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ON TWO DEGREE–AND–DISTANCE–BASED GRAPH INVARIANTS

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A b s t r a c t. Let G be a connected graph with vertex set $V(G)$. For $u, v \in V(G)$, by $d(v)$ and $d(u,v)$ are denoted the degree of the vertex v and the distance between the vertices u and v. A much studied degree–and–distance–based graph invariant is the degree distance, defined as $DD = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]\, d(u,v)$. A related such invariant is $ZZ = \sum_{\{u,v\} \subseteq V(G)} [d(u) \times d(v)]\, d(u,v)$. If G is a tree, then both DD and ZZ are linearly related with the Wiener index $W = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$. We show how these relations can be extended in the case when $d(u)$ and $d(v)$ are replaced by $f(u)$ and $f(v)$, where f is any function of the corresponding vertex. We also give a few remarks concerning the discovery of DD and ZZ.

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1. *Introduction and historical remarks*

Let G be a connected graph of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The degree of the vertex $x \in V(G)$, denoted by $d_G(x) = d(x)$, is the number of first neighbors of x in the graph G. The distance of the vertices $x, y \in V(G)$, denoted by $d_G(x,y) = d(x,y)$ is the length of (= number of edges in) a shortest path in G, connecting x and y.

In this paper we are concerned with two degree–and–distance–based graph invariants, namely with the *degree distance* defined as

$$DD = DD(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v)]\, d(u,v) \tag{1.1}$$

and another closely related invariant, defined as

$$ZZ = ZZ(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) \times d(v)]\, d(u,v)\,. \tag{1.2}$$

In additions, we recall the definition of the *Wiener index*:

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)\,.$$

The Wiener index was introduced in 1947 by Harold Wiener [32] and since then became one of the most extensively studied distance–based graph invariants; for details see [7, 14, 26, 27].

The degree distance, as defined by Eq. (1.1), was put forward by Dobrynin and Kochetova in 1994 [8]. In the meantime, this degree–and–distance–based graph invariant became a popular topic for mathematical studies; for details see the recent papers [23, 6, 17, 1, 33] and the references cited therein.

However, five years before the concept of degree distance was conceived, Schultz considered a seemingly unrelated quantity, which he named *molecular topological index*, and defined as [28]

$$MTI = \sum_{k=1}^{n} \left[\begin{pmatrix} d(v_1) \\ d(v_2) \\ \vdots \\ d(v_n) \end{pmatrix} \mathbf{A} + \mathbf{D} \right]_k$$

where $\mathbf{A} = (a_{ij})$ and $\mathbf{D} = (d_{ij})$ are the adjacency and distance matrices. Recall that

$$a_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

whereas $d_{ij} = d(v_i, v_j)$.

Bearing in mind that

$$\begin{pmatrix} d(v_1) \\ d(v_2) \\ \vdots \\ d(v_n) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \mathbf{A}$$

one immediately sees that

$$\sum_{k=1}^{n} \left[\begin{pmatrix} d(v_1) \\ d(v_2) \\ \vdots \\ d(v_n) \end{pmatrix} \mathbf{A} \right]_k = \sum_{k=1}^{n} d(v_k)^2$$

which is just the classical first Zagreb index (for details see [12]). The other term in the expression for MTI is equal to

$$\begin{aligned} \sum_{k=1}^{n} \left[\begin{pmatrix} d(v_1) \\ d(v_2) \\ \vdots \\ d(v_n) \end{pmatrix} \mathbf{D} \right]_k &= \sum_{k=1}^{n} \left[\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \mathbf{AD} \right]_k = \sum_{k=1}^{n} \sum_{i=1}^{n} \big[\mathbf{AD}\big]_{ik} \\ &= \sum_{k=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}\, d_{jk} = \sum_{k=1}^{n} \sum_{j=1}^{n} d(v_j)\, d(v_j, v_k)\,. \end{aligned}$$

