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Research Article

On spectral properties of neighborhood second Zagreb matrix of graphs

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Abstract: Let G be a simple graph with vertex set $V(G) = \{1, 2, \dots, n\}$ and $\delta(i) = \Sigma_{\{i,j\}\in E(G)} d(j)$, where $d(j)$ is the degree of the vertex j in G. Inspired by the second Zagreb matrix and neighborhood first Zagreb matrix of a graph, we introduce the neighborhood second Zagreb matrix of G, denoted by $N_F(G)$. It is the $n \times n$ matrix whose ij-th entry is equal to $\delta(i)\delta(j)$, if i and j are adjacent in G and 0, otherwise. The neighborhood second Zagreb spectral radius $\rho_{N_F}(G)$ is the largest eigenvalue of $N_F(G)$. The neighborhood second Zagreb energy $\mathcal{E}(N_F)$ of the graph G is the sum of the absolute values of the eigenvalues of $N_F(G)$. In this paper, we obtain some spectral properties of $N_F(G)$. We provide sharp bounds for $\rho_{N_F}(G)$ and $\mathcal{E}(N_F)$, and obtain the corresponding extremal graphs.

Keywords: Graph, neighborhood second Zagreb matrix, spectral radius, eigenvalues, Zagreb index.

AMS Subject classification: 05C50, 05C09, 05C92.

1. Introduction

Let G be a simple graph with vertex set $V(G) = \{1, 2, \dots, n\}$ and edge set $E(G)$. If two vertices i and j are adjacent, we denote it by $i \sim j$. The edge between i and j is denoted by $\{i, j\}$. The *adjacency matrix* of G is defined as the $n \times n$ matrix $A(G) = [a_{ij}]$, where $a_{ij} = 1$, if i and j are adjacent in G and 0, otherwise. Since $A(G)$ is a real symmetric matrix, all its eigenvalues are real. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be the eigenvalues of $A(G)$ arranged in nonincreasing order. The largest eigenvalue $\mu_1(G)$

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of $A(G)$ is called the *spectral radius* of G and is denoted by $\rho(G)$. The *neighborhood set* of a vertex i in G is defined as the collection of vertices that are adjacent to i, and it is denoted by $N_G(i)$. Let $d(i)$ denote the degree of the vertex i. Note that $d(i) = |N_G(i)|$.

Let M be a complex $m \times n$ matrix with singular values $\sigma_1(M) \geq \sigma_2(M) \geq \cdots \geq \sigma_n(M)$. The *energy* of M is defined by Nikiforov [21] as the sum of the singular values of the matrix M, that is, $\mathcal{E}(M) = \sum_{i=1}^{n} \sigma_i(M)$. Note that if M is an $n \times n$ Hermitian matrix with eigenvalues $\mu_1(M) \geq \mu_2(M) \geq \cdots \geq \mu_n(M)$, then the singular values of M are the moduli of $\mu_i(M)$ taken in descending order. In [21], the author provided bounds on the energy of M using matrix norms. Gutman [8] introduced the *energy* of a graph G as $\mathcal{E}(A)$, where $A(G)$ is the adjacency matrix of G, that is, $\mathcal{E}(A) = \sum_{i=1}^{n} |\mu_i|$.

The graph energy has been extensively studied; see, for example [4, 16, 30, 32]. For some recent developments on the bounds for the graph energy, see [6, 23, 26] and the references therein.

In mathematical chemistry, a *topological index* for a graph is defined as $I_F(G) = \sum_{\{i,j\} \in E(G)} F(d(i), d(j))$, where F is a suitable chosen function with the property that $F(x, y) = F(y, x)$. Topological indices are crucial for describing and characterizing the molecular structure; see [9]. Weiner [28] introduced the first topological index, known as *Weiner index* to calculate the boiling points of alkanes. In [12], Gutman and Trinajstić observed that in the approximate expression for total π-electron energy two terms occur:

$$M_1(G) = \sum_{i=1}^{n} d(i)^2 \text{ and } M_2(G) = \sum_{\{i,j\} \in E(G)} d(i)d(j).$$

Later, Todeschini and Consonni [27] named M_1 and M_2 as the *first Zagreb index* and the *second Zagreb index*. See also the article by Nikolić et al. [22] for more background. In [5], Doslic et al. proved that

$$M_1(G) = \sum_{\{i,j\} \in E(G)} d(i) + d(j) = \sum_{i=1}^{n} d(i)^2.$$

For more information about the mathematical properties of the first and second Zagreb indices, see [10, 14, 17, 22].

Let $\delta(i) = \sum_{\{i,j\} \in E(G)} d(j)$ be the sum of the degrees of the vertices that are adjacent to i. Interestingly, for a graph G on n vertices,

$$\sum_{i=1}^{n} \delta(i) = M_1(G).$$

Ghorbani and Hosseinzadeh [7] introduced the neighborhood versions of the first and second Zagreb indices of G as

$$M_1'(G) = \sum_{\{i,j\} \in E(G)} \delta(i) + \delta(j) \quad \text{and} \quad M_2'(G) = \sum_{\{i,j\} \in E(G)} \delta(i)\delta(j),$$

respectively, and computed them for an infinite family of nanostar dendrimers. The index $M_1'(G)$ is called the neighborhood first Zagreb index and the index $M_2'(G)$ is called the neighborhood second Zagreb index. In [20], Mondal et al. investigated the chemical applicability of $M_2'(G)$ and found that $M_2'(G)$ has a significant correlation with entropy and acentric factor in comparison with $M_1(G)$ and $M_2(G)$.

Given a graph G and a topological index $I_F(G)$, we can always associate a matrix A_F to the graph G in the following way [15].

$$(A_F)_{ij} = \begin{cases} F(d(i), d(j)), & \text{if } \{i, j\} \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

In [15], Rad et al. introduced the first Zagreb matrix and the second Zagreb matrix of a graph by taking $F(d(i), d(j)) = d_i + d_j$ and $F(d(i), d(j)) = d_i d_j$, respectively, and defined the corresponding energies, named as the *first Zagreb energy* and the *second Zagreb energy*. It was observed that the first Zagreb energy and the first Zagreb index depend on the eigenvalues of the first Zagrb matrix similar to the case of adjacency matrix. The authors also obtain bounds for the first Zagreb energy and the Zagreb Estrada index. In [25], Rakshith investigated the properties of edge-Zagreb energy. Recently, Zhan et al. [30] studied the second Zagreb matrix (naming it as the edge-Zagreb matrix). The authors obtained bounds on the spectral radius of the second Zagreb matrix and the energy, and characterized the extremal graphs.

