

M-POLYNOMIAL BASED MATHEMATICAL FORMULATION OF THE (a, b) -NIRMALA INDEX AND ITS BOUNDS

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Abstract Topological indices are graph-invariant numerical parameters that characterize the topology of a graph. Numerous topological indices have been developed and many of them have played an essential role in forecasting the chemical, pharmacological, and other characteristics of molecular graphs. In early 2022, a new topological index was introduced depending on the degree of end vertices of an edge in a graph and was named the (a, b) -Nirmala index. In this paper, we formulate the (a, b) -Nirmala index in terms of M-polynomial of a graph χ and present its correlation with several related previously defined well-known degree-dependent topological indices of χ . Moreover, we derive the value of the (a, b) -Nirmala index for some standard graphs. Additionally, we determine some general bounds for the (a, b) -Nirmala index of χ .

1 Introduction

Let $\chi = (V(\chi), E(\chi))$ be a connected, simple and finite graph, where $V(\chi)$ signifies the vertex set and $E(\chi)$ signifies the edge set. The *order* and *size* of graph χ are generally the cardinalities of $V(\chi)$ and $E(\chi)$, respectively. The number of edges of a graph χ that are incident to the vertex $t \in V(\chi)$ is known as the *degree* of a vertex t and is represented by $d(t)$. If two vertices t' and t'' of a graph χ are connected with each other by an edge then we denote it by $t't''$ (or $t''t'$). We denote the maximum and minimum degree of a graph χ by Δ and δ . A graph assembled from disjoint replicas of χ_1 and χ_2 by joining every vertex of χ_1 to every vertex of χ_2 is called a *join* of two graphs χ_1 and χ_2 and is denoted by $\chi_1 \vee \chi_2$. The *Cartesian product* of graphs χ_1 and χ_2 is a graph, represented by $\chi_1 \square \chi_2$ has the vertex set $V(\chi_1 \square \chi_2) = V(\chi_1) \times V(\chi_2) = \{(t, t') : t \in \chi_1, t' \in \chi_2\}$ and the edge set $E(\chi_1 \square \chi_2) = \{(t'_1, t'_2)(t''_1, t''_2) : t'_1 = t''_1 \text{ and } t'_2 t''_2 \in E(\chi_2), \text{ or } t'_2 = t''_2 \text{ and } t'_1 t''_1 \in E(\chi_1)\}$. For more details, please see [1, 2].

The subfield of mathematical chemistry that has a significant impact on the advancement of the chemical sciences is known as Chemical Graph Theory (CGT). A topological index for a molecular structure is a single number that reveals the structural properties of a molecular graph. Several molecular descriptors, also known as topological indices, have seen usefulness in theoretical chemistry, particularly in QSPR¹/QSAR² research [3]. QSPR modeling was performed in [4, 5] to predict the physico-chemical properties of several COVID-19 drugs through regression analysis. Very recently, the chemical applicability of different novel degree-based topological indices was tested in the articles [6, 7]. In Table 1, we assemble some familiar degree-dependent topological indices with their notations and formulas.

¹Quantitative structure property relationship.

²Quantitative structure activity relationship.

Table 1. Some familiar degree-dependent topological indices of a graph χ .

Sl. No.	Topological Index	Notation	Formula of Topological Indices
1.	First Zagreb Index [8]	$M_1(\chi)$	$\sum_{t't'' \in E(\chi)} d(t') + d(t'')$
2.	Harmonic Index [9]	$H(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{2}{d(t') + d(t'')}$
3.	Sum-connectivity Index [10]	$S(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{1}{\sqrt{d(t') + d(t'')}}$
4.	Inverse Sum (Indeg) Index [11]	$ISI(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{d(t')d(t'')}{d(t') + d(t'')}$
5.	Sombor Index [12, 13]	$SO(\chi)$	$\sum_{t't'' \in E(\chi)} \sqrt{d(t')^2 + d(t'')^2}$
6.	Modified Sombor Index [14]	${}^m SO(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{1}{\sqrt{d(t')^2 + d(t'')^2}}$
7.	p -Sombor Index [15]	$SO_p(\chi)$	$\sum_{t't'' \in E(\chi)} (d(t')^p + d(t'')^p)^{1/p}$
8.	K_1 Index [16]	$K_1(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{\sqrt{2}}{\sqrt{d(t')^2 + d(t'')^2}}$
9.	Misbalance Prodeg Index [17]	$MPI(\chi)$	$\sum_{t't'' \in E(\chi)} (\sqrt{d(t')} + \sqrt{d(t'')})$
10.	Nirmala Index [18]	$N(\chi)$	$\sum_{t't'' \in E(\chi)} \sqrt{d(t') + d(t'')}$
11.	First Inverse Nirmala Index [19]	$IN_1(\chi)$	$\sum_{t't'' \in E(\chi)} \sqrt{\frac{1}{d(t')} + \frac{1}{d(t'')}}$
12.	Second Inverse Nirmala Index [19]	$IN_2(\chi)$	$\sum_{t't'' \in E(\chi)} \frac{1}{\sqrt{\frac{1}{d(t')} + \frac{1}{d(t'')}}}$
13.	Forgotten Index [20]	$F(\chi)$	$\sum_{t't'' \in E(\chi)} d(t')^2 + d(t'')^2$
14.	Hyper-Zagreb Index [21]	$HM(\chi)$	$\sum_{t't'' \in E(\chi)} (d(t') + d(t''))^2$
15.	Dharwad Index [22]	$D(\chi)$	$\sum_{t't'' \in E(\chi)} \sqrt{d(t')^3 + d(t'')^3}$

