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Extremal problems for trees with given segment sequence

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ABSTRACT

A segment of a tree T is a path whose end vertices have degree 1 or at least 3, while all internal vertices have degree 2. The lengths of all the segments of T form its segment sequence, in analogy to the degree sequence. We address a number of extremal problems for the class of all trees with a given segment sequence. In particular, we determine the extremal trees for the number of subtrees, the number of matchings and independent sets, the graph energy, and spectral moments.

1. Introduction

So-called topological indices are graph invariants that map a graph to a real number, usually serving as descriptors of the graph structure. Throughout the years numerous topological indices have been introduced, motivated by various applications. To give one example, the *Wiener index* of a graph G is defined as the sum of all distances between pairs of vertices in G:

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

where $d_G(u, v)$ (or simply $d(u, v)$ when there is no ambiguity) is the distance between u and v. Several further examples will be given later.

Particular attention has been given to extremal problems. Here, the general question is: given a family of graphs $\mathcal{G}$, what can be said about graphs in $\mathcal{G}$ which attain the maximum and minimum values of a given graph invariant? To give a simple example, it is known that the maximum and minimum of the Wiener index are attained by the path and the star respectively (see [8, Equation (3)]) if the family of all trees is considered.

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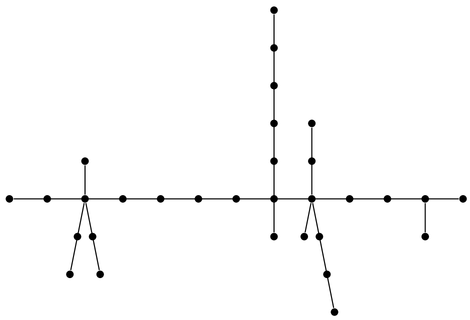

Fig. 1. A quasi-caterpillar with segment sequence (5,5,3,3,2,2,2,2,1,1,1,1,1,1).

Fig. 2. The trees $O(11, 7)$ and $E(11, 8)$.

A recent paper by Lin and Song [19] considered the family of all trees with a given *segment sequence*, and this family will also be the main object of study in our paper. Let us first define the concept of a segment sequence. We write $P(v, w)$ for the unique path between two vertices v and w of a tree T, and $E(P(v, w))$ for its edge set. A *segment* of a tree T is a path $P(v, w)$ in T with the property that each of the ends (v and w) is either a leaf or a *branching vertex* (vertex whose degree is at least 3) and that all internal vertices of the path have degree 2. The segment sequence of T is the non-increasing sequence of the lengths of all segments of T, see Fig. 1 for an example. If $(l_1, l_2, \dots, l_m)$ is the segment sequence of a tree, then the number of edges is $l_1 + l_2 + \cdots + l_m$, and consequently the number of vertices is $l_1 + l_2 + \cdots + l_m + 1$.

Segments can be thought of as building blocks of a tree, and there are, for example, several formulas that allow for the efficient calculation of the Wiener index based on segment lengths, see [8, Section 5]. This was also one of the motivations to study extremal problems for trees with given segment sequence.

Starlike trees play a special role in this context. For a given segment sequence $(l_1, l_2, \dots, l_m)$, the starlike tree $S(l_1, l_2, \dots, l_m)$ is the tree with exactly one vertex of degree ≥ 3 formed by identifying one end of each of the m segments. It was shown in [19] that $S(l_1, l_2, \dots, l_m)$ minimizes the Wiener index among all trees with segment sequence $(l_1, l_2, \dots, l_m)$.

To find the tree with segment sequence $(l_1, l_2, \dots, l_m)$ that *maximizes* the Wiener index turns out to be somewhat more complicated, and it leads naturally to the notion of *quasi-caterpillars*. A quasi-caterpillar is a tree with the property that all its branching vertices lie on a path, see Fig. 1. It was shown in [4] that the tree maximizing the Wiener index among all trees with a given segment sequence is necessarily always a quasi-caterpillar, answering a question that was posed in [19]. Some further properties of the maximizing quasi-caterpillar were determined in [4] as well.

Similar questions on trees with given number of segments were also discussed in [19]. It was shown that, among trees with m segments, the Wiener index is minimized by the balanced starlike tree $ST(n, m)$, defined as the unique starlike tree $S(l_1, \dots, l_m)$ of order n that satisfies $|l_i - l_j| \leq 1$ for all $i, j \in \{1, 2, \dots, m\}$.

Again, the maximization problem is slightly more complicated and was settled in [4]. For given n and m, we define trees $O(n, m)$ (for odd m) and $E(n, m)$ (for even m) respectively. The graph $O(n, m)$ is obtained from a path $v_0 v_1 \dots v_\ell$ of length $\ell = n - \frac{m+1}{2}$ by attaching a total of $\frac{m-1}{2}$ leaves to vertices $v_1, v_2, \dots, v_{\lfloor (m-1)/4 \rfloor}$ and $v_{\ell-1}, v_{\ell-2}, \dots, v_{\ell-\lceil (m-1)/4 \rceil}$, see Fig. 2 (left) for the case $n = 11, m = 7$. Note that $O(n, m)$ has exactly m segments.

Likewise, $E(n, m)$ is a tree with n vertices and m segments (m even) obtained from a path $v_0 v_1 \dots v_\ell$ of length $\ell = n - \frac{m}{2} - 1$ by attaching a total of $\frac{m}{2}$ leaves to vertices $v_1, v_2, \dots, v_{\lfloor (m-2)/4 \rfloor}$ and $v_{\ell-1}, v_{\ell-2}, \dots, v_{\ell-\lceil (m-2)/4 \rceil}$, where two leaves are attached to vertex v_1 (so that it becomes the only vertex of degree 4), see Fig. 2 (right) for the case $n = 11, m = 8$.

It was proven in [4] that $O(n, m)$ (resp. $E(n, m)$) always has the greatest Wiener index among trees with n vertices and m segments, for odd (resp. even) m.

The main aim of this paper is to prove several similar results for other graph invariants. The first of these invariants, and the one we will study most thoroughly, is the *number of subtrees* of a tree T, denoted by $F(T)$. The study of extremal problems involving $F(T)$ started in [23,24]. The star was found to have the greatest number of subtrees, while the path has the least number of subtrees. Special families of trees have been considered as well, notably trees with given degree sequence [4,30,29,22], but also others (trees with given number of leaves, bipartition, domination number, etc.) [17].

It is known that a not yet fully understood relation between $F(T)$ and the Wiener index $W(T)$ exists. Indeed, for the family of all trees and many special families of trees (e.g. trees with given degree sequence), it is known that the extremal structure that minimizes $F(T)$ also maximizes $W(T)$ and/or vice versa. The correlation between various graph invariants was studied in [25], and $F(T)$ and $W(T)$ were found to be strongly negatively correlated.

Just like the number of subtrees, most of the other invariants we study in this paper are also based on counting certain substructures. For a rooted tree B, let $\mathrm{m}(B, k)$ be the number of matchings of B with cardinality k and $\mathrm{M}(B, x) =$