Neighbourhood status connectivity indices of graphs

H. S. Ramane¹ and Kavita Bhajantri ²*

Abstract
Let $G$ be a simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The status of a vertex $u$ denoted by $\sigma(u)$ is the sum of the distance between the vertex $u$ and all other vertices in a graph $G$ and $S_\sigma(u)$ be the sum of the status of the neighbours of the vertex $u$ in $G$. In this paper, we have defined the first and second neighbourhood status connectivity indices of graph $G$ as $NS_1(G) = \sum_{uv \in E(G)} [S_\sigma(u) + S_\sigma(v)]$ and $NS_2(G) = \sum_{uv \in E(G)} [S_\sigma(u)S_\sigma(v)]$ respectively. These indices are computed for some standard graphs and further obtained the bounds for these indices.

Keywords
Distance, status of a vertex, neighbourhood status of a vertex, neighbourhood status connectivity indices.

AMS Subject Classification
05C09, 05C12, 05C92

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Contents

1 Introduction .................................................. 86
2 Neighbourhood status connectivity indices of some graphs ............................................. 87
3 Bounds for the neighbourhood status connectivity indices .............................................. 89
4 Regression analysis ............................................. 89
5 Acknowledgements ............................................. 90
References ......................................................... 91

1. Introduction

Topological indices are numerical parameters of a molecular graph which characterize bonding topology of a molecule and are necessarily structure invariant. Mathematical models based on Quantitative Structure Property Relationships (QSPR) and Quantitative Structure Activity Relationships (QSAR) have been studied in [3].

Let $G$ be a simple connected graph with $n$ vertices and $m$ edges. Let $V(G)$ be the vertex set of a graph $G$ and $E(G)$ be the edge set of a graph $G$. The edge connects to vertices $u$ and $v$ is denoted by $uv$. The number of vertices adjacent to vertex $v$ is termed as degree of a vertex $v$ and is denoted by $d(v)$. If all the vertices of $G$ have same degree equal to $r$, then $G$ is called a regular graph of degree $r$. The distance between the vertices $u$ and $v$, denoted by $d(u,v)$, is the length of the shortest path joining $u$ and $v$ in $G$. The maximum distance between any pair of vertices in $G$ is called the diameter of $G$ and is denoted by $diam(G)$. The status [8] of a vertex $u \in V(G)$ is defined as the sum of its distance from every other vertex in $V(G)$ and is denoted by $\sigma(u)$. That is,

$$\sigma(u) = \sum_{v \in V(G)} d(u,v).$$

The first and second Zagreb indices of a graph $G$ are defined respectively as [4]

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

and  

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

The Zagreb indices were used in the structure property model [6]. Recent results on the Zagreb indices can be found in [2, 6, 7, 9, 10, 15].

The first and second status connectivity indices of a graph $G$ are defined as [12]

$$S_1(G) = \sum_{uv \in E(G)} [\sigma(u) + \sigma(v)]$$

and  

$$S_2(G) = \sum_{uv \in E(G)} \sigma(u)\sigma(v).$$
The \textit{neighbourhood degree sum} \(S(u)\) of a vertex \(u \in V(G)\) is defined as the sum of the degree of neighbours of vertex \(u\) in \(G\).

The \textit{Neighbourhood first and second Zagreb indices} of a graph \(G\) are defined as \cite{14}

\[
NM_1(G) = \sum_{v \in V(G)} (S(v))^2 \quad \text{and} \quad NM_2(G) = \sum_{u \in V(G)} S(u)S(v).
\]

Motivated by the invariant like neighbourhood first and second Zagreb indices, we define first neighbourhood status connectivity index \(NS_1(G)\) and second neighbourhood status connectivity index \(NS_2(G)\) of a connected graph \(G\) as:

\[
NS_1(G) = \sum_{uv \in E(G)} [S\sigma(u) + S\sigma(v)] \quad (1.1)
\]
and

\[
NS_2(G) = \sum_{uv \in E(G)} S\sigma(u)S\sigma(v) \quad (1.2)
\]
where \(S\sigma(u) = \sum_{v \in u} \sigma(v), v \sim u\) means \(v\) is adjacent to \(u\).

