

On Van Degrees of Vertices and Van Indices of Graphs

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Abstract: Topological indices have been used to modeling biological and chemical properties of molecules in quantitative structure property relationship studies and quantitative structure activity studies. All the degree based topological indices have been defined via classical degree concept. In this paper we define two novel degree concepts for a vertex of a simple connected graph: Van degree and reverse Van degree. And also we define Van and reverse Van indices of a simple connected graph by using the Van degrees concepts. We compute the Van and reverse Van indices for well-known simple connected graphs such as paths, stars, complete graphs and cycles.

Keywords: Van Degrees, Reverse Van Degrees, Van Indices, Reverse Van Indices, Topological Indices, QSAR, QSPR

1. Introduction

Graph theory has many applications to modeling real world situations from the basic sciences to engineering and social sciences. Chemical graph theory has an important effect on the development of the chemical sciences by using topological indices. A topological index, which is a graph invariant it does not depend on the labeling or pictorial representation of the graph, is a numerical parameter mathematically derived from the graph structure. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physicochemical properties or biological activity. These indices are used in quantitative structure property relations (QSPR) research. Topological indices are important tools for analyzing some physicochemical properties of molecules without performing any experiment. The first distance based topological index was proposed by Wiener (1947) for modeling physical properties of alkanes, and after him, hundred topological indices were defined by chemists and mathematicians and so many properties of chemical structures were studied [1]. More than forty years ago Gutman & Trinajstić (1971) defined Zagreb indices which are degree based topological indices [2]. These topological indices were proposed to be measures of branching of the carbon-atom skeleton in [3]. The Randić and Zagreb indices are the most used topological indices in

chemical and mathematical literature so far. For detailed discussions of both these indices and other well-known topological indices, we refer the interested reader [4-14] and references therein. In 1998, Estrada *et al* modelled the enthalpy of formation of alkanes by using atom-bond connectivity (ABC) index [15]. The ABC index for a connected graph G defined as;

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u) \times \deg(v)}} \quad (1)$$

There are many open problems related to ABC index in the mathematical chemistry literature. We refer the interested reader the studies of the last two years [16-20].

In 2009, Vukičević and Furtula defined geometric-arithmetic (GA) index and compared GA index with the well-known Randić index [21]. The authors showed that the GA index give better correlation to modelling standard enthalpy of vaporization of octane isomers. The GA index for a connected graph G defined as;

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\deg(u) \times \deg(v)}}{\deg(u) + \deg(v)} \quad (2)$$

After that many studies related to GA index were conducted in view of mathematical chemistry and QSPR researches [22-26].

The harmonic index was defined by Zhong in 2012 [27]. The H index for a connected graph G defined as;

$$H(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)} \quad (3)$$

The relationships between harmonic index and domination like parameters were investigated by Li *et al.* [28] We refer the interested reader for the article related to H index by Ilić and the references therein [29].

The sum-connectivity index (χ) were defined by Zhou and Trinajstić in 2009 [30]. The χ index for a connected graph G defined as;

$$\chi(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v))^{-1/2} \quad (4)$$

Farahani computed the sum-connectivity index of carpa designed cycle [31] and Akhter *et al* investigated the sum-connectivity index of cacti [32].

As of now in the chemical and mathematical literature all degree based topological indices have been defined by using classical degree concept.

In this study our aim is to define two novel degree concepts namely, Van degrees and reverse Van degrees. Also by using Van and reverse Van degrees, we define the first, the second and the third Van and reverse Van indices for a simple connected graph. We choose the name “Van” inspired by the well-known Zagreb indices. Van is the most beautiful city from the eastern Anatolian region of Turkey.

2. Van Degrees and Van Indices

In this section we give basic definitions and facts about above mentioned graph invariants. 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 , $N[v]$.

For a vertex v , $S_v = \sum_{u \in N(v)} \deg(u)$. For convince, we name S_v as “the sum degree of v ” or briefly “sum degree”. For a vertex v , $M_v = \prod_{u \in N(v)} \deg(u)$. For convince, we name M_v as “the multiplication degree of v ” or briefly “multiplication degree”.

Definition 2.1. The Van degree of a vertex v of a simple connected graph G defined as;

$$van(v) = \frac{\sum_{u \in N(v)} \deg(u)}{\prod_{u \in N(v)} \deg(u)} = \frac{S_v}{M_v} \quad (5)$$

Definition 2.2. The reverse Van degree of a vertex v of a simple connected graph G defined as;

$$rvan(v) = \frac{\prod_{u \in N(v)} \deg(u)}{\sum_{u \in N(v)} \deg(u)} = \frac{M_v}{S_v} \quad (6)$$

