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NEIGHBOURHOOD DEGREE MATRIX OF A GRAPH

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ABSTRACT. In this note, we define a new graph matrix called neighbourhood degree matrix of a graph G and study its properties. The relations connecting this matrix with some degree-based topological indices are investigated. In addition, we present bounds for the spectral radius of neighbourhood degree matrix and neighbourhood degree energy of graphs and we express the neighbourhood degree energy of some transformation graphs in terms of neighbourhood degree energy of the graph considered for the transformation.

1. Introduction

Throughout this paper, by a graph G we mean a finite undirected graph without loops and multiple edges. Basic graph theoretic terminologies and notations can be found in [2, 4, 9, 11].

Let $G = (V, E)$ be a graph of order n and size m. Let $V(G) = \{v_1, v_2, ..., v_n\}$ be the vertex set and $E(G) = \{e_1, e_2, ..., e_m\}$ be an edge set of G. The *degree* $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident to it in G. For a vertex $v_i, i = 1, 2, ..., n$, we denote $d_i = d_G(v_i)$. The graph G is *r-regular* if and only if the degree of each vertex in G is r.

Topological indices are numerical values associated with the molecular graphs. In mathematical chemistry, these graph invariants are known as molecular descriptors. Topological indices play a vital role in mathematical chemistry specially, in chemical documentation, isomer discrimination, quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. *Wiener index* is the first topological index used by Wiener [19] in the year 1947, to calculate boiling point of paraffins. Later, Gutman et al. [7] defined *Zagreb indices* in 1972, which now are most popular and have many applications in chemistry. The first and second Zagreb indices of a graph G are defined respectively as follows:

$$M_1(G) = \sum_{v_i \in V(G)} d_G(v_i)^2 \text{ and } M_2(G) = \sum_{v_i v_j \in E(G)} d_G(v_i) \cdot d_G(v_j).$$

The multiplicative versions of these two Zagreb indices are defined in [17, 18] as

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$$\Pi_1(G) = \prod_{v_i \in V(G)} d_G(v_i)^2 \text{ and } \Pi_2(G) = \prod_{v_iv_j \in E(G)} d_G(v_i) \cdot d_G(v_j).$$

The vertex-degree-based graph invariant,

$$F(G) = \sum_{v_i \in V(G)} d_G(v_i)^3 = \sum_{v_iv_j \in E(G)} [d_G(v_i)^2 + d_G(v_j)^2]$$

was encountered in [7]. This index is called "forgotten topological index"[5]. Randić [13] introduced the most chemically efficient topological index called *Randić index* which is defined as

$$R(G) = \sum_{v_iv_j \in E(G)} [d_G(v_i) \cdot d_G(v_j)]^{-\frac{1}{2}}.$$

Later, Bollobás et al. in [3] extended this concept to *general product-connectivity index* which is defined as

$$R_\alpha(G) = \sum_{v_iv_j \in E(G)} [d_G(v_i) \cdot d_G(v_j)]^\alpha, \quad \alpha \in \mathbb{R}.$$

For an $\alpha \in \mathbb{R}$, the *first general Zagreb index* [12] of a graph G is defined as

$$M_1^\alpha(G) = \sum_{v_i \in V(G)} d_G(v_i)^\alpha.$$

2. Motivation

In literature of graph matrices, we can find huge number of matrices associated with graph namely, adjacency matrix, Laplacian matrix, maximum degree matrix etc. One can refer [4, 8] for graph matrices. Recently, the concepts of degree sum matrix [14], degree exponent matrix [15] etc., were put forward. Nowhere we find a matrix defined with its entry as the degree of the vertex rather we can see some of them have used one, or maximum degree, or minimum degree, or degree exponent etc., which is quite interesting. To study effect of the degree of vertices on the matrix and its properties, we now define the *neighbourhood degree matrix* of a graph G as an $n \times n$ matrix $ND(G) = [(nd)_{ij}]$, whose elements are defined as

$$(nd)_{ij} = \begin{cases} d_j & if \;\; v_iv_j \in E(G), \\ 0 & otherwise. \end{cases}$$

Let I be the identity matrix and J be the matrix whose all entries are equal to 1. The *neighbourhood degree polynomial* of a graph G is defined as

$$P_{ND}(G; \xi) = det(\xi I - ND(G)).$$

The *eigenvalues* $\xi_i, i = 1, 2, ..., n$ of the matrix $ND(G)$ are called the *neighbourhood degree eigenvalues* of G and their collection is called the *neighbourhood degree spectra* of G. If G is an *r-regular* graph, then $ND(G) = rA(G)$, where $A(G)$ is an adjacency matrix of G. The *neighbourhood degree energy* $E_{ND}(G)$ of a graph G is defined as

$$E_{ND}(G) = \sum_{i=1}^{n} |\xi_i|.$$

The *norm* [1] of a matrix is the square root of the sum of squares of all entries in the matrix.

Interestingly, the neighbourhood degree matrix is useful to find various novel topological indices, to say a few Zagreb indices, forgotten topological index, first general Zagreb index and general product-connectivity index etc. We can observe that the