Very recently, the M-polynomial based derivation formulas for Nirmala and GQ - QG indices are determined in [23, 24]. The Nordhaus-Gaddum-type inequalities for the Nirmala Indices were investigated in [25]. A comparative study between Nirmala and Sombor indices based on their applicability, degeneracy and smoothness were supervised in [26]. Furthermore, the Nirmala indices-based entropy measure for silicon-carbide network was studied in the paper [27].

In early 2022, Nandargi and Kulli introduced a new degree-dependent topological index known as the (a, b) -Nirmala index [28] for a graph χ and is defined as

$$N_{a,b}(\chi) = \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2} \right)^b. \quad (1.1)$$

Usually, we estimate the topological indices by using their respective mathematical formulas. At present, the algebraic approach in the calculation of topological indices is more notable and beneficent. Several graph polynomials in the literature of CGT were introduced for the computation of different classes of topological indices. The M-polynomial [29] is one of those polynomials which was developed by Deutsch and Klavžar in 2015 for determining the degree-dependent topological indices.

Definition 1.1 ([29]). The M -polynomial of a graph χ is expressed as

$$M(\chi; r, s) = \sum_{\delta \leq i \leq j \leq \Delta} m_{i,j} r^i s^j,$$

where $\delta = \min\{d(t) | t \in V(\chi)\}$, $\Delta = \max\{d(t) | t \in V(\chi)\}$ and $m_{i,j}$ is the number of edges $t't'' \in E(\chi)$ such that $d(t') = i$, $d(t'') = j$ ($i, j \geq 1$).

In 2011, Deng et al. [30] defined the degree-dependent topological index as a graph invariant,

abbreviated as $I(\chi)$ and described it as

$$I(\chi) = \sum_{t't'' \in E(\chi)} f(d(t'), d(t'')), \quad (1.2)$$

where $f(r, s) \geq 0$ is a real function of r and s such that $f(r, s) = f(s, r)$ and it essentially depends on the mathematical formula of the corresponding topological index. Therefore, $I(\chi)$ can also be rewritten as

$$I(\chi) = \sum_{i \leq j} m_{i,j} f(i, j). \quad (1.3)$$

Different graph polynomials are estimated for several graphs and molecular structures [31–40].

Our Contributions

In this article, we focus on estimating significant results on a recently introduced degree-dependent topological index, named the (a, b) -Nirmala index [28] for a graph χ . In Section 2, we propose the M-polynomial based formula of the (a, b) -Nirmala index by introducing some new operators. There are numerous well-known degree-dependent topological indices in the literature which are listed in Table 1. We endeavour to establish a correlation between the (a, b) -Nirmala index and the tabulated degree-dependent topological indices of a graph χ . Section 3 deals with computing the (a, b) -Nirmala index for different types of graphs such as path graph, cycle graph, complete graph, complete bipartite graph, wheel graph, star graph, book graph, ladder graph and friendship graph by using our proposed (in Section 2) M-polynomial based formula of the (a, b) -Nirmala index. Moreover, in Section 4, we put forward some bounds on the (a, b) -Nirmala index in terms of the order, degree and size of a graph χ , and also in terms of the degree sequence and size of the graph. Lastly, we conclude in Section 5.

2 Derivation Formula for the (a, b) -Nirmala Index From M-polynomial and Its Relation With Other Indices

In this section, we formulate the M-polynomial based compact derivation formula for finding the (a, b) -Nirmala index of a graph χ . For this purpose, we require one of the previously defined operators $J(f(r, s)) = f(r, r)$, which was introduced in [29]. Besides, we propose some more operators that are needed to establish the above formula. They are

$$V_r^\alpha(f(r^i, s^j)) = f(r^{i\alpha}, s^j),$$

$$V_s^\alpha(f(r^i, s^j)) = f(r^i, s^{j\alpha}),$$

$$\text{and } T_r^\beta(f(r^i, s^j)) = \left(r \frac{\partial f(r^i, s^j)}{\partial r} \right)^\beta \cdot (f(r^i, s^j))^{1-\beta},$$

where $i, j \in \mathbb{N} \cup \{0\}$, $\alpha, \beta \in \mathbb{R}$, and \mathbb{N}, \mathbb{R} are the set of natural and real numbers, respectively.

