

On ev -Degree and ve -Degree Topological Indices

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ABSTRACT

Recently two new degree concepts have been defined in graph theory: ev -degree and ve -degree. Also the ev -degree and ve -degree Zagreb and Randić indices have been defined very recently as parallel of the classical definitions of Zagreb and Randić indices. It was shown that ev -degree and ve -degree topological indices can be used as possible tools in QSPR researches [2]. In this paper, we define the ve -degree and ev -degree Narumi–Katayama indices, investigate the predicting power of these novel indices and extremal graphs with respect to these novel topological indices. Also we give some basic mathematical properties of ev -degree and ve -degree Narumi-Katayama and Zagreb indices.

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1. INTRODUCTION

Topological indices have important place in theoretical chemistry. Many topological indices were defined by using vertex degree concept. The Zagreb and Randić indices are the most used degree based topological indices so far in mathematical and chemical literature among the all topological indices. Very recently, Chellali, Haynes, Hedetniemi and Lewishave published a seminal study: On ve -degrees and ev -degrees in graphs [1]. The authors defined two novel degree concepts in graph theory; ev -degrees and ve -degrees and investigate some basic mathematical properties of both novel graph invariants with regard to graph regularity and irregularity [1]. After given the equality of the total ev -degree and total ve -degree for any graph, also the total ev -degree and the total ve -degree were stated as in relation to the first Zagreb index. It was proposed in the article that the chemical applicability of the total ev -degree (and the total ve -degree) could be an interesting problem in view of chemistry and chemical graph theory. In the light of this suggestion, one of the

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present author has carried these novel degree concepts to chemical graph theory by defining the ev -degree and ve -degree Zagreb and Randić indices [2]. It was compared these new group ev -degree and ve -degree indices with the other well-known and most used topological indices in literature such as; Wiener, Zagreb and Randić indices by modeling some physicochemical properties of octane isomers [2]. It was shown that the ev -degree Zagreb index, the ve -degree Zagreb and the ve -degree Randić indices give better correlation than Wiener, Zagreb and Randić indices to predict the some specific physicochemical properties of octanes [2]. Also it was given the relations between the second Zagreb index and ev -degree and ve -degree Zagreb indices and some mathematical properties of ev -degree and ve -degree Zagreb indices [2]. In this paper we define the ve -degree and ev -degree Narumi–Katayama indices, investigate the predicting power of these novel indices and extremal graphs with respect to these topological indices. Also we give some basic mathematical properties of ev -degree and ve -degree Zagreb indices.

A graph $G = (V, E)$ consists of two nonempty sets V and 2-element subsets of V namely E . The elements of V are called vertices and the elements of E are called edges. For a vertex v , $\deg(v)$ show the number of edges that incident to v . The set of all vertices which adjacent to v is called the open neighborhood of v and denoted by $N(v)$. If we add the vertex v to $N(v)$, then we get the closed neighborhood of v , $N[v]$.

The first and second Zagreb indices [3] defined as follows: The first Zagreb index of a connected graph G , defined as,

$$M_1 = M_1(G) = \sum_{u \in V(G)} \deg(u)^2 = \sum_{uv \in E(G)} (\deg(u) + \deg(v)).$$

and the second Zagreb index of a connected graph G , defined as

$$M_2 = M_2(G) = \sum_{uv \in E(G)} \deg(u) \cdot \deg(v).$$

The authors investigated the relationship between the total π -electron energy on molecules and Zagreb indices [3]. For the details see the references [4–6]. Randić investigated the measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons via Randić index [7]. The Randić index of a connected graph G defined as;

$$R = R(G) = \sum_{uv \in E(G)} (\deg(u) \cdot \deg(v))^{-1/2}.$$

We refer the interested reader to [8–10] and the references therein for the up to date arguments about the Randić index.