Mondal et al. [19] investigated the neighborhood version of the first Zagreb matrix and the corresponding energy. Inspired by the neighborhood first Zagreb matrix, we introduce the neighborhood version of the second Zagreb matrix of a graph G, denoted by $N_F(G)$ (or simply by N_F), which is defined as the $n \times n$ matrix $N_F(G) = [n_{i,j}]$, where

$$n_{ij} = \begin{cases} \delta(i)\delta(j), & \text{if } \{i, j\} \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

Observe that $N_F(G)$ is a real, symmetric matrix. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $N_F(G)$ arranged in nonincreasing order. The largest eigenvalue of $N_F(G)$ is called *neighborhood second Zagreb spectral radius* of G and is denoted by $\rho_{N_F}(G)$. The spectrum of $N_F(G)$ is defined as $S(G) = (\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G))$. Similar to the classical graph energy, the neighborhood second Zagreb energy is defined as

$$\mathcal{E}(N_F) = \sum_{i=1}^{n} |\lambda_i|.$$

In this article, we study the neighborhood second Zagreb matrix and its eigenvalues. Given a graph, first we obtain some fundamental properties of the neighborhood second Zagreb matrix of G. It has been observed that $N_F(G)$ satisfies many spectral properties similar to the adjacency matrix of G. It is well known that G is bipartite if and only if the spectrum of $A(G)$ is symmetric about the origin. Interestingly, the same is true for the neighborhood second Zagreb matrix. We prove that a graph G is bipartite if and only if the spectrum of $N_F(G)$ is symmetric about the origin. The spectral radius $A(G)$ and the energy of a graph corresponding to $A(G)$ are well studied. We consider the neighborhood second Zagreb spectral radius and the neighborhood second Zagreb energy of G, and obtain several bounds in terms of different graph parameters. The extremal graphs are also characterized.

The paper is organized as follows: Section 2 contains some known results that will be used to prove our main results in the subsequent sections. In Section 3, we prove some properties of the neighborhood second Zagreb matrix. In Section 4, we study the spectral properties of N_F related to graph structure. We obtain the bounds for the spectral radius of N_F and characterize the respective extremal graphs. In Section 5, we provide bounds for the neighborhood second Zagreb energy using $\det(N_F)$, trace of N_F^2, $M_2'(G)$, and $\delta(i)$, and then identify the extremal graphs.

2. Preliminaries

This section contains some known results that will be used later. We use the notations C_n, K_n, S_n, K_{n_1,n_2} to denote the cycle, complete graph, star, and complete bipartite graph of order n, respectively. By kG, we denote k copies of G. By $\mathbf{0}$, we denote the zero matrix of an appropriate size. We begin with the following result on singular values of the sum of two matrices.

Theorem 1. (Day and So [4]) *Let A and B be two $n \times n$ matrices. Then*

$$\sum_{i=1}^{n} \sigma_i(A+B) \leq \sum_{i=1}^{n} \sigma_i(A) + \sum_{i=1}^{n} \sigma_i(B).$$

The equality holds if and only if there exists a unitary matrix P such that both PA and PB are positive semidefinite matrices.

The following result on energy of a blocked matrix is proved by Gutman et al. in [11].

Lemma 1. (Gutman et al. [11]) *Let C be a symmetric matrix of the form*

$$C = \begin{pmatrix} \mathbf{0} & A & \mathbf{0} \\ A^T & \mathbf{0} & B \\ \mathbf{0} & B^T & \mathbf{0} \end{pmatrix},$$

where A and B are two real rectangular matrices. Then

$$\mathcal{E}(C) \leq 2\mathcal{E}(A) + 2\mathcal{E}(B).$$

The equality holds if and only if $AB = \mathbf{0}$.

The following two lemmas provide bounds on the spectral radius of a connected graph G.

Lemma 2. (Collatz and Sinogowitz [3], Yuan [29]) *Let G be a connected graph on n vertices and m edges. Then*

$$\frac{2m}{n} \leq \rho(G) \leq \sqrt{2m-n+1}.$$

The equality in the left-hand side inequality holds if and only if G is regular, and the equality in the right-hand side inequality holds if and only if $G \cong S_n$ or $G \cong K_n$.

Lemma 3. (Collatz and Sinogowitz [3], Zhou [31]) *Let G be a graph on n vertices and $d_{max} = \max\{d(i) : i \in V(G)\}$. Then*

$$\sqrt{\frac{M_1(G)}{n}} \leq \rho(G) \leq d_{max}.$$

The equality in the left-hand side inequality holds if and only if G is a regular or semiregular graph. If G is a connected graph, then the equality in the right-hand side inequality holds if and only if G is regular.

The following two crucial results on the spectral radius of irreducible nonnegative matrices are proved in [13] and [2], respectively.

Theorem 2. (Horn and Johnson [13]) *Let $A = (a_{ij})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius $\rho(A)$. Then*

$$\min_{1\leq i\leq n} \sum_{j=1}^{n} a_{ij} \leq \rho(A) \leq \max_{1\leq i\leq n} \sum_{j=1}^{n} a_{ij}.$$

The equality on the left and right-hand sides of inequalities holds if and only if the row sums of A are equal.

Theorem 3. (Brouwer and Haemers [2]) *Let A be an $n\times n$ irreducible nonnegative matrix with spectral radius $\rho(A)$. Suppose that $a \in \mathbb{R}$, and $x \geq 0$, $x \neq 0$. If $Ax \leq ax$, then $a \geq \rho(A)$.*

The following result is based on the number of distinct eigenvalues of an irreducible nonnegative symmetric matrix.

Theorem 4. (Liu and Shiu [18]) *Let A be an $n \times n$ $(n \geq 2)$ irreducible nonnegative symmetric matrix. Let α_1 be the maximum eigenvalue of A and x be the unit Perron-Frobenius eigenvector of A. Then A has t $(2 \leq t \leq n)$ distinct eigenvalues if and only if there exist $t-1$ real numbers $\alpha_2, \ldots, \alpha_t$ with $\alpha_1 > \alpha_2 > \cdots > \alpha_t$ such that*

$$\prod_{i=2}^{t} (A - \alpha_i I_n) = \prod_{i=2}^{t} (\alpha_1 - \alpha_i) x x^T.$$

Moreover, $\alpha_1 > \alpha_2 > \cdots > \alpha_t$ are exactly the t distinct eigenvalues of A.

