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# Nirmala energy

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**Abstract:** A novel vertex-degree-based topological invariant, called Nirmala index, was recently put forward, defined as the sum of the terms $\sqrt{d(u)+d(v)}$ over all edges $uv$ of the underlying graph, where $d(u)$ is the degree of the vertex $u$. Based on this index, we now introduce the respective "Nirmala matrix", and consider its spectrum and energy. An interesting finding is that some spectral properties of the Nirmala matrix, including its energy, are related to the first Zagreb index.

**Keywords:** Nirmala index; Degree (of vertex); Energy (of graph); Zagreb index.

**MSC:** 05C50; 05C07; 05C92.

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## 1. Introduction

In this paper we consider simple graphs, i.e., graphs without directed, weighted, or multiple edges, and without self-loops. Let $G$ be such a graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Let $|\mathbf{V}(G)| = n$ and $|\mathbf{E}(G)| = m$ be the number of vertices and edges of $G$. By $uv \in \mathbf{E}(G)$ we denote the edge of $G$, connecting the vertices $u$ and $v$. The degree (= number of first neighbors) of a vertex $u \in \mathbf{V}(G)$ is denoted by $d(u)$. For other graph-theoretical notions, the readers are referred to textbooks [1–3].

In the mathematical and chemical literature, several dozens of vertex-degree-based graph invariants of the form

$$TI(G) = \sum_{uv\in\mathbf{E}(G)} F\big(d(u),d(v)\big) \tag{1}$$

have been and are currently studied, where $F(x,y)$ is an appropriately chosen function with the property $F(x,y) = F(y,x)$. The oldest such invariant, conceived as early as in the 1970s, is the *first Zagreb index*, $Zg$ [4]. Among the newest such invariants are the *Sombor index*, $SO$ [5,6] and the *Nirmala index*, $N$ [7,8]. These are defined as

$$Zg = Zg(G) = \sum_{uv\in\mathbf{E}(G)} \big[d(u)+d(v)\big], \tag{2}$$

$$SO = SO(G) = \sum_{uv\in\mathbf{E}(G)} \sqrt{d(u)^2+d(v)^2}, \tag{3}$$

$$N = N(G) = \sum_{uv\in\mathbf{E}(G)} \sqrt{d(u)+d(v)}\,. \tag{4}$$

Recall that $Zg$ if often written in the form

$$Zg(G) = \sum_{u\in\mathbf{V}(G)} d(u)^2$$

which, of course, is equivalent to (2). The Sombor index (3) is constructed by using Euclidean metrics [5,6]. By comparing (3) and (4), it is seen that the Nirmala index is a somewhat simplified variant of the Sombor index.

Let the vertices of the graph $G$ be labeled by $1, 2, \ldots, n$. Then the $(0,1)$-adjacency matrix of $G$, denoted by $\mathbf{A}(G)$, is defined as the symmetric square matrix of order $n$, whose $(i,j)$-elements is

$$\mathbf{A}(G)_{ij} = \begin{cases} 1 & \text{if } ij \in \mathbf{E}(G), \\ 0 & \text{if } ij \notin \mathbf{E}(G), \\ 0 & \text{if } i = j\,. \end{cases}$$

The eigenvalues of $\mathbf{A}(G)$ form the spectrum of the graph $G$. For details of spectral graph theory, see [9].

Some time ago [10], it was attempted to combine spectral graph theory with the theory of vertex-degree-based graph invariants. For this, using formula (1), an adjacency-matrix-type square symmetric matrix $\mathbf{A}_F(G)$ was introduced, whose $(i,j)$-elements are defined as

$$\mathbf{A}_F(G)_{ij} = \begin{cases} F\big(d(i), d(j)\big) & \text{if } ij \in \mathbf{E}(G), \\ 0 & \text{if } ij \notin \mathbf{E}(G), \\ 0 & \text{if } i = j\,. \end{cases}$$

The theory based on the matrix $\mathbf{A}_F$ and its spectrum was recently elaborated in some detail [11,12].

