On Some Mathematical Properties of Nirmala Index

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Abstract. Recently, a novel degree based topological index was introduced, named
Nirmala index. In this paper, we obtain upper and lower bounds on the Nirmala index, by
using various graph parameters.

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1. Introduction

A molecular graph is a graph such that its vertices correspond to the atoms and the edges
to the bonds. Chemical Graph Theory is a branch of Mathematical Chemistry, which has
an important effect on the development of the Chemical Sciences. A topological index is
a numerical parameter mathematically derived from the graph structure. Several such
topological indices have been considered in Theoretical Chemistry and have found many
applications, especially in QSPR/QSAR study, see [1-3].

Let $G=(V(G), E(G))$ be a finite, simple, connected graph. Let $d_G(u)$ be the degree
of a vertex $u$ in $G$. We refer [4] for undefined notations and terminologies.

Nowadays, several hundreds of topological indices have been and are being
studied in the mathematical chemistry literature [5,6]. Of these, the so-called sum-
connectivity index is defined as [7]

$$SCI(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$ 

For details of the study of $SCI$, see [8-10] and the references cited therein. Soon after
$SCI$ was introduced, also its “general” version

$$SCI_\alpha(G) = \sum_{u,v \in E(G)} \left[ d_G(u) + d_G(v) \right]^\alpha$$

was considered [11,12]. Evidently, $SCI_\alpha(G) = SCI(G)$ for $\alpha = -1/2$. For details on
mathematical properties of $SCI_\alpha$ see [13-15] and the references cited therein.
Quite recently, the so-called Sombor index was put forward, defined as 
\[ SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}. \]
Ref. [16] was soon followed by a series of publications [17-26].

Inspired by work on Sombor indices, Kulli introduced the Nirmala index [27] of a (molecular) graph \( G \) as follows:
\[ N(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}. \] (1)

It is immediately seen that the Nirmala index is the reverse version of the sum-connectivity index. In addition, the Nirmala index is a special case of the general sum-connectivity index, for \( \alpha = \pm 1/2 \).

In the literature there are several more graph invariants whose form is similar to the Nirmala index. In [28], Vukičević and M. Gašperov introduced the misbalance rodeg index of a graph \( G \), defined as
\[ MRI(G) = \sum_{uv \in E(G)} \left| \sqrt{d_G(u)} - \sqrt{d_G(v)} \right|. \]

In a recent paper [29], Kulli considered two more vertex degree based indices, named first and second \((a,b)\)-KA indices and these are defined as
\[ KA_{a,b}^1(G) = \sum_{uv \in E(G)} \left[ d_G(u)^a + d_G(v)^a \right]^b, \]
\[ KA_{a,b}^2(G) = \sum_{uv \in E(G)} \left[ d_G(u)^a d_G(v)^a \right]^b \]
Where \( a \) and \( b \) are real numbers. Needless to say that \( KA_{a,1}^1(G) = N(G) \) for \( a = 1 \) and \( b = +1/2 \).

Here we define the misbalance prodeg index of a graph \( G \) as
\[ MPI(G) = \sum_{uv \in E(G)} \left[ \sqrt{d_G(u)} + \sqrt{d_G(v)} \right]. \]
For \( a=\frac{1}{2}, b=1 \), \( KA_{a,b}^1 \) is equal to the misbalance prodeg index.

In addition, we define the double reverse Randić index of a graph \( G \) as
\[ DR(G) = \sum_{uv \in E(G)} \left[ d_G(u) d_G(v) \right]^{1/4} \]
For \( a=1, b=\frac{1}{4} \), \( KA_{a,b}^2 \) is equal to the double reverse Randić index.

In this paper, we obtain upper and lower bounds on the Nirmala index of graphs by using some graph parameters.

2. Results
As usual, denote by \( P_n \), \( S_n \), and \( K_n \) be the \( n \)-vertex path, star, and complete graph.

Theorem 1. Let \( G \) be a connected \( n \)-vertex graph. Let \( T \) be an \( n \)-vertex tree. Then
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(i) \( N(P_n) \leq N(T) \leq N(S_n) \)

(ii) \( N(P_n) \leq N(G) \leq N(K_n) \)

with equalities if and only if \( T \equiv P_n \) or, and \( G \equiv P_n \) or \( G \equiv K_n \).