Theorem 2.1. *Let $\chi = (V(\chi), E(\chi))$ be a graph, then the expression of the (a, b) -Nirmala index in terms of its M-polynomial $M(\chi; r, s)$ is given by*

$$N_{a,b}(\chi) = \frac{1}{2^b} T_r^b J V_s^a V_r^a M(\chi; r, s)|_{r=1}$$

Proof. From the definition of M-polynomial, we have

$$M(\chi; r, s) = \sum_{i \leq j} m_{i,j} r^i s^j$$

Let us now calculate the following term,

$$\begin{aligned}
 \frac{1}{2^b} T_r^b J V_s^a V_r^a M(\chi; r, s) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a \left\{ \sum_{i \leq j} m_{i,j} r^i s^j \right\} \\
 &= \frac{1}{2^b} \sum_{i \leq j} T_r^b J V_s^a V_r^a \{ m_{i,j} r^i s^j \} \\
 &= \frac{1}{2^b} \sum_{i \leq j} T_r^b J V_s^a \{ m_{i,j} r^{i^a} s^j \} \\
 &= \frac{1}{2^b} \sum_{i \leq j} T_r^b J \{ m_{i,j} r^{i^a} s^{j^a} \} \\
 &= \frac{1}{2^b} \sum_{i \leq j} T_r^b \{ m_{i,j} r^{i^a + j^a} \} \\
 &= \frac{1}{2^b} \sum_{i \leq j} \left\{ r \frac{\partial}{\partial r} \left(m_{i,j} r^{i^a + j^a} \right) \right\}^b \cdot \left\{ m_{i,j} r^{i^a + j^a} \right\}^{1-b} \\
 &= \frac{1}{2^b} \sum_{i \leq j} \left\{ (i^a + j^a) m_{i,j} r^{i^a + j^a} \right\}^b \cdot \left\{ m_{i,j} r^{i^a + j^a} \right\}^{1-b} \\
 &= \frac{1}{2^b} \sum_{i \leq j} (i^a + j^a)^b m_{i,j} r^{i^a + j^a} \\
 &= \sum_{i \leq j} \left(\frac{i^a + j^a}{2} \right)^b m_{i,j} r^{i^a + j^a}. \tag{2.1}
 \end{aligned}$$

We can now rewrite the mathematical definition of the (a, b) -Nirmala index, by using Equations 1.2 and 1.3, as

$$N_{a,b}(\chi) = \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2} \right)^b = \sum_{i \leq j} \left(\frac{i^a + j^a}{2} \right)^b m_{i,j} \tag{2.2}$$

where, $m_{i,j}(\chi)$ is the number of edges $t't'' \in E(\chi)$ such that $d(t') = i, d(t'') = j$ ($i, j \geq 1$). Therefore, from Equations 2.1 and 2.2, we have

$$N_{a,b}(\chi) = \frac{1}{2^b} T_r^b J V_s^a V_r^a M(\chi; r, s)|_{r=1}.$$

□

Now, we propose some correlations between the previously known standard degree-dependent topological indices (as reported in Table 1) and the (a, b) -Nirmala index for a certain set of values of a and b . The results mentioned in the following corollary are immediate from the mathematical definitions of the indices mentioned in Table 1, Equation 1.1 and Theorem 2.1.

Corollary 2.2. *The well-known degree-dependent topological indices are linked with the (a, b) -Nirmala index for a certain set of values of a and b , as*

- (i) $M_1(\chi) = 2N_{1,1}(\chi) = T_r^1 J V_s^1 V_r^1 M(\chi; r, s)|_{r=1}$,
- (ii) $H(\chi) = N_{1,-1}(\chi) = 2T_r^{-1} J V_s^1 V_r^1 M(\chi; r, s)|_{r=1}$,
- (iii) $S(\chi) = \frac{1}{\sqrt{2}} N_{1,-\frac{1}{2}}(\chi) = T_r^{-1/2} J V_s^1 V_r^1 M(\chi; r, s)|_{r=1}$,
- (iv) $ISI(\chi) = \frac{1}{2} N_{-1,-1}(\chi) = T_r^{-1} J V_s^{-1} V_r^{-1} M(\chi; r, s)|_{r=1}$,
- (v) $SO(\chi) = \sqrt{2} N_{2,\frac{1}{2}}(\chi) = T_r^{1/2} J V_s^2 V_r^2 M(\chi; r, s)|_{r=1}$,