Because of

$$\sum_{k=1}^{n} \sum_{j=1}^{n} d(v_j)\, d(v_j, v_k) = \sum_{k=1}^{n} \sum_{j=1}^{n} d(v_k)\, d(v_k, v_j) = \sum_{k=1}^{n} \sum_{j=1}^{n} d(v_k)\, d(v_j, v_k)$$

the above expression can be rewritten as

$$\frac{1}{2} \sum_{k=1}^{n} \sum_{j=1}^{n} \big[d(v_j) + d(v_k)\big] d(v_j, v_k) = \sum_{k<j} \big[d(v_j) + d(v_k)\big] d(v_j, v_k)$$

which coincides with the degree distance, Eq. (1.1). Therefore,

$$MTI = \sum_{k=1}^{n} d(v_k)^2 + DD$$

an identity, the existence of which was not recognized for a long time.

The fact that in the case of acyclic graphs, there is a simple linear relation between MTI and the Wiener index was first noticed in [24], and then mathematically proven by Klein [18]. An independent proof was offered by the present author [11]. All this happened before the publication of the Dobrynin–Kochetova article [8]. The respective result can be stated as:

Theorem 1.1 ([18, 11]). *Let T be a tree of order n. Then its degree distance and Wiener index are related as*

$$DD(T) = 4\,W(T) - n(n-1)\,. \tag{1.3}$$

The author of [11] noticed that by means of his proof technique, an identity analogous to Eq. (1.3) can be deduced for the graph invariant in which the sum $d(u)+d(v)$ is replaced by $d(u) \times d(v)$. Thus, for the quantity ZZ defined via Eq. (1.2), the following result could be verified:

Theorem 1.2 ([11]). *Let T be a tree of order n. Then*

$$ZZ(T) = 4\,W(T) - (2n-1)(n-1)\,. \tag{1.4}$$

The degree–and–distance–based graph invariant ZZ appeared in the paper [11] for the first time. The sole reason for its introduction was to point out the analogy between Eqs. (1.3) and (1.4). No name for this invariant was proposed.

When Todeschini and Consonni produced their *Handbooks of Molecular Descriptors* [30, 31], they mentioned in it the quantity ZZ and named it *Gutman index*. This inadequate and unjustified name was eventually accepted in the mathematical and chemical literature [2, 10, 16, 19, 21, 22, 29, 5, 9, 4, 20, 25, 3].

2. *Extending Theorems 1.1*

Let G be a graph and $V(G)$ its vertex set. Let f be a function that associates a real number $f(v)$ to every vertex $v \in V(G)$. Bearing in mind Eq. (1.1), we consider a generalized version of degree distance, defined as

$$DD_{gen} = DD_{gen}(G) = \sum_{\{u,v\} \subseteq V(G)} [f(u) + f(v)]\, d(u,v)\,. \tag{2.1}$$

We are interested in extending Theorem 1.1 so as to hold also to DD_{gen}. For this, we need some preparations.

Let T be a tree of order n, thus possessing $n-1$ edges. Let Let $e \in E(T)$ be an edge of T. Let the end vertices of e be x and y. Divide the vertices of T into two disjoint sets $V_1(e)$ and $V_2(e)$ so that

$$\begin{aligned} V_1(e) &= \{v \in V(T) \mid d(v,x) < d(v,y)\}, \\ V_2(e) &= \{v \in V(T) \mid d(v,x) > d(v,y)\}\,. \end{aligned}$$

Then $V_1(e) \cap V_2(e) = \emptyset$, $V_1(e) \cup V_2(e) = V(T)$, and therefore, $|V_1(e)| + |V_2(e)| = n$.

