d'_i. Then

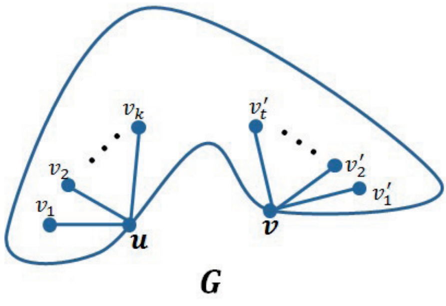

Figure 1. Non-adjacent vertices u and v

$$\begin{aligned}
\sigma(G) &= \sigma(G - \{u,v\}) + \sum_{i=1}^{k} (k - d_i)^2 + \sum_{i=1}^{t} (t - d'_i)^2 \\
&= \sigma(G - \{u,v\}) + k \cdot k^2 - 2k \sum_{i=1}^{k} d_i + \sum_{i=1}^{k} d_i^{\,2} + t \cdot t^2 - 2t \sum_{i=1}^{t} d'_i + \sum_{i=1}^{t} (d'_i)^2 .
\end{aligned}$$

Now add a new edge e to join u and v as in Fig. 2.

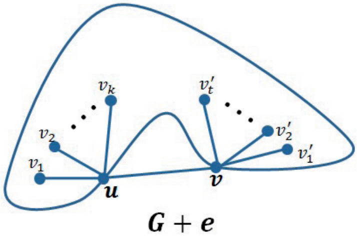

Figure 2. The graph $G+e$

Then,

$$\begin{aligned}\sigma(G+e) &= \sigma(G-\{u,v\}) + (d_u+1-d_1)^2 + \cdots + (d_u+1-d_k)^2 \\ &+ (d_v+1-d'_1)^2 + \cdots + (d_v+1-d'_t)^2 + (d_u-d_v)^2\end{aligned}$$

and hence

$$\sigma(G+e) - \sigma(G) = k+t+2\left[k^2+t^2-\sum_{i=1}^{k} d_i - \sum_{i=1}^{t} d'_i\right] + (k-t)^2$$

which is clearly even as $k+t$ and $(k-t)^2$ have the same parity.

Case $ii)$ Let us add a new edge e to join a vertex $v \in G$ to a new pendent vertex $v \notin V(G)$ as in Fig. 3:

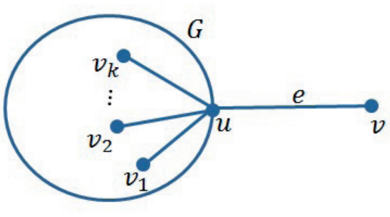

Figure 3. A graph with a pendent edge

Let the degree of u in G be denoted by $d_u = k$ and let $N_G(u) = \{v_1, \ldots, v_k\}$ with d_i denoting the degree of v_i. Then

$$\sigma(G) = \sigma(G-u) + k^3 + \sum_{i=1}^{k} d_i{}^2 - 2k\sum_{i=1}^{k} d_i$$

and

$$\sigma(G+e) = \sigma(G-u) + k^3 + 3k^2 + k + \sum_{i=1}^{k} {d_i}^2 - 2k\sum_{i=1}^{k} d_i - 2\sum_{i=1}^{k} d_i$$

implying that

$$\sigma(G+e) - \sigma(G) = k(3k+1) - 2\sum_{i=1}^{k} d_i$$

which is again an even integer. ■

Corollary 2.1. *Let G be a simple graph. Let a vertex u of G be joined to a new vertex $v \notin V(G)$ by a new pendent edge e. Then $\sigma(G+e) = \sigma(G)$ if and only if*

$$\sum_{v\in N(u)} d_v = \frac{k(3k+1)}{2}\,.$$

Proof. By the second proof of Theorem 2.1, $\sigma(G+e) = \sigma(G) = k(3k+1) - 2\sum_{i=1}^{k} d_i$. ■

If the vertex u is pendent, we have

Corollary 2.2. *Let G be a simple graph. Let a pendent vertex u of G be joined to a new pendent vertex $v \notin V(G)$ by a new pendent edge e. Then $\sigma(G+e) = \sigma(G)$ iff $d_v = 2$.*

Proof. By easy computation. ■

Corollary 2.2 means that if we have a pendent path of length at least 2 in a graph G and if we add a new edge to the pendent end of this path, then the sigma index does not change. This enables us to omit the branches of length more than 2 when calculating the sigma index, see Fig. 4.