The following inequality on nonnegative real numbers is proved in [32].

Lemma 4. (Zhou et al. [32]) *Let $a_1, a_2, \ldots, a_n$ be nonnegative real numbers. Then*

$$n\Big[\frac{1}{n}\sum_{i=1}^{n} a_i - \Big(\prod_{i=1}^{n} a_i\Big)^{\frac{1}{n}}\Big] \le n\sum_{i=1}^{n} a_i - \Big(\sum_{i=1}^{n}\sqrt{a_i}\Big)^2 \le n(n-1)\Big[\frac{1}{n}\sum_{i=1}^{n} a_i - \Big(\prod_{i=1}^{n} a_i\Big)^{\frac{1}{n}}\Big].$$

3. Properties of neighborhood second Zagreb matrix

This section contains some fundamental properties of the neighborhood second Zagreb matrix of a graph similar to the adjacency matrix. Given a graph G, let us start with the trace of the powers of N_F. Let L_k be the k-th spectral moment of N_F, that is, $L_k = tr(N_F^k) = \sum_{i=1}^{n} \lambda_i^k$. Then observe that $L_0 = tr(N_F^0) = n$ and $L_1 = tr(N_F) = 0$. Further, it can be shown that

$$L_2 = tr(N_F^2) = 2\sum_{i\sim j} \delta^2(i)\delta^2(j), \tag{3.1}$$

$$L_3 = tr(N_F^3) = 6\sum_{i\sim j\sim k\sim i} \delta^2(i)\delta^2(k)\delta^2(j), \tag{3.2}$$

$$L_4 = tr(N_F^4) = \sum_{i=1}^{n}\sum_{j=1}^{n}\Big(\sum_{k:i\sim k\sim j} \delta(i)\delta^2(k)\delta(j)\Big)^2. \tag{3.3}$$

Let G be a graph on n vertices. A *linear subgraph* H of G is a disjoint union of some edges and some cycles in G. Let $\phi_A(G;x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n$ be the characteristic polynomial of $A(G)$. Then $a_0 = 1, a_1 = 0$ and a_2 is the number of edges in G. In general, we have (see [1])

$$a_k = \sum_{H\in\mathcal{H}_k} (-1)^{c_1(H)+c(H)}(2)^{c(H)},\ k = 1, 2, \ldots, n,$$

where $\mathcal{H}_k$ is the set of all linear subgraphs H of G of size k, and $c_1(H)$ denotes the number of components of size 2 in H and $c(H)$ denotes the number of cycles in H.

A similar description can be given for the coefficients of the characteristic polynomial of the neighborhood second Zagreb matrix of G. Let $\phi_{N_F}(G;x) = b_0x^n + b_1x^{n-1} + \cdots + b_{n-1}x + b_n$ be the characteristic polynomial of $N_F(G)$. Then, $b_0 = 1$ and the other coefficients of $\phi_{N_F}(G;x)$ can be expressed in the following way.

Theorem 5. *Let G be a graph on n vertices, and $\phi_{N_F}(G;x) = b_0x^n + b_1x^{n-1} + \cdots + b_{n-1}x + b_n$ be the characteristic polynomial of $N_F(G)$. Then*

$$b_k = \sum_{H\in\mathcal{H}_k} (-1)^{c_1(H)+c(H)}2^{c(H)} \prod_{v\in V(H)} \delta^2(v),\ \ k = 1, 2, \ldots, n,$$

where $\mathcal{H}_k$ is the set of all linear subgraphs H of G of size k.

Proof. Observe that b_k is equal to $(-1)^k$ times the sum of all $k \times k$ principal minors of N_F and each $k \times k$ principal minor is of the form

$$Q = \begin{vmatrix} 0 & \delta(i_1)\delta(i_2) & \cdots & \delta(i_1)\delta(i_k) \\ \delta(i_2)\delta(i_1) & 0 & \cdots & \delta(i_2)\delta(i_k) \\ \vdots & \vdots & \ddots & \vdots \\ \delta(i_k)\delta(i_1) & \delta(i_k)\delta(i_2) & \cdots & 0 \end{vmatrix}.$$

By Leibniz's formula for determinant, we have

$$Q = \sum_{\pi} sgn(\pi)\delta(i_1)\delta(\sigma(i_1))\cdots\delta(i_k)\delta(\sigma(i_k)),$$

where the summation is over all permutations of $1, 2, \ldots, k$.

Consider a nonzero term of the form $\delta(i_1)\delta(\sigma(i_1))\cdots\delta(i_k)\delta(\sigma(i_k))$. Since π admits a cycle decomposition, such a term corresponds to an edge joining i and j in G as well as some cycles in G. Thus, each nonzero term in the summation arises from a set $\mathcal{H}_k$ of all linear subgraphs H of G of size k. Note that $sgn(\pi)$ is $(-1)^{k-c_1(H)-c(H)}$ and each linear subgraph gives rise to $2^{c(H)}$ terms in the summation. Since each cycle can be associated with a cyclic permutation in two ways, the term $\delta(i_1)\delta(\sigma(i_1))\cdots\delta(i_k)\delta(\sigma(i_k))$ equals to $(\delta(i_1)\delta(i_2)\cdots\delta(i_k))^2$. Thus,

$$b_k = (-1)^k \sum_{H\in\mathcal{H}_k} (-1)^{k-c_1(H)-c(H)} 2^{c(H)} \prod_{j=1}^{k} \delta^2(i_j) = \sum_{H\in\mathcal{H}_k} (-1)^{c_1(H)+c(H)} 2^{c(H)} \prod_{v\in V(H)} \delta^2(v).$$

□

As a consequence of the above result, we have the following corollary that depicts a nice relationship between the determinant of the neighborhood second Zagreb matrix and the determinant of the adjacency matrix of a graph G.