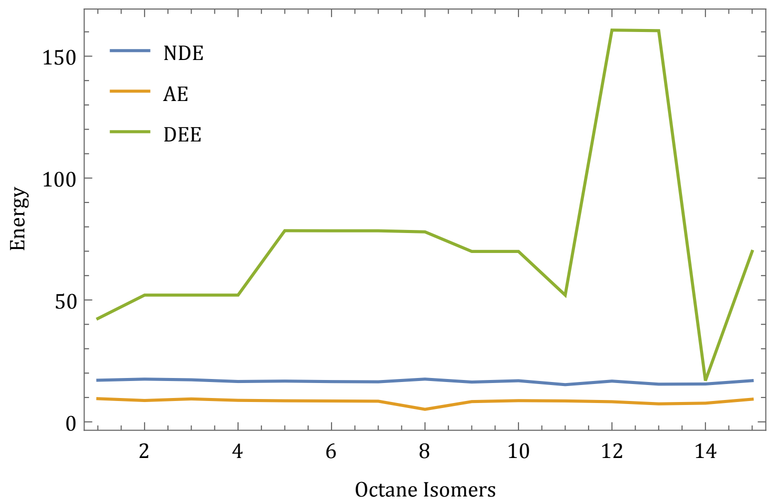

FIGURE 1. The plot showing the comparision between neighbourhood degree energy (NDE), adjacency energy (AE), and the degree exponent energy (DEE) of octane isomers.

matrix operations are simpler than the vertex partitions and edge partitions which are required to find these degree-based topological indices. The neighbourhood degree energy lies between the energy $E_A(G)$ of a graph G corresponding to its adjacency matrix and the degree exponent energy $E_{DE}(G)$. i.e.,

$$E_A(G) \leq E_{ND}(G) \leq E_{DE}(G). \tag{2.1}$$

The equality for left hand side of (2.1) holds, if G is 1-regular and the equality for right hand side of (2.1) holds, for K_2. We compare these three energies of *octane isomers* and the comparision is shown in Figure 1.

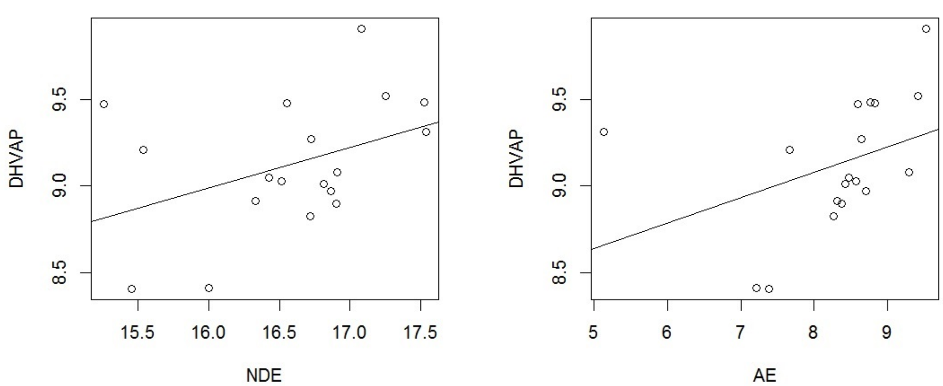

FIGURE 2. Scatter diagram of DHVAP on NDE and on AE super imposed by the fitted regression line.

TABLE 1. Experimental values of the DHVAP and the corresponding value of NDE and AE of octane isomers.

Alkane	**DHVAP**	**NDE**	**AE**
n-octane	9.915	17.0791	9.51754
2-methyl-heptane	9.484	17.5271	8.76257
3-methyl-heptane	9.521	17.2538	9.40926
4-methyl-heptane	9.483	16.5543	8.82843
3-ethyl-hexane	9.476	15.2603	8.5872
2,2-dimethyl-hexane	8.915	16.3291	8.31285
2,3-dimethyl-hexane	9.272	16.7234	8.64705
2,4-dimethyl-hexane	9.029	16.5169	8.56519
2,5-dimethyl-hexane	9.051	16.4258	8.47214
3,3-dimethyl-hexane	8.973	16.8636	8.70531
3,4-dimethyl-hexane	9.316	17.536	5.14115
2-methyl-3-ethyl-pentane	9.209	15.5382	7.66299
3-methyl-3-ethyl-pentane	9.081	16.9097	9.2915
2,2,3-trimethyl-pentane	8.826	16.7167	8.26113
2,2,4-trimethyl-pentane	8.402	15.4548	7.38465
2,3,3-trimethyl-pentane	8.897	16.9018	8.37513
2,3,4-trimethyl-pentane	9.014	16.8129	8.42429
2,2,3,3-tetramethylbutane	8.41	16	7.2111

Now, we discuss the linear regression analysis of NDE and AE with standard enthalpy of vaporization (DHVAP) of octane isomers. The NDE and AE are tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. The dataset of octane isomers(columns 1 and 2 of Table 1) are taken from above web link whereas the last two column of Table 1 are computed by definition of NDE and AE, respectively. Here, the correlation between standard enthalpy of vaporization (DHVAP) and NDE is **0.4054488** (See Fig. 2) while the correlation between standard enthalpy of vaporization (DHVAP) and AE is **0.3866829** (See Fig. 2). Therefore, the correlation of NDE with DHVAP is better than that of the adjacency energy (AE).

All these observations regarding the neighbourhood degree matrix motivated us to define and study its properties. The graph obtained by identification of the grah G with the graph H is denoted by $G \cdot H$ [9].

Example 1. *subsectionExample If $G = K_2 \cdot K_3$ (see Figure 3(a)) is a graph, then the neighbourhood degree matrix is:*

$$ND(G) = \begin{bmatrix} 0 & 3 & 0 & 0 \\ 1 & 0 & 2 & 2 \\ 0 & 3 & 0 & 2 \\ 0 & 3 & 2 & 0 \end{bmatrix},$$

the neighbourhood degree polynomial is: $P_{ND}(G;\xi) = \xi^4 - 19\xi^2 - 24\xi - 12$,
neighbourhood degree eigenvalues are: $\xi_1 \approx 4.842, \xi_2 \approx 0.384, \xi_3 = -2.000$ *and* $\xi_4 \approx -3.226$,
neighbourhood degree energy of G is: $E_{ND}(G) \approx 10.452$,