The forgotten topological index for a connected graph G is defined as,

$$F = F(G) = \sum_{u \in V(G)} \deg(u)^3 = \sum_{uv \in E(G)} (\deg(u)^2 + \deg(v)^2).$$

It was showed in [11] that the predictive power of the forgotten topological index is very close to the first Zagreb index for the entropy and eccentric factor. For further studies about the forgotten topological index we refer to the interested reader [11–13] and references therein.

In the 1980s, Narumi and Katayama considered the production of the degrees of vertices

$$NK = NK(G) = \prod_{v \in V(G)} \deg(v)$$

and named it the “simple topological index” [14]. Later for this graph invariant, the name “Narumi-Katayama index” was used in [15–17]. The extremal graphs with respect to NK index was studied by Gutman and Ghorbani [15], Zolfi and Ashrafi [20]. Some relations between the Narumi-Katayama index and the first Zagreb index were introduced in the more recent paper [21].

Multiplicative version of the first Zagreb index of a connected graph was defined by Eliasi et. al. in [22] as:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{uv \in E(G)} (\deg(u) + \deg(v)).$$

For detailed discussions of the multiplicative version of Zagreb indices, we refer the interested reader to [23] and the references cited therein.

In the following section, we will give basic definitions of ev -degree and ve -degree concepts, ve -degree and ev -degree Zagreb indices and as well as the basic mathematical properties of these novel topological indices. And also we give the definitions of ev -degree and ve -degree Narumi-Katayama indices.

2. VE-DEGREE AND EV-DEGREE CONCEPTS AND CORRESPONDING TOPOLOGICAL INDICES

In this section we give the definitions of ev -degree and ve -degree concepts which were given by Chellali et al. in [1] and the definitions and properties of ev -degree and ve -degree topological indices.

Definition 2.1 [1] *Let G be a connected graph and $v \in V(G)$. The ve -degree of the vertex v , $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed neighborhood of v . For convenience we prefer to show the ve -degree of the vertex v , by c_v .*

Definition 2.2 [1] *Let G be a connected graph and $e = uv \in E(G)$. The ev -degree of the edge e , $deg_{ev}(e)$, equals the number of vertices of the union of the closed neighborhoods of u and v . For convenience we prefer to show the ev -degree of the edge $e = uv$, by c_e or c_{uv} .*

Definition 2.3 [1] *Let G be a connected graph and $v \in V(G)$. The total ev -degree of the graph G is defined as $T_e = T_e(G) = \sum_{e \in E(G)} c_e$ and the total ve -degree of the graph G is defined as $T_v = T_v(G) = \sum_{v \in V(G)} c_v$.*

Observation 2.4 [1] *For any connected graph G , $T_e(G) = T_v(G)$.*

Observation 2.5 [1] *For any triangle free connected graph G , $c_e = c_{uv} = \deg(u) + \deg(v)$.*

The following theorem states the relationship between the first Zagreb index and the total ve -degree of a connected graph G .

Theorem 2.6 [1] *For any connected graph G , $T_e(G) = T_v(G) = M_1(G) - 3n(G)$, where $n(G)$ denotes the total number of triangles in G .*

In [1], the authors suggested the idea that to carry these novel degree concepts to mathematical chemistry. One of the present author following this suggestion defined ev -degree and ve -degree Zagreb indices and showed that these novel group Zagreb and Randić indices give better correlation than well-known topological indices such as; Wiener, Zagreb and Randić indices to modeling some physicochemical properties of octane isomers [2]. And now, we give the definitions and some basic mathematical properties of ev -degree and ve -degree Zagreb indices which were given in [2].

