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On Steiner degree distance of trees

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ABSTRACT

Let G be a connected graph, and u, v, w its vertices. By d_u is denoted the degree of the vertex u, by $d(u, v)$ the (ordinary) distance of the vertices u and v, and by $d(u, v, w)$ the Steiner distance of u, v, w. The degree distance DD of G is defined as the sum of terms $[d_u + d_v]\, d(u, v)$ over all pairs of vertices of G. As early as in the 1990s, a linear relation was discovered between DD of trees and the Wiener index. We now consider SDD, the Steiner–distance generalization of DD, defined as the sum of terms $[d_u + d_v + d_w]\, d(u, v, w)$ over all triples of vertices of G. Also in this case, a linear relation between SDD and the Wiener index could be established.

1. Introduction

In graph theory applied to chemical problems, a large number of molecular structure descriptors, so-called “*topological indices*”, has been studied [38], aimed as representing certain chemically interesting structural features of the underlying molecules. Many of these descriptors are defined in terms of vertex degrees (for details see [10,17,20,38]) and equally many in terms of distance between vertices (for details see [13,21,38,41]). There are also several degree-and-distance-based topological indices [11,12,38,40]. Among these, the *degree distance*, put forward by Dobrynin and Kochetova [15], attracted much attention of researchers, and has been subject to a legion of studies; see the recent papers [2–5,16,24,32,33,42] and the references cited therein.

For a graph G with vertex set $V(G)$, the degree distance is defined as [15]

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

where d_u is the degree (= number of first neighbors) of the vertex $u \in V(G)$, and $d(u, v)$ is the distance between the vertices $u, v \in V(G)$ (= the number of edges in a shortest path connecting u and v).

At this point we recall that the Wiener index is defined as

$$W = W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)\,. \tag{2}$$

For details on the theory of this classical, almost 70 years old, distance–based graph invariant see the surveys [14,35,41] and the recent papers [23,26–28,37]. Observe that if the graph G is regular of degree r, then $DD(G) = 2r\, W(G)$. In 1947, together

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with the index W also the so-called Wiener polarity index was introduced [39], equal to the number of pairs of vertices at distance 4; for more details see [30,31,43] and the references cited therein.

A few years before the paper [15] was published, Schultz considered a seemingly unrelated quantity, which he named "*molecular topological index*" (*MTI*). For a graph G of order n whose adjacency and distance matrices are $\mathbf{A}(G)$ and $\mathbf{D}(G)$, respectively, the molecular topological index is defined as [36]

$$MTI(G) = \sum_{i=1}^{n} \Big(\mathbf{d}(G) \big[\mathbf{A}(G) + \mathbf{D}(G) \big] \Big)_i$$

where $\mathbf{d}(G)$ is the column vector of vertex degrees. It is not difficult to verify [19] that

$$MTI(G) = DD(G) + \sum_{u \in V(G)} d_u^2 \,. \tag{3}$$

Within the study of *MTI*, it was noticed [34] that in the case of acyclic graphs, there is a simple linear relation between *MTI* and the Wiener index, which we state here as:

Theorem 1. *Let T be a tree of order n, and let DD and W the topological indices defined via Eqs. (1) and (2). Then*

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

The first mathematical proof of the identity (4) was given by Klein [25]. An independent proof was offered by the present author [19]. All this happened before the publication of the Dobrynin–Kochetova article [15].

In this paper, we first propose a generalization of the degree distance by using the concept of Steiner distance. Then we show that for the three-center Steiner degree distance, a result analogous to Theorem 1 holds.

2. Steiner distance and Steiner degree distances

The Steiner[1] distance of a graph was put forward in 1989 by Chartrand et al. [7]. It is a natural and consequent generalization of the classical graph distance. For a connected graph G with vertex set $V(G)$, let S be a subset of $V(G)$ containing at least two vertices. Then the *Steiner distance* $d(S)$ of the vertices in S (or simply the distance of S) is the minimum number of edges of a connected subgraph of G that contains all vertices from S. This subgraph is necessarily a tree (and is referred to as a Steiner tree).

If $S = \{u, v\}$, i.e., if $|S| = 2$, then the Steiner distance reduces to the ordinary distance between the vertices u and v, i.e., $d(S) \equiv d(u, v)$. More details on Steiner distance can be found in [1,6,7,18].

Bearing in mind the definition (2) of the Wiener index, it is reasonable to consider a series of its generalizations, namely [8,9,22,29]

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d(S) \quad ; \quad k = 2, 3, \ldots, n$$

where, of course, $SW_2(G) \equiv W(G)$.

In the same manner, starting from Eq. (1), we can construct the generalized versions of the degree distance as

$$SDD_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left[\sum_{v \in S} d_v \right] d(S) \quad ; \quad k = 2, 3, \ldots, n \tag{5}$$

in which case, again, SDD_2 will coincide with the ordinary degree distance. Observe that if the graph G is regular of degree r, then $SDD_k(G) = kr\,W(G)$.

It is purposeful that SDD_k be referred to as the *k-center Steiner degree distance*. In what follows, we shall be particularly interested in the 3-center Steiner degree distance, which can be expressed as

$$SDD_3(G) = \sum_{\substack{\{u,v,w\} \subseteq V(G) \\ |\{u,v,w\}|=3}} [d_u + d_v + d_w] \, d(u, v, w) \,.$$

3. Steiner degree distance of trees

Let G be a connected graph on n vertices, with vertex set $V(G)$. Let e be an edge of G, with x and y being its end-vertices. Divide the vertices of G into three sets:

$$\mathcal{N}_1(e) = \{ v \in V(G) \,|\, d(v, x) < d(v, y) \}$$

[1] Jakob Steiner (1795–1863), Swiss mathematician.