MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 273-292

ISSN 0340 - 6253

Greedy Trees, Caterpillars, and Wiener–type Graph Invariants

Nina S. Schmuck[a*], **Stephan G. Wagner**[b†], **Hua Wang**[c]

[a] Institut für Mathematik B
Technische Universität Graz
Steyrergasse 30, 8010 Graz, Austria
nina.schmuck@tugraz.at

[b] Department of Mathematical Sciences
Stellenbosch University
Private Bag X1, Matieland 7602, South Africa
swagner@sun.ac.za

[c] Department of Mathematical Sciences
Georgia Southern University
Statesboro, GA 30460, USA
hwang@georgiasouthern.edu

(Received July 15, 2011)

Abstract

The extremal questions of maximizing or minimizing various distance-based graph invariants among trees with a given degree sequence have been vigorously studied. In many cases, the so-called greedy tree and the caterpillar are found to be extremal. In this note, we show a "universal property" of the greedy tree with a given degree sequence, namely that the number of pairs of vertices whose distance is at most k is maximized by the greedy tree for all k. This rather strong assertion immediately implies, and is equivalent to, the minimality of the greedy trees with respect to graph invariants of the form $W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$ for any nonnegative, nondecreasing function f. With different choices of f, one directly solves the minimization problems of distance-based graph invariants including the

*N. Schmuck is supported by the Austrian Science Foundation FWF, project S9606, that is part of the Austrian National Research Network "Analytic Combinatorics and Probabilistic Number Theory".

†This material is based upon work supported financially by the National Research Foundation of South Africa under grant number 70560.

classical Wiener index, the Hyper-Wiener index and the generalized Wiener index. We also consider the maximization of some of such invariants among trees with a given degree sequence. These problems turned out to be more complicated. Analogous to the known case of the Wiener index, we show that $W_f(T)$ is maximized by a caterpillar for any increasing and convex function f. This result also leads to a partial characterization of the structure of the extremal caterpillars. Through a similar approach, the maximization problem of the terminal Wiener index is also addressed.

1 Introduction

In organic chemistry, to develop a quantitative structure-activity relationship (QSAR) and to establish the mathematical basis for connections between molecular structures and physico-chemical properties, chemists and mathematicians are increasingly using a class of graph invariants, known as topological indices, as powerful tools that relate a chemical compound's molecular graph with its characteristics. Among these topological indices, a number of *distance-based* graph invariants received great attention.

One of the most classic and well-studied distance-based graph invariants is the *Wiener index*, which was introduced by and named after Wiener [25]. The Wiener index of a graph G is the sum of the distances between all pairs of vertices, denoted by

$$W(G) = \sum_{\{v,w\} \subseteq V(G)} d(v,w),$$

where $d(v,w)$ is the distance between two vertices $v, w \in V(G)$.

Trees are typically one of the first special classes of graphs to be studied—see [7] for a survey on the Wiener index of trees. In this paper, we are interested in trees with prescribed degree sequence and graph invariants like the Wiener index and its generalization

$$W_\alpha(G) = \sum_{\{v,w\} \subseteq V(G)} d(v,w)^\alpha$$

as well as the *hyper-Wiener index*, which is defined as follows:

Let v and w be vertices in a tree and denote by $n(v,w)$ the number of vertices u (including v itself) for which the unique path from u to w passes through v. Then the hyper-Wiener index is defined as

$$WW(G) = \sum_{\{v,w\} \subseteq V(G)} n(v,w) n(w,v),$$

which can easily be proven to be equal to

$$WW(G) = \sum_{\{v,w\}\subseteq V(G)} \binom{d(v,w)+1}{2}, \tag{1}$$

an expression that makes sense for arbitrary graphs [13].

The *terminal Wiener index* [9] is defined in an analogous way to the Wiener index, but the vertices v and w in the sum have to be leaves.

There are several other similar graph invariants, see for instance [10, 11, 15] for further examples.

In the past, the extremal graphs/trees that maximize or minimize a certain distance-based graph invariant have been studied for various categories of graphs including general graphs/trees, graphs/trees with prescribed maximum degree, diameter, matching and independence numbers, etc. [6, 8, 9, 11, 12, 14, 15, 17, 24, 26].