Definition 2.7 [2] *Let G be a connected graph and $e \in E(G)$. The ev -degree Zagreb index of the graph G is defined as $S = S(G) = \sum_{e \in E(G)} c_e^2$.*

Definition 2.8 [2] *Let G be a connected graph and $v \in V(G)$. The first ve -degree Zagreb alpha index of the graph G is defined as $S^\alpha = S^\alpha(G) = \sum_{v \in V(G)} c_v^2$.*

Definition 2.9 [2] *Let G be a connected graph and $uv \in E(G)$. The first ve -degree Zagreb beta index of the graph G is defined as $S^\beta = S^\beta(G) = \sum_{uv \in E(G)} (c_u + c_v)$.*

Definition 2.10 [2] *Let G be a connected graph and $uv \in E(G)$. The second ve -degree Zagreb index of the graph G is defined as $S^\mu = S^\mu(G) = \sum_{uv \in E(G)} c_u c_v$.*

Definition 2.11 [2] *Let G be a connected graph and $uv \in E(G)$. The ve -degree Randić index of the graph G is defined as $R^\alpha = R^\alpha(G) = \sum_{uv \in E(G)} (c_u c_v)^{-1/2}$.*

And now we restate the some basic properties of ev -degree and ve -degree Zagreb indices which were given in [2].

Lemma 2.12 [2] *Let T be a tree and $v \in V(T)$ then, $c_v = \sum_{u \in N(v)} \deg(u)$.*

Theorem 2.13 [2] Let T be a tree with the vertex set $V(T) = \{v_1, v_2, \dots, v_n\}$ then, $S^\beta(T) = 2M_2(T)$.

Theorem 2.14 [2] Let G be a triangle free connected graph, then; $S(G) = F(G) + 2M_2(G)$.

Corollary 2.15 Let T be a tree then, $S(T) = F(T) + S^\beta(T)$.

And now we give the definitions of *ev*-degree and *ve*-degree Narumi-Katayama indices for a graph G .

Definition 2.16 The *ve*-Narumi-Katayama index of a graph G is defined with the following equation $NK_{ve} = NK_{ve}(G) = \prod_{v \in V(G)} C_v$.

If a graph has an isolated vertex, its $NK_{ve} = 0$ which is the minimal value of NK_{ve} . We take the graphs without isolated vertices in the following results which will be introduced in the section four.

Definition 2.17 The *ev*-Narumi-Katayama index of a graph G is defined with the following equation $NK_{ev} = NK_{ev}(G) = \prod_{e \in E(G)} C_e$.

In the next section we investigate the predicting power of these novel topological indices and after that we investigate some mathematical properties of these novel indices.

3. NEW TOOLS FOR QSPR RESEARCHES: THE *EV*-NARUMI-KATAYAMA INDEX AND THE *VE*-NARUMI-KATAYAMA INDEX

In this section we compare the Narumi-Katayama index and its corresponding versions of the *ev*-Narumi-Katayama and *ve*-Narumi-Katayama indices with each other by using strong correlation coefficients acquired from the chemical graphs of octane isomers. We get the experimental results at the www.moleculardescriptors.eu (see Table 1). The following physicochemical features have been modeled:

- Entropy,
- Acentric factor (AcenFac),
- Enthalpy of vaporization (HVAP),
- Standard enthalpy of vaporization (DHVAP).

We select those physicochemical properties of octane isomers for which give reasonably good correlations, i.e. the absolute value of correlation coefficients are larger

than 0.8959 (see Table 2). Also we find the Narumi-Katayama index of octane isomers values at the www.molecularDescriptors.eu (see Table 3). We also calculate and show the *ev*-Narumi-Katayama and the *ve*-Narumi-Katayama indices of octane isomers values in Table 3.

Table 1. Some physicochemical properties of octane isomers.

