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# FIRST NEIGHBORHOOD STRESS INDEX FOR GRAPHS

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Abstract. We propose a new topological index for graphs, referred to as the first neighborhood stress index, which is defined based on the neighborhood stresses of individual vertices. Various inequalities involving this index are derived, and some results are proven. Additionally, the first neighborhood stress index values are calculated for certain well-known graphs. This study further explores the chemical relevance of the first neighborhood stress index by applying regression analysis to a dataset of 22 benzenoid hydrocarbons. Through logarithmic regression models, we assess the relationship between the first neighborhood stress index and multiple physicochemical properties of these hydrocarbons.

## 1. Introduction

We refer to the textbook of Harary [3] for standard terminology and concepts in graph theory. This article will provide non-standard information when needed.

Let $G = (V, E)$ represent a graph that is finite, simple, connected, and undirected. The degree of a vertex $v$ in $G$ is denoted by $\deg(v)$. A shortest path (or geodesic) between two vertices $u$ and $v$ in $G$ is a path that connects $u$ and $v$ using the fewest possible edges. We say that a graph geodesic $P$ passes through a vertex $v$ in $G$ if $v$ is an internal vertex of $P$, meaning that $v$ is part of the path but not one of its endpoints.

The concept of stress of a node (node) in a network (graph) has been introduced by Shimbel as centrality measure in 1953 [21]. This centrality measure has applications in biology, sociology, psychology, etc., (See [6, 19]). The stress of a node $v$ in a graph $G$, denoted by $\mathrm{str}_G(v)$ $\mathrm{str}(v)$, is the number of geodesics passing through it. We denote the maximum stress among all the nodes of $G$ by $\Theta_G$ and minimum stress among all the nodes of $G$ by $\theta_G$. Further, the concepts of stress number of a graph and stress regular graphs have been studied by Bhargava et al. in their paper [2]. A graph $G$ is called $k$-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$.
Neighborhood of a vertex $v$ is defined as

$$N_G(v) = \{u \in V(G) \mid uv \in E(G)\}.$$

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We introduce a novel index known as the neighborhood stress of a vertex $v$, denoted by $N_s(v)$. This index is defined as the sum of the stresses of the adjacent vertices of $v$, formally expressed as:

$$N_s(v) = \sum_{u \in N_G(v)} str(u)$$

In this study, we explore finite, simple, and connected graphs, which will collectively be referred to as graphs. Let $G$ denote a particular graph, and let $N$ represent the total number of geodesics in $G$ with length at least 2. Driven by the stress on vertices and the associated indices, we introduce a novel topological index known as the first neighborhood stress index. We derive several inequalities, establish fundamental results, and compute this index for various well-known graphs. Additionally, we investigate the chemical relevance of the first neighborhood stress index by applying regression analysis to a dataset of 22 benzenoid hydrocarbons, exploring its correlation with a range of physicochemical properties. For new stress/degree based topological indices, we suggest the reader to refer the papers [1, 4, 5, 7–18, 20, 22, 23].

## 2. First neighborhood stress index

**Definition 2.1.** The first neighborhood stress index of a graph $G$ is defined as

$$NS_1(G) = \sum_{v \in V(G)} N_s(v)^2 \tag{2.1}$$

**Definition 2.2.** A graph $G$ is called $k$- neighborhood stress regular if $N_s(v) = k$ for all $v \in V(G)$

**Example 2.3.** Consider the graph $G$ given in Figure 1.

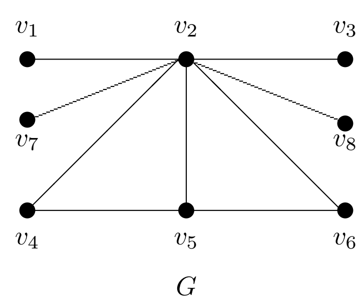


FIGURE 1. A graph $G$

The neighborhood stresses of the nodes of $G$ are as follows:
$N_s(v_1) = 19, N_s(v_2) = 1, N_s(v_3) = 19, N_s(v_4) = 20, N_s(v_5) = 19$
$N_s(v_6) = 20, N_s(v_7) = 19, N_s(v_8) = 19.$

First neighborhood stress index of $G$ is:

$$NS_1(G) = 19^2 + 1^2 + 19^2 + 20^2 + 19^2 + 20^2 + 19^2 + 19^2 = 2606$$

**Corollary 2.4.** *If there is no geodesic of length* $\geq 2$ *in a graph* $G$*, then* $NS_1(G) = 0$*. Moreover, for a complete graph* $K_n$*,* $NS_1(G)(K_n) = 0$*.*