- (vi) ${}^mSO(\chi) = \frac{1}{\sqrt{2}}N_{2,-\frac{1}{2}}(\chi) = T_r^{-1/2}JV_s^2V_r^2M(\chi; r, s)|_{r=1}$,
- (vii) $SO_p(\chi) = 2^{1/p}N_{p,\frac{1}{p}}(\chi) = T_r^{1/p}JV_s^pV_r^pM(\chi; r, s)|_{r=1}$,
- (viii) $K_1(\chi) = N_{2,-\frac{1}{2}}(\chi) = \sqrt{2}T_r^{-1/2}JV_s^2V_r^2M(\chi; r, s)|_{r=1}$,
- (ix) $MPI(\chi) = 2N_{\frac{1}{2},1}(\chi) = T_r^1JV_s^{1/2}V_r^{1/2}M(\chi; r, s)|_{r=1}$,
- (x) $N(\chi) = \sqrt{2}N_{1,\frac{1}{2}}(\chi) = T_r^{1/2}JV_s^1V_r^1M(\chi; r, s)|_{r=1}$,
- (xi) $IN_1(\chi) = \sqrt{2}N_{-1,\frac{1}{2}}(\chi) = T_r^{1/2}JV_s^{-1}V_r^{-1}M(\chi; r, s)|_{r=1}$,
- (xii) $IN_2(\chi) = \frac{1}{\sqrt{2}}N_{-1,-\frac{1}{2}}(\chi) = T_r^{-1/2}JV_s^{-1}V_r^{-1}M(\chi; r, s)|_{r=1}$,
- (xiii) $F(\chi) = 2N_{2,1}(\chi) = T_r^1JV_s^2V_r^2M(\chi; r, s)|_{r=1}$,
- (xiv) $HM(\chi) = 4N_{1,2}(\chi) = T_r^2JV_s^1V_r^1M(\chi; r, s)|_{r=1}$,
- (xv) $D(\chi) = \sqrt{2}N_{3,\frac{1}{2}}(\chi) = T_r^{1/2}JV_s^3V_r^3M(\chi; r, s)|_{r=1}$.

3 Computing the (a, b)-Nirmala Index for Certain Standard Graphs

In this section, we calculate the (a, b)-Nirmala index for certain standard graphs using our proposed derivation formula (mentioned in Theorem 2.1) through their respective M-polynomials. The following theorem lists all such M-polynomials of our interest.

Theorem 3.1 ([41, 42]). *Let χ be a graph. Then the expression of the M-polynomials for the graphs are as follows.*

- (i) *If $\chi = P_n$ is a path graph, then $M(P_n; r, s) = 2rs^2 + (n - 3)r^2s^2$,*
- (ii) *If $\chi = C_n$ is a cycle graph, then $M(C_n; r, s) = nr^2s^2$,*
- (iii) *If $\chi = K_n$ is a complete graph, then $M(K_n; r, s) = \frac{n(n-1)}{2}r^{n-1}s^{n-1}$,*
- (iv) *If $\chi = K_{n_1,n_2}$ is a complete bipartite graph, then $M(K_{n_1,n_2}; r, s) = n_1n_2r^{n_1}s^{n_2}$,*
- (v) *If $\chi = W_n = C_n \vee K_1$ is a wheel graph, then $M(W_n; r, s) = nr^3s^3 + nr^3s^n$,*
- (vi) *If $\chi = S_n = K_{1,n}$ is a star graph, then $M(S_n; r, s) = nr^3s^n$,*
- (vii) *If $\chi = B_n = S_n \square P_2 = K_{1,n} \square K_2$ is a book graph, then $M(B_n; r, s) = nr^2s^2 + 2nr^2s^{n+1} + r^{n+1}s^{n+1}$,*
- (viii) *If $\chi = L_n = P_n \square P_2$ is a ladder graph, then $M(L_n; r, s) = 2r^2s^2 + 4r^2s^3 + (3n - 8)r^3s^3$,*
- (ix) *If $\chi = F_n = K_1 \vee nK_2$ is a friendship graph, then $M(F_n; r, s) = nr^2s^2 + 2nr^2s^{2n}$.*

Theorem 3.2. *Let $M(\chi; r, s)$ be the M-polynomial of a graph χ . Then the (a, b)-Nirmala index of χ is*

- (i) $N_{a,b}(\chi) = 2\left(\frac{1+2^a}{2}\right)^b + (n - 3)2^{ab}$, for the path graph $\chi = P_n$,
- (ii) $N_{a,b}(\chi) = n2^{ab}$, for the cycle graph $\chi = C_n$,
- (iii) $N_{a,b}(\chi) = \frac{1}{2}n(n - 1)^{ab+1}$, for the complete graph $\chi = K_n$,
- (iv) $N_{a,b}(\chi) = n_1n_2\left(\frac{n_1^a+n_2^a}{2}\right)^b$, for the complete bipartite graph $\chi = K_{n_1,n_2}$,
- (v) $N_{a,b}(\chi) = n3^{ab} + n\left(\frac{3^a+n^a}{2}\right)^b$, for the wheel graph $\chi = W_n = C_n \vee K_1$,
- (vi) $N_{a,b}(\chi) = n\left(\frac{1+n^a}{2}\right)^b$, for the star graph $\chi = S_n = K_{1,n}$,

$$(vii) \ N_{a,b}(\chi) = (n+1)^{ab} + 2n \left(\frac{2^a + (n+1)^a}{2} \right)^b + n2^{ab}, \quad \text{for the book graph } \chi = B_n = S_n \square P_2 = K_{1,n} \square K_2,$$

$$(viii) \ N_{a,b}(\chi) = 2 \times 2^{ab} + 4 \left(\frac{2^a + 3^a}{2} \right)^b + (3n-8)3^{ab}, \quad \text{for the ladder graph } \chi = L_n = P_n \square P_2,$$

$$(ix) \ N_{a,b}(\chi) = n2^{ab} + 2n \left(\frac{2^a + (2n)^a}{2} \right)^b, \quad \text{for the friendship graph } \chi = F_n = K_1 \vee nK_2.$$

Proof. We derive the value of the (a, b) -Nirmala index for the graph χ under consideration using the M-polynomial based derivation formula of the (a, b) -Nirmala index

$$N_{a,b}(\chi) = \frac{1}{2^b} T_r^b J V_s^a V_r^a M(\chi; r, s) |_{r=1}.$$

The M-polynomial expressions of the respective graphs are listed in Theorem 3.1.

