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GUTMAN INDEX – A CRITICAL PERSONAL ACCOUNT

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Dedicated to Aleksandar Ivić (1949–2020)

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A b s t r a c t. In the recent literature there are numerous publications concerned with a graph invariant named "Gutman index" (ZZ). In this paper, some details about the discovery of ZZ are explained. In particular, it is pointed out that the name for ZZ is a result of negligence, caused by a sloppy reading of the article in which ZZ was mentioned for the first time. The main mathematical properties of ZZ are presented. The reasons why ZZ became popular among scholars doing research in graph theory and mathematical chemistry are discussed, and the practical applicability of ZZ (which is minor) commented.

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1. *Introduction*

In this paper we are concerned with a graph invariant

$$ZZ = ZZ(G) = \sum_{\{u,v\} \subseteq \mathbf{V}(G)} \big[d(u) \times d(v)\big]\, d(u,v) \tag{1.1}$$

and with two other closely related invariants

$$DD = DD(G) \quad = \sum_{\{u,v\}\subseteq \mathbf{V}(G)} \big[d(u) + d(v)\big]\, d(u,v) \tag{1.2}$$

$$W = W(G) \quad = \sum_{\{u,v\}\subseteq \mathbf{V}(G)} d(u,v) \tag{1.3}$$

where G denotes a graph of order n with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$, and where $d(x) = d(x|G)$ is the degree (number of first neighbors) of the vertex $x \in \mathbf{V}(G)$, whereas $d(x,y) = d(x,y|G)$ is the distance between the vertices $x,y \in \mathbf{V}(G)$ (= length of a shortest path connecting x and y). Throughout this paper it is assumed that G is connected, and $n \geq 2$.

Most of our considerations pertain to trees. Recall that a tree is a connected graph with n vertices and $m = n-1$ edges. Trees are graphs without cycles.

In the current chemical and mathematical literature, several hundred graph invariants are being considered, viewed to be molecular structure descriptors, and claimed to be related with some physical, chemical, pharmacological, or toxicological property of the underlying chemical compounds. These are usually referred to as "*topological indices*". Among them are also ZZ, XX, and W. The index DD is called *degree distance*, W is called *Wiener index*, whereas the name of ZZ will be disclosed later.

2. *History: before* ZZ

The Wiener index W, Eq. (1.3), is the oldest among topological indices. It was put forward by Harold Wiener in 1947 [23]. After a latent period of ca. 25 years, an extensive study of W started [4, 12, 24], and is still happening (see e.g., [2, 3, 13]).

In 1989, Harry Schultz introduced a new topological index, and named it "*molecular topological index*" (MTI) [16]. Eventually, the same author and the members of his family published a whole series of papers [17], [18], etc. [19], proposing additional graph invariants similar to MTI. Therefore, the colleagues did not consider these new topological indices as something serious, their later study was minor, and is by now almost completely abandoned.

In 1994, Andrey Dobrynin and Amide Kochetova conceived the degree distance DD, Eq. (1.2) [5]. This index was viewed as a modification of the Wiener index. Namely, the Wiener index is the sum of all distances in the considered graph, each distance having the same weight. The idea of Dobrynin and Kochetova was to increase the effect of branched vertices (whose distance is usually small), or – what is the same – to diminish the effect of pairs of vertices at greater distance.

It seems that the authors of [5] were not aware of the paper [16]. Anyway, MTI and DD are closely related as

$$DD(G) = MTI(G) - \sum_{u \in \mathbf{V}(G)} d(u|G)^2 \,. \tag{2.1}$$

For details on MTI and the relation (2.1), see [7].

In the 1990s and later, DD became a popular topic for mathematical studies, see the recent papers [1, 10, 15, 22], and also [26, 32], as well as the references cited therein.

In the case of trees, in the early 1990s, a simple linear relation between MTI and W was discovered. This regularity was first reported in [14], and was obtained by means of computer–aided numerical calculations. Its rigorous mathematical proof was given by Douglas Klein [11]. All this happened before the publication of the Dobrynin–Kochetova article [5]. If we bear in mind Eq. (2.1), then the respective result can be stated as:

Theorem 2.1. *Let T be a tree of order n. Then its molecular topological index, degree distance, and Wiener index are related as*

$$\begin{aligned} MTI(G) &= 4\,W(T) - n(n-1) + \sum_{u \in \mathbf{V}(G)} d(u|G)^2 \\ DD(T) &= 4\,W(T) - n(n-1)\,. \end{aligned} \tag{2.2}$$

3. *History: towards* $\boldsymbol{ZZ}$

In the early 1990s there was no e-mail, and scholars had to communicate by regular mail (later dubbed “snail-mail”). There were telephone and fax, but for a poor Serbian scientist, these were too expensive to be used. Interestingly, these technical details resulted in the formulation of the ZZ-index and the discovery of Theorem 3.1.