\section{2. Neighbourhood status connectivity indices of some graphs}

If \(G\) is a connected, regular graph of degree \(r\) and \(\text{diam}(G) \leq 2\) then \(NS_1(G) = rS_1(G)\) and \(NS_2(G) = r^2S_2(G)\).

\textbf{Theorem 2.1.} Let \(G\) be a connected graph with \(n\) vertices and \(m\) edges, and \(\text{diam}(G) \leq 2\). Then

\[
NS_1(G) = (2n - 2)M_1(G) - 2M_2(G) \quad (2.1)
\]
and

\[
NS_2(G) = (2n - 2)^2M_2(G) - (2n - 2)NM_1(G)
+ NM_2(G). \quad (2.2)
\]

\textbf{Proof.} If \(\text{diam}(G) \leq 2\) then \(d(u)\) number of vertices at distance 1 from the vertex \(u\) and the remaining \((n - 1 - d(u))\) vertices are at distance 2. Therefore \(S\sigma(u) = d(u)(2n - 2) - S(u),\) where \(S(u)\) is the sum of the degrees of the neighbours of vertex \(u\). Therefore

\[
NS_1(G) = \sum_{uv \in E(G)} [S\sigma(u) + S\sigma(v)]
= \sum_{uv \in E(G)} [d(u)(2n - 2) - S(u) + d(v)(2n - 2) - S(v)]
+ \sum_{uv \in E(G)} [(2n - 2)(d(u) + d(v)) - (S(u) + S(v))]
= (2n - 2) \sum_{uv \in E(G)} (d(u) + d(v))
- \sum_{uv \in E(G)} (S(u) + S(v))
= (2n - 2)M_1(G) - 2M_2(G)
\]
and

\[
NS_2(G) = \sum_{uv \in E(G)} S\sigma(u)S\sigma(v)
= (d(u)(2n - 2) - S(u))(d(v)(2n - 2) - S(v))
= \sum_{uv \in E(G)} [(2n - 2)^2(d(u)d(v))
- (2n - 2)[d(u)S(v) + d(v)S(u)] + S(u)S(v)]
= (2n - 2)^2 \sum_{uv \in E(G)} d(u)d(v) -
(2n - 2) \sum_{uv \in E(G)} [d(u)S(v) + d(v)S(u)]
+ \sum_{uv \in E(G)} S(u)S(v)
= (2n - 2)^2M_2(G) - (2n - 2)NM_1(G) + NM_2(G).
\]

\textbf{Corollary 2.2.} For a connected regular graph \(G\) of degree \(r\)
on \(n\) vertices and \(\text{diam}(G) \leq 2\),

\[
NS_1(G) = 2nr^2(n - 1) - nr^3
\]

and

\[
NS_2(G) = \frac{nr^5}{2} + 2nr^3[r(1 - n) + (n - 1)^2].
\]

\textbf{Corollary 2.3.} For a complete graph \(K_n\) on \(n\) vertices

\[
NS_1(K_n) = n(n - 1)^3 \quad \text{and} \quad NS_2(K_n) = \frac{n^2}{2}(n - 1)^3.
\]

\textbf{Proposition 2.4.} For a complete bipartite graph \(K_{p,q}\)

\[
NS_1(K_{p,q}) = 2pq(p^2 + q^2) - 2pq(p + q) + 2p^2q^2
\]

and

\[
NS_2(K_{p,q}) = p^2q^2[(p + q - 1)(2p + 2q - 4) + p].
\]

\textbf{Proof.} The graph \(K_{p,q}\) has \(n = p + q\) vertices and
\(\text{diam}(K_{p,q}) \leq 2\). Also

\[
M_1(K_{p,q}) = pq(p + q),
\]
\[
M_2(K_{p,q}) = (pq)^2,
\]
\[
NM_1(K_{p,q}) = p^2q^2(p + q),
\]
and
\[
NM_2(K_{p,q}) = p^3q^3.
\]

Therefore by Theorem 2.1

\[
NS_1(K_{p,q}) = 2pq(p^2 + q^2) - 2pq(p + q) + 2p^2q^2
\]

and

\[
NS_2(K_{p,q}) = p^2q^2[(p + q - 1)(2p + 2q - 4) + p].
\]
Proposition 2.5. For a cycle $C_n$ on $n \geq 3$ vertices

$$NS_1(C_n) = \begin{cases} 4n^2 & \text{if } n \text{ is even} \\ 2n \left\lfloor \frac{n^2}{2} \right\rfloor & \text{if } n \text{ is odd} \end{cases}$$

and

$$NS_2(C_n) = \begin{cases} 4n^3 & \text{if } n \text{ is even} \\ n \left(\left\lfloor \frac{n^2}{2} \right\rfloor\right)^2 & \text{if } n \text{ is odd.} \end{cases}$$