**Proof:** For any \( uv \in E(T) \) it is \( d_T(u) + d_T(v) \leq n \). Equality for all edges holds if and only if \( T \equiv S_n \). This implies the right-hand side of (i). The path is the only tree for which \( d_T(u) \leq 2 \) holds for all vertices. \( d_T(u) + d_T(v) = 3 \) holds for two edges, whereas \( d_T(u) + d_T(v) = 4 \) holds for the other \( n - 3 \) edges. Therefore, the path has smallest Nirmala index among all trees.

In the case of graphs, the greatest possible value of \( d_T(u) + d_T(v) \) is \( (n-1) + (n-1) \), which happens at all edges of the complete graph. In addition, the complete graph has the greatest number of edges. The right-hand side of (ii) follows.

By deleting an edge from a graph \( G \), the degree of two of its vertices is diminished. In addition, the resulting graph has fewer number of edges. Therefore, its Nirmala index is strictly smaller. If the edges are deleted so that the resulting graph remains connected, then we finally arrive at a tree. Thus, a connected graph with smallest Nirmala index must be a tree. From (i) follows that this tree is the path, implying the left-hand side of (ii).

**Corollary 0.** Suppose that \( n \geq 3 \). Then \( N(P_n) = 2n - 6 + 2\sqrt{3} \), \( N(S_n) = (n - 1)\sqrt{n} \), and \( N(K_n) = \left(\frac{n}{2}\right) \sqrt{2n - 2} \).

In the following theorem, we establish upper and lower bounds on \( N(G) \) in terms of \( n, \Delta(G), \delta(G) \).

**Theorem 2.** Let \( G \) be connected graph of order \( n \), size \( m \) with the maximum degree \( \Delta \) and minimum degree \( \delta \). Then

\[
\text{(i)} \quad \sqrt{2\delta(G)}m \leq N(G) \leq \sqrt{2\Delta(G)}m
\]

\[
\text{(ii)} \quad \frac{n\delta(G)^{3/2}}{\sqrt{2}} \leq N(G) \leq \frac{n\Delta(G)^{3/2}}{\sqrt{2}}
\]

with equality (left and right) if and only if \( G \) is regular.

**Proof:** From the definition of the Nirmala index, Eq. (1), and \( \delta \leq d_G(u) \leq \Delta \), one directly gets (i).

It is known that

\[
\sum_{u \in V(G)} d_G(u) = 2m
\]

From which it follows

\[
n\delta(G) \leq 2m \leq n\Delta(G)
\]
with equality (left and right) if and only if $G$ is regular. Combining this with (i) we get (ii), with equality (left and right) if and only if $G$ is regular.

In the following theorems, we obtain further upper and lower bounds on Nirmala index.

**Theorem 3.** Let $G$ be a connected graph with the maximum degree $\Delta$ and minimum degree $\delta$. Then

$$\frac{1}{\sqrt{\Delta}}SO(G) \leq N(G) \leq \frac{1}{\sqrt{\delta}}SO(G).$$

Equality (left and right) holds if and only if $G$ is regular.

**Proof:**

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \leq \sum_{uv \in E(G)} \sqrt{\Delta d_G(u) + \Delta d_G(v)}$$

$$= \Delta \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)} = \Delta N(G)$$

from which the left-hand side inequality follows. The right-hand side inequality is obtained analogously.

**Theorem 4.** Let $G$ be a connected graph of order $n$ and size $m$. Then

$$\frac{1}{\sqrt{2}}MPI(G) \leq N(G) \leq MPI(G).$$

Equality on the left-hand side holds if and only if $d_G(u) = d_G(v)$ for any edge $uv \in E(G)$

Equality on the right-hand side holds if and only if $G \cong K_n$.

**Proof:** Let $a$ and $b$ be any two non-negative real numbers. Then

$$\sqrt{a + b} \geq \frac{1}{\sqrt{2}}(\sqrt{a} + \sqrt{b})$$

with equality if and only if $a = b$.

If $a = d_G(u)$ and $b = d_G(v)$, then the above inequality becomes

$$\sqrt{d_G(u) + d_G(v)} \geq \frac{1}{\sqrt{2}}\left(\sqrt{d_G(u)} + \sqrt{d_G(v)}\right).$$

By the definition of Nirmala index, we have

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)} \geq \frac{1}{\sqrt{2}}\left(\sqrt{d_G(u)} + \sqrt{d_G(v)}\right) = \frac{1}{\sqrt{2}}MPI(G).$$

Equality in left hand side holds if and only if $d_G(u) = d_G(v)$ for any edge $uv \in E(G)$.