Due to the restrictions on the degrees of the vertices in a molecular graph, which correspond to the valences of the atoms in a compound, and to the fact that a large amount of chemical compounds have acyclic structures, it is of natural interest to consider trees with degree restrictions (see for instance [8, 16, 19, 22, 23, 27, 28]), in particular trees with prescribed degree sequence.

In regard to maximizing or minimizing the above mentioned distance-based invariants over all trees with prescribed degree sequence, it has been proven that the minimum is obtained for the "greedy tree" in the cases of the Wiener [22, 23, 28] and terminal Wiener index [20]. On the other hand, it was shown that the greedy tree maximizes the spectral radius [1]. For completeness, we present a formal definition of the *greedy tree*:

Definition 1 (Greedy trees). With given vertex degrees, the greedy tree is achieved through the following "greedy algorithm":

i) Label the vertex with the largest degree as v (the root);

ii) Label the neighbors of v as v_1, v_2, ..., assign the largest degrees available to them such that $\deg(v_1) \geq \deg(v_2) \geq \cdots$;

iii) Label the neighbors of v_1 (except v) as v_{11}, v_{12}, ... such that they take all the largest degrees available and that $\deg(v_{11}) \geq \deg(v_{12}) \geq \cdots$, then do the same for v_2, v_3, ...;

iv) Repeat (iii) for all the newly labeled vertices, always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

For example, Figure 1 displays a greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$.

The extremality of the greedy tree was proven through rather different approaches, sometimes even for the same graph invariant (i.e. in the case of the Wiener index). How-

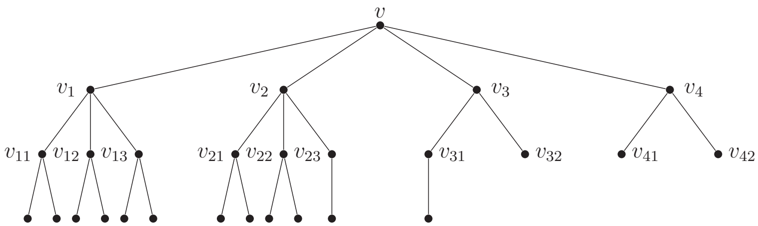

Figure 1: A greedy tree.

ever, from the "greedy" construction of a greedy tree, it is natural to ask for a universal property that may shed some light on these observations. We will show that the number of pairs of vertices whose distance is at most k is maximized by the greedy tree for all k. This property turns out to be equivalent to the minimality of the greedy tree with respect to general graph invariants of the form

$$W_f(T) = \sum_{\{u,v\}\subseteq V(T)} f(d(u,v))$$

for any nonnegative and nondecreasing function f. As some special cases, solutions to the minimization problems of the Wiener index, its generalized form, and the hyper-Wiener index follow immediately. The results regarding the generalized Wiener index and the hyper-Wiener index are, to the best of our knowledge, not in the literature. We will also present some discussions on the consequences from considering small values of k.

The maximization problem is somewhat more complicated. In the special case of the Wiener index, it has been proven that the problem can be reduced to the study of caterpillars [19].

Definition 2 (Caterpillars). A caterpillar is a tree with the property that a path remains if all leaves are deleted. E.g. Figure 2 shows a caterpillar with degree sequence $(6, 5, 4, 4, 2, 1, 1, \ldots, 1)$. We call the path that is formed by the non-leaves the *backbone* of the caterpillar.

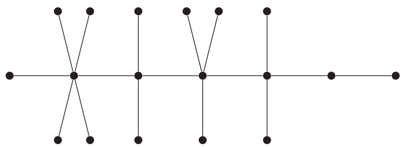

Figure 2: A caterpillar.

We will see in this note that a general conclusion can be drawn in this regards as well: $W_f(T)$ is maximized by a caterpillar for any increasing and convex function f.

Furthermore, a partial characterization of the trees that maximizes $W_f(T)$ follows from these results.

However, a complete characterization of the extremal trees seems impossible. For the Wiener index, Zhang et. al. [27] first pointed out the complexity of the question and studied cases for trees with few internal vertices. An efficient algorithm was recently provided in [4].

Through similar approaches as for $W_f(T)$, we also discuss the maximization of the terminal Wiener index. As a result, the same algorithm as in [4] can be used to find a solution.

The "universal property" of the greedy tree and its consequences will be discussed in Section 2. For the maximization problems and caterpillar, we study $W_f(T)$ in Section 3 and the terminal Wiener index in Section 4.

