

Sigma Index and Forgotten Index of the Subdivision and r -Subdivision Graphs

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Abstract

Topological graph indices are defined and used by mathematicians and chemists to obtain some chemical properties of a molecule under consideration by calculating the related topological index obtained from the graph modelling the molecule. This saves one from a lot of laboratory work and its labor and cost. In this paper, we concentrate on two of these topological graph indices, namely the sigma index and the forgotten index of a graph. We calculate these two indices for the subdivision and r -subdivision graphs and give examples for some well-known graph classes.

1 Introduction

In this paper, we take $G = (V, E)$ as a simple, connected and undirected graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. That means, we do not allow loops or multiple edges. For a vertex $v \in V(G)$, the degree of v is denoted by $d_G(v)$ or briefly by $d(v)$, if there is no possible confusion. As a special case, a vertex with degree one is called a pendant vertex. As usual, we denote by P_n , C_n , S_n , K_n , $K_{a,b}$ and $T_{a,b}$ the path, cycle, star, complete, complete bipartite and tadpole graphs, respectively.

Topological graph indices which are very useful graph invariants are defined and used in many areas to study several properties of different objects such as atoms and molecules. These indices

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can be classified into several classes according to their way of definition: by means of matrices, by means of vertex degrees, by means of distances, etc.

Two of the most frequently used vertex degree-based topological graph indices are the first and second Zagreb indices defined by

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

These indices were defined by Gutman and Trinajstić, [9], in 1972. Some results on the first Zagreb index together with some other indices were given in [4]. In [5], the multiplicative versions of these indices are studied. These indices are calculated in [10] for some graph operations. Some relations between Zagreb indices and some other indices such as ABC, GA and Randić indices are obtained in [11]. Zagreb indices of subdivision graphs were studied in [13] and these were calculated for the line graphs of the subdivision graphs in [12]. A more generalized version of subdivision graphs is called r -subdivision graphs and Zagreb indices of r -subdivision graphs are calculated in [15]. These indices are calculated for several important graph classes in [14].

In this paper, we particularly deal with two of the vertex degree based graph indices which had not appeared in the literature as much as they deserve. The F -index of a graph G denoted by $F(G)$ or $M_3(G)$ is defined as the sum of the cubes of the degrees of the vertices of the graph. The total π -electron energy depends on the degree based sums $M_1(G)$ and

$$F(G) = \sum_{u \in V(G)} d_G^3(u).$$

These indices were first appeared in the study of structure-dependency of total π -electron energy in 1972, [9]. The first index, as we have already seen, was later named as the first Zagreb index and the second sum has never been further studied. In a recent paper, this sum was named as the forgotten index by Furtula and Gutman, [7], and it was shown to have an exceptional applicative potential.

If all vertices of a graph have the same degree, then the graph is called 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 called irregular. Irregularity may occur slightly or strongly. As a result of this, several measures for irregularity have been defined and used by some authors. Some of those measures are in terms of vertex degrees. The most thoroughly investigated ones are the Albertson index (which is also called irregularity index, third Zagreb index or Kekule index)

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

see [2], [6], [8], and the Bell index

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

see [3] and [8].

There is yet another irregularity index in literature. Although it was mentioned that this index may have important applicative properties, [1] and [8], there is no further investigation about it. The second author studied this index and its properties, especially the inverse problem for it, in [16]. In this paper, this index is going to be called as the sigma index which is going to be denoted by σ in resemblance with the standard deviation in statistics and defined by

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

Most of the topological graph indices have several applications in various areas including chemical graph theory due to their advantages over existing experimental methods with high costs. In recent years, a large number of topological indices have been defined and utilized for chemical documentation, isomer discrimination, molecular complexity, chirality, similarity, QSAR/QSPR, drug design and database selection, lead optimization, etc. The pharmaceutical industry contributed towards increased interest in molecular descriptors because of the necessity to reduce the expenditure involved in synthesis, in vitro, in vivo, or clinical testing of new medicinal compounds.