(i) **For the path graph P_n :** $M(P_n; r, s) = 2rs^2 + (n-3)r^2s^2$

$$\begin{aligned} N_{a,b}(P_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(P_n; r, s) |_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (2rs^2 + (n-3)r^2s^2) |_{r=1} \\ &= \frac{1}{2^b} T_r^b J (2rs^{2^a} + (n-3)r^{2^a}s^{2^a}) |_{r=1} \\ &= \frac{1}{2^b} T_r^b (2r^{1+2^a} + (n-3)r^{2^a+2^a}) |_{r=1} \\ &= \frac{1}{2^b} \left(2(1+2^a)^b r^{1+2^a} + (n-3)(2^a+2^a)^b r^{2^a+2^a} \right) \Big|_{r=1} \\ &= 2 \left(\frac{1+2^a}{2} \right)^b + (n-3)2^{ab}. \end{aligned}$$

(ii) **For the cycle graph C_n :** $M(C_n; r, s) = nr^2s^2$

$$\begin{aligned} N_{a,b}(C_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(C_n; x, y) |_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (nr^2s^2) |_{r=1} \\ &= \frac{1}{2^b} T_r^b J (nr^{2^a}s^{2^a}) |_{r=1} \\ &= \frac{1}{2^b} T_r^b (nr^{2^a+2^a}) |_{r=1} \\ &= \frac{1}{2^b} n(2^a+2^a)^b r^{2^a+2^a} |_{r=1} \\ &= n2^{ab}. \end{aligned}$$

(iii) **For the complete graph K_n :** $M(K_n; r, s) = \frac{n(n-1)}{2} r^{n-1} s^{n-1}$

$$\begin{aligned} N_{a,b}(K_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(K_n; r, s) |_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a \left(\frac{n(n-1)}{2} r^{n-1} s^{n-1} \right) \Big|_{r=1} \\ &= \frac{n(n-1)}{2^{b+1}} T_r^b J V_s^a V_r^a (r^{n-1} s^{n-1}) |_{r=1} \end{aligned}$$

$$\begin{aligned}
 &= \frac{n(n-1)}{2^{b+1}} T_r^b J(r^{(n-1)^a} s^{(n-1)^a})|_{r=1} \\
 &= \frac{n(n-1)}{2^{b+1}} T_r^b (r^{2(n-1)^a})|_{r=1} \\
 &= \frac{n(n-1)}{2^{b+1}} (2(n-1)^a)^b r^{2(n-1)^a}|_{r=1} \\
 &= \frac{1}{2} n(n-1)^{ab+1}.
 \end{aligned}$$

(iv) **For the complete bipartite graph K_{n_1, n_2} :** $M(K_{n_1, n_2}; r, s) = n_1 n_2 r^{n_1} s^{n_2}$

$$\begin{aligned}
 N_{a,b}(K_{n_1, n_2}) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(K_{n_1, n_2}; r, s)|_{r=1} \\
 &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (n_1 n_2 r^{n_1} s^{n_2})|_{r=1} \\
 &= \frac{n_1 n_2}{2^b} T_r^b J V_s^a V_r^a (r^{n_1} s^{n_2})|_{r=1} \\
 &= \frac{n_1 n_2}{2^b} T_r^b J (r^{n_1^a} s^{n_2^a})|_{r=1} \\
 &= \frac{n_1 n_2}{2^b} T_r^b (r^{n_1^a + n_2^a})|_{r=1} \\
 &= \frac{n_1 n_2}{2^b} (n_1^a + n_2^a)^b r^{n_1^a + n_2^a}|_{r=1} \\
 &= n_1 n_2 \left(\frac{n_1^a + n_2^a}{2} \right)^b.
 \end{aligned}$$

(v) **For the wheel graph W_n :** $M(W_n; r, s) = nr^3 s^3 + nr^3 s^n$

$$\begin{aligned}
 N_{a,b}(W_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(W_n; r, s)|_{r=1} \\
 &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (nr^3 s^3 + nr^3 s^n)|_{r=1} \\
 &= \frac{1}{2^b} T_r^b J (nr^{3^a} s^{3^a} + nr^{3^a} s^{n^a})|_{r=1} \\
 &= \frac{1}{2^b} T_r^b (nr^{3^a + 3^a} + nr^{3^a + n^a})|_{r=1} \\
 &= \frac{1}{2^b} (n(3^a + 3^a)^b r^{3^a + 2^a} + n(3^a + n^a)^b r^{3^a + n^a})|_{r=1} \\
 &= n3^{ab} + n \left(\frac{3^a + n^a}{2} \right)^b.
 \end{aligned}$$

