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Maximizing Wiener index for trees with given vertex weight and degree sequences☆

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A B S T R A C T

The Wiener index is maximized over the set of trees with the given vertex weight and degree sequences. This model covers the traditional "unweighed" Wiener index, the terminal Wiener index, and the vertex distance index. It is shown that there exists an optimal caterpillar. If weights of internal vertices increase in their degrees, then an optimal caterpillar exists with weights of internal vertices on its backbone monotonously increasing from some central point to the ends of the backbone, and the same is true for pendent vertices. A tight upper bound of the Wiener index value is proposed and an efficient greedy heuristics is developed that approximates well the optimal index value. Finally, a branch and bound algorithm is built and tested for the exact solution of this NP-complete problem.

1. Nomenclature

This section introduces the basic graph-theoretic notation. The *vertex set* and the *edge set* of a simple connected undirected graph G are denoted with $V(G)$ and $E(G)$ respectively, and the *degree* (i.e., the number of incident edges) of vertex $v \in V(G)$ in graph G is denoted with $d_G(v)$. Let $W(G)$ be the set of *pendent vertices* (those having degree one) of graph G, and let $M(G) := V(G) \backslash W(G)$ be the set of its *internal vertices*. Connected graph T with $|E(T)| = |V(T)| - 1$ is called a *tree*. Let $\mathcal{T}$ denote the set of all trees.

Definition 1. A tree is called a *path* if it has exactly two pendent vertices.

Definition 2. A tree is a *caterpillar* if removing pendent vertices and their incident edges makes a path (called the *backbone* of this caterpillar).

Definition 3. A tree is called a *star* if it has at most one internal vertex.

Definition 4. In a *starlike tree* the degree of at most one vertex exceeds 2.

Definition 5. The *centroid* is a midpoint of the longest path in the tree.

Graph G is called *vertex-weighted* if non-negative weight is assigned to each its vertex. The weight of vertex $v \in V(G)$ in graph G is denoted as $\mu_G(v)$. Let $\mathcal{WT}$ stand for the set of all vertex-weighted trees.

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Let us consider monotone decreasing natural sequence $d_i, i = 1, \ldots, n,$ and non-negative sequence $\mu_i, i = 1, \ldots, n,$ of the same length and introduce corresponding column vectors $\mathbf{d} = (d_1, \ldots, d_n)^T$, $\mathbf{w} = (\mu_1, \ldots, \mu_n)^T$.

Definition 6. Tree T *has degree sequence* $\mathbf{d}$ if its vertices can be indexed from v_1 to v_n such that $d_T(v_i) = d_i$, $i = 1, \ldots, n$. Let $\mathcal{T}(\mathbf{d})$ be the set of trees with degree sequence $\mathbf{d}$.

It is known that $\mathcal{T}(\mathbf{d})$ is not empty, if and only if

$$d_1 + \ldots + d_n = 2(n-1). \tag{1}$$

Definition 7. Vertex-weighted tree $T \in \mathcal{WT}$ *has vertex degree sequence* $\mathbf{d}$ *and vertex weight sequence* $\mathbf{w}$ if its vertices can be indexed from v_1 to v_n such that $d_T(v_i) = d_i$, $\mu_T(v_i) = \mu_i$ for all $i = 1, \ldots, n$. Let $\mathcal{WT}(\mathbf{w}, \mathbf{d})$ be the set of all such trees.

Without loss of generality assume that if $d_i = d_j$ and $i < j$, then $\mu_i \ge \mu_j$.

Definition 8. Weight sequence $\mathbf{w}$ is *monotone* in degree sequence $\mathbf{d}$, if from d_i, $d_j \ge 2$, $i < j$, it follows that $\mu_i \ge \mu_j$.

For any pair of vertices $u, v \in V(G)$ of connected graph G let $d_G(u, v)$ be the distance (the number of edges in the shortest path) between vertices u and v in graph G. Then *the Wiener index* of graph G is defined as

$$WI(G) := \frac{1}{2} \sum_{u,v \in V(G)} d_G(u, v). \tag{2}$$

2. Introduction

Graph invariants (also known as topological indices) play an important role in algebraic graph theory providing numeric measures for various structural properties of graphs. The Wiener index (2) is probably the most renowned graph invariant. It measures "compactness" of a connected graph [1]; for instance, a *star* has the minimum value of the Wiener index among all trees of the given order, while a *path* has the maximum value of WI. The most "compact" (i.e., the one minimizing the Wiener index) tree with the given vertex degree sequence is a "greedy" balanced tree, in which all distances from leaves to the *centroid* differ by at most unity while vertex degrees do not decrease towards the centroid [2,3].

The *Wiener index for graphs with weighted vertices* was proposed in [4]. It can be defined as

$$VWWI(G) := \frac{1}{2} \sum_{u,v \in V(G)} \mu_G(u)\mu_G(v)d_G(u, v), \tag{3}$$

where $d_G(u, v)$ is the distance between vertices u and v in graph G, while $\mu_G(u)$ and $\mu_G(v)$ are, respectively, real weights of graph vertices u and v.

VWWI is used to foster calculation of the Wiener index [5], to predict boiling and melting points of various compounds [6,7]. In particular, in [7] the search of an alcohol isomer with the minimum normal boiling point was reduced to the minimization of VWWI over the set of trees with the given vertex weight and degree sequences.

It is shown in [8] that if weights of internal vertices do not decrease in their degrees, then the most "compact" (the one minimizing VWWI) tree with the given vertex weight and degree sequences is the, so called, *generalized Huffman tree*. It is efficiently constructed by joining sequentially sub-graphs of the minimum weight.

The problem of the Wiener index maximization appeared a bit more complex. It is known that an extremal tree is some caterpillar [9] (i.e., a tree that makes a path, called a *backbone*, after deletion of all its pendent vertices); vertex degrees first do not increase and then do not decrease while one moves from one to the other end of the backbone [2]. An efficient dynamic programming algorithm assigns internal vertices to positions on the backbone of an optimal caterpillar [10].

In this article, the problem of the maximum Wiener index over the set of trees with the given vertex weight and degree sequences is solved for the case of internal vertex weights being monotone in degrees. This problem appears NP-complete (the classic partition problem reduces to its special case). It is shown that, similarly to the partition problem, complexity of the maximization problem for WI and VWWI is a result of asymmetry of the vertex set. If for each distinct combination of the weight and the degree the number of vertices having this weight and degree is even (although one internal and/or one pendent vertex with minimum weight may be unmatched), then VWWI is maximized by a symmetric caterpillar, in which vertices are placed mirror-like with respect to its center in the order of increasing weights. For the general case an analytical upper bound is proposed, the greedy heuristic algorithm and the economic branch and bound scheme are constructed, and their performance is evaluated for random weight and degree sequences.

3. Literature review

Since its appearance in 1947 [11] the Wiener index remains one of the most discussed graph invariants. On the one hand, its mathematical properties have been comprehensively studied (see surveys in [1,12]). On the other hand, its relation is established to many physical and chemical properties of compounds of different classes ([13–16] and many others). Many papers that appeared in recent decades investigate extremal graphs that deliver the minimum or the maximum of the Wiener index over various sets of graphs [2,3,17–21] along with its lower and upper bounds. In particular, a relation is