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On some degree-and-distance-based graph invariants of trees

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ABSTRACT

Let G be a connected graph with vertex set $V(G)$. For $u, v \in V(G)$, $d(v)$ and $d(u,v)$ denote 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 (usually called "Gutman index") is $ZZ = \sum_{\{u,v\}\subseteq V(G)} [d(u)\cdot d(v)]\, d(u,v)$. 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 examine the difference $DD - ZZ$ for trees and establish a number of regularities.

1. Introduction

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

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

$$DD = DD(G) = \sum_{\{u,v\}\subseteq V(G)} \Big[d(u)+d(v)\Big]\, d(u,v) \tag{1}$$

and another closely related invariant, defined as

$$ZZ = ZZ(G) = \sum_{\{u,v\}\subseteq V(G)} \Big[d(u)\cdot d(v)\Big]\, d(u,v). \tag{2}$$

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

$$W = W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v). \tag{3}$$

The Wiener index was introduced in 1947 by Harold Wiener [15] and since then became one of the most extensively studied distance–based graph invariants; for details see the surveys [3,17] and the recent papers [7,9–11,14].

The degree distance, as defined by Eq. (1), was put forward by Dobrynin and Kochetova in 1994 [4]. In the meantime, this degree–and–distance–based graph invariant became a popular topic for mathematical studies; for details see the recent papers [1,2,5,12,16,18] and the references cited therein.

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The fact that in the case of trees there is a simple linear relation between DD and the Wiener index was first noticed in [13], and then mathematically proven by Klein [8]. An independent proof was offered by one of the present authors [6]. The respective result can be stated as:

Theorem 1 [6,8]**.** *Let T be a tree of order n. Then its degree distance and Wiener index are related as*

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

In [6], it was noticed that an identity analogous to Eq. (4) holds if the sum $d(u) + d(v)$ is replaced by $d(u) \cdot d(v)$:

Theorem 2 [6]**.** *Let T be a tree of order n. Then*

$$ZZ(T) = 4W(T) - (2n-1)(n-1). \tag{5}$$

Theorem 2 was the sole reason for considering the invariant ZZ, namely the multiplicative analogue of degree distance. Eventually and unfortunately, this invariant is nowadays referred to as the *Gutman index*.

Combining Eqs. (4) and (5), one immediately realizes that $DD(T) - ZZ(T) = (n-1)^2$. Curiously, whereas both Eqs. (4) and (5) were discovered in the 1990s, the fact that their difference depends solely on the number of vertices of the underlying tree seems to have so far eluded attention. We state the same observation in a slightly different manner:

Corollary 3. *Let T be a tree of order n. Then the expression*

$$\sum_{\{u,v\} \subseteq V(T)} \Big[d_T(u) + d_T(v) - d_T(u)\, d_T(v) \Big]\, d_T(u,v)$$

is independent of the structure of T, and is equal to $(n-1)^2$.

2. Elaborating Corollary 3

In the case of trees, it is purposeful to divide the Wiener index, Eq. (3), into two parts as $W = W_{ex} + W_{in}$, where

$$W_{ex} = W_{ex}(T) = \sum_{\substack{\{u,v\} \subseteq V(T) \\ \min\{d(u),d(v)\}=1}} d_T(u,v) \tag{6}$$

$$W_{in} = W_{in}(T) = \sum_{\substack{\{u,v\} \subseteq V(T) \\ \min\{d(u),d(v)\}\geq 2}} d_T(u,v).$$

We refer to these as to the "*external*" and "*internal*" Wiener index of the tree T. Evidently, the external Wiener index pertains to the distances between pairs of vertices of T, of which at least one is pendent.

Note now that the term $d(u) + d(v) - d(u)\, d(v)$ is equal to unity if either $d(u) = 1$ or $d(v) = 1$, equal to zero if $d(u) = d(v) = 2$, and negative–valued in all other cases.

Define an auxiliary quantity Θ as

$$\Theta = \Theta(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ \min\{d(u),d(v)\}\geq 2}} \Big[d_G(u)\, d_G(v) - d_G(u) - d_G(v) \Big]\, d_G(u,v)$$

and note that its value is non-negative for all graphs G.

Bearing in mind the above, Corollary 3 can be re-stated as:

Corollary 4. *Let T be a tree of order n. Then*

$$DD(T) - ZZ(T) = W_{ex}(T) - \Theta(T) = (n-1)^2$$

i.e.,

$$W_{ex}(T) = (n-1)^2 + \Theta(T)\,.$$

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

Theorem 5. *Let T be a tree of order n. Then*

$$W_{ex}(T) \geq (n-1)^2\,.$$

Equality holds if and only if $T \cong S_n$ *or* $T \cong P_n$ *for all* $n \geq 2$.

Proof. The inequality in Theorem 5 is a direct consequence of $\Theta(T) \geq 0$. Equality $\Theta(T) = 0$ happens in two cases:

(a) if the tree T does not have a pair of non-pendent vertices, and
(b) if all non-pendent vertices of the tree T are of degree two.