In this paper, we examine a special case of $\mathbf{A}_F$, associated with the Nirmala index $N(G)$. We call it *Nirmala matrix*, denote it by $\mathbf{A}_N$, and define via

$$\mathbf{A}_N(G)_{ij} = \begin{cases} \sqrt{d(i) + d(j)} & \text{if } ij \in \mathbf{E}(G), \\ 0 & \text{if } ij \notin \mathbf{E}(G), \\ 0 & \text{if } i = j\,. \end{cases} \tag{5}$$

The eigenvalues of $\mathbf{A}_N(G)$ are denoted by $\nu_1, \nu_2, \ldots, \nu_n$, and are said to form the *Nirmala spectrum* of the graph $G$. The *Nirmala characteristic polynomial* is defined as

$$\phi_N(G, \lambda) = \det\big(\lambda\, \mathbf{I}_n - \mathbf{A}_N(G)\big),$$

in analogy to the ordinary characteristic polynomial [9]

$$\phi(G, \lambda) = \det\big(\lambda\, \mathbf{I}_n - \mathbf{A}(G)\big),$$

where $\mathbf{I}_n$ is the unit matrix of order $n$. Recall that $\nu_i$, $i = 1, 2, \ldots, n$, are the zeros of $\phi_N(G, \lambda)$, i.e., satisfy the condition $\phi_N(G, \nu_i) = 0$.

## 2. Spectral properties of the Nirmala matrix

**Lemma 1.** *Let $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$ be the Nirmala eigenvalues of the graph $G$. Then $\sum_{i=1}^{n} \nu_i = 0$ and $\sum_{i=1}^{n} \nu_i^2 = 2\, Zg(G)$ where $Zg$ is the first Zagreb index (2).*

**Proof.** The first equality is a direct consequence of $\mathbf{A}_N(G)_{ii} = 0$ for all $i = 1, 2, \ldots, n$. The second equality is obtained from (5) as follows: Suppose that the vertices of $G$ are labeled by $1, 2, \ldots, n$. Then

$$\begin{aligned} \sum_{i=1}^{n} \nu_i^2 &= Tr\, \mathbf{A}_N(G)^2 \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{A}_N(G)_{ij}\, \mathbf{A}_N(G)_{ji} \\ &= 2 \sum_{ij \in \mathbf{E}(G)} \mathbf{A}_N(G)_{ij}\, \mathbf{A}_N(G)_{ji} \\ &= 2 \sum_{ij \in \mathbf{E}(G)} \sqrt{d(i) + d(j)}\, \sqrt{d(j) + d(i)} \\ &= 2 \sum_{ij \in \mathbf{E}(G)} \big[d(i) + d(j)\big] = 2\, Zg(G)\,. \end{aligned}$$

□

Recalling that the sum of squares of the eigenvalues of the ordinary adjacency matrix is equal to $2m$, from Lemma 1 we see that in the spectral theory of Nirmala matrix, the the first Zagreb index will play the same role as the number of edges plays in the ordinary spectral graph theory.

**Lemma 2.** *Let $\nu_1$ be the greatest Nirmala eigenvalue. Then*

$$\nu_1 \geq \frac{2\,N(G)}{n}$$

*where $N(G)$ is the Nirmala index (4). Equality is attained if and only if the graph $G$ is regular.*

**Proof.** According to the Rayleigh–Ritz variational principle, if $\mathbf{X}$ is any $n$-dimensional column-vector, then

$$\frac{\mathbf{X}^T\,\mathbf{A}_N(G)\,\mathbf{X}}{\mathbf{X}^T\,\mathbf{X}} \leq \nu_1\,.$$

Setting $\mathbf{X} = (1,1,\ldots,1)^T$, we get

$$\mathbf{X}^T\,\mathbf{A}_N(G)\,\mathbf{X} = \sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_N(G)_{ij} = 2\sum_{ij\in\mathbf{E}(G)}\mathbf{A}_N(G)_{ij} = 2\sum_{ij\in\mathbf{E}(G)}\sqrt{d(i)+d(j)} = 2\,N(G)$$

and

$$\mathbf{X}^T\,\mathbf{X} = n\,.$$

In the case of regular graphs, $\mathbf{X} = (1,1,\ldots,1)^T$ is an eigenvector of $\mathbf{A}_N(G)$, corresponding to the eigenvalue $\nu_1$. Then, and only then, equality in Lemma 2 holds. □