According to Wiener's theorem [7, 32],

$$W(T) = \sum_{e \in E(T)} |V_1(e)| \cdot |V_2(e)| \,. \tag{2.2}$$

Consider now formula (2.1), and apply in to a tree T. Any two vertices u and v of a tree are connected by a unique path. This path contains $d(u,v)$ edges. According to (2.1), DD_{gen} is equal to the sum of terms $f(u) + f(v)$, added as many time as many edges are on the (unique) path connecting u and v. These sums can be divided into contributions associated with a particular edge e, which are equal to

$$|V_2(e)| \sum_{u \in V_1(e)} f(u) + |V_1(e)| \sum_{v \in V_2(e)} f(v) \,.$$

Their summation over all edges results in DD_{gen}. Thus we arrive at:

Theorem 2.1. *Let T be a tree with edge set $E(T)$, and the sets $V_1(e), V_2(e)$ as defined above. Then the generalized degree distance of T obeys the relation*

$$DD_{gen}(T) = \sum_{e \in E(T)} \left[|V_2(e)| \sum_{u \in V_1(e)} f(u) + |V_1(e)| \sum_{v \in V_2(e)} f(v) \right] . \tag{2.3}$$

We now consider two simplest special cases of Eq. (2.3).

If $f(v) \equiv 1$, then

$$\sum_{u \in V_1(e)} f(u) = |V_1(e)| \qquad \text{and} \qquad \sum_{v \in V_2(e)} f(v) = |V_2(e)| \,.$$

Bearing in mind Wiener's theorem, Eq. (2.2), we get:

Corollary 2.1. *If $f(v) \equiv 1$, then Eq.* (2.3) *reduces to*

$$DD_{gen}(T) = 2\,W(T) \,.$$

Corollary 2.2. *If $f(v) = d(v)$, then Eq.* (2.1) *reduces to Eq.* (1.3)*, i.e., Theorem* 1.1 *is a special case of Theorem* 2.1.

PROOF. Let T be a tree and e its edge. The subgraph obtained by deleting e from T consists of two disconnected trees, T_1 and T_2, such that $V(T_1) = V_1(e)$ and $V(T_2) = V_2(e)$. Then,

$$\sum_{u \in V_1(e)} d_T(u) = 1 + \sum_{u \in V(T_1)} d_{T_1}(u) = 1 + 2\,|E(T_1)| = 1 + 2\big(|V_1(e)| - 1\big) = 2\,|V_1(e)| - 1$$

and analogously,

$$\sum_{v \in V_2(e)} d_T(v) = 2\,|V_2(e)| - 1\,.$$

Substituting these relations into Eq. (2.3), we get

$$\begin{aligned}
DD_{gen} &= \sum_{e \in E(T)} \Big[|V_2(e)|\,(2\,|V_1(e)| - 1) + |V_1(e)|\,(2\,|V_2(e)| - 1) \Big] \\
&= \sum_{e \in E(T)} \Big[4|V_1(e)| \cdot |V_2(e)| - (|V_1(e)| + |V_2(e)|) \Big] \\
&= 4 \sum_{e \in E(T)} |V_1(e)| \cdot |V_2(e)| - \sum_{e \in E(T)} n \\
&= 4\,W(T) - n(n-1),
\end{aligned}$$

where we used Wiener's formula (2.2) and the fact that T has $n-1$ edges.

3. *Extending Theorems 1.2*

The considerations leading to the extension of Theorem 1.2 are analogous to those presented in the preceding section. Therefore, we state the respective results without proofs.

Let, as before, G be a graph and $V(G)$ its vertex set. Let f be a function that associates a real number $f(v)$ to every vertex $v \in V(G)$. Bearing in mind Eq. (1.2), we consider a generalized version of the ZZ index, defined as

$$ZZ_{gen} = ZZ_{gen}(G) = \sum_{\{u,v\} \subseteq V(G)} \big[f(u) \times f(v) \big]\, d(u,v)\,. \tag{3.1}$$

Theorem 3.1. *Let T be a tree with edge set $E(T)$, and the sets $V_1(e), V_2(e)$ as defined in the preceding section. Then the generalized ZZ index of T obeys the relation*

$$ZZ_{gen}(T) = \sum_{e \in E(T)} \left[\sum_{u \in V_1(e)} f(u) \times \sum_{v \in V_2(e)} f(v) \right]. \tag{3.2}$$

We again consider two simplest special cases of Eq. (3.2).