(vi) **For the star graph S_n :** $M(S_n; r, s) = nr s^n$

$$\begin{aligned}
 N_{a,b}(S_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(S_n; r, s)|_{r=1} \\
 &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (nr s^n)|_{r=1} \\
 &= \frac{1}{2^b} T_r^b J (nr s^{n^a})|_{r=1} \\
 &= \frac{1}{2^b} T_r^b (nr^{1+n^a})|_{r=1} \\
 &= \frac{1}{2^b} (n(1 + n^a)^b r^{1+n^a})|_{r=1} \\
 &= n \left(\frac{1 + n^a}{2} \right)^b.
 \end{aligned}$$

(vii) **For the book graph B_n :** $M(B_n; r, s) = nr^2s^2 + 2nr^2s^{n+1} + r^{n+1}s^{n+1}$

$$\begin{aligned} N_{a,b}(B_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(B_n; r, s)|_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (nr^2s^2 + 2nr^2s^{n+1} + r^{n+1}s^{n+1})|_{r=1} \\ &= \frac{1}{2^b} T_r^b J (nr^{2a}s^{2a} + 2nr^{2a}s^{(n+1)a} + r^{(n+1)a}s^{(n+1)a})|_{r=1} \\ &= \frac{1}{2^b} T_r^b (nr^{2a+2a} + 2nr^{2a+(n+1)a} + r^{2(n+1)a})|_{r=1} \\ &= \frac{1}{2^b} (n(2^a + 2^a)^b r^{2a+2a} + 2n(2^a + (n+1)^a)^b r^{2a+(n+1)a} + (2(n+1)^a)^b r^{2(n+1)a})|_{r=1} \\ &= n2^{ab} + 2n \left(\frac{2^a + (n+1)^a}{2} \right)^b + (n+1)^{ab}. \end{aligned}$$

(viii) **For the ladder graph L_n :** $M(L_n; r, s) = 2r^2s^2 + 4r^2s^3 + (3n-8)r^3s^3$

$$\begin{aligned} N_{a,b}(L_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(L_n; r, s)|_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (2r^2s^2 + 4r^2s^3 + (3n-8)r^3s^3)|_{r=1} \\ &= \frac{1}{2^b} T_r^b J (2r^{2a}s^{2a} + 4r^{2a}s^{3a} + (3n-8)r^{3a}s^{3a})|_{r=1} \\ &= \frac{1}{2^b} T_r^b (2r^{2a+2a} + 4r^{2a+3a} + (3n-8)r^{3a+3a})|_{r=1} \\ &= \frac{1}{2^b} (2(2^a + 2^a)^b r^{2a+2a} + 4(2^a + 3^a)^b r^{2a+3a} + (3n-8)(3^a + 3^a)^b r^{3a+3a})|_{r=1} \\ &= 2^{ab+1} + 4 \left(\frac{2^a + 3^a}{2} \right)^b + (3n-8)3^{ab}. \end{aligned}$$

(ix) **For the friendship graph F_n :** $M(F_n; r, s) = nr^2s^2 + 2nr^2s^{2n}$

$$\begin{aligned} N_{a,b}(F_n) &= \frac{1}{2^b} T_r^b J V_s^a V_r^a M(F_n; r, s)|_{r=1} \\ &= \frac{1}{2^b} T_r^b J V_s^a V_r^a (nr^2s^2 + 2nr^2s^{2n})|_{r=1} \\ &= \frac{1}{2^b} T_r^b J (nr^{2a}s^{2a} + 2nr^{2a}s^{(2n)a})|_{r=1} \\ &= \frac{1}{2^b} T_r^b (nr^{2a+2a} + 2nr^{2a+(2n)a})|_{r=1} \\ &= \frac{1}{2^b} (n(2^a + 2^a)^b r^{2a+2a} + 2n(2^a + (2n)^a)^b r^{2a+(2n)a})|_{r=1} \\ &= n2^{ab} + 2n \left(\frac{2^a + (2n)^a}{2} \right)^b. \end{aligned}$$

□

4 Some Results on the Bounds of the (a, b) -Nirmala Index

This section deals with certain interesting outcomes regarding the bounds of the (a, b) -Nirmala Index of a graph χ in terms of some of its graph-theoretic parameters.

4.1 Bounds in Terms of Order, Degree and Size of a Graph χ

Theorem 4.1. *Let χ be a connected, simple, undirected graph with n vertices and m edges. If δ and Δ are the minimum and maximum degrees of a vertex of a graph χ . Then*

- (i) $m(\delta)^{ab} \leq N_{a,b}(\chi) \leq m(\Delta)^{ab}$,
- (ii) $\frac{1}{2}n(\delta)^{ab+1} \leq N_{a,b}(\chi) \leq \frac{1}{2}n(\Delta)^{ab+1}$

and equality (left and right) occurs if and only if χ is a regular graph.

