European Journal of Combinatorics 41 (2014) 79–99

Contents lists available at ScienceDirect

European Journal of Combinatorics

journal homepage: www.elsevier.com/locate/ejc

The distances between internal vertices and leaves of a tree ☆

Hua Wang

Department of Mathematical Sciences, Georgia Southern University, Statesboro, GA 30460, USA

ARTICLE INFO

Article history:
Received 31 March 2013
Accepted 30 March 2014
Available online 16 April 2014

ABSTRACT

Distance-based graph invariants have been of great interest and extensively studied. The classic Wiener index was proposed in biochemistry and defined to be the sum of distances between all pairs of vertices. The sum of distances between all pairs of leaves, named the Gamma index and the terminal Wiener index respectively, was motivated from both biochemistry and phylogenetic reconstruction. The studies of such distance-based graph invariants include, for instance, the "middle part" of a tree, the extremal structures with given constraints, the extremal values of ratios of the distance function at the "middle part" and leaves. In particular, when considering the extremal structures, correlations between the Wiener index and other graph invariants have been discovered and general methods have been developed. Other related graph invariants include the number of subtrees or leaf containing subtrees (corresponding to the "acceptable residue configurations"), subforests, root-containing subtrees (in relation to the antichains in a Hasse diagram with the structure of a rooted tree), to name a few.

As has been repeatedly mentioned in earlier works, it is of both mathematical interests and practical importance to generalize the current studies to other distance-based graph invariants. The sum of distances between internal vertices has been considered and many similar results have been obtained.

On the other hand, a natural similar concept is the sum of distances between internal vertices and leaves. It has been proposed in different literatures. In this paper we conduct a relatively comprehensive study of this concept, providing results analogous to those of the aforementioned studies. We start with identifying the "middle part" of a tree with respect to the total distance from

☆ This work was partially supported by a grant from the Simons Foundation (#245307).
E-mail address: hwang@georgiasouthern.edu.

http://dx.doi.org/10.1016/j.ejc.2014.03.014

leaves. Then the extremal ratios with respect to the distance from leaves are examined and the structures achieving the extremal ratios are characterized. Lastly, we provide extremal trees under different constraints that maximize or minimize the sum of all such distances.

1. Introduction and previous work

The study of distances between vertices of a tree probably started from the classic *Wiener index* [25], one of the most well used chemical indices that correlate a chemical compound's structure (the "molecular graph") with the compound's physical–chemical properties. The Wiener index, introduced in 1947, is defined as the sum of distances between all pairs of vertices, namely that

$$W(T) = \sum_{v,u \in V(T)} d(v,u) = \frac{1}{2} \sum_{v \in V(T)} d(v)$$

where

$$d(v) = \sum_{u \in V(T)} d(v,u)$$

is called the *distance* of v. Although defined for general graphs, the consideration of these concepts in trees is of interests because of the applications in acyclic molecular structures.

A natural sibling concept, the distances between leaves, was only brought to our attention recently. The sum of all such distances, i.e.,

$$\sum_{v,u \in L(T)} d(v,u)$$

where $L(T)$ denotes the set of leaves of T, was proposed independently as the *Gamma index* [19] (from the study of "Tree Bisection and Reconnection" neighborhood in phylogeny reconstruction) and the *terminal Wiener index* [8] (for similar purpose as the original Wiener index).

With the presence of the distance between all vertices and the distance between all leaves, a concept named the *spinal index* naturally arose. The spinal index is defined as the sum of the distances between all internal vertices [2]. It is easy to see that the spinal index of a tree T is essentially the Wiener index of the "skeleton" $T - L(T)$ of T, hence it is not surprising that many studies of the Wiener index can be easily generalized to the spinal index [4].

Of course, the Wiener index is simply the sum of the Gamma index, the spinal index, and the sum of all distances between internal vertices and leaves in a tree, the last one of which, we define as

$$K(T) = \sum_{u \in V(T)-L(T),\, v \in L(T)} d(u,v).$$

As a related notation, let

$$K_T(v) = \sum_{u \in L(T)} d(u,v)$$

denote the *leaf-distance* of v. Evidently we have

$$K(T) = \sum_{v \in V(T)-L(T)} K_T(v).$$

The concepts $K(T)$ and $K_T(v)$ have been frequently mentioned in related literatures. See, for instance, [17]. More details in this regard will be incorporated in the rest of this section. As natural and