2 Greedy trees

We show that the greedy tree defined in Definition 1 is indeed greedy with respect to the distances in the following sense.

Theorem 2.1. *Let $d_1 \geq d_2 \geq \cdots \geq d_n$ be positive integers such that $\sum_i d_i = 2(n-1)$, and let k be another arbitrary positive integer. Among all trees with degree sequence $(d_1, d_2, \ldots, d_n)$, the greedy tree has the largest number $p_k(T)$ of pairs (u,v) of vertices such that $d(u,v) \leq k$.*

Before we come to a proof of this result, let us state the following important consequence.

Corollary 2.2. *Let $f(x)$ be any nonnegative, nondecreasing function of x. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

is minimized by the greedy tree among all trees with given degree sequence.

Proof. Simply note that

$$W_f(T) = \sum_{k \geq 0} (f(k+1) - f(k)) \left| \{\{u,v\} \subseteq V(T) : d(u,v) > k\} \right|,$$

and that $f(k) - f(k-1)$ is nonnegative for all k (we set $f(0) = 0$). ■

Remark 1. The above corollary includes, in addition to the classical Wiener index ($f(x) = x$), the hyper-Wiener index ($f(x) = \frac{x(x+1)}{2}$) and the generalized Wiener index with $f(x) = x^\alpha$.

Remark 2. Corollary 2.2 does not only follow from Theorem 2.1, it is actually equivalent, as can be seen by considering the function

$$f_k(x) = \begin{cases} 0 & x \le k, \\ 1 & x > k. \end{cases}$$

Then it is easy to show that

$$W_{f_k}(T) = \binom{n}{2} - p_k(T)$$

for any tree T of order n, so that p_k is maximized if $W_{f_k}(T)$ is minimized and vice versa.

The proof of Theorem 2.1 is obtained in two steps: first we prove that subtrees of optimal trees (that maximize p_k) can be assumed to be greedy in a certain sense. This is applied to prove the so-called semi-regularity property from [20], from which the theorem follows. Let us start with two lemmas regarding rooted and edge-rooted trees. We fix the outdegrees on each level and only allow "reshuffling" on each level. It turns out that we can always obtain an optimal tree that satisfies the "level-greedy" property stated in Definition 3 below with respect to any root by means of this reshuffling operation. Finally we will see that optimal trees with this "level-greedy" property (with the restriction of outdegrees at each level) are indeed greedy trees defined in Definition 1.

Definition 3 (Level-greedy trees). For $i = 0, 1, \ldots, H$, let multisets $\{a_{i1}, a_{i2}, \ldots, a_{i\ell_i}\}$ of nonnegative numbers be given such that $\ell_0 = 1$ and

$$\ell_{i+1} = \sum_{j=1}^{\ell_i} a_{ij}.$$

Assume that the elements of each multiset are sorted, i.e. $a_{i1} \ge a_{i2} \ge \cdots \ge a_{i\ell_i}$. The level-greedy tree (with height H) corresponding to this sequence of multisets is the rooted tree whose j-th vertex at level i has outdegree a_{ij}.

Likewise, if sorted multisets $\{a_{i1}, a_{i2}, \ldots, a_{i\ell_i}\}$ of nonnegative numbers are given for $i = 0, 1, \ldots, H$ such that $\ell_0 = 2$ and

$$\ell_{i+1} = \sum_{j=1}^{\ell_i} a_{ij},$$

then the level-greedy tree corresponding to this sequence of multisets is the edge-rooted tree (i.e. there are two vertices at level 0, connected by an edge) whose j-th vertex at level i has outdegree a_{ij}.

Every greedy tree is clearly also level-greedy (with respect to any root vertex), but the converse is not true (i.e. a tree can be level-greedy with respect to a certain root without being a greedy tree). For example, Figure 3 shows a level-greedy tree corresponding to the following sequence of multisets: $\{a_{01} = 3\}$, $\{a_{11} = 4, a_{12} = 2, a_{13} = 1\}$, $\{2, 2, 2, 1, 1, 0, 0\}$, $\{1, 1, 0, 0, 0, 0, 0, 0\}$ and $\{0, 0\}$.