This paper is planned as follows: In Section 2, sigma indices of subdivision and r -subdivision graphs are calculated and these numbers are also obtained for some well-known graph classes. In Section 3, the forgotten index of subdivision and r -subdivision graphs are calculated and similar examples are given for the same graph classes. Some relations between these indices are given.

2 Sigma index of subdivision and r -subdivision graphs

Recall that the subdivision graph $S(G)$ of a graph G is the graph obtained from G by replacing each of its edges by a path of length 2, or equivalently by inserting an additional vertex into each edge of G . The subdivision graph of the cycle graph is illustrated in Figure 1.

Subdivision graphs are used to obtain several mathematical and chemical properties of more complex graphs from more basic graphs and there are many results on these graphs.

Figure 2 shows the molecular graph of the transition state of the first step of the nucleophilically unassisted solvolysis of protonated 2-endo- and 2-exo-norbornanol. There are three critical points: nuclear attractor critical point, bond critical point and ring critical point.

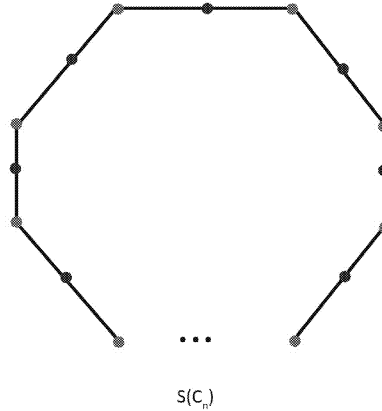


Figure 1: Subdivision of the cycle graph C_n

There are several papers dealing with some topological indices, mainly several Zagreb indices and coindices, of the subdivision graphs of some graphs. In [12], the Zagreb indices of the line graphs of the subdivision graphs were studied. In [13], Zagreb indices of the subdivision graphs were calculated. In [14], all 10 versions of Zagreb indices and coindices of subdivision graphs of certain graph types were calculated. Similarly, in [17], Zagreb indices and multiplicative Zagreb indices of subdivision graphs of double graphs which are obtained by taking another copy of the given graph and joining all vertices in one to all neighbour vertices in the other were found. In [17], this time, Zagreb indices and multiplicative Zagreb indices of subdivision graphs of double graphs were studied.

When the graph G is regular, we have an immediate result about the sigma index of G :

Lemma 2.1. *If G is a regular graph, then*

$$\sigma(G) = 0.$$

The following is a useful relation giving the sigma index in terms of the forgotten index and the second Zagreb index:

Theorem 2.1. *For any simple connected graph G , we have*

$$\sigma(G) = F(G) - 2M_2(G).$$

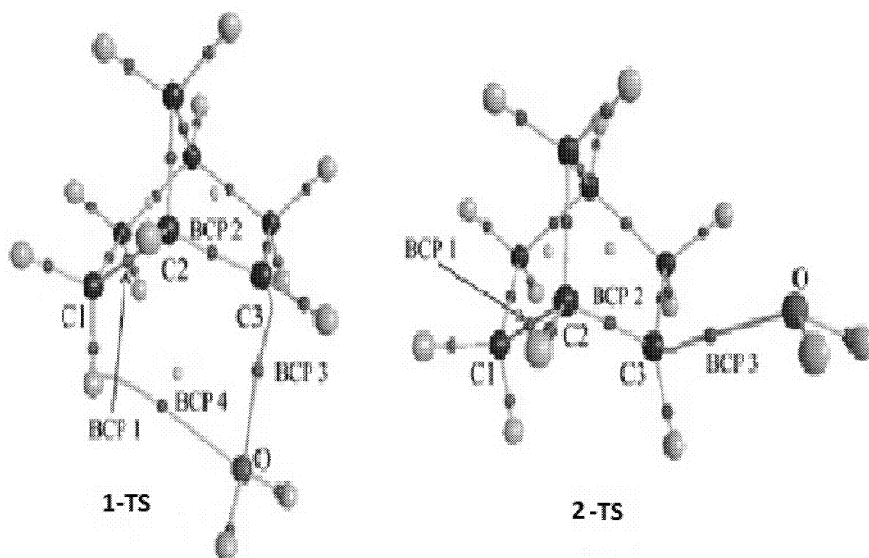


Figure 2: Molecular graphs of the transition state of solvolysis of 2-endo- and 2-exo-norbornanols