Proof. The sum of the status of neighbours of each vertex $u$ in $C_n$, for even number of vertices is $S_\sigma(u) = 2n$. Therefore

$$NS_1(C_n) = \sum_{uv \in E(G)} [S_\sigma(u) + S_\sigma(v)] = \sum_{uv \in E(G)} (2n + 2n) = 4n^2$$

and

$$NS_2(C_n) = \sum_{uv \in E(G)} S_\sigma(u)S_\sigma(v) = \sum_{uv \in E(G)} (2n)(2n) = 4n^3.$$ 

The sum of the status of neighbours of vertex $u$ in $C_n$ for odd number of vertices is $S_\sigma(u) = \left\lfloor \frac{n^2}{2} \right\rfloor$, where $\left\lfloor \cdot \right\rfloor$ represents the greatest integer function. Therefore

$$NS_1(C_n) = \sum_{uv \in E(G)} [S_\sigma(u) + S_\sigma(v)] = \sum_{uv \in E(G)} \left\lfloor \frac{n^2}{2} \right\rfloor + \left\lfloor \frac{n^2}{2} \right\rfloor = 2n \left\lfloor \frac{n^2}{2} \right\rfloor$$

and

$$NS_2(C_n) = \sum_{uv \in E(G)} S_\sigma(u)S_\sigma(v) = \sum_{uv \in E(G)} \left(\left\lfloor \frac{n^2}{2} \right\rfloor\right)^2 = n \left(\left\lfloor \frac{n^2}{2} \right\rfloor\right)^2.$$ 

A wheel $W_{n+1}$ is a graph obtained from the cycle $C_n$, $n \geq 3$, by adding a new vertex and making it adjacent to all the vertices of $C_n$.

Proposition 2.6. For a wheel $W_{n+1}$, $n \geq 3$

$$NS_1(W_{n+1}) = 2n(n^2 + 6n - 9)$$

and

$$NS_2(W_{n+1}) = 2n(5n^3 - n^2 + 21n + 18).$$

Proof. The wheel $W_{n+1}$ has $n+1$ vertices and $diam(W_{n+1}) \leq 2$. Therefore

$$M_1(W_{n+1}) = n^2 + 9n, \\
M_2(W_{n+1}) = 3n^3 + 9n, \\
NM_1(G) = n^3 + 21n^2 + 36n,$$

and $NM_2(W_{n+1}) = 4n^3 + 30n^2 + 36n$.

Substituting these in Eqs. (2.1) and (2.2) result follows.

A friendship graph (or Dutch windmill graph) $F_n$, $n \geq 2$, is a graph that can be constructed by coalescence $n$ copies of the cycle $C_3$ of length 3 with a common vertex. It has $2n + 1$ vertices and $3n$ edges.

**Figure 1. Wheel**

Proposition 2.7. For a friendship graph $F_n$, $n \geq 2$,

$$NS_1(F_n) = 8n(2n^2 + 2n - 1)$$

and

$$NS_2(F_n) = 4n(24n^3 - 11n^2 - 2n + 1).$$

Proof. For friendship graph $F_n$,

$$M_1(F_n) = 4n^2 + 8n, \\
M_2(F_n) = 8n^2 + 4n, \\
NM_1(G) = 8n^3 + 32n^2 + 8n,$$

and $NM_2(F_n) = 20n^3 + 24n^2 + 4n$.

Also $diam(F_n) = 2$. Therefore by Theorem 2.1 the result follows.
3. Bounds for the neighbourhood status connectivity indices

**Theorem 3.1.** Let $G$ be a connected graph with $n$ vertices and let $\text{diam}(G) = D$. Then,

$$(2n - 2)M_1(G) - 2M_2(G) \leq NS_1(G) \leq D(D - 1)M_1(G) - (1 - D)2M_2(G)$$

and

$$(2n - 2)^2 M_2(G) - (2n - 2)NM_1(G) + NM_2(G) \leq NS_2(G) \leq D^2(D - 1)^2 M_2(G) - (D^2 - D^3)NM_1(G) + (1 - D)^2NM_2(G),$$

with equality holds both sides if and only if $\text{diam}(G) \leq 2$.

