Advanced Studies in Contemporary Mathematics
31 (2021), No. 2, pp. 163 - 173

www.jangjeon.or.kr
http://dx.doi.org/10.17777/ascm2021.31.2.163

STRESS INDICES OF GRAPHS

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Abstract. The stress of a vertex in a graph had been introduced by Shimbel in 1953 as the number of geodesics (shortest paths) passing through it. A topological index of a chemical structure (molecular graph) is a number that correlates given chemical structure with a chemical reactivity or physical property. In this paper, we introduce two new topological indices for graphs called first and second stress indices by means of the notion of stress of a vertex. Further, we establish some inequalities, prove some fundamental results and compute these stress indices for some standard graphs. These two indices are expected to give new applications in chemistry and social science problems as the notion of stress of a vertex depends on the geodesics passing through that vertex and may lead to new notions related to graphs.

2010 Mathematics Subject Classification. 05C05, 05C07, 05C30.

Keywords and phrases. Graph, stress index, neighborhood, stress of a vertex, geodesic.

1. Introduction

For standard terminology and notions in graph theory, we follow the textbook of Harary [4]. The non-standard notions will be given as and when required.

Let $G = (V, E)$ be a finite and undirected graph. The distance between two vertices u and v in G, denoted by $d(u, v)$, is the number of edges in a shortest path (called a graph geodesic) connecting them. We say that a graph geodesic P is passing through a vertex v in G if v is an internal vertex of P. The degree of a vertex v in G is denoted by $d_G(v)$ or $d(v)$.

The concept of stress of a vertex in a network (graph) has been introduced by Shimbel as a centrality measure in 1953, [7]. This centrality measure has applications in biology, sociology, psychology, etc., (see e.g. [5, 6]). The stress of a vertex v in a graph G, denoted by $\mathrm{str}_G(v)$ or briefly by $\mathrm{str}(v)$ if there is no possibility of confusion, is the number of geodesics passing through it. We denote the maximum stress amongst all the vertices of G by Θ_G and minimum stress among all the vertices of G by θ_G. The concepts of stress number of a graph and stress regular graphs have been studied by K. Bhargava, N. N. Dattatreya, and R. Rajendra in their paper [1]. A graph G is k-stress regular if $str(v) = k$ for all $v \in V(G)$.

The first and second Zagreb indices have been defined by means of the degrees of vertices in a graph to explain some properties of chemical compounds at molecular level, [2, 3]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a simple graph G are defined by

$$M_1(G) = \sum_{v\in V(G)} d(v)^2, \tag{1}$$

$$M_2(G) = \sum_{uv\in E(G)} d(u)d(v). \tag{2}$$

There are several variants of these two indices. By the motivation of these two indices, in this paper, we introduce two new topological indices for graphs called the first stress index and the second stress index by means of the stresses of vertices. Further, we establish some inequalities and compute both stress indices for some standard graphs.

2. Stress indices of graphs

Definition 2.1. *The first stress index $S_1(G)$ and the second stress index $S_2(G)$ of a simple graph G are defined by*

$$S_1(G) = \sum_{v\in V(G)} str(v)^2, \tag{3}$$

$$S_2(G) = \sum_{uv\in E(G)} str(u)str(v). \tag{4}$$

Observation. From the Definition 2.1, it follows that, for any graph $G = (V, E)$, we have

$$|V|\theta_G^2 \leq S_1(G) \leq |V|\Theta_G^2$$

and

$$|E|\theta_G^2 \leq S_2(G) \leq |E|\Theta_G^2.$$

Example 2.1. *We compute the stress indices of hydrogen-depleted molecular graph G of 1-Ethyl-2-methylcyclobutane C_7H_{14}. We label the vertices of G (See Fig. 1). The stresses of the vertices of G are as follows: $str(a) = 2$, $str(b) = 9$, $str(c) = 3$, $str(d) = 12$, $str(e) = 6$, $str(f) = 0$ and $str(g) = 0$. The first and second stress indices of G are*

$$\begin{aligned} S_1(G) &= 2^2 + 9^2 + 3^2 + 12^2 + 6^2 + 0^2 + 0^2 \\ &= 274, \\ S_2(G) &= 2\cdot 9 + 2\cdot 3 + 9\cdot 0 + 9\cdot 12 + 3\cdot 12 + 12\cdot 6 + 6\cdot 0 \\ &= 240. \end{aligned}$$