Corollary 1. *Let G be a graph on n vertices. Let A and N_F be the adjacency matrix and the neighborhood second Zagreb matrix of G, respectively. Then*

$$\det(N_F) = \prod_{i=1}^{n} \delta^2(i)\det(A).$$

Proof. Note that $b_n = (-1)^n \det(N_F)$ and $\det(A) = \sum_{H\in\mathcal{H}_n} (-1)^{n-c_1(H)-c(H)} 2^{c(H)}$. By Theorem 5

$$b_n = \sum_{H\in\mathcal{H}_n} (-1)^{c_1(H)+c(H)} 2^{c(H)} \prod_{i=1}^{n} \delta^2(i),$$

where the summation is over all permutations of $1, 2, \ldots, n$. Thus,

$$\det(N_F) = \prod_{i=1}^{n} \delta^2(i) \sum_{H\in\mathcal{H}_n} (-1)^{n-c_1(H)-c(H)} 2^{c(H)} = \prod_{i=1}^{n} \delta^2(i)\det(A).$$

□

A *matching* M of size k in a graph G is a set of k independent edges. The cardinality of a maximum matching in G is called the *matching number* of G and is denoted by $m(G)$. Let $\mathcal{M}_k(G)$ denote the set of all matchings of size k in G. A matching in G is called a *perfect matching* if every vertex of G is incident to an edge of the matching. For an edge $e = \{i, j\}$ of G, let $w(e) = \delta(i)\delta(j)$ be the *neighborhood weight* of the edge e. Denote

$$J_2^{(k)}(G) = \sum_{\{e_{i_t}:1\leq t\leq k\}\in\mathcal{M}_k(G)} \left(w(e_{i_1})w(e_{i_2})\cdots w(e_{i_k})\right)^2.$$

It is known that the rank of the adjacency matrix of a tree is related to the matching number $m(T)$. For a tree T on n vertices, the multiplicity of its 0 as an eigenvalue of $A(T)$ is $n - 2m(T)$. Further, $A(T)$ is nonsingular if and only if T has a perfect matching, and in this case, the perfect matching is unique. We provide a similar result for the neighborhood second Zagreb matrix $N_F(T)$ in the following corollary.

Corollary 2. *Let T be a tree on n vertices, and $\phi_{N_F}(T; x) = x^n + b_1x^{n-1} + b_2x^{n-2} + \cdots + b_{n-1}x + b_n$. Then*

(i) $b_{2k+1} = 0$ *and* $b_{2k+2} = (-1)^{k+1}J_2^{(k+1)}(T)$, *for* $k = 0, 1, \ldots$;

(ii) *the multiplicity of* 0, *as an eigenvalue of* $N_F(T)$ *is* $n - 2m(T)$;

(iii) $N_F(T)$ *is nonsingular if and only if* T *has a perfect matching.*

Proof. Since T has no cycles, (i) follows from Theorem 5. Now, using (i) we have

$$\begin{aligned}\phi_{N_F}(T; x) &= x^n - J_2^{(1)}x^{n-2} + \cdots + (-1)^l J_2^{(l)}x^{n-2l},\\ &= x^{n-2l}(x^{2l} - J_2^{(1)}x^{2l-2} + \cdots + (-1)^l J_2^{(l)}).\end{aligned}$$

Since T has maximum matching l, $J_2^{(l)} \neq 0$. Hence, we have (ii). If T has a perfect matching, then $l = \frac{n}{2}$ and hence (iii) follows from (ii). □

4. Spectral properties of the neighborhood second Zagreb matrix

Let G be a graph on n vertices. In this section, we discuss some properties of the eigenvalues of $N_F(G)$ and obtain bounds for the spectral radius of $N_F(G)$. It is well known that a graph G is bipartite if and only if the eigenvalues of $A(G)$ are symmetric about the origin. The same holds for the eigenvalues of the neighborhood second Zagreb matrix of a bipartite graph. This is proved in our next result, along with some other interesting properties of the eigenvalues of $N_F(G)$.

Proposition 1. *Let G be a graph on n vertices with no isolated vertices. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A(G)$ and $N_F(G)$, respectively. Then the following are true.*

(i) *G is bipartite if and only if $\lambda_i = -\lambda_{n-i+1}$, for $i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$.*

(ii) *If G is r-regular, then $\lambda_i = r^4 \mu_i$, for $i = 1, 2, \ldots, n$. Moreover, if $G \cong K_n$, then $\lambda_1 = (n-1)^5$ and $\lambda_2 = \cdots = \lambda_n = -(n-1)^4$.*

(iii) *If G is a (r, s)-semiregular bipartite graph, then $\lambda_i = r^2 s^2 \mu_i$, for $i = 1, 2, \ldots, n$. Moreover, if $G \cong K_{n_1,n_2}$, where $n_1 + n_2 = n$, then $\lambda_1 = -\lambda_n = n_1^2 n_2^2 \sqrt{n_1 n_2}$ and $\lambda_2 = \cdots = \lambda_{n-1} = 0$.*

Proof. (i) If G is a bipartite graph, then with a suitable labelling of its vertices corresponding to the bipartition, $N_F(G)$ can be written as

$$N_F(G) = \begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}.$$

Assume (λ, Z) be an eigenpair of $N_F(G)$, where $Z = (z_1, z_2)^T$. Then, observe that $(-\lambda, Z^*)$ is also an eigenpair of $N_F(G)$, where $Z^* = (z_1, -z_2)^T$. Thus, $\lambda_i = -\lambda_{n-i+1}$ for $i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. Conversely, if $\lambda_i = -\lambda_{n-i+1}$ for $i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$, let $\lambda_1, \lambda_2, \ldots, \lambda_k, -\lambda_k, -\lambda_{k-1}, \ldots, -\lambda_1$ be the nonzero eigenvalues of $N_F(G)$. Then the characteristic polynomial of $N_F(G)$

$$\phi_{N_F}(G; x) = x^{n-2k}(x^2 - \lambda_1^2) \cdots (x^2 - \lambda_k^2).$$

Thus, $b_{2k+1} = 0$, $k = 0, 1, \ldots$. Hence, G has no odd cycles and is bipartite.

(ii) If G is r-regular, then $N_F(G) = r^4 A(G)$. Hence, $\lambda_i = r^4 \mu_i$ for $i = 1, 2, \ldots, n$. Now, if $G \cong K_n$, then $r = n-1$, $\mu_1 = (n-1)$ and $\mu_2 = \cdots = \mu_n = -1$. Thus, $\lambda_1 = (n-1)^5$ and $\lambda_2 = \cdots = \lambda_n = -(n-1)^4$.