In that time, the present author (I.G.) learned about the result that later was published in [14], and was told that Klein has a proof. He sent a letter to Klein (to USA), asking him for details of the proof. Indeed, Klein promptly replied and sent to I.G. his (in that time unpublished) proof. The time between sending a letter to Klein and receiving his reply, in the best case, could be a few weeks. In this period, I.G. decided to construct a proof himself, just to show that he too could do the same. It happened that Klein’s and I. G.’s proofs of Theorem 2.1 were completely different [11, 6].

Working on his proof of Theorem 2.1, I. G. noticed that a fully analogous results could be obtained if the summations $\big[d(u) + d(v)\big]$ in Eq. (1.2) is replaced by multiplication $\big[d(u) \times d(v)\big]$. This could be stated as:

Theorem 3.1. *Let T be a tree of order n. Then the ZZ-index, Eq.* (1.1)*, and Wiener index are related as*

$$ZZ(T) = 4\,W(T) - (2n-1)(n-1)\,. \tag{3.1}$$

I.G.'s proofs of Theorems 2.1 and 3.1 were eventually published in [6]. As a curiosity, we mention that [6] appeared immediately after the Dobrynin–Kochetova article [5].

Important: The graph invariant ZZ appeared in the paper [6] for the first time. In [6], it was clearly indicated that ZZ is not a newly proposed topological index, but that it was mentioned only because of its curios analogy with MTI and DD, Eqs. (2.2) and (3.1). To comprehend this, one only would need to read the paper [6] with a necessary understanding. Unfortunately, this was not always the case.

In the "*Handbooks of Molecular Descriptors*" by Todeschini and Consonni [20] the quantity ZZ was included among topological indices. Even worse, it was named "*Gutman index*". This reveals the sloppiness and lack of care in which the *Handbook* was compiled. The same failure was repeated in its next edition [21].

As one could expect, the inadequate and unjustified name for ZZ was eventually accepted in the mathematical and chemical literature, and is nowadays in standard use. The articles [25]–[64] have "Gutman index" in their titles, whereas the same name for ZZ is used in many more papers.

For readers who speak Serbian, ZZ-index should be pronounced as "zez-indeks", which then will get a proper and deserved meaning.

4. *Mathematical properties of ZZ-index*

Let S_n and P_n denote, respectively, the star and path of order n.

Theorem 4.1 ([44])**.** (a) *Among trees of order n, the star S_n, and only the star, has minimal value of the ZZ-index.*

(b) *Among trees of order n, the path P_n, and only the path, has maximal value of the ZZ-index.*

(c) *If T is a tree of order n, $T \ncong S_n, P_n$, then*

$$(n-1)(2n-3) = ZZ(S_n) < ZZ(T) < ZZ(P_n) = \frac{1}{3}(n-1)(2n^2-4n+3)\,.$$

PROOF.Theorem 4.1 directly follows from Eq. (3.1) and the earlier known bounds for the Wiener index of trees [4, 24]. □

It could be shown [9] that the star S_n has minimal ZZ-index among all connected graphs with n vertices. The search for the graph(s) with maximal ZZ [9], did not yield a conclusive result.

The result for degree distance, analogous to Theorem 4.1, reads:

Theorem 4.2. (a) *Among trees of order n, the star S_n, and only the star, has minimal degree distance.*

(b) *Among trees of order n, the path P_n, and only the path, has maximal degree distance.*

(c) *If T is a tree of order n, $T \ncong S_n, P_n$, then*

$$(n-1)(3n-4) = DD(S_n) < DD(T) < DD(P_n) = \frac{1}{3}\, n(n-1)(2n-1)\,.$$

The most remarkable result in the theory of ZZ-index is Theorem 4.3, which is a straightforward consequence of Eqs. (2.2) and (3.1).

Theorem 4.3. *If T is a tree of order n, then*

$$DD(T) - ZZ(T) = (n-1)^2\,.$$

A detailed analysis of Theorem 4.3 can be found in [9].

This surprising and counterintuitive result shows that the difference of degree distance and ZZ-index is insensitive of any structural detail of the underlying tree, and depends only on its order. In other words, the expression

$$\sum_{\{u,v\}\subseteq \mathbf{V}(G)} \big[d(u|T) + d(v|T) - du(u|T)\, d(v|T)\big]\, d(u,v|T)$$

is independent of both vertex degrees and distances of a tree T, and depends only of the number of vertices of T.