Definition 2.3. The first Van index of a simple connected graph G defined as;

$$Van^1(G) = \sum_{v \in V(G)} van(v)^2 \quad (7)$$

Definition 2.4. The second Van index of a simple

connected graph G defined as;

$$Van^2(G) = \sum_{uv \in E(G)} van(u)van(v) \quad (8)$$

Definition 2.5. The third Van index of a simple connected graph G defined as;

$$Van^3(G) = \sum_{uv \in E(G)} [van(u) + van(v)] \quad (9)$$

Definition 2.6. The first reverse Van index of a simple connected graph G defined as;

$$Van^{1r}(G) = \sum_{v \in V(G)} rvan(v)^2 \quad (10)$$

Definition 2.4. The second reverse Van index of a simple connected graph G defined as;

$$Van^{2r}(G) = \sum_{uv \in E(G)} rvan(u)rvan(v) \quad (11)$$

Definition 2.5. The third reverse Van index of a simple connected graph G defined as;

$$Van^{3r}(G) = \sum_{uv \in E(G)} [rvan(u) + rvan(v)] \quad (12)$$

Proposition 2.6. Let K_n be a complete graph with n vertices ($n \geq 3$). Then;

- a. $Van^1(K_n) = \frac{n}{(n-1)^{2(n-3)}}$
- b. $Van^2(K_n) = \frac{n}{2(n-1)^{2n-7}}$
- c. $Van^3(K_n) = \frac{n}{(n-1)^{n-4}}$
- d. $Van^{1r}(K_n) = n(n-1)^{2(n-3)}$
- e. $Van^{2r}(K_n) = \frac{1}{2}n(n-1)^{(2n-5)}$
- f. $Van^{3r}(K_n) = n(n-1)^{n-2}$

Proof. Let $v \in K_n$. Then $S_v = (n-1)(n-1) = (n-1)^2$ and $M_v = (n-1)^{n-1}$. Therefore $van(v) = \frac{S_v}{M_v} = \frac{1}{(n-1)^{n-3}}$ and $rvan(v) = \frac{M_v}{S_v} = (n-1)^{n-3}$. We can begin to compute since all the vertices of complete graph have same Van degree and reverse Van degree.

- a. $Van^1(K_n) = \sum_{v \in V(K_n)} van(v)^2 = \frac{n}{(n-1)^{2(n-3)}}$
- b. $Van^2(K_n) = \sum_{uv \in E(K_n)} van(u)van(v) = \frac{n}{2(n-1)^{2n-7}}$
- c. $Van^3(K_n) = \sum_{uv \in E(K_n)} [van(u) + van(v)] = \frac{n}{(n-1)^{n-4}}$
- d. $Van^{1r}(K_n) = \sum_{v \in V(K_n)} rvan(v)^2 = n(n-1)^{2(n-3)}$
- e. $Van^{2r}(K_n) = \sum_{uv \in E(K_n)} rvan(u)rvan(v) = \frac{1}{2}n(n-1)^{(2n-5)}$
- f. $Van^{3r}(K_n) = \sum_{uv \in E(K_n)} [rvan(u) + rvan(v)] = n(n-1)^{n-2}$

Proposition 2.7. Let C_n be a cycle graph with n vertices ($n \geq 3$). Then;

- a. $Van^1(C_n) = n$
- b. $Van^2(C_n) = n$
- c. $Van^3(C_n) = 2n$
- d. $Van^{1r}(C_n) = n$
- e. $Van^{2r}(C_n) = n$
- f. $Van^{3r}(C_n) = 2n$

Proof. Let $v \in C_n$. Then $S_v = 2 + 2 = 4$ and $M_v = 2 \cdot 2 = 4$. Therefore $van(v) = \frac{S_v}{M_v} = 1$ and $rvan(v) = \frac{M_v}{S_v} = 1$. We

can begin to compute since all the vertices of cycle graph have same Van degree and reverse Van degree.

- a. $Van^1(C_n) = \sum_{v \in V(C_n)} van(v)^2 = n$
- b. $Van^2(C_n) = \sum_{uv \in E(C_n)} van(u)van(v) = n$
- c. $Van^3(C_n) = \sum_{uv \in E(C_n)} [van(u) + van(v)] = 2n$
- d. $Van^{1r}(C_n) = \sum_{v \in V(C_n)} rvan(v)^2$
- e. $Van^{2r}(C_n) = \sum_{uv \in E(C_n)} rvan(u)rvan(v) = n$
- f. $Van^{3r}(C_n) = \sum_{uv \in E(C_n)} [rvan(u) + rvan(v)] = 2n$

Proposition 2.8. Let P_n be a path graph with n vertices ($n \geq 3$). Then;

- a. $Van^1(P_n) = n + 5/2$
- b. $Van^2(P_n) = n + 1$
- c. $Van^3(P_n) = 4n - 4$
- d. $Van^{1r}(P_n) = n - 10/9$
- e. $Van^{2r}(P_n) = n - 7/3$
- f. $Van^{3r}(P_n) = 2n - 10/3$