(iii) If G is a (r, s)-semiregular bipartite graph, then $N_F(G) = r^2 s^2 A(G)$. Thus, $\lambda_i = r^2 s^2 \mu_i$ for $i = 1, 2, \ldots, n$. If $G \cong K_{n_1,n_2}$, then $\mu_1 = -\mu_n = \sqrt{n_1 n_2}$ and $\mu_2 = \cdots = \mu_{n-1} = 0$. Thus, $\lambda_1 = -\lambda_n = n_1^2 n_2^2 \sqrt{n_1 n_2}$ and $\lambda_2 = \cdots = \lambda_{n-1} = 0$. □

The following is an interesting characterization.

Lemma 5. *Let G be a graph on n vertices with no isolated vertices. Then $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$ if and only if n is even and $G \cong \frac{n}{2} K_2$.*

Proof. First, assume that G is connected. Then, by the Perron-Frobenius theorem, λ_1 is positive and algebraically simple. So $\lambda_2 < 0$ and $\lambda_2 = -\lambda_1$. Since $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\sum_{i=1}^{n} \lambda_i = 0$. Therefore, we must have $n = 2$ and $G \cong K_2$. Now, if G is disconnected with no isolated vertex, then $\lambda_1 > 0$. Therefore, each connected component of G must be K_2, that is, $G \cong \frac{n}{2} K_2$. The converse is true by using Proposition 1. □

Since $N_F(G)$ is a nonnegative symmetric irreducible matrix, we have an immediate result on the number of distinct eigenvalues of $N_F(G)$ by applying Theorem 4.

Lemma 6. *Let G be a connected graph on $n \geq 2$ vertices, and λ_1 be the largest eigenvalue of $N_F(G)$ and x be its corresponding unit eigenvector. Then $N_F(G)$ has t $(2 \leq t \leq n)$ distinct eigenvalues if and only if there exist $t-1$ real numbers $\lambda_2, \ldots, \lambda_t$ with $\lambda_1 > \lambda_2 > \cdots > \lambda_t$ such that*

$$\prod_{i=2}^{t}(N_F(G) - \lambda_i I_n) = \prod_{i=2}^{t}(\lambda_1 - \lambda_i)xx^T.$$

Moreover, $\lambda_1 > \lambda_2 > \cdots > \lambda_t$ are exactly t distinct $N_F(G)$ eigenvalues.

The above result provides an equivalent condition for a connected graph with $t \geq 2$ distinct neighborhood second Zagreb eigenvalues. As an application, the characterization of a connected graph with two distinct $N_F(G)$ eigenvalues is given below.

Theorem 6. *Let G be a connected graph on n vertices. Then $N_F(G)$ has exactly two distinct eigenvalues if and only if $G \cong K_n$.*

Proof. If $G \cong K_n$, then from Proposition 1, $N_F(G)$ has two distinct eigenvalues. Conversely, suppose that $\lambda_1 > \lambda_2$ are two distinct eigenvalues of $N_F(G)$. By Lemma 6, $N_F(G) = \lambda_2 I_n + (\lambda_1 - \lambda_2)xx^T$. Since x is a positive eigenvector, the off-diagonal entries of $N_F(G)$ are nonzero. Thus, $G \cong K_n$. □

Next, we discuss the neighborhood second Zagreb spectral radius of graphs. The following result shows that the complete graph K_n has the maximum neighborhood second Zagreb spectral radius among all connected graphs on n vertices.

Theorem 7. *Let G be a connected graph on n vertices. Then*

$$\rho_{N_F}(G) \leq (n-1)^5.$$

The equality holds if and only if $G \cong K_n$.

Proof. For a connected graph G on n vertices $\delta(i) \leq (n-1)^2$, for each vertex $i \in V(G)$. Taking y as all ones vector, we have

$$(N_F(G)y)_i = \sum_{\{i,j\} \in E(G)} \delta(i)\delta(j) \leq (n-1)^5.$$

Now, using Theorem 3, we have $\rho_{N_F}(G) \leq (n-1)^5$. If equality holds, then for each pair of vertices i and j, $\delta(i)\delta(j) = (n-1)^4$, simultaneously, with the fact that $\delta(i) \leq (n-1)^2$. Hence $G \cong K_n$. □

The following result shows that $K_{\frac{n}{2},\frac{n}{2}}$ has the maximum neighborhood second Zagreb spectral radius among all connected bipartite graphs on n vertices when n is even.

Theorem 8. *Let G be a connected bipartite graph on $n = 2k$ vertices where $k \in \mathbb{N}$. Then*

$$\rho_{N_F}(G) \leq \left(\frac{n}{2}\right)^5.$$

The equality holds if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Let G be a connected bipartite graph on n vertices with a partition of the vertex set as (V_1, V_2), where V_1 and V_2 contain n_1 and n_2 vertices, respectively, and $n = n_1 + n_2$. We have $\delta(i) \leq n_1 n_2 \leq \left(\frac{n}{2}\right)^2$, for each vertex $i \in V(G)$. Taking y as all ones vector, we have

$$(N_F(G)y)_i = \sum_{\{i,j\}\in E(G)} \delta(i)\delta(j) \leq \sum_{\{i,j\}\in E(G)} n_1^2 n_2^2 \leq \left(\frac{n}{2}\right)^5.$$

Then using Theorem 3, we have $\rho_{N_F}(G) \leq \left(\frac{n}{2}\right)^5$.

If equality holds, then for each pair of vertices i and j, $\delta(i)\delta(j) = n_1^2 n_2^2 = \left(\frac{n}{2}\right)^4$, simultaneously, with the fact that $\delta(i) \leq n_1 n_2 \leq \left(\frac{n}{2}\right)^2$. Hence, $G \cong K_{\frac{n}{2},\frac{n}{2}}$. □

For a graph G on vertices $1, 2, \ldots, n$, let $\delta_{min} = \min\{\delta(i) : i \in V(G)\}$ and $\delta_{max} = \max\{\delta(i) : i \in V(G)\}$. Thus, we have $\delta(i)\delta(j) \geq \delta_{min}^2$ and $\delta(i)\delta(j) \leq \delta_{max}^2$, for all edges $\{i, j\}$ in G. The following result shows a nice relationship between the spectral radius of the neighborhood second Zagreb matrix of G and the spectral radius of $A(G)$.