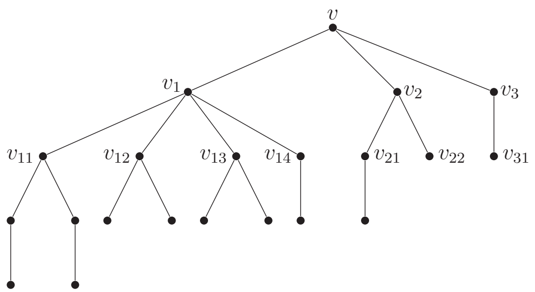

Figure 3: A level-greedy tree.

Lemma 2.3. *Consider the set of all rooted trees whose outdegrees at each level i are given by a multiset $\{a_{i1}, a_{i2}, \ldots, a_{i\ell_i}\}$ as in Definition 3. Among all such trees, the level-greedy tree maximizes the value of $p_k(T)$.*

Proof. For fixed i and j, consider the number of pairs of vertices (u, v) with $d(u, v) \leq k$ such that u is at level i and v is at level j. If $i + j \leq k$, then all possible pairs satisfy the distance condition. Otherwise, a vertex u at level i and a vertex v at level j satisfy $d(u, v) \leq k$ if and only if they have the same ancestor at level $\lceil (i + j - k)/2 \rceil$. Let us therefore count the number of pairs (u, v) of vertices such that u is at level i, v is at level j with a common ancestor at level $r = \lceil (i + j - k)/2 \rceil$. To this end, we denote by w_1, w_2, …, w_m the vertices at level r, and by x_1, x_2, …, x_m and y_1, y_2, …, y_m the number of their respective successors at level i and level j. Then the number of pairs we have to count is

$$x_1y_1 + x_2y_2 + \cdots + x_my_m$$

if $i \neq j$, and otherwise

$$\binom{x_1}{2} + \binom{x_2}{2} + \cdots + \binom{x_m}{2}.$$

In the latter case, however, since the sum $x_1 + x_2 + \cdots + x_m$ is constant under reshuffling, maximizing this sum is equivalent to maximizing

$$x_1^2 + x_2^2 + \cdots + x_m^2 = x_1y_1 + x_2y_2 + \cdots + x_my_m,$$

so the case $i = j$ can be treated along the same lines. Under all possible "reshuffled" trees, it is clear that the level-greedy tree maximizes $x_1 + x_2 + \cdots + x_h$ and $y_1 + y_2 + \cdots + y_h$ for all $1 \le h \le m$. Hence the result will follow as a consequence of the following simple lemma, whose proof is given for completeness:

Lemma 2.4. *Suppose that the sequences $(x_1, x_2, \ldots, x_m)$, $(y_1, y_2, \ldots, y_m)$, $(x'_1, x'_2, \ldots, x'_m)$ and $(y'_1, y'_2, \ldots, y'_m)$ of nonnegative real numbers satisfy*

$$\sum_{j=1}^{h} x_j \ge \sum_{j=1}^{h} x'_{\sigma(j)} \qquad \textit{and} \qquad \sum_{j=1}^{h} y_j \ge \sum_{j=1}^{h} y'_{\sigma(j)} \tag{2}$$

for all $1 \le h \le m$ and all permutations σ of $\{1, 2, \ldots, m\}$. Then

$$x_1 y_1 + x_2 y_2 + \cdots + x_m y_m \ge x'_1 y'_1 + x'_2 y'_2 + \cdots + x'_m y'_m. \tag{3}$$

Proof of Lemma 2.4. Suppose that x'_1, x'_2, …, x'_m and y'_1, y'_2, …, y'_m are such that the sum

$$x'_1 y'_1 + x'_2 y'_2 + \cdots + x'_m y'_m$$

is a maximum under the given restrictions (since the inequalities define a compact set, this is possible). By the rearrangement inequality, we may assume that $x'_1 \ge x'_2 \ge \cdots \ge x'_m$ and $y'_1 \ge y'_2 \ge \cdots \ge y'_m$. Let h be the smallest index such that

$$x_1 + x_2 + \cdots + x_h > x'_1 + x'_2 + \cdots + x'_h,$$

and let $\epsilon > 0$ be the difference between the two sides of the inequality. Replacing x'_h by $x'_h + \epsilon$ and x'_{h+1} by $x'_{h+1} - \epsilon$, we obtain a new $(2m)$-tuple of numbers satisfying the requirements, while the sum

$$x'_1 y'_1 + x'_2 y'_2 + \cdots + x'_m y'_m$$

changes by $\epsilon(y'_h - y'_{h+1}) \ge 0$. We can repeat this argument until we end up with $x_1 = x'_1$, $x_2 = x'_2$, …, $x_m = x'_m$, $y_1 = y'_1$, $y_2 = y'_2$, …, $y_m = y'_m$. This proves the lemma. ∎