*Proof.* If there is no geodesic of length $\geq 2$ in a graph $G$, then $N_s(v) = 0$. Hence we have $NS_1(G) = 0$.
In $K_n$, there is no geodesic of length $\geq 2$ and so $NS_1(K_n) = 0$. □

**Theorem 2.5.** *For a graph* $G$*,* $NS_1(G) = 0$ *iff* $G$ *is complete.*

*Proof.* Assume that $NS_1(G) = 0$. By Definition 2.1, this implies that $N_s(v) = 0$ for every vertex $v \in V(G)$, which in turn means that $\mathrm{str}(v) = 0$ for all $v \in V(G)$. If the number of vertices in $G$, denoted $|V(G)|$, is either 1 or 2, then $G$ must be a complete graph, specifically $G \cong K_1$ or $G \cong K_2$. Now, assume $|V(G)| > 2$. Let $u$ and $v$ be two distinct vertices in $G$. We aim to show that $u$ and $v$ must be adjacent. Suppose for the sake of contradiction that $u$ and $v$ are not adjacent. Then there exists a geodesic between $u$ and $v$ that passes through at least one intermediate vertex $w$. This would imply $\mathrm{str}(w) \geq 1$, which contradicts our initial assumption that $\mathrm{str}(v) = 0$ for all vertices. Therefore, $u$ and $v$ must be adjacent, which implies that $G$ is a complete graph.
Conversely, suppose $G$ is a complete graph. By Definition 2.1, it follows that $NS_1(G) = 0$.

□

**Proposition 2.6.** *For the complete bipartite* $K_{m,n}$*,*

$$NS_1(K_{m,n}) = \frac{m^2n^2\left[m(m-1)^2 + n(n-1)^2\right]}{4}.$$

*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,

$$N_s(v_i) = \frac{n.m(m-1)}{2} \text{ for } 1 \leq i \leq m \tag{2.2}$$

and

$$N_s(u_j) = \frac{m.n(n-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.3}$$

Using (2.2) and (2.3) in the Definition 2.1, we have

$$\begin{aligned}
NS_1(K_{m,n}) &= \sum_{i=1}^{m} N_s(v_i)^2 + \sum_{j=1}^{n} N_s(u_j)^2 \\
&= \sum_{i=1}^{m} \left[\frac{nm(m-1)}{2}\right]^2 + \sum_{j=1}^{n} \left[\frac{mn(n-1)}{2}\right]^2 \\
&= \frac{mn^2m^2(m-1)^2}{4} + \frac{nm^2n^2(n-1)^2}{4} \\
&= \frac{m^2n^2\left[m(m-1)^2 + n(n-1)^2\right]}{4}.
\end{aligned}$$

□

**Proposition 2.7.** *For the star graph $K_{1,n}$ on $n+1$ vertices*

$$NS_1(K_{1,n}) = \frac{n^3(n-1)^2}{4}.$$

*Proof.* In a star graph $K_{1,n}$ , internal vertex has neighborhood stress zero and remaining $n$ have neighborhood stress $\frac{n(n-1)}{2}$ By the Definition 2.1, we have

$$\begin{aligned} NS_1(G) &= \sum_{v \in V(G)} N_s(v)^2 \\ &= \sum_{v \in V(G)} \left[\frac{n(n-1)}{2}\right]^2 \\ &= \frac{n^3(n-1)^2}{4}. \end{aligned}$$

□

**Proposition 2.8.** *If $G=(V,E)$ is a $k$-neighborhood stress regular graph, then*

$$NS_1(G) = k^2|V|.$$

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

$$N_s(v) = k \text{ for all } v \in V(G).$$

By the Definition 2.1, we have

$$\begin{aligned} NS_1(G) &= \sum_{v \in V(G)} N_s(v)^2 \\ &= \sum_{v \in V(G)} k^2 \\ &= k^2|V|. \end{aligned}$$

□

**Corollary 2.9.** *For a cycle $C_n$,*

$$NS_1(C_n) = \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{16}, & \textit{if } n \textit{ is odd;} \\ \dfrac{n^3(n-2)^2}{16}, & \textit{if } n \textit{ is even.} \end{cases}$$