Proof. By the definition, we have

$$\begin{aligned}
 \sigma(G) &= \sum_{uv \in E(G)} (d_u - d_v)^2 \\
 &= \sum_{uv \in E(G)} (d_u^2 + d_v^2) - 2 \sum_{uv \in E(G)} d_u d_v \\
 &= \sum_{w \in V(G)} d_w^3 - 2 \sum_{uv \in E(G)} d_u d_v \\
 &= F(G) - 2M_2(G).
 \end{aligned}$$

□

In a similar way to the subdivision graphs, the r -subdivision graph of G denoted by $S^r(G)$ is defined by adding r vertices to each edge by Togan, Yurttas and Cangul in [15]. They had calculated the first and second Zagreb indices and multiplicative Zagreb indices of graphs. They had also given some relations between these numbers.

Lemma 2.2. *Sigma index stays invariant for all the r -subdivision graphs $S^r(G)$ where $r = 1, 2, 3, \dots$. That is, for any simple connected graph G ,*

$$\sigma(S^r(G)) = \sigma(S(G)).$$

Proof. Consider an edge uv of G . Let d_u and d_v be the degrees of the vertices u and v , respectively. We obtain the subdivision graph $S(G)$ of G by adding a vertex w to the edge uv (and a new vertex to each of all other edges of G . As dealing with the edge uv is enough to complete the proof, we shall not put the extra vertices on the other edges).

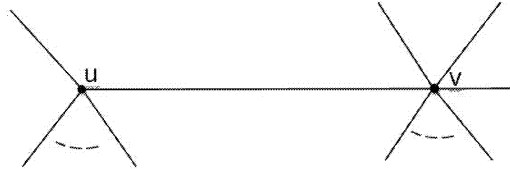


Figure 3: A graph G

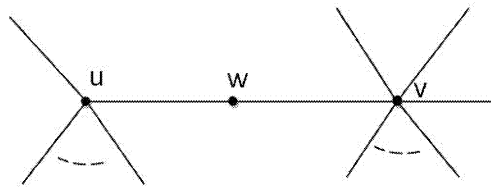


Figure 4: The subdivision graph $S(G)$

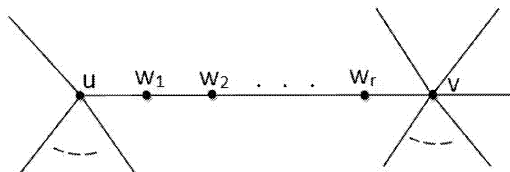


Figure 5: The r -subdivision graph $S^r(G)$

As in Figure 4, the part of $\sigma(S(G))$ corresponding to the edge uv is $(d_u - d_w)^2 + (d_w - d_v)^2$ which is equal to $(d_u - 2)^2 + (d_v - 2)^2$ as $d_w = 2$, and the part of $\sigma(S^r(G))$ corresponding to the edge uv is $(d_u - d_{w_1})^2 + (d_{w_1} - d_{w_2})^2 + \dots + (d_{w_{r-1}} - d_{w_r})^2 + (d_{w_r} - d_v)^2$ which is equal to $(d_u - 2)^2 + (d_v - 2)^2$ as $d_{w_i} = 2$ for each $i = 1, 2, \dots, r$. The result then follows. \square

Theorem 2.2. For any graph G

$$\sigma(S^r(G)) = \sum_{u \in V(G)} d_u(d_u - 2)^2.$$

Proof. By Lemma 2.2, it is enough to calculate $\sigma(S(G))$. Consider an edge uv as above.