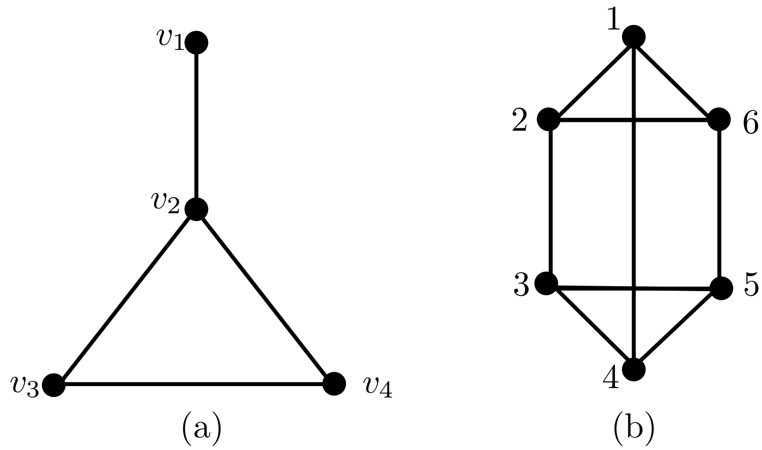

FIGURE 3. **(a)** The graph $G = K_2 \cdot K_3$ and **(b)** the graph H.

and the energy corresponding to adjacency matrix is: $E_A(G) \approx 4.96239$,
and the degree exponent energy is: $E_{DE}(G) \approx 29.2916$.

Example 2. *If H (see Figure 3(b)) is a 3-regular graph, then the neighbourhood degree matrix is:*

$$ND(H) = \begin{bmatrix} 0 & 3 & 0 & 3 & 0 & 3 \\ 3 & 0 & 3 & 0 & 0 & 3 \\ 0 & 3 & 0 & 3 & 3 & 0 \\ 3 & 0 & 3 & 0 & 3 & 0 \\ 0 & 0 & 3 & 3 & 0 & 3 \\ 3 & 3 & 0 & 0 & 3 & 0 \end{bmatrix},$$

the neighbourhood degree polynomial is: $P_{ND}(H;\xi) = \xi^6 - 81\xi^4 - 108\xi^3 + 972\xi^2$,
neighbourhood degree eigenvalues are: $\xi_1 = 9, \xi_2 = 3, \xi_3 = 0, \xi_4 = 0, \xi_5 = -6, \xi_6 = -6$,
the neighbourhood degree energy of H is: $E_{ND}(H) = 24$,
the energy corresponding to adjacency matrix is: $E_A(H) = 8$,
and the degree exponent energy is: $E_{DE}(H) = 270$.

3. PROPERTIES OF NEIGHBOURHOOD DEGREE MATRIX OF A GRAPH

Observation 1. *In the matrix $ND(G)$, the degree d_i of vertex $v_i \in V(G)$ appears d_i times in the i^{th} column.*

Theorem 3.1. *If G is a simple (n,m)-graph, then*

(i) *The principal diagonal entries of $ND(G)$ are zeros.*
(ii) $Trace(ND(G)) = 0$.
(iii) $\sum_{i=1}^{n}\sum_{j=1}^{n}(nd)_{ij} = \sum_{i=1}^{n} d_G(v_i)^2 = M_1(G)$.
(iv) $[Norm(ND(G))]^2 = F(G)$.
(v) $\sum_{i=1}^{n}\sum_{j=1}^{n}(nd)_{ij}^{\alpha} = \sum_{i=1}^{n} d_G(v_i)^{\alpha} = M_1^{\alpha}(G)$.

(vi) $\prod_{i=1}^{n}\prod_{j=1}^{n}(nd)_{ij} = \prod_{i=1}^{n} d_G(v_i)^2 = \Pi_1(G)$.

Proof. The results (i) and (ii) are immediate from the definition of neighbourhood degree matrix. From Observation 1, we get

$$\sum_{i=1}^{n}(nd)_{ij} = d_j^2 \qquad for \quad j = 1, 2, ..., n.$$

Therefore,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(nd)_{ij} = \sum_{i=1}^{n} d_i^2 = M_1(G).$$

And

$$[Norm(ND(G))]^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}(nd)_{ij}^2 = \sum_{i=1}^{n} d_i(d_i^2) = F(G).$$

Similarly, one can easily obtain the result (v) and (vi). □

Theorem 3.2. *If G is an r-regular graph, then*

$$ND(G) = rA(G),$$

where $A(G)$ is an adjacency matrix of G.

Proof. If G is an r-regular graph, then $ND(G) = [(nd)_{ij}]$, whose elements are defined as

$$(nd)_{ij} = \begin{cases} r & if \;\; v_iv_j \in E(G), \\ 0 & otherwise. \end{cases}$$

From this fact one can observe that

$$(nd)_{ij} = ra_{ij},$$

where a_{ij} are the entries in the adjacency matrix $A(G)$ of the graph G. Thus, we can have the desired result. □

Theorem 3.3. *If G is a complete graph of order n, then*

$$P_{ND}(G;\xi) = (\xi - (n-1)^2)(\xi + n - 1)^{n-1}.$$

Proof. Suppose G is a complete graph. Then we have

$$ND(G) = (n-1)(J_n - I_n),$$

where J_n is the matrix of order n whose all entries are $1's$. From which we can arrive at the desired result. □

Theorem 3.4. *The sum of 2×2 principal minors of $ND(G)$ equals the negative of second Zagreb index of G.*

Proof. Clearly for a graph G, $ND(G)$ is a square matrix with zeros on the principal diagonal. For $i \neq j$, the principal submatrix of $ND(G)$ formed by the rows and the columns i, j is the zero matrix, if $v_iv_j \notin E(G)$ (nonadjacent vertices). Otherwise, it equals $\begin{bmatrix} 0 & d_j \\ d_i & 0 \end{bmatrix}$. The determinant of this submatrix is $-d_id_j$. Thus, the sum of 2×2 principal minors of $ND(G)$ equals

$$-\sum_{v_iv_j \in E(G)} d_i \cdot d_j = -M_2(G).$$

□

Corollary 3.5. *The product of* 2×2 *principal minors of* $ND(G)$ *equals the negative of second multiplicative Zagreb index of* G *if* m *(i.e., the number of edges of* G*) is odd and it equals second multiplicative Zagreb index of* G *otherwise.*

Corollary 3.6. *If* G *is an* r*-regular graph, then the sum of* 2×2 *principal minors of* $ND(G)$ *equals* $-r^2|E(G)|$.