Molecule	Entropy	AcenFac	HVAP	DHVAP
n-octane	111.70	0.39790	73.19	9.915
2-methyl-heptane	109.80	0.37792	70.30	9.484
3-methyl-heptane	111.30	0.37100	71.30	9.521
4-methyl-heptane	109.30	0.37150	70.91	9.483
3-ethyl-hexane	109.40	0.36247	71.70	9.476
2,2-dimethyl-hexane	103.40	0.33943	67.70	8.915
2,3-dimethyl-hexane	108.00	0.34825	70.20	9.272
2,4-dimethyl-hexane	107.00	0.34422	68.50	9.029
2,5-dimethyl-hexane	105.70	0.35683	68.60	9.051
3,3-dimethyl-hexane	104.70	0.32260	68.50	8.973
3,4-dimethyl-hexane	106.60	0.34035	70.20	9.316
2-methyl-3-ethyl-pentane	106.10	0.33243	69.70	9.209
3-methyl-3-ethyl-pentane	101.50	0.30690	69.30	9.081
2,2,3-trimethyl-pentane	101.30	0.30082	67.30	8.826
2,2,4-trimethyl-pentane	104.10	0.30537	64.87	8.402
2,3,3-trimethyl-pentane	102.10	0.29318	68.10	8.897
2,3,4-trimethyl-pentane	102.40	0.31742	68.37	9.014
2,2,3,3-tetramethylbutane	93.06	0.25529	66.20	8.410

Table 2. Topological indices of octane isomers.

Molecule	Nar	<i>ev</i> Nar	<i>ve</i> Nar
n-octane	4.159	9.129	9.129
2-methyl-heptane	3.871	9.640	9.757
3-methyl-heptane	3.871	9.575	9.575
4-methyl-heptane	3.871	9.575	9.510
3-ethyl-hexane	3.871	9.510	9.352
2,2-dimethyl-hexane	3.466	10.491	10.738
2,3-dimethyl-hexane	3.584	10.045	10.098
2,4-dimethyl-hexane	3.584	10.085	10.163
2,5-dimethyl-hexane	3.584	10.150	10.386
3,3-dimethyl-hexane	3.466	10.386	10.450
3,4-dimethyl-hexane	3.584	9.980	9.940
2-methyl-3-ethyl-pentane	3.584	9.980	9.911
3-methyl-3-ethyl-pentane	3.466	10.281	10.240
2,2,3-trimethyl-pentane	3.178	10.869	11.075
2,2,4-trimethyl-pentane	3.178	11.002	11.298
2,3,3-trimethyl-pentane	3.178	10.828	11.010
2,3,4-trimethyl-pentane	3.296	10.515	10.658
2,2,3,3-tetramethylbutane	2.773	11.736	12.210

Table 3. The correlation coefficients between new and old topological indices and some physicochemical properties of octane isomers.

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.9398	0.9700	0.8959	0.9410
<i>ve</i> -Nar	-0.9192	-0.9092	-0.9236	-0.9490
<i>ev</i> -Nar	-0.9369	-0.9486	-0.9202	-0.9568

Table 4. The squares of correlation coefficients between topological indices and some physicochemical properties of octane isomers.

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.8832	0.9409	0.8026	0.8854
<i>ve</i> -Nar	0.8449	0.8266	0.8530	0.9006
<i>ev</i> -Nar	0.8778	0.8998	0.8468	0.9154

Note that the all values in Table 2 are given by using natural logarithm. It can be seen from the Table 2 that the most convenient indices which are modeling the Entropy, Enthalpy of vaporization (HVAP), Standard enthalpy of vaporization (DHVAP) and Acentric factor (AcenFac) are Narumi-Katayama index (S) for entropy and Acentric Factor, *ve*-Narumi-Katayama index for the Enthalpy of vaporization (HVAP) and *ev*-Narumi-Katayama index for the Standard enthalpy of vaporization (DHVAP), respectively. But notice that the Narumi-Katayama index show the positive strong correlation and the *ve*-Narumi-Katayama and the *ev*-Narumi-Katayama indices show the negative strong correlation. Because of this fact we can compare these graph invariants with each other by using the squares of correlation coefficients for ensure the compliance between the positive and negative correlation coefficients (see Table 4).

The cross-correlation matrix of the indices are given in Table 5.

Table 5. The cross-correlation matrix of the topological indices.