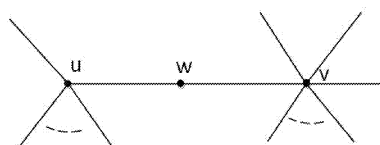


Figure 6: The subdivision graph $S(G)$

For the edge uv , we have $(d_u - d_w)^2 + (d_w - d_v)^2 = (d_u - 2)^2 + (d_v - 2)^2$ in $\sigma(S(G))$. Similarly each edge adds a similar sum to $\sigma(S(G))$. For each $u \in V(G)$, d_u times $(d_u - 2)^2$ is added to $\sigma(S(G))$. Therefore the result follows. \square

Corollary 2.1. For any simple connected graph G with n vertices and m edges, we have

$$\sigma(S^r(G)) = F(G) - 4M_1(G) + 8m.$$

The proof is straightforward.

Example 2.1. The sigma indices of some frequently-used graph classes are given as follows:

$$\sigma(G) = \begin{cases} 2 & \text{if } G = P_n, n \geq 2 \\ 0 & \text{if } G = C_n, n > 2 \\ m \cdot (n - 2)^2 & \text{if } G = S_n, n \geq 2 \\ 0 & \text{if } G = K_n, n \geq 2 \\ (a - b)^2 \cdot ab & \text{if } G = K_{a,b}, a, b \geq 1 \\ 4 & \text{if } G = T_{a,b}, a \geq 3, b \geq 1, \end{cases}$$

$$\sigma(S^r(G)) = \begin{cases} 2 & \text{if } G = P_n, n \geq 2 \\ 0 & \text{if } G = C_n, n > 2 \\ m(1 + (n - 2)^2) & \text{if } G = S_n, n \geq 2 \\ 2m \cdot (n - 3)^2 & \text{if } G = K_n, n \geq 2 \\ (a - 2)^2 \cdot b + (b - 2)^2 \cdot a & \text{if } G = K_{a,b}, a, b \geq 1 \\ 4 & \text{if } G = T_{a,b}, a \geq 3, b \geq 1, \end{cases}$$

The proofs of each one follows easily from the definition of sigma index combinatorically.

3 Forgotten index of subdivision and r -subdivision graphs

Theorem 3.1. *For any simple connected graph G with n vertices and m edges, we have*

$$F(S^r(G)) - F(G) = 8mr.$$

Proof. To obtain $S^r(G)$, one adds r new vertices of degree 2 to each edge. As $|E(G)| = m$, the total number of these new edges is mr . The original vertices in G do not change their degrees in $S^r(G)$. So the total value added to $F(G)$ is $mr \cdot 2^3 = 8mr$. \square

The following result giving the forgotten index of the subdivision graph is an immediate corollary of Theorem 3.1 in case of $r = 1$:

Corollary 3.1. *For any simple connected graph G with n vertices and m edges, the relation between the forgotten index of G and the forgotten index of its subdivision graph is*

$$F(S(G)) - F(G) = 8m.$$

Corollary 3.2. *For any simple connected k -regular graph G , we have*

$$F(G) = nk^3,$$

$$F(S^r(G)) = nk^3 + 8mr.$$

Note that these results are compatible with Theorem 3.1.

Example 3.1. *The forgotten indices of some frequently-used graph classes are given as follows:*

$$F(G) = \begin{cases} 2(4n - 7) & \text{if } G = P_n, n \geq 2 \\ 2^3n & \text{if } G = C_n, n > 2 \\ (n - 1) \cdot (1 + (n - 1)^2) & \text{if } G = S_n, n \geq 2 \\ n \cdot (n - 1)^3 & \text{if } G = K_n, n \geq 2 \\ ab^3 + a^3b & \text{if } G = K_{a,b}, a, b \geq 1 \\ 2^3(a + b - 2) + 28 & \text{if } G = T_{a,b}, a \geq 3, b \geq 1, \end{cases}$$

The proofs of each one follows easily from the definition of forgotten index combinatorically.

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