Also, by the definition of Nirmala index, we have
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\[ N(G) = \sum_{u \in V(G)} \sqrt{d_G(u) + d_G(v)} \]

\[ \geq \sum_{uv \in E(G)} \left( \sqrt{d_G(u)} + \sqrt{d_G(v)} \right) \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right) \]

\[ \leq \sum_{uv \in E(G)} \left( \sqrt{d_G(u)} + \sqrt{d_G(v)} \right) = \text{MPI}(G). \]

Equality holds if and only if \( \sqrt{d_G(u) + d_G(v)} = 0 \) i.e., if and only if \( G \cong \tilde{K}_n \).

In the next theorem, a relationship between the Nirmala index, misbalance Rodeg index, and double reverse Randić index is derived.

**Theorem 5.** Let \( G \) be connected graph of order \( n \geq 2 \) and size \( m \). Then

\[ \frac{1}{\sqrt{2}} \text{MRI}(G) + \sqrt{2} \text{DR}(G) \leq N(G) \leq \text{MRI}(G) + \sqrt{2} \text{DR}(G). \]

Equality in left hand side holds if and only if \( G \cong \tilde{K}_n \). Equality in right hand side holds if and only if \( d_G(u) = d_G(v) \) for any edge \( uv \in E(G) \).

**Proof:** Putting \( a = \left( \sqrt{d_G(u)} + \sqrt{d_G(v)} \right)^2 \) and \( b = 2\sqrt{d_G(u)d_G(v)} \) in inequality (2), we obtain

\[ \frac{1}{\sqrt{2}} \left[ \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2 + 2\sqrt{d_G(u)d_G(v)} \right]^{1/2} \]

\[ \geq \frac{1}{\sqrt{2}} \left[ \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2 \right]^{1/2} + \left( 2\sqrt{d_G(u)d_G(v)} \right)^{1/2} \]

\[ = \frac{1}{\sqrt{2}} \left[ \sqrt{d_G(u) - d_G(v)} + \sqrt{2} (d_G(u)d_G(v))^{1/4} \right]. \]

Thus

\[ N(G) \geq \frac{1}{\sqrt{2}} \left[ \sum_{uv \in E(G)} \sqrt{d_G(u) - d_G(v)} + \sqrt{2} \sum_{uv \in E(G)} (d_G(u)d_G(v))^{1/4} \right]. \]

Therefore

\[ N(G) \geq \frac{1}{\sqrt{2}} \text{MRI}(G) + \sqrt{2} \text{DR}(G). \]

Equality holds if and only if \( \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2 = 2\sqrt{d_G(u)d_G(v)} \), which implies that equality holds if and only if \( G \cong \tilde{K}_n \).

We now prove the second part. Let \( a \) and \( b \) be any two non-negative real numbers. Then it is easy to see that

\[ \sqrt{a+b} \leq \sqrt{a} + \sqrt{b} \]
with equality if and only if $a = 0$ or $b = 0$.

Putting $a = \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2$ and $b = 2\sqrt{d_G(u)d_G(v)}$ in the above inequality, we get

$$\left[ \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2 + 2\sqrt{d_G(u)d_G(v)} \right]^{1/2} \leq \left[ \left( \sqrt{d_G(u)} - \sqrt{d_G(v)} \right)^2 + \left( 2\sqrt{d_G(u)d_G(v)} \right)^{1/2} \right]^{1/2}$$

$$= \left| \sqrt{d_2(u)} - \sqrt{d_2(v)} \right| + \sqrt{2} \left( d_G(u)d_G(v) \right)^{1/4}$$

resulting in

$$N(G) \leq \sum_{uv \in E(G)} \left| \sqrt{d_2(u)} - \sqrt{d_2(v)} \right| + \sqrt{2} \sum_{uv \in E(G)} \left( d_G(u)d_G(v) \right)^{1/4}$$

i.e.,

$$N(G) \leq MRI(G) + \sqrt{2} DR(G).$$

Equality holds if and only if either $d_G(u) - d_G(v) = 0$ or $d_G(u)d_G(v) = 0$. Therefore we conclude that equality holds if and only if $d_G(u) = d_G(v)$ for any edge $uv \in E(G)$.

4. Conclusion

In this study, some upper and lower bounds on the Nirmala index of graphs by using some graph parameters are established.

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