Theorems 2.1 and 3.1 show that the topological indices of the general form

$$\sum_{\{u,v\}\subseteq \mathbf{V}(T)} F\Big(d(u|T), d(v|T)\Big) d(u,v|T)$$

have special properties if either $F(x,y) = x+y$ or $F(x,y) = x \cdot y$. It would be interesting to find other functions $F(x,y)$ for which results analogous or similar to Theorems 2.1 and 3.1 hold [8]. Much work along these lines was done (by the present author), but without any success.

Another direction of research would be to extend the results of Theorems 2.1, 3.1, and 4.3 to cycle–containing graphs. If we exclude the trivial case of regular graphs, then – again – no success has been achieved. In [34] the following extension of Theorem 4.3 was obtained:

Theorem 4.4. *Let G be a connected graph of order n, with m edges and p pendent vertices. Then*

$$DD(G) - ZZ(G) \geq W(G) + (n-p-2)M_2(G) - \frac{1}{2}(n-p-3)M_1(G) - \frac{1}{2}(2m-n)(2m-n+1)(n-p-1) \tag{4.1}$$

where M_1 and M_2 are the first and second Zagreb indices, defined as [20]

$$M_1 = \sum_{u \in \mathbf{V}(G)} d(u)^2 \qquad \textit{and} \qquad M_2 = \sum_{uv \in \mathbf{E}(G)} d(u)\, d(v)\,.$$

Equality in (4.1) *is attained if and only if the distance between any two non-pendent vertices in G is at most* 2.

5. *Epilogue*

More than twenty years passed since the ZZ-index was listed among chemically relevant "topological indices" and unjustly named "Gutman index" [20]. This means that there was a tacit expectation that ZZ will find some application in modeling physical, chemical, pharmacological, or toxicological properties of at least some class of chemical compounds. As argued above, in our opinion, this was a mistake, caused by a careless reading of the paper [6]. Now, twenty years later, it became evident that our conclusion was correct: In no one of the great many papers on the ZZ-index [7, 9, 8], [25]–[64], there is any mention of chemical application. All these papers report mathematical investigations.

What happened and is happening with the ZZ-index is typical for contemporary activities in "applied" graph theory and mathematical chemistry. Scholars who do research in this field of science, usually are not interested whether their (easy) mathematical results have any actual application in chemistry or elsewhere (including "pure" mathematics), but their aim is just to publish one more paper.

REFERENCES

[1] Y. Alizadeh, S. Klavžar, *On the relation between degree distance and eccentric connectivity index*, MATCH Commun. Math. Comput. Chem. **84** (2020) 647–659.

[2] S. Bessy, F. Dross, K. Hriñákov, M. Knor, R. Škrekovski, *Maximal Wiener index for graphs with prescribed number of blocks*, Appl. Math. Comput. **380** (2020) #125274.

[3] S. Bessy, F. Dross, M. Knor, R. Škrekovski, *Graphs with the second and third maximum Wiener indices over the 2-vertex connected graphs*, Discr. Appl. Math. **284** (2020) 195–200.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001) 211–249.

[5] A. A. Dobrynin, A. A. Kochetova, *Degree distance of a graph: A degree analogue of the Wiener index*, J. Chem. Inf. Comput. Sci. **34** (1994) 1082–1086.

[6] I. Gutman, *Selected properties of the Schultz molecular topological index*, J. Chem. Inf. Comput. Sci. **34** (1994) 1087–1089.

[7] I. Gutman, *On two degree-and-distance-based graph invariants*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) **149** (2016) 21–31.

[8] I. Gutman, *On degree–and–distance–based topological indices*, Rev. Roum. Chim. **66** (2021) (to appear).

[9] I. Gutman, B. Furtula, K. C. Das, *On some degree–and–distance–based graph invariants of trees*, Appl. Math. Comput. **289** (2016) 1–6.

[10] H. Hua, H. Wang, X. Hu, *On eccentric distance sum and degree distance of graphs*, Discr. Appl. Math. **250** (2018) 262–275.

[11] D. J. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, *Molecular topological index: A relation with the Wiener index*, J. Chem. Inf. Comput. Sci. **32** (1992) 304–305.

[12] M. Knor, R. Škrekovski, A. Tepeh, *Mathematical aspects of Wiener index*, Ars Math. Contemp. **11** (2016) 327–352.

[13] H. Lin, *Extremal Wiener index of trees with prescribed path factors*, MATCH Commun. Math. Comput. Chem. **83** (2020) 85–94.