## 3. Nirmala energy and its bounds

The energy $En(G)$ of a graph $G$ is, by definition, equal to the sum of the absolute values of the eigenvalues of $\mathbf{A}(G)$. For details on graph energy, see [13]. In analogy to this, we now define the *Nirmala energy* of $G$ as

$$En_N(G) = \sum_{i=1}^{n}|\nu_i|\,. \tag{6}$$

It is no surprise that $En(G)$ and $En_N(G)$ have a number of analogous properties. In what follows, we state two such results.

**Theorem 1** (McClelland–type bound)**.** *If $G$ is a graph on $n$ vertices, with first Zagreb index $Zg(G)$, then*

$$En_N(G) \leq \sqrt{2n\,Zg(G)}$$

*which is the analogue of the McClelland bound $En(G) \leq \sqrt{2nm}$ [14].*

**Proof.** Start with

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(|\nu_i| - |\nu_j|\right)^2 \geq 0$$

and use Equation (6) and the results of Lemma 1.

Equality in Theorem 1 will hold if and only if $|\nu_1| = |\nu_2| = \cdots = |\nu_n|$. Which are the graphs with such a property awaits to be determined. □

**Theorem 2** (Koolen–Moulton–type bound). *Let $G$ be a graph on $n$ vertices, with Nirmala and first Zagreb indices $N(G)$ and $Zg(G)$, respectively. Then*

$$En_N(G) \leq \frac{2\,N(G)}{n} + \sqrt{2(n-1)\left[Zg(G) - \left(\frac{2\,N(G)}{n}\right)^2\right]} \tag{7}$$

*which is the analogue of the Koolen–Moulton bound $En(G) \leq \frac{2m}{n} + \sqrt{2(n-1)\left[m - \left(\frac{2m}{n}\right)^2\right]}$ [15]. If $G$ is bipartite, then*

$$En_N(G) \leq \frac{4\,N(G)}{n} + \sqrt{2(n-2)\left[Zg(G) - 2\left(\frac{2\,N(G)}{n}\right)^2\right]}. \tag{8}$$

**Proof.** We follow the reasoning by Koolen and Moulton [15,16], modified for the Nirmala energy. In an analogous way as in Theorem 1, one can show that

$$\sum_{i=2}^{n} |\nu_i| \leq \sqrt{2(n-1)\,Zg'(G)}$$

where

$$2\,Zg'(G) = \sum_{i=2}^{n} \nu_i^2 = 2\,Zg(G) - \nu_1^2$$

This yields,

$$En_N(G) - |\nu_1| \leq \sqrt{2(n-1)\big(Zg(G) - \nu_1^2\big)}$$

i.e.,

$$En_N(G) \leq \nu_1 + \sqrt{2(n-1)\big(Zg(G) - \nu_1^2\big)}\,. \tag{9}$$

Recall that $\nu_1 > 0$ and thus $|\nu_1| = \nu_1$.

Consider the function

$$f(x) = x + \sqrt{2(n-1)\big(Zg(G) - x^2\big)}\,.$$

It monotonously decreases in the interval $(a,b)$ where $a = \sqrt{2Zg(G)/n}$ and $b = \sqrt{2Zg(G)}$. Therefore, the inequality (9) remains valid if on its right–hand side, $\nu_1$ is replaced by $2\,N(G)/n$, see Lemma 2. This results in the bound (7).

The bound (8) is obtained analogously [17], by taking into account that for bipartite graphs $\nu_i = -\nu_{n+1-i}$ holds for $i = 1, 2, \ldots, n$, and therefore $|\nu_n| = \nu_1$.