Figure 4. Tadpole graphs with equal σ indices

Similarly, if we have a cycle of length k within G which has $k-1$ vertices of degree 2, then we can replace this cycle with a triangle, see Fig. 5. We shall call this replacement a cyclic reduction.

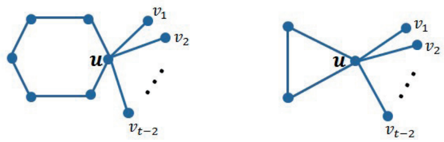

Figure 5. Cyclic reduction keeps σ unchanged: both graphs have equal σ-values

In general, if we have a sequence of adjacent vertices $v_1, v_2, \ldots, v_q$ of degree 2, we can replace this $v_1 - v_q$ path by an edge connecting v_1 to v_q. Similarly, we call this replacement a path reduction, see Fig. 6.

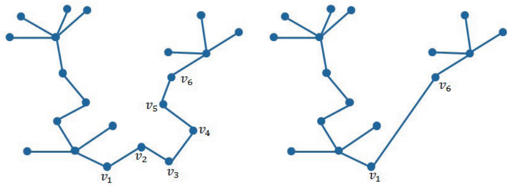

Figure 6. Path reduction keeps σ unchanged: both graphs have equal σ-values

The above specified two reductions enable one to calculate $\sigma(G)$ by determining the σ-value of a graph much smaller than G.

Theorem 2.2. *Let $S_{r,k}$ be the double star depicted in Fig. 7. Let the degrees of two adjacent central vertices u, v be $d_u = k \geq 3, d_v = r \geq 1$. The sigma index of $S_{r,k}$ is then given by*

$$\sigma(S_{r,k}) = (k-1)^3 + k^2 + (r-1)^3 + r^2 - 2kr\,.$$

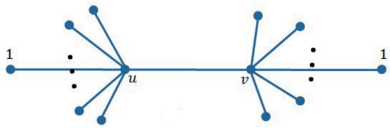

Figure 7. The double star graph $S_{r,k}$

Similar results can be given for $d_u \geq 1, d_v \geq 3$.

Proof. Consider the following graphs in Figs. 8, 9, and 10:

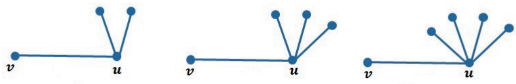

Figure 8. The graphs $S_{1,3}$, $S_{1,4}$, and $S_{1,5}$

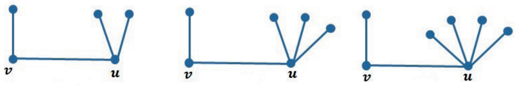

Figure 9. The graphs $S_{2,3}$, $S_{2,4}$, and $S_{2,5}$

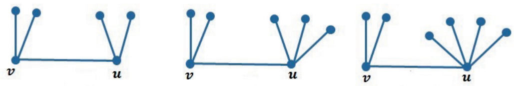

Figure 10. The graphs $S_{3,3}$, $S_{3,4}$, and $S_{3,5}$

Consider the graphs $S_{1,k}$. It is easy to see that

$$\sigma(S_{1,k}) = (k-1)^2 \cdot k = k^3 - 2k^2 + k],.$$

In an analogous manner we can obtain the following formulas:

$$\begin{aligned}
\sigma(S_{2,k}) &= k^3 - 2k^2 - k + 4 \\
\sigma(S_{3,k}) &= k^3 - 2k^2 - 3k + 16 \\
\sigma(S_{4,k}) &= k^3 - 2k^2 - 5k + 42 \\
\sigma(S_{5,k}) &= k^3 - 2k^2 - 7k + 88 \\
\sigma(S_{6,k}) &= k^3 - 2k^2 - 9k + 160\,.
\end{aligned}$$

It is not difficult to see that the coefficient of k in $\sigma(S_{r,k})$ is $3-2r$. To find the constant term, say a_r, which only depends on r, note that the following formula is satisfied:

$$a_{r+1} = a_r + 12 + \sum_{i=1}^{r-2}(6i+8)\,.$$

Therefore we conclude that

$$a_{r+1} = a_r + 3r^2 - r + 2\,.$$

After telescopic sum, we obtain the general formula for the constant term of $\sigma(S_{r,k})$ as

$$a_r = (r-1)(r^2 - r + 2)\,.$$

Hence the result follows. ∎

Note that $\sigma(S_{r,k})$ increases according to the following relations when we move to the right and down in Figs. 8, 9 and 10:

Corollary 2.3. $\sigma(S_{r,k+1}) - \sigma(S_{r,k}) = 3k^2 - k - 2(r-1)$.