Example 2.2. *Consider the graph G given in Fig. 2. The stresses of the vertices of G are as follows: $str(v_1) = str(v_3) = str(v_7) = str(v_8) = 0$, $str(v_2) = 19$, $str(v_5) = 1$ and $str(v_4) = str(v_6) = 0$. Hence the first and second stress indices of G are*

$$\begin{aligned} S_1(G) &= 0^2 + 19^2 + 0^2 + 0^2 + 1^2 + 0^2 + 0^2 + 0^2 \\ &= 362, \\ S_2(G) &= 0\cdot 19 + 19\cdot 0 + 19\cdot 0 + 19\cdot 1 + 19\cdot 0 + 19\cdot 0 + 19\cdot 0 + 0\cdot 1 + 1\cdot 0 \end{aligned}$$

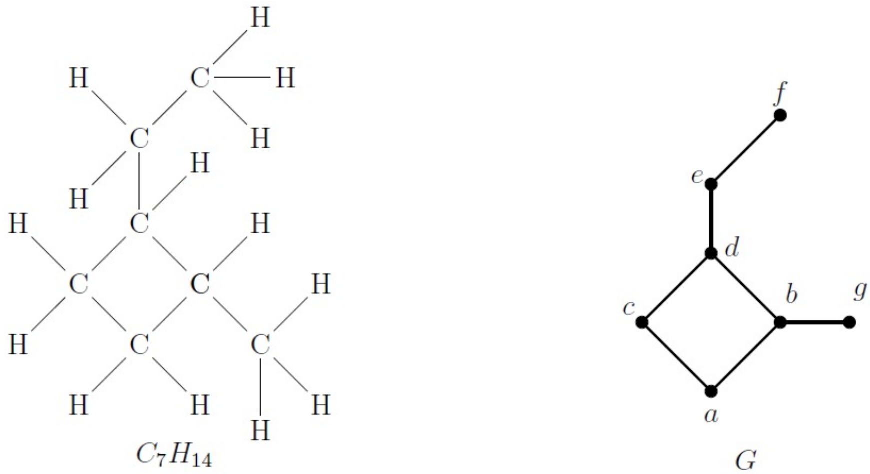

Figure 1: 1-Ethyl-2-methylcyclobutane C_7H_{14} and the corresponding hydrogen-depleted molecular graph G

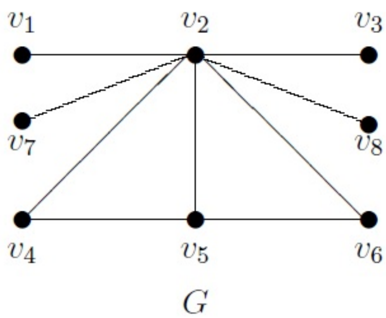

Figure 2: A graph G

$= 19.$

Proposition 2.1. *Let N be the number of geodesics of length ≥ 2 in a graph G. Then*

$$0 \leq S_1(G) \leq N^2(|V| - q) \leq N^2(|V| - p) \tag{5}$$

and

$$0 \leq S_2(G) \leq N^2(|E| - t) \leq N^2(|E| - p) \tag{6}$$

where q is the number of vertices with zero stress, p is the number of pendant vertices (which is the same as pendant edges) and t is the number of edges with at least one end vertex of zero stress in G.