Finding the conditions under which equality holds in (7) and (8) is difficult and we leave this question unanswered. □

## 4. Nirmala spectrum and energy of trees

In order to determine some of the main spectral properties of the Nirmala matrix of a tree, recall that the (ordinary) characteristic polynomial of a tree $T$ is of the form [9,18,19]

$$\phi(T,\lambda) = x^n + \sum_{k\geq 1} (-1)^k\, m(T,k)\, \lambda^{n-2k}$$

where $m(T,k)$ stands for the number of $k$-matchings (= selections of $k$ mutually independent edges) in the tree $T$. By definition, $m(T,1) = m = n-1$.

According to the Sachs coefficient theorem [9,20], for the Nirmala characteristic polynomial an analogous expression would hold, namely

$$\phi_N(T,\lambda) = x^n + \sum_{k\geq 1} (-1)^k\, m_N(T,k)\, \lambda^{n-2k}\,.$$

The term $m_N(T,k)$ is equal to the sum of weights coming from all $k$-matchings of $T$. Each particular $k$-matching contributes to $m_N(T,k)$ by the product of the squares of the terms $\sqrt{d(u)+d(v)}$, pertaining to the edges contained in that matching. Thus, let $M$ be a distinct $k$-matching of $T$, and let $\mathcal{M}(k)$ be the set of all such $k$-matchings. Recall that for $k \geq 1$, $\mathcal{M}(k)$ consists of $m(T,k)$ elements, i.e., $|\mathcal{M}(k)| = m(T,k)$.

The weight of $M$ is equal to

$$\prod_{uv\in\mathbf{E}(M)} \left[\sqrt{d(u)+d(v)}\right]^2 = \prod_{uv\in\mathbf{E}(M)} \left[d(u)+d(v)\right]$$

and therefore

$$m_N(T,k) = \sum_{M\in\mathcal{M}(k)} \prod_{uv\in\mathbf{E}(M)} \left[d(u)+d(v)\right] \tag{10}$$

provided $\mathcal{M}(k) \neq \varnothing$, and $m_N(T,k) = 0$ If $\mathcal{M}(k) = \varnothing$.

As seen, the structure-dependency of the Nirmala characteristic polynomial (i.e., of its coefficients) is perplexed, and by no means easy to comprehend. Yet, we have the following simple result.

The signature of the spectrum is the number of positive, zero, and negative eigenvalues.

**Theorem 3.** *The spectrum and Nirmala spectrum of a tree have equal signatures.*

**Proof.** Because both the spectrum and the Nirmala spectrum of $T$ are symmetric w.r.t. zero, it suffices to show that both spectra have equal number of zero eigenvalues.

If $\mathcal{M}(k)$ is non-empty, i.e., if $m(T,k) > 0$, then from Equation (10) we conclude that $m_N(T,k) > m(T,k) > 0$, whereas $m_N(T,k) = 0$ if and only if $m(T,k) = 0$. Hence, the multiplicity of zeros of the polynomials $\phi(T,\lambda)$ and $\phi_N(T,\lambda)$ are equal. □

The following Coulson-type formula was obtained for the energy of trees [21,22]:

$$En(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln\left[1 + \sum_{k\geq 1} m(G,k)\, x^{2k}\right] dx$$

From it, far-reaching conclusions on the energy of trees could be deduced [13,22]. The analogous expression for the Nirmala energy is

$$En_N(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln\left[1 + \sum_{k\geq 1} m_N(G,k)\, x^{2k}\right] dx\,.$$

In view of Equation (10), it seems that this formula will be of little use for the study of the structure dependency of Nirmala energy. Yet, because of $d(u)+d(v) > 0$ and $m_N(T,k) > m(T,k)$, we have:

**Theorem 4.** *For any tree $T$ with $n > 1$ vertices, $En_N(T) > En(T)$.*

In connection with Theorem 3, we mention that if $G$ is an $r$-regular graph, then $\mathbf{A}_N(G) = \sqrt{2r}\,\mathbf{A}(G)$ and therefore $En_N(G) = \sqrt{2r}\,En(G)$. Establishing the relations between $En_N(G)$ and $En(G)$ for non-regular cycle-containing graphs remains a task for the future. We anyway conjecture that $En_N(G) > En(G)$ holds in the general case.

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