On Van Degrees of Vertices and Van Indices of Graphs

Süleyman Ediz*, Mesut Semiz

Department of Mathematics Education, Faculty of Education, Yüzüncü Yıl University, Van, Turkey

Email address: suleymanediz@yyu.edu.tr (S. Ediz), mesutsemiz@gmail.com (M. Semiz)

*Corresponding author

To cite this article: Süleyman Ediz, Mesut Semiz. On Van Degrees of Vertices and Van Indices of Graphs. Mathematics and Computer Science. Vol. 2, No. 4, 2017, pp. 35-38. doi: 10.11648/j.mcs.20170204.11

Received: May 11, 2017; Accepted: May 27, 2017; Published: July 7, 2017

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 alcanes, 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 alcanes by using atom- bond connectivity (ABC) index [15]. The ABC index for a connected graph $G$ defined as:

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

(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:

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

(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;
\[ H(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)} \] (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 \( \chi \) were defined by Zhou and Trinajstić in 2009 [30]. The \( \chi \) index for a connected graph \( G \) defined as;

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

Farahani computed the sum-connectivity index of carpa 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 converse, 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 converse, 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;

\[ \text{van}(v) = \frac{\sum_{u \in N(v)} \deg(u)}{\sum_{u \in N(v)} \deg(u)} = \frac{S_v}{M_v} \] (5)

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

\[ \text{rvan}(v) = \frac{\prod_{u \in N(v)} \deg(u)}{\sum_{u \in N(v)} \deg(u)} = \frac{M_v}{S_v} \] (6)

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

\[ \text{Van}^1(G) = \sum_{v \in V(G)} \text{van}(v)^2 \] (7)

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

\[ \text{Van}^2(G) = \sum_{uv \in E(G)} \text{van}(u)\text{van}(v) \] (8)

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

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

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

\[ \text{Van}^1r(G) = \sum_{v \in V(G)} \text{rvan}(v)^2 \] (10)

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

\[ \text{Van}^2r(G) = \sum_{uv \in E(G)} \text{rvan}(u)\text{rvan}(v) \] (11)

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

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

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

a. \( \text{Van}^1(K_n) = \frac{n}{(n-1)^2(n-3)} \)

b. \( \text{Van}^2(K_n) = \frac{n^2}{2(n-1)^2(n-3)} \)

c. \( \text{Van}^3(K_n) = \frac{n^3}{3(n-1)^2(n-3)} \)

d. \( \text{Van}^1r(K_n) = n(n-1)^2(n-3) \)

e. \( \text{Van}^2r(K_n) = \frac{n(n-1)^2(n-3)}{2} \)

f. \( \text{Van}^3r(K_n) = n(n-1)^2(n-3) \)

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

a. \( \text{Van}^1(K_n) = \sum_{v \in V(K_n)} \text{van}(v)^2 = \frac{n}{(n-1)^2(n-3)} \)

b. \( \text{Van}^2(K_n) = \sum_{v \in V(K_n)} \text{van}(u)\text{van}(v) = \frac{n^2}{2(n-1)^2(n-3)} \)

c. \( \text{Van}^3(K_n) = \sum_{v \in V(K_n)} [\text{van}(u) + \text{van}(v)] = \frac{n^3}{3(n-1)^2(n-3)} \)

d. \( \text{Van}^1r(K_n) = \sum_{v \in V(K_n)} \text{rvan}(u)\text{rvan}(v) = n(n-1)^2(n-3) \)

e. \( \text{Van}^2r(K_n) = \sum_{v \in V(K_n)} \text{rvan}(u)\text{rvan}(v) = \frac{n(n-1)^2(n-3)}{2} \)

f. \( \text{Van}^3r(K_n) = n(n-1)^2(n-3) \)

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

a. \( \text{Van}^1(C_n) = n \)

b. \( \text{Van}^2(C_n) = n \)

c. \( \text{Van}^3(C_n) = 2n \)

d. \( \text{Van}^1r(C_n) = n \)

e. \( \text{Van}^2r(C_n) = n \)

f. \( \text{Van}^3r(C_n) = 2n \)

Proof. Let \( v \in C_n \). Then \( S_v = 2 + 2 = 4 \) and \( M_v = 2 + 2 = 4 \). We
can begin to compute since all the vertices of cycle graph
have same Van degree and reverse Van degree.
\[ a. \text{Van}^1(C_n) = \sum_{v \in V(C_n)} \text{van}(v)^2 = n \]
\[ b. \text{Van}^2(C_n) = \sum_{u \in E(C_n)} \text{van}(u) \text{van}(v) = n \]
\[ c. \text{Van}^3(C_n) = \sum_{v \in V(C_n)} [\text{van}(u) + \text{van}(v)] = 2n \]
\[ d. \text{Van}^r(C_n) = \sum_{v \in V(C_n)} \text{rvan}(v)^2 \]
\[ e. \text{Van}^{2r}(C_n) = \sum_{u \in E(C_n)} \text{rvan}(u) \text{rvan}(v) = n \]
\[ f. \text{Van}^{3r}(C_n) = \sum_{u \in E(C_n)} [\text{rvan}(u) + \text{rvan}(v)] = 2n \]

Proposition 2.8. Let \( P_n \) be a path graph with \( n \) vertices
\((n \geq 3)\). Then;
\[ a. \text{Van}^1(P_n) = n + 5/2 \]
\[ b. \text{Van}^2(P_n) = n + 1 \]
\[ c. \text{Van}^3(P_n) = 4n - 4 \]
\[ d. \text{Van}^r(P_n) = n - 10/9 \]
\[ e. \text{Van}^{2r}(P_n) = n - 7/3 \]
\[ f. \text{Van}^{3r}(P_n) = 2n - 10/3 \]

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

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

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.