*Proof.* For any node $v$ in $C_n$, we have,

$$N_s(v) = \begin{cases} \dfrac{(n-1)(n-3)}{4}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{4}, & \text{if } n \text{ is even.} \end{cases}$$

Hence $C_n$ is

$$\begin{cases} \dfrac{(n-1)(n-3)}{4}\text{-neighborhood stress regular}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{4}\text{-neighborhood stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

Since $C_n$ has $n$ nodes and $n$ edges, by Proposition 2.8, we have

$$NS_1(C_n) = n \times \begin{cases} \dfrac{(n-1)^2(n-3)^2}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^2(n-2)^2}{16}, & \text{if } n \text{ is even.} \end{cases}$$
$$= \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^3(n-2)^2}{16}, & \text{if } n \text{ is even.} \end{cases}$$

□

**Proposition 2.10.** *For the path $P_n$ on $n$ nodes*

$$NS_1(P_n) = 2(n-2)^2 + \sum_{i=2}^{n-1} \left[(i-2)(n+1-i) + i(n-1-i)\right]^2.$$

*Proof.* Let $P_n$ be the path with node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 2).

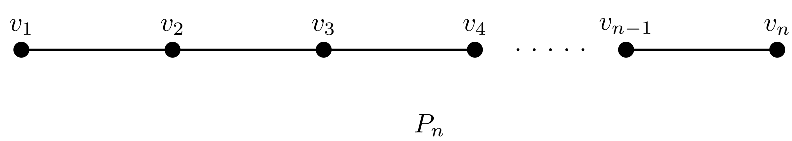


FIGURE 2. The path $P_n$ on $n$ nodes.

We have ,

$$N_s(v_i) = \begin{cases} (i-2)(n+1-i) + i(n-1-i), & \text{if } 1<\text{i} < n \text{ ;} \\ (n-2), & \text{if } i\text{=1 or } i\text{=n.} \end{cases}$$

Thus by the Definition 2.1, we have

$$\begin{aligned} NS_1(P_n) &= N_s(v_1)^2 + N_s(v_n)^2 + \sum_{i=2}^{n-1} N_s(v_i)^2 \\ &= (n-2)^2 + (n-2)^2 + \sum_{i=2}^{n-1} \left[(i-2)(n+1-i) + i(n-1-i)\right]^2 \\ &= 2(n-2)^2 + \sum_{i=2}^{n-1} \left[(i-2)(n+1-i) + i(n-1-i)\right]^2. \end{aligned}$$

□

**Proposition 2.11.** *For a fan graph $F_{n+1} = P_n + K_1$ , $n \geq 3$ on $n+1$ vertices*

$$NS_1(F_{n+1}) = (n-2)^2 + 4\left[\frac{n^2-3n+4}{2}\right]^2 + (n-4)\left[\frac{n^2-3n+6}{2}\right]^2.$$

*Proof.* A fan graph $F_{n+1} = P_n + K_1$ where $V(K_1) = v_0$ and Let $P_n$ be the path with node sequence $v_1, v_2, \ldots, v_n$.
we have

$$N_s(v_i) = \begin{cases} \frac{n^2-3n+6}{2}, & \text{if } 3 \le i \le n-2\ ; \\ \frac{n^2-3n+4}{2}, & \text{if } i = 1, 2, n-1, n. \end{cases}$$

and

$$N_s(v_0) = (n-2)$$

Thus by the Definition 2.1, we have

$$\begin{aligned} NS_1(F_{n+1}) &= N_s(v_0)^2 + N_s(v_1)^2 + N_s(v_2)^2 + N_s(v_{n-1})^2 + N_s(v_n)^2 + \sum_{i=3}^{n-2} N_s(v_i)^2 \\ &= (n-2)^2 + 4\left[\frac{n^2-3n+4}{2}\right]^2 + \sum_{i=3}^{n-2}\left[\frac{n^2-3n+6}{2}\right]^2 \\ &= (n-2)^2 + 4\left[\frac{n^2-3n+4}{2}\right]^2 + (n-4)\left[\frac{n^2-3n+6}{2}\right]^2 \end{aligned}$$