Proof. If N is the number of all geodesics of length ≥ 2 in a graph G, then by the definition of stress of a vertex, for any vertex v in G, $0 \leq str(v) \leq N$.

Hence by the Definition 2.1, we have

$$0 \leq S_1(G) \leq N^2(|V| - q) \tag{7}$$

where q is the number of vertices with zero stress in G. Let p be the number of pendant vertices in G. Since the stress of a pendant vertex in a graph is zero, $p \leq q$ and so

$$N^2(|V| - q) \leq N^2(|V| - p) \tag{8}$$

Now, (5) follows from the inequalities (7) and (8).

By a similar argument as above, we can establish (6). □

Corollary 2.2. *If there is no geodesic of length ≥ 2 in a graph G, then $S_1(G) = S_2(G) = 0$. In particular, for a complete graph K_n, $S_1(K_n) = S_2(K_n) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.1, we have $S_1(G) = S_2(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and the result follows. □

Theorem 2.3. *For a graph G, $S_1(G) = 0$ if and only if the neighbours of every vertex induce a complete subgraph of G.*

Proof. Suppose that $S_1(G) = 0$. Then by Eq. (3), $str(v)^2 = 0$ for all $v \in V(G)$. Hence $str(v) = 0$ for all $v \in V(G)$. Let $v \in V(G)$. We need to show that neighbors of v induce a complete subgraph of G. If v is a pendant vertex, then there is nothing to prove. Suppose that v is not a pendant vertex. We claim that any two neighbouring vertices are adjacent in G. If there are two neighbours u and w of v that are not adjacent in G, then uvw is a graph geodesic passing through v, which implies $str(v)^2 \geq 1$, a contradiction. Hence our claim holds. Thus neighbours of v induce a complete subgraph of G. Since v is arbitrary in $V(G)$, the neighbours of every vertex induce a complete subgraph of G.

Conversely, suppose that neighbours of every vertex in G induce a complete subgraph of G. Let $v \in V(G)$. Since neighbors of v induce a complete subgraph of G, any two neighbouring vertices are adjacent and so there is no geodesic of length ≥ 2 passing through v. Since v is an arbitrary vertex in G, by the Corollary 2.2, it follows that $S_1(G) = 0$. □

Theorem 2.4. *If the neighbours of every vertex induce a complete subgraph of G, then $S_2(G) = 0$.*

Proof. Suppose that the neighbours of every vertex in G induce a complete subgraph of G. Let $v \in V(G)$. Since the neighbors of v induce a complete subgraph of G, any two neighbouring vertices of v are adjacent and so there is no geodesic of length ≥ 2 passing through v. Since v is an arbitrary vertex in G, by Corollary 2.2, it follows that $S_2(G) = 0$. □

Remark 2.1. *Converse of Theorem 2.4 is not true in general. For a counter-example, consider the path P_3 on 3 vertices:*

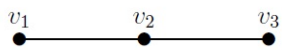

Figure 3: The path P_3

The stresses of the vertices of P_3 are as follows: $str(v_1) = str(v_3) = 0$ and $str(v_2) = 1$. Then the second stress index of P_3 is

$$S_2(P_3) = str(v_1)str(v_2) + str(v_2)str(v_3) = 0 \cdot 1 + 1 \cdot 0 = 0.$$

But here, v_1 and v_3 are the only neighbors of v that are not adjacent to each other but they do not induce a complete subgraph of P_3.