Corollary 3.7. *If* $K_{a,b}$ *is a complete bipartite graph, then the sum of* 2×2 *principal minors of* $ND(K_{a,b})$ *equals* $-(ab)^2$.

Corollary 3.8. *The sum of* $\alpha^{th}, (\alpha\in\mathbb{R})$ *powers of* 2×2 *principal minors of* $ND(G)$ *equals* $(-1)^\alpha R_\alpha(G)$*, where* $R_\alpha(G)$ *is the general product-connectivity index of* G*. If* $\alpha=-\frac{1}{2}$ *, then we get Randić index of* G*.*

Theorem 3.9. *For any positive integer* n*, the neighbourhood degree eigenvalues of* K_n *are* $(n-1)^2$ *with multiplicity* 1 *and* $-(n-1)$ *with multiplicity* $(n-1)$*.*

Proof. First consider J_n, the $n\times n$ matrix with all entries equals 1. It is a symmetric, rank 1 matrix, and hence it has only one nonzero eigenvalue which must equals the trace. Thus, the eigenvalues of J_n are n with multiplicity 1 and 0 with multiplicity $(n-1)$. Since $ND(K_n)=(n-1)(J_n-I_n)$, the eigenvalues of $ND(K_n)$ must be $(n-1)^2$ with multiplicity 1 and $-(n-1)$ with multiplicity $(n-1)$. □

Theorem 3.10. *For any positive integers* a *and* b*, the neighbourhood degree eigenvalues of a complete bipartite graph* $K_{a,b}$ *are* $ab, -ab$*, and* 0 *with multiplicity* $(a+b-2)$*.*

Proof. To prove this, we consider

$$ND(K_{a,b})=\begin{bmatrix} 0 & J^a_{ab} \\ J^b_{ba} & 0 \end{bmatrix},$$

where J^x_{mn} is a matrix of order $m\times n$ with all entries equal to x.
Now,

$$rank[ND(K_{a,b})]=rank[J^a_{ab}]+rank[J^b_{ba}]=2.$$

Hence, $ND(K_{a,b})$ must have precisely two nonzero eigenvalues. These must be of the form ξ and $-\xi$, since the trace of $ND(K_{a,b})=0$. The sum of 2×2 principal minors of $ND(K_{a,b})$ equals $-(ab)^2$. This sum also equals the product of the eigenvalues, taken two at a time, which is $-\xi^2$. Thus, $\xi^2=(ab)^2$ and the eigenvalues must be $ab, -ab$, and 0 with multiplicity $(a+b-2)$. □

Let $G=(V,E)$ is a graph with vertex set $V(G)$ and an edge set $E(G)$. An *elementary subgraph* H of G is a subgraph of G which has either an edge or a cycle as its components. Denote by $r(H)$ and $c(H)$, the number of components in a subgraph H which are edges and cycles, respectively. The graph G and its elementary subgraphs with n vertices where $n=2,3,4$ are shown in figure 4.

Theorem 3.11. *If* G *is an* r*-regular graph with* n *vertices* $\{1,2,...,n\}$ *and* $ND(G)$ *is the neighbourhood degree matrix of* G*, then*

$$det(ND(G))=r^n\sum(-1)^{n-r(H)-c(H)}2^{c(H)},$$

where the summation is taken over all spanning elementary subgraphs H *of* G*.*

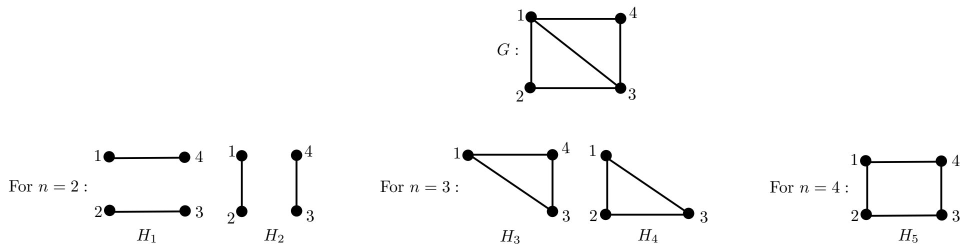

FIGURE 4. The graph G and its elementary subgraphs.

Proof. If G an r regular graph, then from Theorem 3.2 we have

$$ND(G) = rA(G).$$

Therefore,

$$det(ND(G)) = r^n \sum_{\pi} sgn(\pi) a_{1\pi(1)}...a_{n\pi(n)},$$

where the summation is taken over all permutations π of 1,2,...,n.
Consider a term $a_{1\pi(1)}...a_{n\pi(n)}$, which is nonzero. Since π admits a cycle decomposition, such a term will correspond to an edge joining v_i and v_j in G which are reflecting some 2-cycles (ij) of π, as well as some cycles of higher order, which corresponds to the cycles in G where $\pi(i) \neq i$ for any i. Thus, each elementary subgraph of G with vertex set $V(G)$ gives rise to a nonzero term in the summation. Suppose spanning elementary subgraph H corresponds to the term $a_{1\pi(1)}...a_{n\pi(n)}$. The sign of π is $(-1)^{n-r(H)-c(H)}2^{c(H)}$.