Index	Nar	<i>ve</i> -Nar	<i>ev</i> -Nar
Nar	1.0000		
<i>ve</i> -Nar	-0.9901	1.0000	
<i>ev</i> -Nar	-0.9715	0.9931	1.0000

It can be shown from the Table 5 that the absolute value of the minimum correlation efficient among the indices is 0.9715 which is indicate strong correlation among all these indices. From the above arguments, we can say that the ve -Narumi-Katayama index and ev -Narumi-Katayama index are possible tools for QSPR researches.

4. MAIN RESULTS

In this section, we firstly give some basic mathematical properties of ve -degree, ev -Narumi-Katayama and ve -Narumi-Katayama indices. Secondly, we investigate certain mathematical properties of ev -degree and ve -degree Zagreb indices.

Lemma 4.1. *Let G be a connected graph, then $\sum_{v \in V(G)} n_v = \sum_{e \in E(G)} n_e = 3n(G)$, where n_v , n_e , $n(G)$ denote the number of triangles in G containing the vertex v , the number of triangles in G containing the edge e and the total number of triangles in G , respectively.*

Proof. The second part of this equality were given in [1]. The first part comes from that since every triangle consists of three vertices and edges, we count every triangle exactly three times for each vertex. Since the total number of triangles in the graph G will not be changed, the desired result acquired easily. \square

Lemma 4.2. *Let G be a connected graph and $v \in V(G)$, then $c_v = \sum_{u \in N(v)} \deg(u) - n_v$.*

Proof. From the Definition 2.1, we know that c_v equals the number of different edges incident to any vertex of $N(v)$. Therefore $c_v = \sum_{u \in N(v)} \deg(u)$ if v does not lie in a triangle. But if v belongs a triangle then the edge that does not incident to v of this triangle must be counted twice in the sum $\sum_{u \in N(v)} \deg(u)$. Therefore we must minus one from the sum $\sum_{u \in N(v)} \deg(u)$ for we find the exact number of different edges incident to $N(v)$. Thus if v lies in more than one triangle then we must minus n_v from the the sum $\sum_{u \in N(v)} \deg(u)$ for we find the exact number of different edges incident to $N(v)$. \square

Corollary 4.3. *For the n -vertex triangle graph G , the ve -degree Narumi-Katayama index $NK_{ve}(G)$ is calculated by the following equation:*

$$NK_{ve}(G) = \prod_{v \in V} (\sum_{u \in N(v)} \deg(u)).$$

Example 4.4. *Consider the P_2 path graph $c_{v_1} = c_{v_2} = 1$ and $NK_{ve}(P_2) = 1$. For P_3 path graph $c_{v_1} = c_{v_2} = c_{v_3} = 2$ and $NK_{ve}(P_3) = 8$. For P_4 , $c_{v_1} = c_{v_4} = 2$ and $c_{v_2} = c_{v_3} = 3$ so that $NK_{ve}(P_4) = 36$. We take the P_n such that $n \geq 5$. $c_{v_1} = c_{v_n} = 2$ and $c_{v_2} = c_{v_{n-1}} = 3$ and the ve -degree of the other vertices are 4. Therefore $NK_{ve}(P_n) = 9.4^{n-3}$.*

Example 4.5. Consider the C_3 cycle $c_{v_1} = c_{v_2} = c_{v_3} = 3$ and $NK_{ve}(C_3) = 27$. For $n \geq 4$ every cycle 4_{ve} -regular and $NK_{ve}(C_n) = 4^n$.

Example 4.6. Consider the S_n -star graph on n vertices. Every vertices have the same ve -degree such that $(n - 1)$. This means $NK_{ve}(S_n) = (n - 1)^n$.

Example 4.7. Consider the K_n -complete graph with n vertices. K_n is a m_{ve} -regular graph with the size $m = n(n - 1)/2$. Therefore, $NK_{ve}(K_n) = m^n$.

Proposition 4.8. Let G be a graph with n vertices, then $NK_{ve}(G) \leq NK_{ve}(K_n)$.