Corollary 2.4. $\sigma(S_{r+1,k}) - \sigma(S_{r,k}) = 3r^2 - r - 2(k-1)$.

Note that moving to right (respectively down) in Figs. 8, 9, and 10 means that we are adding a new pendent vertex (and edge) to u (respectively v). Hence we can obtain the σ index of $S_{r,k}$ for large r and k in terms of smaller r and k's.

3 Inverse problem for sigma index

Inverse problems are encountered in many areas of science, and naturally in mathematics. Graph–theoretical problems of this kind are also interesting. The inverse problem for topological indices is concerned with the existence of a graph whose index is equal to a given non-negative integer. This problem. representing the beginning of what nowadays is referred to as the inverse problem for graph indices, seems to be first proposed in [17]. In [25], 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. In [31], Wagner showed that each integer greater than 469 is the Wiener index of a special graph class called starlike trees. In [32], all 49 positive integer values which are not the Wiener index of any graph are listed. Some more results for the Wiener index can be found in [3] and [9].

In [19], the inverse problem for four topological indices was studied. Recently, in [29], the inverse problem for the second Zagreb index $M_2(G)$, forgotten index $F(G)$, and hyper–Zagreb index $HM(G)$ was completely solved. In particular, the authors of [29] 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 were established.

In this paper, we study the inverse problem for σ index, which is one of the irregularity indices. Our methodology depends on the following crucial observations:

Transformation 3.1. *Let G be a graph possessing adjacent vertices u, v of degree 3. Construct the graph G^* by inserting a new vertex x of degree 2 on the edge connecting u and v, cf. Fig. 11.*

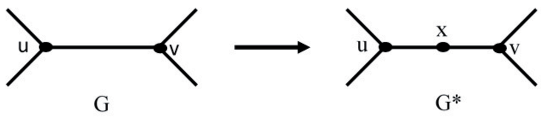

Figure 11. Transformation 3.1

Lemma 3.1. *For any graph G having two adjacent vertices of degree 3,*

$$\sigma(G^*) = \sigma(G) + 2\,.$$

That is, applying Transformation 3.1 increases the sigma index of a graph G satisfying the given degree conditions by 2.

Proof. Let u and v be two adjacent vertices of the graph G having degree $d_u = d_v = 3$. Let us add a vertex x of degree 2 on the edge uv. Then

$$\sigma(G) = \sum_{\substack{rs \in E(G) \\ rs \neq uv}} (d_r - d_s)^2$$

and

$$\sigma(G^*) = (d_u - d_x)^2 + (d_x - d_v)^2 + \sum_{\substack{rs \in E(G^*) \\ rs \neq ux, xv}} (d_r - d_s)^2 = 1^2 + 1^2 + \sum_{\substack{rs \in E(G) \\ rs \neq uv}} (d_r - d_s)^2$$

implying the result. ∎

Transformation 3.2. *Let G and G^* be as in Transformation 3.1. Construct the graph G^{**} by attaching a new pendent vertex y to the vertex x of G^*, cf. Fig. 12.*

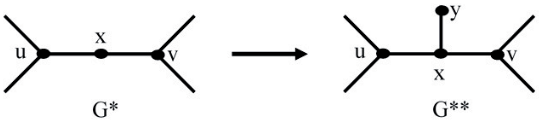

Figure 12. Transformation 3.2

Lemma 3.2. *Let G and G^* be as in Transformation 3.1. Then*

$$\sigma(G^{**}) = \sigma(G) + 4\,.$$

That is, applying Transformation 3.2 increases the sigma index of a graph G satisfying the given degree conditions by 4.