**Proof.** Lower bound: For any vertex $u$ of $G$, there are $d(u)$ vertices which are at distance 1 from $u$ and the remaining $(n - 1 - d(u))$ vertices are at distance at least 2. Therefore

$$\sigma(u) \geq d(u) + (n - 1 - d(u)) = 2n - 2 - d(u).$$

Let $v_1, v_2, \ldots, v_k$ be the neighbours of $u$ and let $d(v_i) = d_i$, $i = 1, 2, \ldots, k$, where $k = d(u)$. Therefore

$$S_\sigma(u) \geq 2n - 2 - d_1 + 2n - 2 - d_2 + \cdots + 2n - 2 - d_k = d(u)(2n - 2) - \sum_{i=1}^{k} d_i = d(u)(2n - 2) - S(u).$$

Therefore

$$NS_1(G) = \sum_{uv \in E(G)} [S_\sigma(u) + S_\sigma(v)] \geq (2n - 2) \sum_{uv \in E(G)} [d(u) + d(v)] - \sum_{uv \in E(G)} [S(u) + S(v)] = (2n - 2)M_1(G) - 2M_2(G)$$

and

$$NS_2(G) = \sum_{uv \in E(G)} S_\sigma(u)S_\sigma(v) \geq (2n - 2)^2 \sum_{uv \in E(G)} (d(u)d(v)) - (2n - 2) \sum_{uv \in E(G)} [d(u)S(v) + d(v)S(u)] + \sum_{uv \in E(G)} (S(u)S(v)) = (2n - 2)^2 M_2(G) - (2n - 2)NM_1(G) + NM_2(G).$$

Upper bound: For any vertex $u$ of $G$, there are $d(u)$ vertices which are at distance 1 from $u$ and the remaining $(n - 1 - d(u))$ vertices are at distance at most $D$. Therefore

$$\sigma(u) \leq d(u) + D(n - 1 - d(u)) = D(n - 1) - (D - 1)d(u)$$

and

$$S_\sigma(u) \leq D(n - 1) - (1 - D)d_1 + D(n - 1) - (1 - D)d_2 + \cdots + D(n - 1) - (1 - D)d_k = d(u)(D(n - 1)) - (1 - D)\sum_{i=1}^{k} d_i = d(u)(D(n - 1) - (1 - D)S(u)).$$

Therefore

$$NS_1(G) = \sum_{uv \in E(G)} [S_\sigma(u) + S_\sigma(v)] \leq \sum_{uv \in E(G)} [D(D - 1)(d(u) + d(v))] - (1 - D)(S(u) + S(v))] = D(D - 1)M_1(G) - 2(1 - D)M_2(G)$$

and

$$NS_2(G) = \sum_{uv \in E(G)} S_\sigma(u)S_\sigma(v) \leq D^2(D - 1)^2 \sum_{uv \in E(G)} (d(u)d(v)) - (D^2 - D^3) \sum_{uv \in E(G)} [d(u)S(v) + d(v)S(u)] + (1 - D)^2 \sum_{uv \in E(G)} (S(u)S(v)) = D^2(D - 1)^2 M_2(G) - (D^2 - D^3)NM_1(G) + (1 - D)^2NM_2(G).$$

\[ \square \]

4. Regression analysis

![Figure 3. Molecular graphs of benzenoid hydrocarbons under consideration.](image)
Table 1. The values of boiling points and neighbourhood status connectivity indices of 21 benzenoid hydrocarbons.