Proof. Note that contribution each edge is positive. Hence, $NK_{ve}(G)$ reaches its maximum value for the complete graphs. \square

Proposition 4.9. For the P_n -path graph with n vertices such that $n \geq 4$, $NK_{ve}(P_n) = NK_{ev}(P_n) = 9.4^{n-3}$.

Proof. We have already known that $NK_{ve}(P_n) = 9.4^{n-3}$ from the Example 4.4. There are $n - 3$ edges with their ev -degrees equal 4 and 2 edges with their ev -degrees equal 3 for the n -vertex path. Therefore, the proof is complete. \square

Proposition 4.10. For the cycle C_n on n vertices such that $n \geq 4$, $NK_{ve}(C_n) = NK_{ev}(C_n) = 4^n$.

Proof. From the Example 4.5 we can directly write that $NK_{ve}(C_n) = 4^n$. Clearly, from the definition of ev -degree, every edge of C_n is 4_{ev} -regular. The proof comes from this fact. \square

Proposition 4.11. For the S_n -star graph with n vertices such that $n \geq 4$, $NK_{ev}(S_n) = n^{n-1} < NK_{ve}(S_n) = (n - 1)^n$.

Proof. We make the proof by induction on n . For $n = 4$, $NK_{ev}(S_4) = 4^3 = 64 < NK_{ve}(S_4) = 3^4 = 81$, as desired. We assume that the claim is true for $n = k$ and we will show that it is true $n = k + 1$. For $n = k$, $k^{k-1} < (k - 1)^k$ is equivalent to

$$\left(1 + \frac{1}{k-1}\right)^{k-1} < k - 1$$

and for $n = k + 1$, $(k + 1)^k < k^{k+1}$. Thus we want to show that

$$\left(1 + \frac{1}{k}\right)^k < k. \left(1 + \frac{1}{k}\right)^k < \left(1 + \frac{1}{k-1}\right)^k = \left(1 + \frac{1}{k-1}\right)^{k-1} \left(1 + \frac{1}{k-1}\right) < (k - 1) \frac{k}{k-1} = k.$$

So, the proof is complete. \square

Theorem 4.12. (a) The n -vertex tree with maximal NK_{ve} is S_n such that $NK_{ve}(S_n) = (n - 1)^n$.
 (b) The n -vertex unicyclic graph with the maximal NK_{ve} is $S_n + e$ (depicted in Figure 1) such that $NK_{ve}(S_n + e) = n^3(n - 1)^{n-3}$.
 (c) The n -vertex bicyclic graph with the maximal NK_{ve} is Z_n (depicted in Figure 1) such that $NK_{ve}(Z_n) = (n + 1)^4(n - 1)^{n-4}$.



Figure 1. The graphs $S_n + e$ and Z_n .

Theorem 4.13. (a) The n -vertex tree with minimal NK_{ve} is P_n ($n \geq 4$) such that $NK_{ve}(P_n) = 9 \cdot 4^{n-3}$.
 (b) The n -vertex unicyclic graph with the minimal NK_{ve} is R_n (depicted in Figure 2) such that $NK_{ve}(R_n) = 2 \cdot 3 \cdot 5^2 \cdot 4^{n-4}$.
 (c) The n -vertex bicyclic graph with the minimal NK_{ve} is T_n (depicted in Figure 2) such that $NK_{ve}(T_n) = 5^4 \cdot 4^{n-4}$.

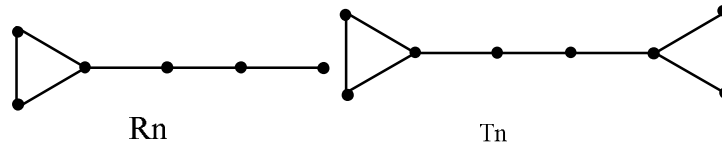


Figure 2. Graphs which are used for Theorem 2.