Proof. Let G be as in Lemma 3.1. Construct G^{**} as described by Transformation 3.2. In Fig. 12, we have $d_u = d_v = d_x = 3$ and $d_y = 1$. We then have

$$\sigma(G^{**}) = (d_u - d_x)^2 + (d_x - d_v)^2 + (d_x - d_y)^2 + \sum_{\substack{rs \in E(G^*) \\ rs \neq ux, xv, xy}} (d_r - d_s)^2 = 0^2 + 0^2 + 2^2 + \sum_{\substack{rs \in E(G) \\ rs \neq uv}} (d_r - d_s)^2$$

which together with the proof of Lemma 3.1 implies the result. ■

The following result answers the inverse problem for σ index:

Theorem 3.1. *For all non-negative integers k, there exists at least one graph G with $\sigma(G) = 2k$.*

Proof. Note first that any regular graph has σ index equal to 0. So we can start with a 3-regular graph G_0 of order at least 2 to satisfy the degree conditions. Let u and v be two adjacent vertices. Evidently, $\sigma(G_0) = 0$. Construct the graph G_1 by applying Transformation 3.1 to G_0. Then

$$\sigma(G_1) = \sigma(G_0) + 2 = 2\,.$$

Construct the graph G_2 by applying Transformation 3.2 to G_1. Then

$$\sigma(G_2) = \sigma(G_1) + 2 = \sigma(G_0) + 2 \cdot 2 = 4\,.$$

Now note that the graph G_2 obtained by successively applying Transformations 3.1 and 3.2 to the graph G_0 possesses two new pairs of adjacent vertices of degree 3: u, x and

x, v, see Fig. 12. Therefore we can apply Transformation 3.1 to G_2 gives a new graph G_3 and by Lemma 3.1, we get

$$\sigma(G_3) = \sigma(G_2) + 2 = \sigma(G_0) + 3 \cdot 2 = 6\,.$$

Now apply the Transformation 3.2 to G_3 to reach to a graph G_4. Evidently,

$$\sigma(G_4) = \sigma(G_3) + 2 = \sigma(G_0) + 4 \cdot 2 = 8\,.$$

Continuing in this fashion, we arrive at graphs $G_5, G_6, G_7, \ldots, G_k, \ldots$ for which $\sigma(G_k) = 2k$. That is, σ can take all non-negative even integer values. ■

Transformation 3.3. *Let G be a graph possessing a vertex v of degree $d \geq 2$. Let $u_1, u_2, \ldots, u_d$ be the vertices of G adjacent to v. Construct the graph $G^\dagger$ by replacing vertex v with a complete graph K_d on d vertices. Thus, if the vertices of this complete graph are $v_1, v_2, \ldots, v_d$, then in $G^\dagger$, v_i is adjacent with u_i, for $i = 1, 2, \ldots, d$, cf. Fig. 13.*

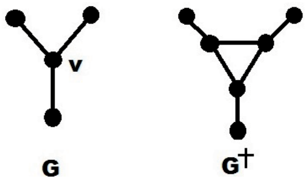

Figure 13. Transformation 3.3 with $d = 3$

Lemma 3.3. *For any graph G different than null graph and K_2,*

$$\sigma(G^\dagger) = \sigma(G)\,.$$

That is, applying Transformation 3.3 preserves the sigma index.

The proof is straightforward.

Clearly, Transformation 3.3 can be repeatedly applied infinitely many times, resulting in the following corollary:

Corollary 3.1. *For each fixed non-negative integer k, there exists infinitely many connected graphs G with $\sigma(G) = 2k$.*

Transformation 3.4. *Let G be a graph possessing a vertex v of degree 2. Let the neighbors of v be u_1, u_2. Construct the graph G^{Δ} by inserting new vertices (of degree 2) on the edges vu_1 and vu_2, and by attaching a two-vertex path to v, cf. Fig. 14.*

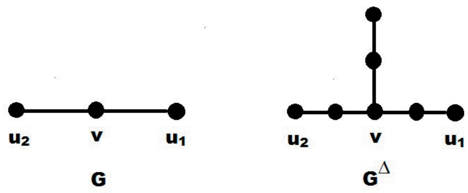

Figure 14. Transformation 3.4

Lemma 3.4. *For any graph G different than the null graph and K_2,*

$$\sigma(G^{\Delta}) = \sigma(G) + 4\,.$$

That is, applying Transformation 3.4 to all graphs except for null graphs and K_2, increases the sigma index by 4.

The proof is by computation.