<table>
<thead>
<tr>
<th>Benzenoid hydrocarbon</th>
<th>BP in °C</th>
<th>NS₁</th>
<th>NS₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>218</td>
<td>1058</td>
<td>25169</td>
</tr>
<tr>
<td>2</td>
<td>338</td>
<td>2924</td>
<td>124691</td>
</tr>
<tr>
<td>3</td>
<td>340</td>
<td>5936</td>
<td>419749</td>
</tr>
<tr>
<td>4</td>
<td>431</td>
<td>6034</td>
<td>430484</td>
</tr>
<tr>
<td>5</td>
<td>429</td>
<td>5526</td>
<td>364014</td>
</tr>
<tr>
<td>6</td>
<td>440</td>
<td>6230</td>
<td>456331</td>
</tr>
<tr>
<td>7</td>
<td>496</td>
<td>7838</td>
<td>637940</td>
</tr>
<tr>
<td>8</td>
<td>493</td>
<td>7524</td>
<td>581944</td>
</tr>
<tr>
<td>9</td>
<td>547</td>
<td>9938</td>
<td>914035</td>
</tr>
<tr>
<td>10</td>
<td>542</td>
<td>9826</td>
<td>690093</td>
</tr>
<tr>
<td>11</td>
<td>535</td>
<td>9701</td>
<td>972375</td>
</tr>
<tr>
<td>12</td>
<td>536</td>
<td>10896</td>
<td>1141262</td>
</tr>
<tr>
<td>13</td>
<td>531</td>
<td>10704</td>
<td>1098206</td>
</tr>
<tr>
<td>14</td>
<td>519</td>
<td>10792</td>
<td>1126775</td>
</tr>
<tr>
<td>15</td>
<td>590</td>
<td>12564</td>
<td>1304760</td>
</tr>
<tr>
<td>16</td>
<td>592</td>
<td>12558</td>
<td>1357544</td>
</tr>
<tr>
<td>17</td>
<td>596</td>
<td>13328</td>
<td>1532092</td>
</tr>
<tr>
<td>18</td>
<td>594</td>
<td>13328</td>
<td>1531500</td>
</tr>
<tr>
<td>19</td>
<td>595</td>
<td>12362</td>
<td>1312520</td>
</tr>
</tbody>
</table>

In [12] The correlation between the boiling point (BP) of benzenoid hydrocarbons with status connectivity indices (S₁, S₂), eccentric connectivity indices (ξ₁, ξ₂) and with the Wiener index (W) is reported. In this section we analyze the correlation between the boiling point of benzenoid hydrocarbons and neighbourhood status connectivity indices.

Data of the boiling point of the benzenoid hydrocarbons represented in Fig. 3 has taken from [11]. The scatter plots between BP and indices NS₁, NS₂ are shown in Figs. 4 and 5. The lines of the regression from the data given in Table 1 are

\[
BP = 261.769(±14.421) + 0.027(±0.002)NS₁ \quad (4.1)
\]

\[
BP = 336.279(±18.394) + 0.0001(±0.001)NS₂ \quad (4.2)
\]

From Tables 2 and 3, we observe that the model (4.1) shows that the correlation of the experimental boiling point of benzenoid hydrocarbons with first neighbourhood status connectivity index is better (R = 0.969) than the correlation with other distance based indices given in [12]. The linear model (4.2) is also good (R = 0.911) compared to the other models in the Table 2.

Table 2. Correlation coefficient and standard error of the estimation of BP with status connectivity indices (S₁, S₂), eccentric connectivity indices (ξ₁, ξ₂) and Wiener index (W).

<table>
<thead>
<tr>
<th>Index</th>
<th>Correlation Coefficient (R) with boiling point</th>
<th>Standard error of the estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>S₁</td>
<td>0.968</td>
<td>23.866</td>
</tr>
<tr>
<td>S₂</td>
<td>0.916</td>
<td>41.206</td>
</tr>
<tr>
<td>ξ₁</td>
<td>0.927</td>
<td>38.525</td>
</tr>
<tr>
<td>ξ₂</td>
<td>0.826</td>
<td>57.848</td>
</tr>
<tr>
<td>W</td>
<td>0.904</td>
<td>43.815</td>
</tr>
</tbody>
</table>

Table 3. Correlation coefficient and standard error of the estimation of BP with NS₁ and NS₂.

<table>
<thead>
<tr>
<th>Index</th>
<th>Correlation Coefficient (R) with boiling point</th>
<th>Standard error of the estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>NS₁</td>
<td>0.969</td>
<td>25.309</td>
</tr>
<tr>
<td>NS₂</td>
<td>0.911</td>
<td>42.243</td>
</tr>
</tbody>
</table>

Figure 4. Scatter plot between the boiling point (BP) and the first neighbourhood status connectivity index (NS₁)

Figure 5. Scatter plot between the boiling point (BP) and the second neighbourhood status connectivity index (NS₂)

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