Theorem 9. *Let G be a graph. Then*

$$\rho(G)\delta_{min}^2 \leq \rho_{N_F}(G) \leq \rho(G)\delta_{max}^2.$$

The equalities on the left and right-hand sides hold if and only if G is regular.

Proof. Consider the unit eigenvector X corresponding to the eigenvalue $\rho_{N_F}(G)$ of $N_F(G)$. Now, applying the Rayleigh-Ritz theorem, we have

$$\begin{aligned}\rho_{N_F}(G) = X^T N_F X &= 2 \sum_{\{i,j\}\in E(G)} \delta(i)\delta(j) x_i x_j \\ &\leq 2\delta_{max}^2 \sum_{\{i,j\}\in E(G)} x_i x_j = \delta_{max}^2 X^T A X \leq \rho(G)\delta_{max}^2.\end{aligned}$$

Thus, $\rho_{N_F}(G) \leq \rho(G)\delta_{max}^2$. If equality holds, then $\delta_{max} = \delta(i)$ for all $i \in V(G)$, which implies G is regular.

Similarly, by taking a unit eigenvector Y corresponding to the eigenvalue $\rho(G)$ of $A(G)$ and applying the Rayleigh-Ritz theorem, we have

$$\begin{aligned}\rho_{N_F}(G) &\geq Y^T N_F Y = 2 \sum_{\{i,j\}\in E(G)} \delta(i)\delta(j) y_i y_j \\ &\geq 2\delta_{min}^2 \sum_{\{i,j\}\in E(G)} y_i y_j = \delta_{min}^2 Y^T A Y = \rho(G)\delta_{min}^2.\end{aligned}$$

Thus, $\rho_{N_F}(G) \geq \rho(G)\delta_{min}^2$. If equality holds, then $\delta_{min} = \delta(i)$ for all $i \in V(G)$, which implies G is regular. □

The following result is a direct consequence of the above result and Lemma 2.

Corollary 3. *Let G be a connected graph on n vertices and m edges. Then*

$$\frac{2m\delta_{min}^2}{n} \leq \rho_{N_F}(G) \leq \delta_{max}^2\sqrt{2m-n+1}.$$

The equality on the left-hand side inequality holds if and only if G is regular, and the equality on the right-hand side of the inequality holds if and only if $G \cong K_n$.

The following result is a direct consequence of Theorem 9 and Lemma 3.

Corollary 4. *Let G be a connected graph on n vertices. Then*

$$\delta_{min}^2\sqrt{\frac{M_1}{n}} \leq \rho_{N_F}(G) \leq \delta_{max}^2 d_{max}.$$

The equalities on the left and right-hand sides hold if and only if G is regular.

Let G be a graph on n vertices with vertex set $V(G) = \{1, 2, \ldots, n\}$. Then the *neighborhood second Zagreb degree* of vertex i, denoted by r_i, is defined as $r_i = \sum_{j=1}^{n} n_{ij}$. A graph G is called neighborhood second Zagreb k-regular if $r_i = k$ for all $i = 1, 2, \ldots, n$. The following result provides a bound on $\rho_{N_F}(G)$ that depends on each r_i and the largest entry of $N_F(G)$.

Theorem 10. *Let G be a connected graph on n vertices with the neighborhood second Zagreb degrees $r_1 \geq r_2 \geq \cdots \geq r_n$, and p be the largest entry of $N_F(G)$. Then*

$$\rho_{N_F}(G) \leq \frac{r_i - p + \sqrt{(r_i - p(2i-3))^2 + 4p(i-1)(r_1 - p(i-2))}}{2}.$$

If $i = 1$, then the equality holds if and only if G is neighborhood second Zagreb regular graph. If $2 \leq i \leq n$, then equality holds if and only if the following two conditions are true.

(i) $n_{lj} = p$ *for* $1 \le l \le n$ *and* $1 \le j \le i-1$ *and* $l \ne j$.

(ii) $r_1 = r_2 = \cdots = r_{i-1} \ge r_i = r_{i+1} = \cdots = r_n$.

Proof. If $i = 1$, then the inequality $\rho_{N_F}(G) \le r_1$ is true, and by Theorem 2, equality holds if and only if the row sums of $N_F(G)$ are all equal. For $2 \le i \le n$ the neighborhood second Zagreb matrix $N_F(G)$ can be written as

$$N_F = \begin{pmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{pmatrix},$$

where N_{11} and N_{22} are square matrices of order $i-1$ and $n-i+1$, respectively. Let V be a diagonal matrix of order n whose first $i-1$ diagonal entries are y and the rest diagonal entries are 1, where $y > 1$. Then

$$F = V^{-1} N_F V = \begin{pmatrix} N_{11} & \frac{1}{y} N_{12} \\ y N_{21} & N_{22} \end{pmatrix}.$$

Since F and N_F are similar matrices, we have $\rho_{N_F}(G) = \rho(F)$. Let $c_1, c_2, \ldots, c_n$ be the row sums of matrix F. For $1 \le l \le i-1$,

$$c_l = \sum_{j=1}^{i-1} n_{lj} + \frac{1}{y}\sum_{j=i}^{n} n_{lj} = \frac{1}{y}\sum_{j=1}^{n} n_{lj} + \left(1 - \frac{1}{y}\right)\sum_{j=1}^{i-1} n_{lj} = \frac{1}{y} r_l + \left(1 - \frac{1}{y}\right)\sum_{j=1}^{i-1} n_{lj},$$

and for $i \le l \le n$,

$$c_l = y\sum_{j=1}^{i-1} n_{lj} + \sum_{j=i}^{n} n_{lj} = \sum_{j=1}^{n} n_{lj} + (y-1)\sum_{j=1}^{i-1} n_{lj} = r_l + (y-1)\sum_{j=1}^{i-1} n_{lj}.$$