[14] D. Plavšić, S. Nikolić, N. Trinajstić, D. J. Klein, *Relation between the Wiener index and the Schultz index for several classes of chemical graphs*, Croat. Chem. Acta **66** (1993) 345–353.

[15] B. R. Rakshith, *A note on degree distance index*, Bull. Int. Math. Virt. Inst. **8** (2018) 155–159.

[16] H. P. Schultz, *Topological organic chemistry. 1. Graph theory and topological indices of alkanes*, J. Chem. Inf. Comput. Sci. **29** (1989) 227–228.

[17] H. P. Schultz, E. B. Schultz, T. P. Schultz, *Topological organic chemistry. 2. Graph theory, matrix determinants and eigenvalues and topological indices of alkanes*, J. Chem. Inf. Comput. Sci. **30** (1990) 27–29.

[18] H. P. Schultz, T. P. Schultz, *Topological organic chemistry. 3. Graph theory, binary and decimal adjacency matrices, and topological indices of alkanes*, J. Chem. Inf. Comput. Sci. **31** (1991) 144–147.

[19] H. P. Schultz, T. P. Schultz, *Topological organic chemistry. 12. Whole–molecule Schultz topological indices of alkanes*, J. Chem. Inf. Comput. Sci. **40** (2000) 107–112.

[20] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[21] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009, Vols. 1 & 2.

[22] W. Weng, B. Zhou, *On degree distance of hypergraphs*, MATCH Commun. Math. Comput. Chem. **84** (2020) 629–645.

[23] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947) 17–20.

[24] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, *A survey on graphs extremal with respect to distance–based topological indices*, MATCH Commun. Math. Comput. Chem. **71** (2014) 461–508.

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[25] V. S. Agnes, *Degree distance and Gutman index of corona product of graphs*, Trans. Comb. **4**(3) (2015) 11–23.

[26] B. Ali, M. Imran, M. A. Malik, H. M. A. Siddiqui, A. Bilal, M. R. Farahani, *Gutman index of some derived graphs*, Adv. Appl. Discr. Math. **20** (2019) 165–184.

[27] M. An, L. Xiong, *Two upper bounds for the Gutman indices of (four) F-sums of graphs*, Ars Comb. **143** (2019) 117–134.

[28] V. Andova, D. Dimitrov, J. Fink, R. Škrekovski, *Bounds on Gutman index*, MATCH Commun. Math. Comput. Chem. **67** (2012) 515–524.

[29] M. Arockiaraj, A. J. Shalini, *Extended cut method for edge Wiener, Schultz and Gutman indices with applications*, MATCH Commun. Math. Comput. Chem. **76** (2016) 233–250.

[30] M. Aruvi, V. Piramanantham, R. Muruganandam, *Reciprocal Gutman index of products of complete graphs*, Int. J. Engin. Sci. Res. Technol. **4** (2015) 108–113.

[31] M. Azari, *On the Gutman index of thorn graphs*, Kragujevac J. Sci. **40** (2018) 33–48.

[32] S. Brezovnik, N. Tratnik, *New methods for calculating the degree distance and the Gutman index*, MATCH Commun. Math. Comput. Chem. **82** (2019) 111–132.

[33] S. Chen, *Cacti with the smallest, second smallest, and third smallest Gutman index*, J. Comb. Optim. **31** (2016) 327–332.

[34] K. C. Das, G. Su, L. Xiong, *Relation between degree distance and Gutman index of graphs*, MATCH Commun. Math. Comput. Chem. **76** (2016) 221–232.

[35] L. Feng, *The Gutman index of unicyclic graphs*, Discr. Math. Algor. Appl. **4** (2012) #1250031.

[36] L. Feng, B. Liu, *The maximal Gutman index of bicyclic graphs*, MATCH Commun. Math. Comput. Chem. **66** (2011) 699–708.

[37] M. M. Feng, K. L. Wang, *Extreme values and rankings of Gutman index of double star trees*, J. Sci. Teachers' College Univ. 2017-04 (in Chinese).

[38] W. Gao, L. Liang, Y. Gao, *Total eccentricity, adjacent eccentric distance sum and Gutman index of certain special molecular graphs*, BioTechnology – An Indian Journal **10** (2014) 3837–3845.

[39] H. Guo, B. Zhou, *Properties of degree distance and Gutman index of uniform hypergraphs*, MATCH Commun. Math. Comput. Chem. **78** (2017) 213–220.

[40] Y. Hu, Y. Hou, Z. Ouyang, *The second–minimum Gutman index of the unicyclic graphs with given girth*, Ars Comb. **118** (2015) 293–304.