Theorem 4.14. (a) The n -vertex tree with second maximal NK_{ve} is X_n (depicted in Figure 3) such that $NK_{ve}(X_n) = 2(n - 1)^2(n - 2)^{n-3}$.
 (b) The n -vertex unicyclic graph with second maximal NK_{ve} is $S_n + e + e'$ (depicted in Figure 4) such that $NK_{ve}(S_n + e + e') = 4 \cdot n^3(n - 2)^{n-4}$.
 (c) The n -vertex bicyclic graph with second maximal NK_{ve} is L_n (depicted in Figure 3) such that $NK_{ve}(L_n) = 5 \cdot (n + 1)^2 n^2 (n - 2)^{n-5}$.

Theorem 4.15. (a) The n -vertex tree with second minimal NK_{ve} is the Q -graph (depicted in Figure 5) such that $NK_{ve}(Q) = 2^2 \cdot 3^3 \cdot 5^3 \cdot 4^{n-8}$.
 (b) The n -vertex unicyclic graph with second minimal NK_{ve} is the R -graph (depicted in Figure 6) such that $NK_{ve}(R) = 2 \cdot 3^2 \cdot 5^5 \cdot 4^{n-8}$.

(c) The n -vertex bicyclic graph with second minimal NK_{ve} is the S -graph (depicted in Figure 7) such that $NK_{ve}(S) = 3.5^7 \cdot 4^{n-8}$.

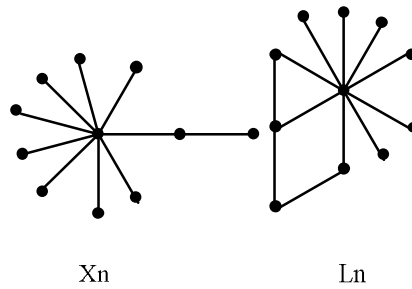


Figure 3. The graph X_n and L_n .

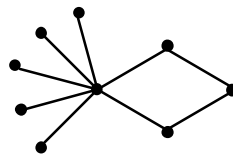


Figure 4. The graph $S_n + e + e'$.

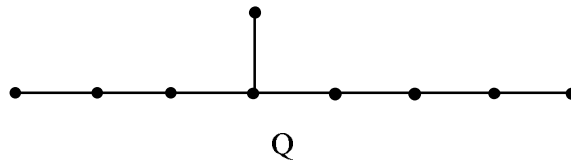


Figure 5. The graph Q .

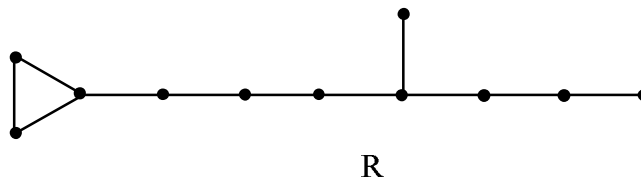


Figure 6. The graph R .

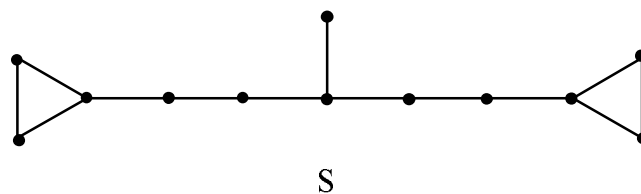


Figure 7. The graph S .

Corollary 4.16. For any triangle-free graph G , $NK_{ev}(G) = \prod_1^*(G)$.

Proof. The proof directly comes from the Observation 2.5, the Definition 2.17 and the definition of multiplicative version of the first Zagreb index. \square

Now, we give some mathematical properties of ev -degree and ve -degree Zagreb indices in terms of the forgotten topological index and the total number of the triangles $n(G)$ of a connected graph G . Before giving propositions, we give following terminologies which be used.