As p is the largest entry of $N_F(G)$, $\sum\limits_{j=1}^{i-1} n_{lj} \le (i-2)p$ for $1 \le l \le i-1$, and $\sum\limits_{j=1}^{i-1} n_{lj} \le (i-1)p$ for $i \le l \le n$. As $y > 1$ and $r_1 \ge r_2 \ge \cdots \ge r_n$, for $1 \le l \le i-1$ we have $c_l \le \frac{1}{y} r_l + \left(1 - \frac{1}{y}\right)(i-2)p$. Equality holds if and only if $n_{lj} = p$, for $1 \le j \le i-1$ and $r_1 = r_l$. Similarly, for $i \le l \le n$, $c_l \le r_l + (y-1)(i-1)p$ and equality holds if and only if $n_{lj} = p$, for $1 \le j \le i-1$ and $r_i = r_l$. Observe that $\max\{c_1, c_2, \ldots, c_n\} \le \max\left\{\frac{1}{y} r_1 + \left(1 - \frac{1}{y}\right)(i-2)p, r_i + (y-1)(i-1)p\right\}$.
Let $\frac{1}{y} r_1 + \left(1 - \frac{1}{y}\right)(i-2)p = r_i + (y-1)(i-1)p$. We have

$$y = \frac{(2i-3)p - r_i + \sqrt{(r_i - p(2i-3))^2 + 4p(i-1)(r_1 - p(i-2))}}{2p(i-1)}.$$

We can choose $y > 1$ for $i \ge 2$ such that

$$\rho_{N_F}(G) \le r_i + (y-1)(i-1)p = \frac{r_i - p + \sqrt{(r_i - p(2i-3))^2 + 4p(i-1)(r_1 - p(i-2))}}{2}.$$

If equality holds, then all the inequalities in the above argument must be equalities. Thus, $r_1 = r_2 = \cdots = r_{i-1} \geq r_i = r_{i+1} = \cdots = r_n$ and $n_{lj} = p$ for $1 \leq l \leq n$ and $1 \leq j \leq i-1$ and $l \neq j$. The converse follows directly. □

The following result gives a bound on $\rho_{N_F}(G)$ using the second spectral moment L_2 of $N_F(G)$.

Lemma 7. *Let G be a connected graph on n vertices. Then*

$$\rho_{N_F}(G) \leq \sqrt{\frac{(n-1)L_2}{n}}.$$

The equality holds if and only if $G \cong K_n$.

Proof. Since $tr(N_F) = \sum_{i=1}^{n} \lambda_i = 0$, we have $\lambda_1^2 = \left(\sum_{i=2}^{n} \lambda_i\right)^2$. Applying Cauchy-Schwartz inequality, we get

$$\lambda_1^2 \leq (n-1)\sum_{i=2}^{n} \lambda_i^2.$$

Since $L_2 = \sum_{i=1}^{n} \lambda_i^2$, we have $\lambda_1^2 \leq (n-1)(L_2 - \lambda_1^2)$. Hence the result follows. If equality holds, then $\lambda_2 = \lambda_3 = \cdots = \lambda_n$. Since the sum of the eigenvalues of $N_F(G)$ is zero, therefore G has two distinct eigenvalues. Thus, from Theorem 6 $G \cong K_n$. Converse can be proved using Proposition 1. □

As a consequence of the above result, and by using the fact that $\sum_{\{i,j\}\in E(G)} (\delta(i)\delta(j))^2 \leq \left(\sum_{\{i,j\}\in E(G)} \delta(i)\delta(j)\right)^2$, we have the following corollary.

Corollary 5. *Let G be a connected graph on n vertices. Then $\rho_{N_F}(G) \leq M_2'\sqrt{\frac{2(n-1)}{n}}$. The equality holds if and only if $G \cong K_2$.*

5. The neighborhood second Zagreb energy of graphs

In this section, we provide bounds on the neighborhood second Zagreb energy of graphs. The following lemma can be proved similarly to Proposition 1.

Lemma 8. *Let G be a graph on n vertices with no isolated vertices. Then the following are true.*

(1) *If G is r-regular, then $\mathcal{E}(N_F) = r^4\mathcal{E}(A)$. Moreover, if $G \cong K_n$, then $\mathcal{E}(N_F) = 2(n-1)^5$, and if $G \cong C_n$, then $\mathcal{E}(N_F) = 16\sum_{k=0}^{n-1} |2\cos(\frac{2\pi k}{n})|$.*

(2) *If G is a (r,s)-semiregular bipartite graph, then $\mathcal{E}(N_F) = r^2s^2\mathcal{E}(A)$. Moreover, if $G = K_{n_1,n_2}$ $(n_1+n_2=n)$, then $\mathcal{E}(N_F) = 2n_1^2n_2^2\sqrt{n_1n_2}$.*

The following lemma provides a relationship between the neighborhood second Zagreb energy and the determinant of the neighborhood second Zagreb matrix.

Lemma 9. *Let G be a graph on $n \geq 2$ vertices. Then*

$$\sqrt{L_2 + n(n-1)(\det N_F)^{\frac{2}{n}}} \leq \mathcal{E}(N_F) \leq \sqrt{(n-1)L_2 + n(\det N_F)^{\frac{2}{n}}}.$$

Proof. We know $L_2 = \sum_{i=1}^{n} \lambda_i^2$. Taking $a_i = \lambda_i^2$ for $i = 1,2,\ldots,n$ on the left-hand side inequality of Lemma 4, we have

$$\sum_{i=1}^{n} \lambda_i^2 - n\Big(\prod_{i=1}^{n} \lambda_i^2\Big)^{\frac{1}{n}} \leq n\sum_{i=1}^{n} \lambda_i^2 - \Big(\sum_{i=1}^{n}|\lambda_i|\Big)^2.$$

Thus, we have

$$L_2 - n(\det(N_F))^{\frac{2}{n}} \leq nL_2 - \mathcal{E}(N_F)^2,$$

which implies that

$$\mathcal{E}(N_F) \leq \sqrt{(n-1)L_2 + n(\det N_F)^{\frac{2}{n}}}.$$

Similarly, if we take $a_i = \lambda_i^2$ for $i = 1,2,\ldots,n$ on the right-hand side inequality of Lemma 4, we have $\mathcal{E}(N_F) \geq \sqrt{L_2 + n(n-1)(\det N_F)^{\frac{2}{n}}}$. □

Let $G(i,j)$ be the spanning subgraph of a graph G, having just a single edge between the vertices i and j. Observe that

$$N_F(G) = \sum_{\{i,j\}\in E(G)} N_F(G(i,j)).$$

In our next result, we give a bound on the neighborhood second Zagreb energy using the neighborhood second Zagreb index.

