Annals of Pure and Applied Mathematics
Vol. 23, No. 2, 2021, 93-99
ISSN: 2279-087X (P), 2279-0888(online)
Published on 23 May 2021
www.researchmathsci.org
DOI: http://dx.doi.org/10.22457/apam.v23n2a06822

Annals of Pure and Applied Mathematics

On Some Mathematical Properties of Nirmala Index

***V.R.Kulli**[*a]* **and** ***Ivan Gutman**[b]*

[a]Department of Mathematics, Gulbarga University
Kalaburgi(Gulbarga) 585 106, India
E-mail:vrkulli@gmail.com

[b]Faculty of Science, University of Kragujevac
34000 Kragujevac, Serbia
E-mail: gutman@kg.ac.rs
[*]Corresponding author

Received 11 April 2021; accepted 12 May 2021

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.

Keywords: Nirmala index, graph, molecular graph.

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C09

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]

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

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

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

was considered [11,12]. Evidently, $SCI_\alpha(G) = SCI(G)$ for $\alpha = -1/2$. For details on mathematical properties of SCI_α see [13-15] and the references cited therein.

Quite recently, the so-called Sombor index was put forward, defined as [16]

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

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:

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_G(u) + d_G(v)}. \tag{1}$$

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 $\alpha = +1/2$.

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

$$KA^1_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a \right]^b,$$

$$KA^2_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a \, d_G(v)^a \right]^b$$

Where *a* and *b* are real numbers. Needless to say that $KA^1_{a,b}(G) = N(G)$ 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 $a=\frac{1}{2}$, $b=1$, $KA^1_{a,b}$ 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 $a=1$, $b=\frac{1}{4}$, $KA^2_{a,b}$ 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

(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 $T \cong P_n$ or, and $G \cong P_n$ or $G \cong K_n$.

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 $T \cong S_n$. 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 $N(K_n) = \binom{n}{2}\sqrt{2n-2}$.

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 Δ and minimum degree δ. Then

(i) $\sqrt{2\delta(G)}m \leq N(G) \leq \sqrt{2\Delta(G)}m$

(ii) $\dfrac{n\delta(G)^{3/2}}{\sqrt{2}} \leq N(G) \leq \dfrac{n\Delta(G)^{3/2}}{\sqrt{2}}$

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 Δ and minimum degree δ. Then

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

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

Proof:

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

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

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

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

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 $G \cong \overline{K}_n$.

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

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

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

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

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

By the definition of Nirmala index, we have

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

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

$$\begin{aligned} N(G) &= \sum_{uv\in E(G)} \sqrt{d_G(u)+d_G(v)} \\ &= \sum_{uv\in E(G)} \left[\left(\sqrt{d_G(u)}+\sqrt{d_G(u)}\right)^2 - 2\sqrt{d_G(u)d_G(v)}\right]^{1/2} \\ &\le \sum_{uv\in E(G)} \left(\sqrt{d_G(u)}+\sqrt{d_G(u)}\right) = MPI(G). \end{aligned}$$

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

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 $n \ge 2$andsize m. Then

$$\frac{1}{\sqrt{2}} MRI(G) + \sqrt{2}\,\mathrm{DR}(G) \le N(G) \le MRI(G) + \sqrt{2}\,\mathrm{DR}(G).$$

Equality in left hand side holds if and only if $G \cong \overline{K}_n$ .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

$$\begin{aligned} &\left[\left(\sqrt{d_G(u)}+\sqrt{d_G(v)}\right)^2 + 2\sqrt{d_G(u)d_G(v)}\right]^{1/2} \\ &\ge \frac{1}{\sqrt{2}}\left[\left(\left(\sqrt{d_G(u)}-\sqrt{d_G(v)}\right)^2\right)^{1/2} + \left(2\sqrt{d_G(u)d_G(v)}\right)^{1/2}\right] \\ &= \frac{1}{\sqrt{2}}\left[\left|\sqrt{d_G(u)}-\sqrt{d_G(v)}\right| + \sqrt{2}\left(d_G(u)d_G(v)\right)^{1/4}\right]. \end{aligned}$$

Thus

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

Therefore

$$N(G) \ge \frac{1}{\sqrt{2}} MRI(G) + \sqrt{2}\,\mathrm{DR}(G).$$

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 $G \cong \overline{K}_n$.

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

$$\sqrt{a+b} \le \sqrt{a} + \sqrt{b}$$

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

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

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.,

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

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.