Theorem 4.17. *Let G be a connected graph, then*

$$S(G) = F(G) + 2M_2(G) - 2 \sum_{uv \in E(G)} (\deg(u) + \deg(v)) n_e + \sum_{e=uv \in E(G)} n_e^2.$$

Proof. We know that $c_{e=uv} = \deg(u) + \deg(v) - n_e$ and $S = S(G) = \sum_{e \in E(G)} c_e^2$. Therefore,

$$\begin{aligned} S &= S(G) = \sum_{e=uv \in E(G)} c_e^2 = (\deg(u) + \deg(v) - n_e)^2 \\ &= \sum_{e=uv \in E(G)} (\deg(u) + \deg(v))^2 - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v)) n_e \\ &\quad + \sum_{e=uv \in E(G)} n_e^2 \\ &= \sum_{e=uv \in E(G)} (\deg(u)^2 + \deg(v)^2) + 2 \sum_{e=uv \in E(G)} \deg(u) \deg(v) \\ &\quad - 2 \sum_{e=uv \in E(G)} (\deg(u) + \deg(v)) n_e + \sum_{e=uv \in E(G)} n_e^2 \\ &= F(G) + 2M_2(G) - 2 \sum_{uv \in E(G)} (\deg(u) + \deg(v)) n_e + \sum_{e=uv \in E(G)} n_e^2. \end{aligned}$$

\square

Theorem 4.18. *Let G be a connected graph, then $S^\beta(G) = 2M_2(G) - 6n(G)$, where $n(G)$ denotes the total number of triangles in G .*

Proof. From the definition of the first ve -degree Zagreb beta index and Lemma 4.2 we get

$$\begin{aligned} S^\beta(G) &= \sum_{uv \in E(G)} (c_u + c_v) \\ &= \sum_{uv \in E(G)} [(\sum_{w \in N(u)} \deg(w) - n_u) + (\sum_{w \in N(v)} \deg(w) - n_v)] \\ &= \sum_{uv \in E(G)} (\sum_{w \in N(u)} \deg(w) + \sum_{w \in N(v)} \deg(w)) - \sum_{uv \in E(G)} (n_u + n_v) \\ &= S^\beta(G) = 2M_2(G) - 6n(G). \end{aligned}$$

\square

Theorem 4.19. *Let G be a connected graph, then*

$$S^\alpha(G) = F(G) - 2 \sum_{v \in V(G)} (\sum_{u \in N(v)} \deg(u) n_v) + \sum_{v \in V(G)} n_v^2$$

where n_v denotes the number of triangles in G containing the vertex v .

Proof. From the definition of the first ve -degree Zagreb alpha index and Lemma 4.2 we get

$$\begin{aligned}
S^\alpha(G) &= \sum_{v \in V(G)} c_v^2 = \sum_{v \in V(G)} \sum_{u \in N(v)} (\deg(u) - n_v)^2 \\
&= \sum_{v \in V(G)} \left[\left(\sum_{u \in N(v)} \deg(u) \right)^2 - 2 \sum_{u \in N(v)} \deg(u) n_v + n_v^2 \right] \\
&= \sum_{v \in V(G)} \left(\sum_{u \in N(v)} \deg(u) \right)^2 - 2 \sum_{v \in V(G)} \left(\sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2 \\
&= \sum_{v \in V(G)} \deg(v)^3 - 2 \sum_{v \in V(G)} \left(\sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2 \\
&= F(G) - 2 \sum_{v \in V(G)} \left(\sum_{u \in N(v)} \deg(u) n_v \right) + \sum_{v \in V(G)} n_v^2.
\end{aligned}$$

□

It is very surprisingly to see that for any triangle free graph the forgotten topological index and the first ve -degree Zagreb alpha index equal each other. The following corollary states this fact.

Corollary 4.20. *Let G be a triangle-free connected graph, then $S^\alpha(G) = F(G)$.*

5. CONCLUSION

In this study we defined ev -degree and ve -degree Narumi-Katayama indices and showed that these novel degree based topological indices can be used possible tools for QSPR researches. Also we investigated some basic mathematical properties of ev -degree and ve -degree Narumi-Katayama and Zagreb indices. It can be interesting to compute the exact value of ev -degree and ve -degree topological indices for some graph operations. It can also be interesting to investigate the ev -degree and ve -degree concepts for the other topological indices for further studies.

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