Proposition 2.5. *For the complete bipartite graph $K_{m,n}$,*

$$S_1(K_{m,n}) = \frac{mn\left[n(n-1)^2 + m(m-1)^2\right]}{4}$$

and

$$S_2(K_{m,n}) = \frac{m^2n^2(m-1)(n-1)}{4}.$$

Proof. Let $V_1 = \{v_1, \ldots, v_m\}$ and $V_2 = \{u_1, \ldots, u_n\}$ be the partite sets of $K_{m,n}$. We have

$$str(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{9}$$

and

$$str(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{10}$$

Substituting (9) and (10) in the Eqns. (3) and (4), we have

$$\begin{aligned}
S_1(K_{m,n}) &= \sum_{v \in V(G)} str(v)^2 \\
&= \sum_{i=1}^{m} str(v_i)^2 + \sum_{j=1}^{n} str(u_j)^2 \\
&= \sum_{j=1}^{m} \left[\frac{n(n-1)}{2}\right]^2 + \sum_{i=1}^{n} \left[\frac{m(m-1)}{2}\right]^2 \\
&= \frac{mn^2(n-1)^2}{4} + \frac{nm^2(m-1)^2}{4} \\
&= \frac{mn\left[n(n-1)^2 + m(m-1)^2\right]}{4}
\end{aligned}$$

and

$$\begin{aligned}
S_2(K_{m,n}) &= \sum_{uv \in E(G)} str(u)str(v) \\
&= \sum_{1 \leq i \leq m,\ 1 \leq j \leq m} str(v_i)str(u_j)
\end{aligned}$$

$$= \sum_{1\le i\le m,\ 1\le j\le n} \left[\frac{n(n-1)}{2}\right]\left[\frac{m(m-1)}{2}\right]$$
$$= mn\left[\frac{n(n-1)}{2}\right]\left[\frac{m(m-1)}{2}\right]$$
$$= \frac{m^2n^2(m-1)(n-1)}{4}.$$

□

Proposition 2.6. *If $G=(V,E)$ is a k-stress regular graph, then*

$$S_1(G) = |V|k^2$$

and

$$S_2(G) = |E|k^2.$$

Proof. Suppose that G is a k-stress regular graph. Then

$$str(v) = k$$

for all $v \in V(G)$. By the Eqns. (3) and (4), we have

$$S_1(G) = \sum_{v\in V(G)} str(v)^2 = \sum_{v\in V(G)} k^2 = |V|k^2$$

and

$$S_2(G) = \sum_{uv\in E(G)} str(u)str(v) = \sum_{uv\in E(G)} k\cdot k = |E|k^2.$$

□

Corollary 2.7. *For a cycle C_n,*

$$S_1(C_n) = S_2(C_n) = \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{64}, & \text{if } n \text{ is odd} \\ \dfrac{n^3(n-2)^2}{64}, & \text{if } n \text{ is even.} \end{cases}$$

Proof. For any vertex v in C_n, we have

$$str(v) = \begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd} \\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Hence C_n is

$$\begin{cases} \dfrac{(n-1)(n-3)}{8}\text{-stress regular}, & \text{if } n \text{ is odd} \\ \dfrac{n(n-2)}{8}\text{-stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

Since C_n has n vertices and n edges, by the Proposition 2.6, we have the result. □

Proposition 2.8. *Let T be a tree on n vertices. Then*

$$S_1(T) = \sum_{v\in I}\left[\sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right]^2$$

and

$$S_2(T) = \sum_{uv\in J}\left[\sum_{1\le i<j\le m(u)} |C_i^u||C_j^u|\right]\left[\sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right]$$

where I is the set of all internal (non-pendant) vertices in T, J is the set of internal (non-pendant) edges in T and the sets $C_1^v, \cdots, C_m^v$ denote the vertex sets of the components of $T - v$ for an internal vertex v of degree $m = m(v)$.