Proof. (i) Since by definition,

$$N_{a,b}(\chi) = \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2} \right)^b,$$

we have

$$\begin{aligned} \sum_{t't'' \in E(\chi)} \left(\frac{\delta^a + \delta^a}{2} \right)^b &\leq \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2} \right)^b \leq \sum_{t't'' \in E(\chi)} \left(\frac{\Delta^a + \Delta^a}{2} \right)^b \\ \Rightarrow m(\delta)^{ab} &\leq \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2} \right)^b \leq m(\Delta)^{ab}. \end{aligned}$$

From the definition of the (a,b)-Nirmala index (see Equation (1.1)), we have

$$m(\delta)^{ab} \leq N_{a,b}(\chi) \leq m(\Delta)^{ab}. \tag{4.1}$$

(ii) Also, the handshaking lemma states that

$$\sum_{t \in V(\chi)} d(t) = 2m.$$

Observe that,

$$\begin{aligned} n\delta &\leq \sum_{t \in V(\chi)} d(t) \leq n\Delta \\ \Rightarrow n\delta &\leq 2m \leq n\Delta. \end{aligned} \tag{4.2}$$

Therefore, from Equations 4.1 and 4.2, we obtain

$$\frac{1}{2}n(\delta)^{ab+1} \leq N_{a,b}(\chi) \leq \frac{1}{2}n(\Delta)^{ab+1}.$$

Furthermore, if χ is a regular graph then $d(t) = \delta = \Delta, \forall t \in V(\chi)$, for which the equality holds for both upper and lower bounds of the (a, b)-Nirmala index of the graph χ . □

4.2 Bounds in Terms of Degree Sequence and Size of a Graph χ

Theorem 4.2. *Let χ be a connected graph of size m with n vertices having degree sequence $(d(t_1), d(t_2), d(t_3), \dots, d(t_n))$, where $d(t_1) \geq d(t_2) \geq \dots \geq d(t_n)$. Let w be the number of vertices of degree $d(t_n)$, and m' be the size of the subgraph induced by these w vertices. Then*

$$\begin{aligned} m' \times (d(t_n))^{ab} + (m - wd(t_n) + m') \times (d(t_{n-w}))^{ab} + (wd(t_n) - 2m') \times \left(\frac{d(t_n)^a + d(t_{n-w})^a}{2} \right)^b \\ \leq N_{a,b}(\chi) \leq \\ m' \times (d(t_n))^{ab} + (m - wd(t_n) + m') \times (d(t_1))^{ab} + (wd(t_n) - 2m') \times \left(\frac{d(t_n)^a + d(t_1)^a}{2} \right)^b. \end{aligned}$$

Proof. Let Υ be the induced subgraph of χ having w vertices of degree $d(t_n)$ and size m' . For any edge $t't''$ in the graph χ , the following cases arise:

- **Case I:** If $t't'' \in E(\Upsilon)$, then

$$\left(\frac{d(t')^a + d(t'')^a}{2}\right)^b = \left(\frac{d(t_n)^a + d(t_n)^a}{2}\right)^b = (d(t_n))^{ab},$$

and note that $|E(\Upsilon)| = m'$.

- **Case II:** If $t't'' \in E(\chi - V(\Upsilon))$, then

$$\begin{aligned} \left(\frac{d(t_{n-w})^a + d(t_{n-w})^a}{2}\right)^b &\leq \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \leq \left(\frac{d(t_1)^a + d(t_1)^a}{2}\right)^b \\ \Rightarrow (d(t_{n-w}))^{ab} &\leq \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \leq (d(t_1))^{ab}, \end{aligned}$$

and observe that in this case $|E(\chi - V(\Upsilon))| = m - wd(t_n) + m'$.

- **Case III:** If $t't'' \in E(\chi)$ with $t' \in V(\Upsilon)$ and $t'' \in V(\chi) - V(\Upsilon)$, or $t' \in V(\chi) - V(\Upsilon)$ and $t'' \in V(\Upsilon)$, then

$$\left(\frac{d(t_n)^a + d(t_{n-w})^a}{2}\right)^b \leq \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \leq \left(\frac{d(t_n)^a + d(t_1)^a}{2}\right)^b,$$

and it follows that the number of edges from the vertex set $V(\Upsilon)$ to $V(\chi) - V(\Upsilon)$ is $wd(t_n) - 2m'$.

Hence, using the above three cases we can write that

$$\begin{aligned} N_{a,b}(\chi) &= \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \\ &\leq m' \times (d(t_n))^{ab} + (m - wd(t_n) + m') \times (d(t_1))^{ab} + (wd(t_n) - 2m') \times \left(\frac{d(t_n)^a + d(t_1)^a}{2}\right)^b, \end{aligned}$$

and

$$\begin{aligned} N_{a,b}(\chi) &= \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \\ &\geq m' \times (d(t_n))^{ab} + (m - wd(t_n) + m') \times (d(t_{n-w}))^{ab} + (wd(t_n) - 2m') \times \left(\frac{d(t_n)^a + d(t_{n-w})^a}{2}\right)^b. \end{aligned}$$

□

Remark 4.3. Observe that the above bounds of the $N_{a,b}(\chi)$ are sharp. It can be easily noted that both the upper and lower bounds of the $N_{a,b}(\chi)$ in Theorem 4.2 are coinciding with the value of the (a, b) -Nirmala index for the path graph $\chi = P_n$ that is,

$$N_{a,b}(P_n) = 2\left(\frac{1+2^a}{2}\right)^b + (n-3)2^{ab},$$

as determined in Theorem 3.2(a).