Finally, each spanning elementary subgraph gives rise to $2^{c(H)}$ terms in the summation, since each cycle can be associated with a cyclic permutation in two ways. All these observations will complete the required proof. □

Theorem 3.12. *If G is an r-regular graph with n vertices $\{1, 2, ..., n\}$ and*

$$P_{ND}(G; \xi) = det(\xi I - ND(G)) = \xi^n + b_1\xi^{n-1} + ... + b_n$$

is the characteristic polynomial of $ND(G)$, then $b_k = r^k \sum(-1)^{r(H)+c(H)}2^{c(H)}$, where the summation is taken over all the elementary subgraphs H of G with k vertices, $k = 1, 2, ..., n$.

Proof. Observe that, b_k is $(-1)^k$ times the sum of the principle minors of $ND(G)$ of order k, $k = 1, 2, ..., n$. By Theorem 3.11, we have the determinant of the sub-matrix of order k of $ND(G)$ as follows:

$$b_k = r^k(-1)^k \sum(-1)^{k-r(H)-c(H)}2^{c(H)},$$

where the summation is taken over all elementary subgraphs H of G with k vertices. □

Remark 3.1. *For an r-regular graph G,*

(i) *The coefficient b_k for $k = 1, 2, ..., n$ also equals the sum of all $k \times k$ minors of $ND(G)$.*
(ii) *$b_1 = 0, b_2 = -mr^2$, $b_3 = -2r^3$(Number of triangles in G) and $b_n = r^n det(A(G))$.*

Corollary 3.13. *Using the notations as in Theorem 3.12, if* $b_{2l+1} = 0, l = 0, 1, ...,$ *then* G *is bipartite.*

Lemma 3.14. *Let* G *be a bipartite graph with neighbourhood degree matrix* $ND(G)$. *If* ξ *is an neighbourhood degree eigenvalue of* G *with multiplicity* l, *then* $-\xi$ *is also an neighbourhood degree eigenvalue of* G *with multiplicity* l.

Proof. Let $V(G) = V_1 \cup V_2$ be two partitions of G. We can make $|V_1| = |V_2|$ by inserting isolated vertices if necessary, which will not affect the required result. Since $ND(G)$ only gets changed in the sense that some rows and columns with all entries equal to zero are appended. Suppose $|V_1| = |V_2| = k$. Then by relabeling the vertices if necessary, we may arrive at $ND(G) = \begin{bmatrix} 0 & B \\ B' & 0 \end{bmatrix}$, where order of B is $k \times k$. Let y be an eigenvector of $ND(G)$ corresponding to ξ. Partition y conformally so that we get

$$\begin{bmatrix} 0 & B \\ B' & 0 \end{bmatrix} \begin{bmatrix} y^{(1)} \\ y^{(2)} \end{bmatrix} = \xi \begin{bmatrix} y^{(1)} \\ y^{(2)} \end{bmatrix}.$$

Also one can easily verify that,

$$\begin{bmatrix} 0 & B \\ B' & 0 \end{bmatrix} \begin{bmatrix} y^{(1)} \\ -y^{(2)} \end{bmatrix} = -\xi \begin{bmatrix} y^{(1)} \\ -y^{(2)} \end{bmatrix}.$$

Thus, $-\xi$ is also an eigenvalue of $ND(G)$. It is also clear that, if there are k linearly independent eigenvectors for ξ, then we can construct k linearly independent eigenvectors for $-\xi$ according to the above said procedure which completes the proof. □

Theorem 3.15. *If* G *is a graph with* n *vertices and* $ND(G)$ *is the neighbourhood degree matrix of* G, *then the following statements are equivalent.*

- (i) G *is bipartite graph.*
- (ii) *if* $P_N D(G; \xi) = \xi^n + b_1 \xi^{n-1} + ... + b_n$ *is the characteristic polynomial of* $ND(G)$, *then* $b_{2k+1} = 0, k = 0, 1, ...$
- (iii) *the NBD-eigenvalues are symmetric with respect to the origin, that is if* ξ *is an NBD-eigenvalue with multiplicity* l, *then* $-\xi$ *is also an NBD-eigenvalue with same multiplicity.*

Proof. From Lemma 3.14, it is immediate that $(i) \implies (iii)$
Now we have to show, $(iii) \implies (ii)$.
Let $\xi_i, -\xi_i$ for $i = 1, 2, ..., l$ be the nonzero *NBD*-eigenvalues. Here $\xi_i, i = 1, 2, ..., l$ are not necessarily distinct. Therefore, zero is also a *NBD*-eigenvalue with multiplicity $(n - 2l)$. Then the characteristic polynomial of $ND(G)$ equals $\xi^{n-2l}(\xi^2 - \xi_1^2), ..., (\xi^2 - \xi_l^2)$ which follows that $b_{2l+1} = 0, k = 0, 1, ...$ and hence (ii) holds.

Finally, it is immediate from Corollary 3.13 that, $(ii) \implies (i)$ which completes the proof. □

4. Bounds for neighbourhood degree energy of a graph

If ξ_i for $i = 1, 2, ..., n$ are the neighbourhood degree eigenvalues of a graph G with n vertices, then

$$\sum_{i=1}^{n} \xi_i = 0 \tag{4.1}$$

and

$$\begin{aligned}\sum_{i=1}^{n}\xi_i^2 &= Trace[(ND(G))^2]\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}(nd)_{ij}\cdot(nd)_{ji}\\ &= 2\sum_{i\sim j}d_j\cdot d_i\\ &= 2\sum_{v_iv_j\in E(G)}d_i\cdot d_j\\ &= 2M_2(G).\end{aligned} \tag{4.2}$$

Theorem 4.1. *If G is a graph of order n, then*

$$\xi_1 \leq \sqrt{\frac{2M_2(G)(n-1)}{n}}, \tag{4.3}$$

where ξ_1 is the neighbourhood degree spectral radius of G.