Proof. We know that a pendant vertex in T has zero stress. Hence we concentrate on internal (non-pendant) vertices and non-pendant edges to compute stress indices. Let v be an internal vertex of T of degree $m = m(v)$. Let $C_1^v, \cdots, C_m^v$ be the components of $T - v$. Since there is only one path between any two vertices in a tree, it follows that

$$str(v) = \sum_{1\le i<j\le m} |C_i^v||C_j^v|.$$

Hence by the Eqns. (3) and (4), we have the required results. □

Corollary 2.9. *For a path graph P_n on n vertices*

$$S_1(P_n) = \frac{n(2n-1)(n-1)^3}{6}$$

and

$$S_2(P_n) = \frac{n(n+1)(n-1)(n-2)(n-3)}{30}.$$

Proof. The proof of this corollary follows by Proposition 2.8. We follow the proof of the Proposition 2.8 to compute the indices. Let P_n be the path graph with vertices $v_1, v_2, \cdots, v_n$ (shown in Fig. 4). We have

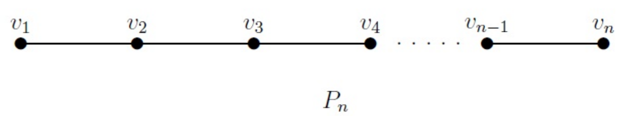

Figure 4: The path P_n on n vertices

$$str(v_i) = (i-1)(n-i),\ 1 \le i \le n.$$

$$S_1(P_n) = \sum_{v\in V(P_n)} str(v)^2 = \sum_{i=1}^{n} str(v_i)^2$$
$$= \sum_{i=1}^{n} (i-1)^2(n-i)^2$$

$$= \frac{n(2n-1)(n-1)^3}{6}$$

and

$$\begin{aligned} S_2(P_n) &= \sum_{uv \in E(P_n)} str(u)str(v) \\ &= \sum_{i=1}^{n-1} str(v_i)str(v_{i+1}) \\ &= \sum_{i=1}^{n-1} (i-1)(n-i)i(n-i-1) \\ &= \frac{n(n+1)(n-1)(n-2)(n-3)}{30}. \end{aligned}$$

□

Proposition 2.10. *Let $Wd(n,m)$ denotes the windmill graph constructed for $n \geq 2$ and $m \geq 2$ by joining m copies of the complete graph K_n at a shared common vertex v. Then*

$$S_1(Wd(n,m)) = \frac{m^2(m-1)^2(n-1)^4}{4}$$

and

$$S_2(Wd(n,m)) = 0.$$

Hence, for the friendship graph F_k on $2k+1$ vertices, we obtain

$$S_1(F_k) = 4k^2(k-1)^2$$

and

$$S_2(F_k) = 0.$$

Proof. Clearly the stress of any vertex other than universal vertex v is zero in $Wd(n,m)$ because the neighbors of that vertex induces a complete subgraph of $Wd(n,m)$. Also, since there are m copies of K_n in $Wd(n,m)$ and their vertices are adjacent to v, it follows that, the only geodesics passing through v are of length 2 only. So, $str(v) = \frac{m(m-1)(n-1)^2}{2}$. Note that there are $m(n-1)$ edges incident on v and the edges that are not incident to v have end vertices of stress zero. Hence by Eqns. (3) and (4), we have

$$S_1(Wd(n,m)) = str(v)^2 = \left[\frac{m(m-1)(n-1)^2}{2}\right]^2 = \frac{m^2(m-1)^2(n-1)^4}{4}$$

and

$$S_2(Wd(n,m)) = 0.$$

Since the friendship graph F_k on $2k+1$ vertices is nothing but $Wd(3,k)$, it follows that

$$S_1(F_k) = \frac{k^2(k-1)^2(3-1)^4}{4} = 4k^2(k-1)^2$$

and

$$S_2(F_k) = 0.$$

□

Proposition 2.11. *Let W_n denote the wheel graph on $n \geq 4$ vertices. Then*

$$S_1(W_n) = \begin{cases} \dfrac{(n-1)(n-4)^2(n^2+12n-12)}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^2(17n^2-132n+259)}{64}, & \text{if } n \text{ is odd} \end{cases}$$

and

$$S_2(W_n)) = \begin{cases} \dfrac{(n-1)(n-2)(n-4)^2(5n-6)}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^3(n-3)(5n-19)}{64}, & \text{if } n \text{ is odd.} \end{cases}.$$