□

**Proposition 2.12.** *Let $Wd(n, m)$ denotes the windmill graph constructed for $n \ge 2$ and $m \ge 2$ by joining $m$ copies of the complete graph $K_n$ at a shared universal node $v$. Then*

$$NS_1(Wd(n, m)) = \frac{m^3(m-1)^2(n-1)^5}{4}.$$

*Hence, for the friendship graph $F_k$ on $2k+1$ nodes,*

$$NS_1(F_k) = 8k^3(k-1)^2.$$

*Proof.* In the wheel graph $W_d(n, m)$, the stress of any vertex other than the central (universal) vertex $v$ is zero. This is because the neighbors of each non-central vertex form a complete subgraph within $W_d(n, m)$. Since there are $m$ copies of $K_n$ (the complete graph on $n$ vertices) in $W_d(n, m)$, and each vertex within these subgraphs is adjacent to the universal vertex $v$, it follows that every geodesic passing through $v$ has a length of 2. As a result, the stress of the central vertex $v$ is given by:

$$\text{str}(v) = \frac{m(m-1)(n-1)^2}{2}.$$

Furthermore, observe that $v$ has $m(n-1)$ incident edges, and all edges not incident to $v$ connect vertices whose stress is zero. Consequently, the neighborhood stress of the universal vertex $v$ is zero, while the neighborhood stress of each non-central vertex is $\frac{m(m-1)(n-1)^2}{2}$. By Definition 2.1, we conclude that

$$NS_1(Wd(n, m)) = m(n-1)N_s(v)^2$$

$$= m(n-1)\left[\frac{m^2(m-1)^2(n-1)^4}{4}\right]$$
$$= \frac{m^3(m-1)^2(n-1)^5}{4}.$$

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

$$NS_1(F_k) = \frac{k^3(k-1)^2(3-1)^5}{4} = 8k^3(k-1)^2.$$

□

**Proposition 2.13.** *Let $W_n$ denotes the wheel graph constructed on $n \geq 5$ nodes. Then*

$$NS_1(W_n) = (n-1)^2 + (n-1)\frac{(n^2-5n+8)^2}{4}$$

*Proof.* In $W_n$ with $n \geq 4$, there are $(n-1)$ peripheral nodes and one central node, say $v$. It is easy to see that

$$\text{str}(v) = \frac{(n-1)(n-4)}{2} \tag{2.4}$$

Let $p$ be a peripheral node. Since $v$ is adjacent to all the peripheral nodes in $W_n$, there is no geodesic passing through $p$ and containing $v$. Hence we have

$$\begin{aligned} \text{str}_{W_n}(p) &= \text{str}_{W_n - v}(p) \\ &= \text{str}_{C_{n-1}}(p) \\ &= 1 \end{aligned} \tag{2.5}$$

Thus we have ,

$$N_s(v) = (n-1)$$

and

$$N_s(p) = \frac{(n-1)(n-4)}{2} + 2$$

Let us denote the set of all the peripheral vertices in $W_n$ by $P$.
Thus by the Definition 2.1, we have

$$\begin{aligned} NS_1(W_n) =& N_s(v)^2 + \sum_{p \in P(G)} N_s(p)^2 \\ =& (n-1)^2 + (n-1)\frac{(n^2-5n+8)^2}{4} \end{aligned}$$

□

## 3. A QSPR Analysis

We carry a QSPR analysis for some physical properties of 22 benzenoid hydrocarbons with first neighborhood stress index of molecular graphs. Table 1 gives the first neighborhood stress index $NS_1(G)$ of molecular graphs and the experimental values for the physical properties - boiling point (BP), $\pi$-electron energy ($\pi$-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR) of benzenoid hydrocarbons.

TABLE 1. First neighborhood stress index($NS_1(G)$), boiling point (BP), $\pi$-electron energy ($\pi$-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR) of benzenoid hydrocarbons