Proof. Let $\xi_1, \xi_2, ..., \xi_n$ are the neighbourhood degree eigenvalues of G. Then by substituting $a_i = 1$ and $b_i = \xi_i$ for $i = 2, 3, ..., n$ in Cauchy-Schwarz inequality [1], we get the desired result as follows:

$$\left(\sum_{i=2}^{n}\xi_i\right)^2 \leq (n-1)\left(\sum_{i=2}^{n}\xi_i^2\right). \tag{4.4}$$

From (4.1) and (4.2), we get

$$\sum_{i=2}^{n}\xi_i = -\xi_1 \quad \textit{and} \quad \sum_{i=2}^{n}\xi_i^2 = 2M_2(G) - \xi_1^2.$$

Therefore, (4.4) becomes

$$(-\xi_1)^2 \leq (n-1)(2M_2(G) - \xi_1^2),$$

which yields the required result. □

Theorem 4.2. [9] *If G is a graph of order n, then*

$$\xi_1 \geq \delta\sqrt{\frac{M_1(G)}{n}}, \tag{4.5}$$

where $\delta = min\{d_i\}$, for $i = 1, 2, ..., n$ and equality holds for regular graphs.

Theorem 4.3. *If G is a graph of order n, then*

$$\sqrt{2M_2(G)} \leq E_{ND}(G) \leq \sqrt{2nM_2(G)}.$$

Proof. Let $\xi_1, \xi_2, ..., \xi_n$ are the neighbourhood degree eigenvalues of G. Then by substituting $a_i = 1$ and $b_i = |\xi_i|$ for $i = 2, 3, ..., n$ in Cauchy-Schwarz inequality [1], we get

$$\begin{aligned}\left(\sum_{i=1}^{n}|\xi_i|\right)^2 &\leq n\sum_{i=1}^{n}|\xi_i|^2\\ E_{ND}(G)^2 &\leq n2M_2(G)\\ E_{ND}(G) &\leq \sqrt{2nM_2(G)}.\end{aligned}$$

Further,

$$E_{ND}(G)^2=\left(\sum_{i=1}^{n}|\xi_i|\right)^2\geq\sum_{i=1}^{n}|\xi_i|^2=2M_2(G).$$

Therefore,

$$E_{ND}(G)\geq\sqrt{2M_2(G)}.$$

Hence,

$$\sqrt{2M_2(G)}\leq E_{ND}(G)\leq\sqrt{2nM_2(G)}.$$

□

Theorem 4.4. *If G is a graph of order n, then*

$$E_{ND}(G)\geq 2\sqrt{M_2(G)}.$$

Equality holds if and only if the graph G has exactly one positive and exactly one negative eigenvalue. This, in turn, is the case if and only if one component of G is complete bipartite graph and all its other components are isolated vertices.

Proof. We know that,

$$\begin{aligned}E_{ND}(G)^2 &= \left(\sum_{i=1}^{n}|\xi_i|\right)^2\\ &= \sum_{i=1}^{n}|\xi_i|^2+2\sum_{i<j}|\xi_i\xi_j|\\ &= 2M_2(G)+2\sum_{i<j}|\xi_i\xi_j|. \qquad (4.6)\end{aligned}$$

Clearly, $M_2(G)\leq\sum_{i<j}|\xi_i\xi_j|$, substituting this in (4.6), we get

$$E_{ND}(G)\geq 2M_2(G)+2M_2(G)=4M_2(G),$$

which yields the required result. □

Theorem 4.5. *If G is an r-regular graph of order n and ξ_i for $i=1,2,...,n$ are the neighbourhood degree eigenvalues of G, then*

(i) $\sum_{i=1}^{n}\xi_i^2=2mr^2$ *where* $m=|E(G)|$.
(ii) $\xi_1\leq\sqrt{\frac{2mr^2(n-1)}{n}}$.
(iii) $E_{ND}(G)=rE_A(G)$ *where $E_A(G)$ is the energy G corresponding to the adjacency matrix.*

Proof. We know that, for an r-regular graph G, $M_2(G) = mr^2$. Therefore, from (4.2) and Theorem 4.2, we get the desired results (i) and (ii).

To prove (iii), consider λ_i for $i = 1, 2, ..., n$ are the eigenvalues of $A(G)$, then clearly $\xi_i = r\lambda_i$ for $i = 1, 2, ..., n$ are the eigenvalues of $ND(G)$.
Note that, for an r-regular graph G from Theorem 3.2, we have

$$ND(G) = rA(G).$$

Therefore,

$$\begin{aligned} E_{ND}(G) &= \sum_{i=1}^{n} |\xi| \\ &= r\sum_{i=1}^{n} |\lambda_i| \\ &= rE_A(G). \end{aligned}$$

□

5. Neighbourhood degree energy of graph operations

Let $A \in R^{m\times n}, B \in R^{p\times q}$. Then the *Kronecker product* of A and B is defined as the matrix

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{bmatrix}$$

Proposition 5.1. [10] *Let $A \in M^m$ and $B \in M^n$. Furthermore, let λ be an eigenvalue of matrix A with corresponding eigenvector x, and μ an eigenvalue of matrix B with corresponding eigenvector y. Then $\lambda\mu$ is an eigenvalue of $A \otimes B$ with corresponding eigenvector $x \otimes y$.*