The following three results are direct consequences of Lemma 3.4:

Corollary 3.2. *There exist trees with $\sigma = 2k$ for all non-negative integers $k \neq 2$.*

Proof. To start with, we know that $\sigma(K_2) = 0$ and $\sigma(P_n) = 2$. We show that σ can take all positive even integer values $6, 8, 10, 12, \ldots$ by means of Lemma 3.4 after finding two graphs with sigma index equal to 6 and 8. Lemma 3.4 then gives two graphs with $\sigma = 6 + 4 = 10$ and $\sigma = 8 + 4 = 12$. Successive applications of the same Lemma give all even integers ≥ 6 as the σ index of a graph. Observe that the graph G^{Δ} in Fig. 14 has $\sigma = 6$ and the graph in Fig. 15 has $\sigma = 8$.

It only remains to show that there is no graph with $\sigma(G) = 4$. For trees which are path graphs at the same time, we know that $\sigma(G) = 2$. So we may assume that G has at least one vertex of degree 3. If G is the star graph S_4, then $\sigma(S_4) = 12$. If we add an extra vertex (of degree 2) to one, two or all three branches of S_4, we obtain $\sigma(G) = 10$, 8, and 6, respectively. As σ has path reduction property, adding more vertices to three branches of S_4 will not change the sigma index. So, when G has a vertex of degree 3,

$\sigma(G)$ cannot be 4. Let us now assume that G has at least one vertex v of degree 4. If at least one vertex u adjacent to v is of degree 2, then the edge uv will contribute 4 to σ. Considering all other edges, σ cannot be 4. If at least one vertex u adjacent to v is of degree 1, then the edge uv will contribute 9 to σ. Finally if all four vertices adjacent to v are of degree 3, then the four edges connecting these vertices to v will contribute 4 to σ. Considering all other edges, σ cannot be 4 again. For graphs having a vertex with degree at least 5, we can use the same idea. ■

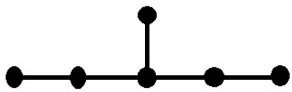

Figure 15. A graph with $\sigma = 8$

Corollary 3.3. *There exist connected unicyclic graphs with* $\sigma = 2k$ *for all non-negative integers* $k \neq 1$.

Proof. By construction. For the cycle graphs C_n, we have $\sigma(C_n) = 0$. Let G_0 be the unicyclic graph obtained by adding a path of length two to any vertex v of a cycle graph C_n, see Fig. 16 with $n = 6$. Then $\sigma(G_0) = 4$.

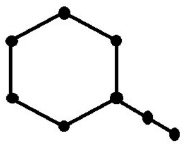

Figure 16. A unicyclic graph with $\sigma = 4$

Let G_1 be the unicyclic graph obtained by adding another path of length two to one of the two adjacent vertices to v which lie on the cycle in G_1, see Fig. 17 with $n = 6$. Then $\sigma(G_1) = 6$.

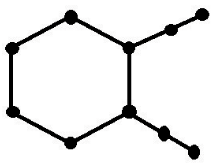

Figure 17. A unicyclic graph with $\sigma = 6$

Let now n be large enough. Continuing adding new paths of length 2 as above, yields the graphs $G_2, G_3, \ldots, G_k, \ldots$ with $\sigma(G_k) = 2k$. ■

Corollary 3.4. *There exist connected bicyclic graphs with $\sigma = 2k$ for all non-negative integers $k \neq 0, 1$.*

Proof. By construction. Let B_2 be the bicyclic graph obtained by gluing two cycle graphs of length not necessarily the same, along one sides of both, see Fig. 18. Then $\sigma(B_2) = 4$.

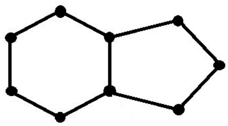

Figure 18. A bicyclic graph with $\sigma = 4$

Let B_3 be the bicyclic graph obtained by adding a path of length two to any vertex v of B_2, see Fig. 19. Then $\sigma(B_3) = 6$.

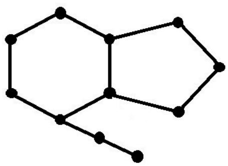

Figure 19. A bicyclic graph with $\sigma = 6$

Let B_4 be the bicyclic graph obtained by adding another path of length two to one of the two neighboring vertices of v on the cycle in B_3, see Fig. 20. Then $\sigma(B_4) = 8$.

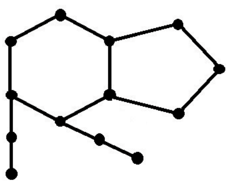

Figure 20. A bicyclic graph with $\sigma = 8$

Continuing the addition of new paths of length 2 as specified above, results in the graphs $B_5, B_6, \ldots, B_k, \ldots$ with $\sigma(B_k) = 2k$. ■

References

[1] H. Abdo, D. Dimitrov, The total irregularity of graphs under graph operations, *Miskolc Math. Notes* **15** (2014) 3–17.