Acknowledgement. The authors are thankful to the reviewer for the valuable suggestions for the paper.

REFERENCES

1. I.Gutman and O.E.Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin (1986).
2. V.R.Kulli, *Multiplicative Connectivity Indices of Nanostructures*, LAP LEMBERT Academic Publishing (2018).
3. J.Devillers and A.T.Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon& Breach, Amsterdam, 1999.
4. V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
5. R.Todeschini and V.Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim (2000).
6. R.Todeschini and V.Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim (2009).
7. B.Zhou and N.Trinajstić, On a novel connectivity index, *Journal of Mathematical Chemistry,* 46 (2009) 1252-1270.
8. B. Lučić, S.Nikolić, N.Trinajstić, B.Zhou and S.Ivaniš Turk, Sum-connectivity index, in: I.Gutman and B.Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications I*, Univ. Kragujevac, Kragujevac (2010), pp. 101-136.
9. R.Xing, B.Zhou and N.Trinajstić, Sum-connectivity index of molecular trees, *Journal of Mathematical Chemistry,* 48 (2010) 583-591.

10. S.Wang, B.Zhou and N.Trinajstić, On the sum-connectivity index, *Filomat*, 25 (2011) 29-42.
11. Z.Du, B.Zhou and N.Trinajstić, Minimum general sum-connectivity indices of unicyclic graphs, *Journal of Mathematical Chemistry,* 48 (2010) 697-703.
12. Z.Du, B.Zhou and N.Trinajstić, On the general sum-connectivity index of trees, *Applied Mathematics Lett*ers, 24 (2011) 402-405.
13. I.Tomescu and S.Kanwal, Ordering trees having small general sum-connectivity index, *MATCH Communications in Mathematical and in Computer Chem*istry, 69 (2013) 535-548.
14. Q.Cui and L.Zhong, On the general sum-connectivity index of trees with given number of pendent vertices, *Discrete Applied Math*ematics, 222 (2017) 213-221.
15. M.R.Alfuraidan, K.C.Das, T.Vetrik and S.Balachandran, General sum-connectivity index of unicyclic graphs with given diameter, *Discrete Applied Mathematics,* 295 (2021) 39-46.
16. I.Gutman, Geometric approach to degree based topological indices: Sombor indices, *MATCH Communications in Mathematical and in Computer Chem*istry, 86 (2021) 11-16.
17. K.C.Das, A.S.Cevik, I.N.Cangul and Y.Shang, On Somborindex, *Symmetry,* 13 (2021) 140.
18. V.R.Kulli, Sombor indices of certain graph operators, *International Journal of Engineering Sciences and Research Technology*, 10(1) (2021) 127-134.
19. V.R.Kulli, Multiplicative Sombor indices of certain nanotubes, *International Journal of Mathematical Archive,* 12 (3) (2021) 1-5.
20. V.R.Kulli, δ-Sombor index and its exponential for certain nanotubes, *Annals of Pure and Applied Mathematics,* 23(1) (2021) 37-42.
21. V.R.Kulli, On Banhatti-Sombor indices, *SSRG International Journal of Applied Chemistry*, 8(1) (2021) 21-25.
22. V.R.Kulli and I. Gutman, Computation of Sombor indices of certain networks, *SSRG International Journal of Applied Chemistry,* 8(1) (2021) 1-5.
23. Z.Lin, L.Miao, and T.Zhon, On the spectral radius, energy and Estrada index of the Sombor matrix of graphs, arXiv: 2102.03960.
24. Z.Lin, T.Zhon, V.R.Kulli and L.Miao, On the first Banhatti-Sombor index, arXiv: 2104.03615v1.
25. I.Milovanović, E.Milovanović and M.Matejić, On some mathematical properties of Sombor indices, *Bulletin of the International Mathematical Virtual Institute,* 11(2) (2021) 341-353.
26. T.Reti, T.Došlić and A.Ali, On the Sombor index of graphs, *Contributions of Mathematics,* 3 (2021) 11-18.
27. V.R.Kulli, Nirmala index, *International Journal of Mathematics Trends and Technology,* 67(3) (2021) 8-12.
28. D. Vukičević and M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta,,* 83 (2010) 243-260.
29. V.R.Kulli, The (a, b)-KA indices of polycyclic aromatic hydrocarbons, and benzenoid systems, *International Journal of Mathematics Trends and Technology,* 65(11) (2019) 115-120.