In fact, the above remark can be generalized as follows.

Theorem 4.4. Let χ be a connected graph having n vertices and size m with the degree of any of its vertex being either Δ or δ . Let w be the number of vertices of degree δ , and m' be the size of the subgraph induced by these w vertices. Then, the (a, b) -Nirmala index of such graph is given by

$$N_{a,b}(\chi) = m' \times (\delta)^{ab} + (m - w\delta + m') \times (\Delta)^{ab} + (w\delta - 2m') \times \left(\frac{\delta^a + \Delta^a}{2}\right)^b.$$

Proof. To prove this equality, let us take Υ as the induced subgraph of χ having w vertices of degree δ and size m' . For any edge $t't''$ in the graph χ , the following cases arise:

- **Case I:** If $t't'' \in E(\Upsilon)$, then

$$\left(\frac{d(t')^a + d(t'')^a}{2}\right)^b = \left(\frac{\delta^a + \delta^a}{2}\right)^b = (\delta)^{ab},$$

and as assumed that, we have $|E(\Upsilon)| = m'$.

- **Case II:** If $t't'' \in E(\chi - V(\Upsilon))$, then

$$\left(\frac{d(t')^a + d(t'')^a}{2}\right)^b = \left(\frac{\Delta^a + \Delta^a}{2}\right)^b = (\Delta)^{ab},$$

and see that for this case, we have $|E(\chi - V(\Upsilon))| = m - w\delta + m'$.

- **Case III:** If $t't'' \in E(\chi)$ with $t' \in V(\Upsilon)$ and $t'' \in V(\chi) - V(\Upsilon)$, or $t' \in V(\chi) - V(\Upsilon)$ and $t'' \in V(\Upsilon)$, then

$$\left(\frac{d(t')^a + d(t'')^a}{2}\right)^b = \left(\frac{\delta^a + \Delta^a}{2}\right)^b,$$

and note that the number of edges from the vertex set $V(\Upsilon)$ to $V(\chi) - V(\Upsilon)$ is $w\delta - 2m'$.

Therefore, combining the above three cases we can write that

$$\begin{aligned} N_{a,b}(\chi) &= \sum_{t't'' \in E(\chi)} \left(\frac{d(t')^a + d(t'')^a}{2}\right)^b \\ &= m' \times (\delta)^{ab} + (m - w\delta + m') \times (\Delta)^{ab} + (w\delta - 2m') \times \left(\frac{\delta^a + \Delta^a}{2}\right)^b. \end{aligned}$$

□

The result in Remark 4.3 is also immediate from the results in Theorem 4.4 by taking $m' = 0$, $\delta = 1$, $\Delta = 2$, $w = 2$, $m = n - 1$.

Another variant of Theorem 4.2 can be stated as follows. Its proof is left as an exercise for the interested reader.

Theorem 4.5. Let χ be a connected graph of size m with n vertices having degree sequence $(d(t_1), d(t_2), d(t_3), \dots, d(t_n))$, where $d(t_1) \geq d(t_2) \geq \dots \geq d(t_n)$. Let w be the number of vertices of degree $d(t_1)$, and m' be the size of the subgraph induced by these w vertices. Then

$$\begin{aligned} &m' \times (d(t_1))^{ab} + (m - wd(t_1) + m') \times (d(t_n))^{ab} + (wd(t_1) - 2m') \times \left(\frac{d(t_1)^a + d(t_n)^a}{2}\right)^b \\ &\leq N_{a,b}(\chi) \leq \\ &m' \times (d(t_1))^{ab} + (m - wd(t_1) + m') \times (d(t_{w+1}))^{ab} + (wd(t_1) - 2m') \times \left(\frac{d(t_1)^a + d(t_{w+1})^a}{2}\right)^b. \end{aligned}$$

5 Conclusion

In the present study, we propounded some remarkable results on the (a, b) -Nirmala index of a connected, simple and finite graph. We first established the M-polynomial based formula of the (a, b) -Nirmala index and thereafter related this index with the already existing standard degree-dependent topological indices. Furthermore, we have calculated the value of the (a, b) -Nirmala index for several well-known graphs. Additionally, we have generated some bounds on the (a, b) -Nirmala index of a graph in terms of some of its graph-theoretic parameters.

The importance of the (a, b) -Nirmala index derives from the fact that their particular cases coincide with the large number of hitherto introduced degree-dependent topological indices for suitably chosen values of the parameters a and b . Hence, by imposing the acquired relation on the bounds of the (a, b) -Nirmala index, we can incorporate these bounds for all the indices which are correlated with the (a, b) -Nirmala index.

Data Availability Statement

My manuscript has no associated data.

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No potential conflict of interest was reported by the authors. All authors have contributed equally.

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