Theorem 11. *Let G be a graph on n vertices with no isolated vertices. Then $\mathcal{E}(N_F) \leq 2M_2'(G)$. The equality holds if and only if n is even and $G \cong \frac{n}{2}K_2$.*

Proof. Note that $\mathcal{E}(N_F(G(i,j))) = 2\delta(i)\delta(j)$. By a repeated application of Theorem 1, we have

$$\mathcal{E}(N_F) \leq 2\sum_{\{i,j\}\in E(G)} \delta(i)\delta(j) = 2M_2'(G).$$

If $G \cong \frac{n}{2}K_2$, it is easy to check that equality occurs. Conversely, if equality holds, that is, $\mathcal{E}(N_F) = 2M_2'(G)$, then we have

$$\sum_{\{i,j\}\in E(G)} \mathcal{E}(N_F(G(i,j))) = \mathcal{E}(N_F) \leq \mathcal{E}(N_F(G(i,j))) + \mathcal{E}\Big(\sum_{\{u,v\}\in E(G)\setminus\{i,j\}} N_F(G(u,v))\Big).$$

Together with Theorem 1, we get

$$\mathcal{E}\Big(\sum_{\{u,v\}\in E(G)\setminus\{i,j\}} N_F(G(u,v))\Big) = \sum_{\{u,v\}\in E(G)\setminus\{i,j\}} \mathcal{E}(N_F(G(u,v))).$$

By repeated application of the above process, we have

$$\mathcal{E}(N_F(G(i_x,j_x)) + N_F(G(i_y,j_y))) = \mathcal{E}(N_F(G(i_x,j_x))) + \mathcal{E}(N_F(G(i_y,j_y))).$$

If no two edges of G are incident, then we are done. Otherwise, if there are two edges, say $e_x = \{i_x, j_x\}$ and $e_y = \{i_y, j_y\}$ and e_x and e_y share a vertex, that is, $j_x = i_y$ then the matrix $N_F(G(i_x,j_x)) + N_F(G(i_y,j_y))$ is permutation similar to a matrix of the form

$$\begin{pmatrix} Z & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \text{ where } Z = \begin{pmatrix} 0 & \delta(i_x)\delta(j_x) & 0 \\ \delta(i_x)\delta(j_x) & 0 & \delta(i_y)\delta(j_y) \\ 0 & \delta(i_y)\delta(j_y) & 0 \end{pmatrix}.$$

Then

$$\mathcal{E}(N_F(G(i_x,j_x)) + N_F(G(i_y,j_y)) = \mathcal{E}(Z).$$

Let $A = \delta(i_x)\delta(j_x)$ and $B = \delta(i_y)\delta(j_y)$. Observe that the structure of the above defined matrix Z and the matrix C in Lemma 1 are the same. Thus using Lemma 1, $AB = 0$. But then, $AB = 0$ holds if and only if either $\{i_x, j_x\} \notin E(G)$ or $\{i_y, j_y\} \notin E(G)$, which is a contradiction. Hence $\{i_x, j_x\}$, and $\{i_y, j_y\}$ do not share a vertex. By applying this process repeatedly, we obtain that n is even and $G \cong \frac{n}{2}K_2$. □

Let $G(i)$ be the spanning subgraph of a graph G, with edges only between the vertices adjacent to i. Then the neighborhood second Zagreb matrix of $G(i)$ has the following form:

$$N_F(G(i)) = \begin{pmatrix} \mathbf{0} & x & \mathbf{0} \\ x' & 0 & y' \\ \mathbf{0} & y & \mathbf{0} \end{pmatrix},$$

where the i-th component of the vector $\begin{pmatrix} x' & 0 & y' \end{pmatrix}$ is $\delta(i)\delta(j)$, if the vertex i is adjacent to j in G, and 0, otherwise. The neighborhood second Zagreb matrix $N_F(G)$ can be expressed in terms of $N_F(G(i))$ as

$$2N_F(G) = \sum_{i=1}^{n} N_F(G(i)).$$

The following result gives another bound on $\mathcal{E}(N_F)$.

Theorem 12. *Let G be a graph on n vertices. Then*

$$\mathcal{E}(N_F) \le \sum_{i=1}^{n} \sqrt{\sum_{\{i,j\}\in E(G)} (\delta(i)\delta(j))^2}.$$

Proof. Applying Theorem 1, we have $2\mathcal{E}(N_F) \leq \sum_{i=1}^{n} \mathcal{E}(N_F(G(i)))$. We know that

$$\mathcal{E}\begin{pmatrix} \mathbf{0} & x & \mathbf{0} \\ x' & 0 & y' \\ \mathbf{0} & y & \mathbf{0} \end{pmatrix} = \mathcal{E}\begin{pmatrix} \mathbf{0} & \mathbf{0} & x \\ \mathbf{0} & \mathbf{0} & y \\ x' & y' & 0 \end{pmatrix} = 2\sqrt{x'x + y'y}.$$

Now, for every vertex i, $x'x + y'y = \sum_{\{i,j\}\in E(G)} (\delta(i)\delta(j))^2$. Thus, $\mathcal{E}(N_F(G(i))) = 2\sqrt{\sum_{\{i,j\}\in E(G)} (\delta(i)\delta(j))^2}$. Hence, $\mathcal{E}(N_F) \leq \sum_{i=1}^{n} \sqrt{\sum_{\{i,j\}\in E(G)} (\delta(i)\delta(j))^2}$. □

6. Conclusion and Scope

In this article, we define the neighborhood second Zagreb matrix $N_F(G)$ and its corresponding energy. We obtain some bounds for the spectral radius and energy of $N_F(G)$, and characterize the extremal graphs. If G is a r-regular graph, then $N_F(G) = r^4A(G)$. Therefore, the spectra of both the matrices $N_F(G)$ and $A(G)$ contain the same information about the graph. The spectrum of $N_F(G)$ may, however, reveal more details about non-regular graphs. Studying the neighborhood second Zagreb matrix may thus lead to nontivial and challenging findings regarding the structure of graphs.

In [24], the authors have given bounds on the first Zagreb index using the signless Laplacian matrix. The neighborhood second Zagreb matrix is merely an illustration of a more general idea that may be applied to various graph matrices. This can be generalized to include several matrices that reflect various structural aspects of graphs. Such generalization is important for examining various matrix representations in graph theory and mathematical chemistry.

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