[2] M. O. Albertson, The irregularity of a graph, *Ars Comb.* **46** (1997) 219–225.

[3] Y. E. A. Ban, S. Bespamyatnikh, N. H. Mustafa, On a conjecture on Wiener index in combinatorial chemistry, in: T. Warnow, B. Zhu (Eds.), *Computing and Combinatorics*, Springer, Berlin, 2003, pp. 509–518.

[4] F. K. Bell, A note on the irregularity of graphs, *Lin. Algebra Appl.* **161** (1992) 45–54.

[5] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Computer Chem.* **78** (2017) 17–100.

[6] K. C. Das, N. Akgunes, M. Togan, A. Yurrtas, I. N. Cangul, A. S. Cevik, On the first Zagreb index and multiplicative graph coindices of graphs, *Ann. Univ. Ovidius Consatnta* **21** (2016) 153–176.

[7] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[8] K. C. Das, A. Yurttas, M. Togan, A. S. Cevik, I. N. Cangul, The multiplicative Zagreb indices of graph operations, *J. Ineq. Appl.* (2013) #90.

[9] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener Index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[10] G. H. Fath–Tabar, I. Gutman, R. Nasiri, Extremely irregular trees, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **145** (2013) 1–8.

[11] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[12] B. Furtula, I. Gutman, Ž. Kovijanić Vukićević, G. Lekishvili, G. Popivoda, On an old/new degree–based topological index, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **40** (2015) 19–31.

[13] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[14] I. Gutman, P. Hansen, H. Melot, Variable neighborhood search for extremal graphs 10. Comparision of irregularity indices for chemical trees, *J. Chem. Inf. Model.* **45** (2005) 222–230.

[15] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[16] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[17] I. Gutman, Y. Yeh, The sum of all distances in bipartite graphs, *Math. Slovaca* **45** (1995) 327–334.

[18] B. Horoldagva, L. Buyantogtokh, S. Dorjsembe, I. Gutman, Maximum size of maximally irregular graphs. *MATCH Commun. Math. Comput. Chem.* **76** (2016) 81–98.

[19] X. Li, Z. Li, L. Wang, The inverse problems for some topological indices in combinatorial chemistry, *J. Comput. Biol.* **10** (2003) 47–55.

[20] V. Lokesha, S. B. Shetty, P. S. Ranjini, I. N. Cangul, Computing ABC, GA, Randić and Zagreb indices, *Enlight. Pure Appl. Math.* **1** (2015) 17–28.

[21] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003), 113–124.

[22] P. S. Ranjini, V. Lokesha, I. N. Cangul, On the Zagreb indices of the line graphs of the subdivision graphs, *Appl. Math. Comput.* **218** (2011) 699–702.

[23] T. Réti, E. Tóth–Laufer, On the construction and comparison of graph irregularity indices, *Kragujevac J. Sci.* **39** (2017) 53–75.

[24] G. H. Shirdel, H. Rezapour, A. M. Sayadi, The hyper–Zagreb index of graph operations, *Iran. J. Math. Chem.* **4** (2013) 213–220.

[25] M. Tavakoli, F. Rahbarnia, Note on properties of first Zagreb index of graphs, *Iran. J. Math. Chem.* **3** (2012) 1–5.

[26] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[27] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009, Vol. 1, Vol. 2.

[28] M. Togan, A. Yurttas, I. N. Cangul, Some formulae and inequalities on several Zagreb indices of r-subdivision graphs, *Enlight. Pure Appl. Math.* **1** (2015) 29–45.

[29] M. Togan, A. Yurttas, I. N. Cangul, Inverse problem for the second Zagreb index and hyper–Zagreb index, (preprint).

[30] M. Togan, A. Yurttas, I. N. Cangul, All versions of Zagreb indices and coindices of subdivision graphs of certain graph types, *Adv. Stud. Contemp. Math.* **26** (2016) 227–236.

[31] S. G. Wagner, A class of trees and its Wiener index, *Acta Appl. Math.* **91** (2006) 119–132.

[32] H. Wang, G. Yu, All but 49 numbers are Wiener indices of trees, *Acta Appl. Math.* **92** (2006) 15–20.