Corollary 3.1. *If $f(v) \equiv 1$, then Eq. (3.2) reduces to*

$$ZZ_{gen}(T) = W(T)\,.$$

Corollary 3.2. *If $f(v) = d(v)$, then Eq.* (3.1) *reduces to Eq.* (1.4)*, i.e., Theorem* 1.2 *is a special case of Theorem* 3.1.

4. *Applications*

A vertex v of a graph G is said to be pendent if $d(v) = 1$. The *terminal Wiener index*, TW is defined as the sum of distances between all pairs of pendent vertices of the underlying graph [15, 13]:

$$TW = TW(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ d(u)=d(v)=1}} d(u,v)\,.$$

Then we have an immediate corollary of Theorem 3.1, analogous to Corollary 3.1:

Corollary 4.1. *Let T be a tree and $TW(T)$ its terminal Wiener index. Let $f(v) = 1$ if the vertex $v \in V(T)$ is pendent, and $f(v) = 0$ otherwise. Then*

$$ZZ_{gen}(T) = TW(T)\,.$$

Let us now examine what happens with $DD_{gen}(T)$ when $f(v)$ is the function specified in Corollary 4.1.

First note an identity, which is an immediate consequence of Eqs. (1.3) and (1.4).

Theorem 4.1. *Let T be a tree of order n. Then*

$$DD(T) - ZZ(T) = (n-1)^2\,. \tag{4.1}$$

Thus, the difference between the indices DD and ZZ is independent of the structure of the tree T, and depends only on the number of its vertices.

Directly from Eqs. (1.1) and (1.2) it follows

$$DD(G) - ZZ(G) = \sum_{\{u,v\} \subseteq V(G)} [d(u) + d(v) - d(u)\,d(v)]\,d(u,v)\,. \tag{4.2}$$

If at least one of the vertices u, v is pendent, then $d(u) + d(v) - d(u)\,d(v) = 1$. If both u and v are of degree 2, then $d(u) + d(v) - d(u)\,d(v) = 0$. In all other cases, $d(u) + d(v) - d(u)\,d(v) < 0$. Bearing this in mind, we get

$$DD(G) - ZZ(G) = STW(G) - \sum_{\substack{\{u,v\} \subseteq V(G) \\ d(u),d(v) \geq 2}} [d(u)\,d(v) - d(u) - d(v)]\,d(u,v)$$

where STW is the *semi-terminal Wiener index*, equal to the sum of distances between pairs of vertices of which at least one is pendent:

$$STW = STW(G) = \sum_{\substack{\{u,v\}\subseteq V(G) \\ \min\{d(u),d(v)\}=1}} d(u,v)\,.$$

Combination of Eqs. (4.1) and (4.2) yields

$$STW(T) = (n-1)^2 + \sum_{\substack{\{u,v\}\subseteq V(T) \\ d(u),d(v)\geq 2}} [d(u)\,d(v) - d(u) - d(v)]\,d(u,v)\,. \tag{4.3}$$

Theorem 4.2. *Let T be a tree of order n and $STW(T)$ its semi-terminal Wiener index. Let S_n and P_n be, respectively, the star and path of order n. Then*

$$STW(T) \leq (n-1)^2,$$

with equality if and only if $T \cong S_n$ or $T \cong P_n$.

PROOF. The inequality holds because the second term on the right–hand side of Eq. (4.3) is positive–valued or equal to zero. Equality will hold if this second term is equal to zero. This will happen in two cases:
(1) if there are no two vertices of degree greater than 1, implying $T \cong S_n$, or
(2) if all non-pendent vertices are of degree two, implying $T \cong P_n$.

Corollary 4.2. *Among trees of a fixed order n, the star and the path have minimal semi-terminal Wiener indices, both equal to $(n-1)^2$.*

It is worth noting that the path is the least branched, whereas the star the most branched tree. Therefore, Corollary 4.2 establishes a quite unusual extremal property of trees.

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