Proof. Let $V(P_n) = \{v_1, v_2, \dots, v_n\}$ and $E(P_n) = \{v_1v_2, v_2v_3, \dots, v_{n-2}v_{n-1}, v_{n-1}v_n\}$. Then $S_{v_1} = S_{v_n} = 2$ and $M_v = 2$. Therefore $van(v_1) = van(v_n) = \frac{S_v}{M_v} = 1$ and $rvan(v_1) = rvan(v_n) = \frac{M_v}{S_v} = 1$. Also $S_{v_2} = S_{v_{n-1}} = 3$ and $M_{v_2} = M_{v_{n-1}} = 2$. Therefore $van(v_2) = van(v_{n-1}) = \frac{S_v}{M_v} = 3/2$ and $rvan(v_2) = rvan(v_{n-1}) = \frac{M_v}{S_v} = 2/3$ and $S_{v_3} = S_{v_4} = \dots = S_{v_{n-3}} = S_{v_{n-2}} = 4$ and $M_{v_3} = M_{v_4} = \dots = M_{v_{n-3}} = M_{v_{n-2}} = 4$. Therefore $van(v_3) = van(v_4) = \dots = van(v_{n-3}) = van(v_{n-2}) = 1$ and $rvan(v_3) = rvan(v_4) = \dots = rvan(v_{n-3}) = rvan(v_{n-2}) = 1$. Note that P_n has n -vertex and $n - 1$ edges.

We can begin our computations.

- a. $Van^1(P_n) = \sum_{v \in V(P_n)} van(v)^2 = 2.1 + 2.9/4 + (n - 4).1 = n + 5/2$
- b. $Van^2(P_n) = \sum_{uv \in E(P_n)} van(u)van(v) = 4.3/2 + (n - 5).1 = n + 1$
- c. $Van^3(P_n) = \sum_{uv \in E(P_n)} [van(u) + van(v)] = 4.5/2 + (n - 5).2 = 2n$
- d. $Van^{1r}(P_n) = \sum_{v \in V(P_n)} rvan(v)^2 = 2.1 + 2.4/9 + (n - 4).1 = n - 10/9$
- e. $Van^{2r}(P_n) = \sum_{uv \in E(P_n)} rvan(u)rvan(v) = 4.2/3 + (n - 5).1 = n - 7/3$
- f. $Van^{3r}(P_n) = \sum_{uv \in E(P_n)} [rvan(u) + rvan(v)] = 4.5/3 + (n - 5).2 = 2n - 10/3$

Proposition 2.8. Let S_n be a star graph with n vertices ($n \geq 3$). Then;

- a. $Van^1(S_n) = n(n - 1)$
- b. $Van^2(S_n) = (n - 1)^2$
- c. $Van^3(S_n) = n(n - 1)$
- d. $Van^{1r}(S_n) = \frac{(n-1)^3+1}{(n-1)^2}$
- e. $Van^{2r}(S_n) = 1$
- f. $Van^{3r}(S_n) = n$

Proof. There are two kind of vertices. For the central vertex v , $deg(v) = n - 1$ and for any pendent vertex u , $deg(u) = 1$. Then $S_v = n - 1$ and $M_v = 1$. Also for any pendent vertex u , $S_u = n - 1$ and $M_u = n - 1$. Therefore

$van(v) = \frac{S_v}{M_v} = n - 1$ and $rvan(v) = \frac{M_v}{S_v} = 1/(n - 1)$. Also $van(u) = \frac{S_u}{M_u} = 1$ and $rvan(u) = \frac{M_u}{S_u} = 1$.

Note that S_n has n -vertex and $n - 1$ edges.

We can begin our computations.

- a. $Van^1(S_n) = \sum_{v \in V(S_n)} van(v)^2 = (n - 1)^2 + (n - 1).1 = n^2 - n = n(n - 1)$
- b. $Van^2(S_n) = \sum_{uv \in E(S_n)} van(u)van(v) = (n - 1).(n - 1).1 = (n - 1)^2$
- c. $Van^3(S_n) = \sum_{uv \in E(S_n)} [van(u) + van(v)] = (n - 1).(n - 1 + 1) = n(n - 1)$
- d. $Van^{1r}(S_n) = \sum_{v \in V(S_n)} rvan(v)^2 = \frac{1}{(n-1)^2} + (n - 1).1 = \frac{(n-1)^3+1}{(n-1)^2}$
- e. $Van^{2r}(S_n) = \sum_{uv \in E(S_n)} rvan(u)rvan(v) = (n - 1).1/(n - 1) = 1$
- f. $Van^{3r}(S_n) = \sum_{uv \in E(S_n)} [rvan(u) + rvan(v)] = (n - 1).(1/(n - 1) + 1) = n$

3. Conclusions

There are many problems for further studies about the Van indices. The mathematical properties and relations between Van indices and other topological indices are interesting problems worth to study. Also QSPR analysis of Van indices may be attract attention of some mathematical chemists.

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