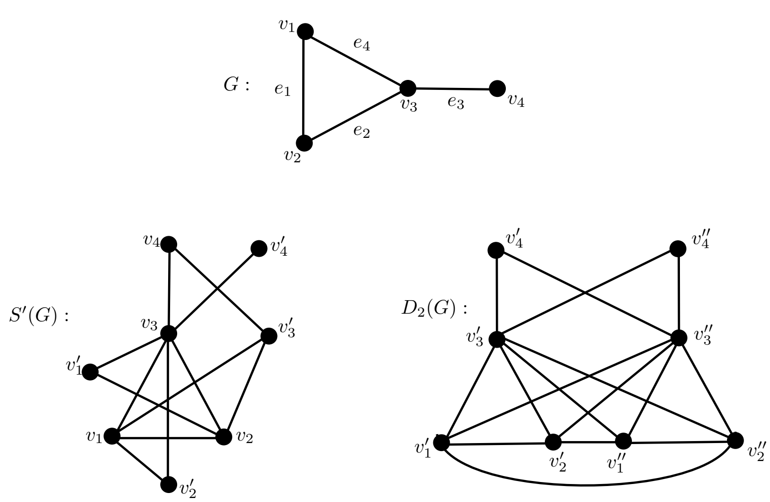

Figure 5. The graph G with its vertex splitting graph $S'(G)$ and shadow graph $D_2(G)$.

Definition 1. *The vertex splitting graph* [16] $S'(G)$ *of a graph* G *is obtained from* G *by adding for each vertex* v *of* G *a new vertex* v' *so that* v' *is adjacent to every vertex that is adjacent to* v *(See figure 5).*

Theorem 5.2. *If* G *is a graph of order* n*, then*

$$E_{ND}(S'(G)) = 2\sqrt{3}E_{ND}(G).$$

Proof. Let $v_1, v_2, ..., v_n$ be the vertices of the graph G. Then its neighbourhood degree matrix is given by

$$ND(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_n \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & \cdots & v_n \end{array} \\ \begin{bmatrix} 0 & nd_{12} & nd_{13} & \dots & nd_{1n} \\ nd_{21} & 0 & nd_{23} & \dots & nd_{2n} \\ nd_{31} & nd_{32} & 0 & \dots & nd_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ nd_{n1} & nd_{n2} & nd_{n3} & \dots & 0 \end{bmatrix} \end{array}$$

Let $u_1, u_2, ..., u_n$ be vertices corresponding to $v_1, v_2, ..., v_n$, which are added in G to obtain $S'(G)$, such that, $N_{v_i}(G) = N_{u_i}(S'(G)), i = 1, 2, ..., n$. Then $ND(S'(G))$ can be written as a block matrix as follows,
$ND(S'(G)) =$

$$\begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_n \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{array} \begin{array}{c} \begin{array}{cccccccccc} v_1 & v_2 & v_3 & \cdots & v_n & u_1 & u_2 & u_3 & \cdots & u_n \end{array} \\ \begin{bmatrix} 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) & 0 & nd_{12} & nd_{13} & \dots & nd_{1n} \\ 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) & nd_{21} & 0 & nd_{23} & \dots & nd_{2n} \\ 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) & nd_{31} & nd_{32} & 0 & \dots & nd_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 & nd_{n1} & nd_{n2} & nd_{n3} & \dots & 0 \\ 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) & 0 & 0 & 0 & \dots & 0 \\ 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) & 0 & 0 & 0 & \dots & 0 \\ 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 & 0 & 0 & 0 & \dots & 0 \end{bmatrix} \end{array}$$

That is,

$$ND(S'(G)) = \begin{bmatrix} 2ND(G) & ND(G) \\ 2ND(G) & 0 \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 2 & 0 \end{bmatrix} \otimes ND(G).$$

Hence,

$$Spec(S'(G)) = \begin{pmatrix} (1-\sqrt{3})\,\xi_i & (1+\sqrt{3})\,\xi_i \\ n & n \end{pmatrix}$$

where $\xi_i, i = 1, 2, ..., n$, are the neighbourhood degree eigenvalues of G, while $(1 \pm \sqrt{3})$ are the eigenvalues of $\begin{bmatrix} 2 & 1 \\ 2 & 0 \end{bmatrix}$. Therefore,

$$\begin{aligned} E_{ND}(S'(G)) &= \sum_{i=1}^{n} \left| \left(1 \pm \sqrt{3}\right) \xi_i \right| \\ &= \sum_{i=1}^{n} |\xi_i| \left[-1 + \sqrt{3} + 1 + \sqrt{3} \right] \\ &= 2\sqrt{3} E_{ND}(G). \end{aligned}$$

□

Corollary 5.3. *If G is an r-regular graph, then*

$$E_{ND}(S'(G)) = 2r\sqrt{3}E_A(G).$$

Definition 2. *The shadow graph [6] $D_2(G)$ of a connected graph G is constructed by taking two copies of G, say G', G'' and joining each vertex v' in G' to the neighbors of the corresponding vertex v'' in G''.*

Theorem 5.4. *If G is a graph of order n, then*

$$E_{ND}(D_2(G)) = 4E_{ND}(G).$$

Proof. Let $v_1, v_2, ..., v_n$ be the vertices of the graph G. Then its neighbourhood degree matrix is given by

$$ND(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_n \end{array} \begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & \cdots & v_n \end{array} \\ \begin{bmatrix} 0 & nd_{12} & nd_{13} & \dots & nd_{1n} \\ nd_{21} & 0 & nd_{23} & \dots & nd_{2n} \\ nd_{31} & nd_{32} & 0 & \dots & nd_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ nd_{n1} & nd_{n2} & nd_{n3} & \dots & 0 \end{bmatrix} \end{array}$$