Proof. In W_n with $n \geq 4$, there are $n-1$ peripheral vertices and one central vertex, say v. It is easy to see that

$$str(v) = \frac{(n-1)(n-4)}{2}. \tag{11}$$

Let p be a peripheral vertex. Since v is adjacent to all the peripheral vertices in W_n, there is no geodesic passing through p and containing v. Hence contributing vertices for $str(p)$ are the remaining peripheral vertices. So, by denoting the cycle $W_n - v$ (on $n-1$ vertices) by C_{n-1}, we have

$$\begin{aligned} str_{W_n}(p) &= str_{W_n - v}(p) \\ &= str_{C_{n-1}}(p) \\ &= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,} \end{cases} \\ &= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases} \end{aligned} \tag{12}$$

Let us denote the set of all the peripheral vertices in W_n by P, the set of all radial edges by R, and the set of all peripheral edges by Q. Note that there are $n-1$ radial edges and $n-1$ peripheral edges in W_n. Substituting Eqns. (11) and (12) in Eqns. (3) and (4), we have

$$\begin{aligned} S_1(W_n) &= str(v)^2 + \sum_{p \in P} str(p)^2 \\ &= \left[\frac{(n-1)(n-4)}{2}\right]^2 + (n-1) \times \begin{cases} \left[\dfrac{(n-2)(n-4)}{8}\right]^2, & \text{if } n \text{ is even;} \\ \left[\dfrac{(n-1)(n-3)}{8}\right]^2, & \text{if } n \text{ is odd} \end{cases} \\ &= \begin{cases} \dfrac{(n-1)^2(n-4)^2}{4} + \dfrac{(n-1)(n-2)^2(n-4)^2}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^2(n-4)^2}{4} + \dfrac{(n-1)^3(n-3)^2}{64}, & \text{if } n \text{ is odd} \end{cases} \end{aligned}$$

$$= \begin{cases} \dfrac{(n-1)(n-4)^2(n^2+12n-12)}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^2(n^3+9n^2-113n+247)}{64}, & \text{if } n \text{ is odd} \end{cases}$$

and

$$\begin{aligned} S_2(W_n)) =& \sum_{xy\in R} str(x)str(y) + \sum_{xy\in Q} str(x)str(y) \\ =&(n-1)str(v)str(p) + (n-1)str(p)^2 \\ =&(n-1) \times \frac{(n-1)(n-4)}{2} \times \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd} \end{cases} \\ &+ (n-1) \times \begin{cases} \left[\dfrac{(n-2)(n-4)}{8}\right]^2, & \text{if } n \text{ is even;} \\ \left[\dfrac{(n-1)(n-3)}{8}\right]^2, & \text{if } n \text{ is odd} \end{cases} \\ =&\begin{cases} \dfrac{(n-1)^2(n-2)(n-4)^2}{16} + \dfrac{(n-1)(n-2)^2(n-4)^2}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^3(n-3)(n-4)}{16} + \dfrac{(n-1)^3(n-3)^2}{64}, & \text{if } n \text{ is odd} \end{cases} \\ =&\begin{cases} \dfrac{(n-1)(n-2)(n-4)^2(5n-6)}{64}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)^3(n-3)(5n-19)}{64}, & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$ □

Conclusion. All graphs considered in this manuscript are simple. We have introduced two new topological indices for graphs called the first and second stress indices by means of the stresses of vertices. Further, we established some inequalities, proved some results and computed these stress indices for some standard graphs. A large number of molecular-graph-based structure descriptors (topological indices) depending on vertex degrees have been defined in literature. But in this paper, we have defined the new topological indices for graphs without using the degrees of vertices. These indices $S_1(G)$ and $S_2(G)$ can be used for other classes of graphs and results in this direction will be reported in subsequent papers. By investigating several properties of these two indices in the forthcoming papers, it may be possible to discover several molecular properties of some chemical molecules.

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