| **Derivatives of benzene** | $NS_1(G)$ | **BP** | **$\pi$-ele** | **MW** | **PO** | **MV** | **MR** |
|---|---|---|---|---|---|---|---|
| Benzene | 216 | 78.8 | 8 | 78.11 | 10.4 | 89.4 | 26.3 |
| Naphthalene | 7344 | 221.5 | 13.683 | 128.17 | 17.5 | 123.5 | 44.1 |
| Phenanthrene | 60656 | 337.4 | 19.448 | 178.23 | 24.6 | 157.7 | 61.9 |
| Anthracene | 65460 | 337.4 | 19.314 | 178.23 | 24.6 | 157.7 | 61.9 |
| Chrysene | 339802 | 448 | 25.192 | 228.3 | 31.6 | 191.8 | 79.8 |
| Benzo[a]anthracene | 318171 | 436.7 | 25.101 | 228.3 | 31.6 | 191.8 | 79.8 |
| Triphenylene | 234300 | 425 | 25.275 | 228.3 | 31.6 | 191.8 | 79.8 |
| Tetracene | 330016 | 436.7 | 25.188 | 228.3 | 31.6 | 191.8 | 79.8 |
| Benzo[a]pyrene | 550848 | 495 | 28.222 | 252.3 | 35.8 | 196.1 | 90.3 |
| Benzo[e]pyrene | 408520 | 467.5 | 28.336 | 252.3 | 35.8 | 196.1 | 90.3 |
| Perylene | 403196 | 467.5 | 28.245 | 252.3 | 35.8 | 196.1 | 90.3 |
| Anthanthrene | 884864 | 497.1 | 31.253 | 276.3 | 40 | 200.4 | 100.8 |
| Benzo[ghi]perylene | 679742 | 501 | 31.425 | 276.3 | 40 | 200.4 | 100.8 |
| Dibenz[a,c]anthracene | 870530 | 518 | 30.942 | 278.3 | 38.7 | 225.9 | 97.6 |
| Dibenz[a,h]anthracene | 1450028 | 524.7 | 30.881 | 278.3 | 38.7 | 225.9 | 97.6 |
| Dibenz[a,j]anthracene | 920250 | 524.7 | 30.88 | 278.3 | 38.7 | 225.9 | 97.6 |
| Picene | 1611582 | 519 | 30.943 | 278.3 | 38.7 | 225.9 | 97.6 |
| Coronene | 1169470 | 525.6 | 34.572 | 300.4 | 44.1 | 204.7 | 111.4 |
| Dibenzo[a,h]pyrene | 2077428 | 552.3 | 33.928 | 302.4 | 42.9 | 230.2 | 108.1 |
| Dibenzo[a,i]pyrene | 2223570 | 552.3 | 33.954 | 302.4 | 42.9 | 230.2 | 108.1 |
| Dibenzo[a,l]pyrene | 1212799 | 552.3 | 34.031 | 302.4 | 42.9 | 230.2 | 108.1 |
| Pyrene | 120048 | 404 | 22.506 | 202.25 | 28.7 | 162 | 72.5 |

**Regression Models.** Using Table 1, a study was carried out with a logarithmic regression model

$$P = A \cdot ln(NS_1(G)) + B,$$

where $P$ is the Physical property , $NS_1(G)$ is the first neighborhood stress index, $B$ is the intercept of the model and $A$ is the coefficient that represents the change in $P$ for a unit change in the logarithm of $NS_1(G)$.

TABLE 2. The correlation coefficient r from logarithmic regression model between first neighborhood stress index and physicochemical properties (BP, $\pi$-ele,MW, PO, MV, MR) of benzenoid hydrocarbons.

| $BP$ | $\pi - ele$ | $MW$ | $PO$ | $MV$ | $MR$ |
|---|---|---|---|---|---|
| 0.99 | 0.961 | 0.967 | 0.957 | 0.965 | 0.957 |

The logarithmic regression models for boiling point , $\pi$-electron energy , molecular weight , polarizability , molar volume , and molar refractivity of benzenoid hydrocarbons are as follows:

$$BP = 54.517 \cdot ln(NS_1(G)) - 241.81 \tag{3.1}$$
$$\pi - ele = 3.1337 \cdot ln(NS_1(G)) - 12.685 \tag{3.2}$$
$$MW = 26.934 \cdot ln(NS_1(G)) - 98.756 \tag{3.3}$$
$$PO = 3.9167 \cdot ln(NS_1(G)) - 15.485 \tag{3.4}$$
$$MV = 16.643 \cdot ln(NS_1(G)) - 17.137 \tag{3.5}$$
$$MR = 9.873 \cdot ln(NS_1(G)) - 38.989 \tag{3.6}$$

From Table 2, it follows that the logarithmic regression models (3.1)-(3.2)-(3.3)-(3.4)-(3.5)-(3.6) can be used as predictive tools.

## 4. Conclusion

Table 2, reveals that the logarithmic regression models (3.1)-(3.2)-(3.3)-(3.4)-(3.5)-(3.6) are useful tools in predicting the physical properties of benzenoid hydrocarbons. It shows that first neighborhood stress index can be used as predictive means in QSPR researches.

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