Let $u_1, u_2, ..., u_n$ be vertices corresponding to $v_1, v_2, ..., v_n$, which are added in G to obtain $D_2(G)$, such that, $N_{v_i}(D_2(G)) = 2N_{v_i}(G) = N_{u_i}(D_2(G)), i = 1, 2, ..., n$. Then $ND(D_2(G))$ can be written as a block matrix as follows,
$ND(S'(G)) =$

$$\begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_n \\ \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{array} \begin{array}{c} \begin{array}{cccccccccc} v_1 & v_2 & v_3 & \cdots & v_n & u_1 & u_2 & u_3 & \cdots & u_n \end{array} \\ \begin{bmatrix} 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) & 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) \\ 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) & 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) \\ 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) & 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 & 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 \\ \\ 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) & 0 & 2(nd_{12}) & 2(nd_{13}) & \dots & 2(nd_{1n}) \\ 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) & 2(nd_{21}) & 0 & 2(nd_{23}) & \dots & 2(nd_{2n}) \\ 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) & 2(nd_{31}) & 2(nd_{32}) & 0 & \dots & 2(nd_{3n}) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 & 2(nd_{n1}) & 2(nd_{n2}) & 2(nd_{n3}) & \dots & 0 \end{bmatrix} \end{array}$$

That is,

$$ND(S'(G)) = \begin{bmatrix} 2ND(G) & 2ND(G) \\ 2ND(G) & 2ND(G) \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \otimes ND(G).$$

Hence,

$$Spec(D_2(G)) = \begin{pmatrix} (4)\,\xi_i & (0)\,\xi_i \\ n & n \end{pmatrix}$$

where $\xi_i, i = 1, 2, ..., n$, are the neighbourhood degree eigenvalues of G, while $4, 0$ are the eigenvalues of $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$. Therefore,

$$\begin{aligned} E_{ND}(S'(G)) &= \sum_{i=1}^{n} |(4+0)\xi_i| \\ &= 4\sum_{i=1}^{n} |\xi_i| \\ &= 4E_{ND}(G). \end{aligned}$$

□

Corollary 5.5. *If G is an r-regular graph, then*

$$E_{ND}(D_2(G)) = 4rE_A(G).$$

6. Conclusion

A new graph matrix is defined in this paper, called neighbourhood degree matrix and the comparison of neighbourhood degree energy with adjacency energy and degree exponent energy are plotted and studied linear regression analysis of neighbourhood degree energy (NDE) and adjacency energy (AE) with standard enthalpy of vaporization (DHVAP). From this matrix, one can easily compute some degree based topological indices namely, first Zagreb index, second Zagreb index, forgotten topological index, first general Zagreb index and general product-connectivity index etc. In addition, we presented bounds for the neighbourhood degree energy and neighbourhood degree spectral radius. The closed forms for neighbourhood degree energy of regular graphs and complete bipartite graphs are obtained. Some relations connecting neighbourhood degree energy to energy corresponding to adjacency matrix of the given graph are discussed. The exact expressions for neighbourhood degree energy of some graph operations are obtained in terms of neighbourhood degree energy of original graph.

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References

[1] S. Bernard, J. M. Child, "Higher Algebra", Macmillan India Ltd., New Delhi, 2001.

[2] J.A. Bondy, U.S.R. Murty, "Graph Theory with Applications", Macmillan, London, 1976.

[3] B. Bollobás, P. Erdös, "Graphs of extremal weights", Ars Combinatorics, Vol. 50, (1998), 225–233.

[4] D. Cvetković, M. Doob, H. Sachs, "Spectra of Graphs-Theory and Applications", Academic Press, New York, 1980.

[5] B. Furtula, I. Gutman, "A forgotten topological index", Journal of Mathematical Chemistry, Vol. 53, (2015), 1184–1190.

[6] J. A. Gallian, "A dynamic survey of graph labeling", Electronic Journal of Combinatorics, Vol. 15, 2008.

[7] I. Gutman, N. Trinajstić, "Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons", Chemical Physics Letters, Vol. 17, (1972), 535–538.

[8] I. Gutman, B. Furtula, "The Total π-Electron Energy Saga", Croatica Chemica Acta, Vol. 90 (3), (2017), 359–368.

[9] F. Harary, "Graph Theory", Addison-Wesley, Reading, 1969.

[10] R. A. Horn, C. R. Johnson, "Topics in matrix analysis", Cambridge University Press, Cambridge, 1991.

[11] V. R. Kulli, "College Graph Theory", Vishwa International Publications, Gulbarga, India, 2012.

[12] X. Li, H. Zhao, "Trees with the first three smallest and largest generalized topological indices", MATCH Communications in Mathematical and in Computer Chemistry, Vol. 50, (2004), 57–62.

[13] M. Randić, "On characterization of molecular branching", Journal of American Chemical Society, Vol. 97, (1975), 6609–6615.

[14] H. S. Ramane,, D. S. Revankar, J. B. Patil, "Bounds for the degree sum eigenvalues and degree sum energy of a graph", International Journal of Pure and Applied Mathematical Sciences, Vol. 6, (2013), 161–167.

[15] H. S. Ramane, S. S. Shinde, "Degree exponent polynomial of graphs obtained by some graph operations ", Electronic Notes in Discrete Mathematics, Vol. 63, (2017), 161–168.

[16] E. Sampathkumar, H. B. Walikar, "On splitting graph of a graph ", Journal of Karnatak University Sciences, Vol. 25 and 26 (combined), (1980-81), 13–16.

[17] R. Todeschini, V. Consonni, "New local vertex invariants and molecular descriptors based on functions of the vertex degrees", MATCH Communications in Mathematical and in Computer Chemistry, Vol. 64, (2010), 359 – 372.

[18] R. Todeschini, D. Ballabio, V. Consonni, "Novel molecular descriptors based on functions of new vertex degrees", [in:] I. Gutman, B. Furtula (eds), Novel molecular structure descriptors – Theory and applications I", University of Kragujevac, (2010), 73 – 100.

[19] H. Wiener, "Strucural determination of paraffin boiling points", Journal of American Chemical Society, Vol. 69, (1947), 17 – 20.

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