[41] V. Kaladevi, G. Kavitha, *Gutman and degree monophonic index of graphs*, Int. J. Innov. Technol. Explor. Engin. **8** (2019) 1982–1989.

[42] S. Kavithaa, V. Kaladevi, *Gutman index and detour Gutman index of pseudo-regular graphs*, . Appl. Math. **2017** (2017) #4180650 (8 pages).

[43] R. Kazemi, L. Meimondari, *Degree distance and Gutman index of increasing trees*, Trans. Comb. **5**(2) (2016) 23–31.

[44] M. Knor, P. Potočnik, R. Škrekovski, *Relationship between the edge–Wiener index and the Gutman index of a graph*, Discr. Appl. Math. **167** (2014) 197–201.

[45] J. Kok, C. Susanth, S. J. Kalayathankal, *A note on the Gutman index of Jaco graph*, Int. J. Pure Appl. Math. **106** (2016) 583–591.

[46] Y. Mao, K. C. Das, *Steiner Gutman index*, MATCH Commun. Math. Comput. Chem. **79** (2018) 779–794.

[47] J. P. Mazorodze, P. Mafuta, S. Munyira, *On the Gutman index and minimum degree of a triangle–free graph*, MATCH Commun. Math. Comput. Chem. **78** (2017) 231–240.

[48] J. P. Mazorodze, S. Mukwembi, T. Vetrík, *On the Gutman index and minimum degree*, Discr. Appl. Math. **173** (2014) 77–82.

[49] J. P. Mazorodze, S. Mukwembi, T. Vetrík, *The Gutman index and the edge-Wiener index of graphs with given vertex–connectivity*, Discuss. Math. Graph Theory **36** (2016) 867–876.

[50] J. Mazorodze, S. Mukwembi, T. Vetrík, *Gutman index, edge-Wiener index and edge-connectivity*, Trans. Comb. **9** (2020) 231–242.

[51] S. Mukwembi, *On the upper bound of Gutman index of graphs*, MATCH Commun. Math. Comput. Chem. **68** (2012) 343–348.

[52] R. Muruganandam, R. S. Manikandan, *Gutman index of some graph operations*, Int. J. Appl. Graph Theory **1**(2) (2017) 1–29.

[53] R. Muruganandam, R. S. Manikandan, M. Aruvi, *The multiplicative version of degree distance and the multiplicative version of Gutman index of strong product of some graphs*, Int. J. Appl. Math. Sci. **9** (2016) 29–40.

[54] R. Muruganandam, R. S. Manikandan, M. Aruvi, *The multiplicative versions of the reciprocal degree distance and the reciprocal Gutman index of some graph products*, Bull. Int. Math. Virt. Inst. **7** (2017) 581–594.

[55] K. Pattabiraman, *Product version of reciprocal Gutman indices of composite graphs*, Creat. Math. Inform. **26** (2017) 211–219.

[56] P. Paulraja, V. S. Agnes, *Gutman index of product graphs*, Discr. Math. Algor. Appl. **6** (2014) #1450058.

[57] R. S. Philipose, P. B. Sarasija, *Gutman index and Harary index of unitary Cayley graphs*, Int. J. Engin. Technol. **7** (2018) 1243–1244.

[58] R. S. Philipose, P. B. Sarasija, *Gutman matrix and Gutman energy of a graph*, Math. Sci. Int. Res. J. **7** (2018) 63–66.

[59] S. Ramakrishnan, J. Baskar Babujee, *Schultz and Gutman indices for graph complements*, Int. J. Pure Appl. Math. **105** (2015) 383–392.

[60] S. Ramakrishnan, J. Baskar Babujee, *Gutman and Schultz indices for nanostar dendrimer*, J. Comput. Theor. Nanosci. **12** (2015) 5449–5456.

[61] A. Sadeghieh, N. Ghanbari, S. Alikhani, *Computation of Gutman index of some cactus chains*, El. J. Graph Theory Appl. **6** (2018) 138–151.

[62] S. Sedghi, N. Shobe, *Degree distance and Gutman index of two graph products*, . Algebra Comb. Discr. Struct. Appl. **7** (2020) 121–140.

[63] Z. Wang, Y. Mao, K. C. Das, Y. Shang, *Nordhaus–Gaddum–type results for the Steiner Gutman index of graphs*, Symmetry **12**(10) (2020) #1711.

[64] L. Zhang, Q. Li, S. Li, M. Zhang, *The expected values for the Schultz index, Gutman index, multiplicative degree–Kirchhoff index and additive degree–Kirchhoff index of a random polyphenylene chain*, Discr. Appl. Math. **282** (2020) 243–256.

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