References

[1] H. Wiener, Structural Determination of Paraffin Boiling
Points, J. Am. Chem. Soc., 69, 17-20, 1947.
[2] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals.
Total π-electron energy of alternant hydrocarbons, Chem.
Phys. Lett., 17, 535-538, 1971.
[3] I. Gutman, B. Ruščić, N. Trinajstić, C. N. Wilcox, Graph
Theory and Molecular Orbitals. XII. Acyclic Polyenes, J.
Chem. Phys. 62, 3399-3405, 1975.
[4] M. Randić, On characterization of molecular branching, J.
Amer. Chem. Soc. 97, 6609–6615, 1975.
[5] Q. Cui, L. Zhong, The general Randić index of trees with
given number of pendent vertices. Appl. Math. Comput. 302,
111-121, 2017.
[6] Z. Chen, G. Su, L. Volkmann, Sufficient conditions on the
zeroth-order general Randić index for maximally edge-
connected graphs. Discrete Appl. Math. 218, 64–70, 2017.
[7] W. Gao, M. K. Jamil, M. R. Farahani, The hyper-Zagreb
index and some graph operations. J. Appl. Math. Comput. 54,
263–275, 2017.
[8] S. Ediz, Reduced second Zagreb index of bicyclic graphs
with pendent vertices. Matematiche (Catania) 71, 135–147,
2016.
[9] S. Ediz, Maximum chemical trees of the second reverse
Zagreb index. Pac. J. Appl. Math. 7, 287–291, 2015.
[10] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index. MATCH Commun. Math. Comput. Chem. 74, 97–101, 2015.

[11] D. Vukičević, J. Sedlar, D. Stevanovic, Comparing Zagreb Indices for Almost All Graphs, MATCH Commun. Math. Comput. Chem. 78, no. 2, 323-336, 2017.

[12] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, New bounds of degree–based topological indices for some classes of c-cyclic graphs, Discr. Appl. Math. 184, 62–75, 2015.

[13] K. C. Das, K. Xu, J. Nam, Zagreb indices of graphs, Front. Math. China 10, 567–582, 2015.

[14] R. M. Tache, On degree–based topological indices for bicyclic graphs, MATCH Commun.

[15] Math. Comput. Chem. 76, 99–116, 2016.

E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. Indian J. Chem. 37A, 849–855, 1998.

[16] L. Zhong, Q. Cui, On a relation between the atom bond connectivity and the first geometric arithmetic indices. Discrete Appl. Math., 185, 249–253, 2015.

[17] A. R. Ashrafi, Z. T. Dehghan, N. Habibi, Extremal atom bond connectivity index of cactus graphs. Commun. Korean Math. Soc. 30, 283–295, 2015.

[18] B. Furtula, Atom bond connectivity index versus Graovac Ghorbani analog. MATCH Commun. Math. Comput. Chem. 75, 233–242, 2016.

[19] D. Dimitrov, On structural properties of trees with minimal atom bond connectivity index II: Bounds on and branches. Discrete Appl. Math. 204, 90–116, 2016.

[20] X. M. Zhang, Y. Yang, H. Wang, X. D. Zhang, Maximum atom bond connectivity index with given graph parameters. Discrete Appl. Math. 215, 208–217, 2016.

[21] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. J. Math. Chem. 46, 1369–1376, 2009.

[22] Y. Yuan, B. Zhou, N. Trinajstić, On geometric arithmetic index. J. Math. Chem. 47, 833–841, 2010.

[23] K. C. Das, On geometric arithmetic index of graphs. MATCH Commun. Math. Comput. Chem. 64, 619–630, 2010.

[24] Z. Raza, A. A. Bhatti, A. Ali, More on comparison between first geometric arithmetic index and atom bond connectivity index. Miskolc Math. Notes 17, 561–570, 2016.

[25] W. Gao, A note on general third geometric arithmetic index of special chemical molecular structures. Commun. Math. Res. 32, 131–141, 2016.

[26] M. An, L. Xiong, G. Su, The k ordinary generalized geometric index. Util. Math., 100; 383–405, 2016.

[27] L. Zhong, The harmonic index for graphs. Applied Mathematics Letters. 25, 561–566, 2012.

[28] J. Li, J. B. Lv, Y. Liu, The harmonic index of some graphs. Bull. Malays. Math. Sci. Soc. 39, 331–340, 2016.

[29] A. Ilić, Note on the harmonic index of a graph. Ars Combin. 128, 295–299, 2016.

[30] B. Zhou, N. Trinajstić, On a novel connectivity index. J. Math. Chem. 46, 1252–1270, 2009.

[31] M. R. Farahani, Randić connectivity and sum connectivity indices for Capra designed of cycles. Pac. J. Appl. Math. 7, 11–17, 2015.

[32] S. Akhter, M. Imran, Z. Raza, On the general sum connectivity index and general Randić index of cacti. J. Inequal. Appl. 300, 2016.