Returning to the proof of Lemma 2.3, let the nondecreasing sequences $(x_1, \ldots, x_m)$, $(y_1, \ldots, y_m)$ be the number of successors at level i and j as described before in a level-greedy tree and let $(x'_1, \ldots, x'_m)$, $(y'_1, \ldots, y'_m)$ be the corresponding sequences for any tree with the same outdegrees on each level. It is easy to see that (2) is satisfied and hence (3) implies that the level-greedy tree indeed maximizes the number of pairs of vertices at levels i and j that have a common ancestor at level $r = \lceil (i + j - k)/2 \rceil$, for every i and j. Hence p_k is maximized by the level-greedy tree. ∎

Lemma 2.5. *Consider the set of all edge-rooted trees whose outdegrees at each level i are given by a multiset $\{a_{i1}, a_{i2}, \ldots, a_{i\ell_i}\}$ as in Definition 3. Among all such trees, the level-greedy tree maximizes the value of $p_k(T)$.*

Proof. Analogous to the previous lemma. ■

Recall that, with a given degree sequence, a tree with the following "semi-regular property" is a greedy tree, as it was shown in [20].

Definition 4 (Semi-regular property). We say that a tree satisfies the semi-regular property if, given any path with non-leaf end vertices $u, v \in V(T)$, the set of subtrees $\{T_u^1, \ldots, T_u^a\}$ attached to u and the set of subtrees $\{T_v^1, \ldots, T_v^b\}$ attached to v (such that $v \notin T_u^i$ and $u \notin T_v^j$ holds for each i and j) satisfy either

$$a \geq b \text{ and } \min\{|V(T_u^1)|, \ldots, |V(T_u^a)|\} \geq \max\{|V(T_v^1)|, \ldots, |V(T_v^b)|\}$$

or

$$b \geq a \text{ and } \max\{|V(T_u^1)|, \ldots, |V(T_u^a)|\} \leq \min\{|V(T_v^1)|, \ldots, |V(T_v^b)|\}.$$

Now we are able to prove the main theorem by showing that for trees maximizing p_k, being level-greedy implies the semi-regular property.

Proof of Theorem 2.1. Let T be any tree that maximizes $p_k(T)$ among all trees with the same degree sequence, and suppose further that T does not yet satisfy the semi-regularity condition. Let v and w be a pair of vertices violating this condition. If the unique path between v and w is of even length, we consider the midpoint of the path as the root of T and apply Lemma 2.3 to the resulting rooted tree. Then v and w are at the same level, and the reshuffling process that yields the level-greedy tree will actually change the shape of T. The value of p_k does not decrease by the lemma. Likewise, if the path between v and w is of odd length, we take the middle edge of the path as the root of T and apply Lemma 2.5.

Since the value of p_k does not necessarily increase strictly, however, we have to make sure that repeated application of the two lemmas does not result in an infinite loop. This is guaranteed by the fact that each "reshuffling step" (i.e. replacing a rooted or edge-rooted tree by the level-greedy tree with the same outdegrees) strictly decreases the Wiener index. Hence the process has to stop, and the "semi-regular" property in Definition 4 has to hold at the end. This implies that we must end up with the greedy tree. ■

Let us specifically consider the special cases $k = 1, 2, 3$. It is easy to see that $p_1(T)$ is just the number of edges of a tree T, and that

$$p_2(T) = \frac{1}{2} \sum_{v \in V(T)} (\deg v)^2,$$

which only depends on the degree sequence. Hence the statement of Theorem 2.1 is void in these two cases. For $k = 3$, we obtain

$$p_3(T) = p_2(T) + \sum_{\{v,w\} \in E(T)} (\deg v - 1)(\deg w - 1)$$
$$= \sum_{\{v,w\} \in E(T)} (\deg v)(\deg w) - \frac{1}{2} \sum_{v \in V(T)} (\deg v)^2 + |E(T)|,$$

so that maximizing $p_3(T)$ among all trees with given degree sequence amounts to maximizing

$$\sum_{\{v,w\} \in E(T)} (\deg v)(\deg w),$$

an invariant which is also known as *second Zagreb index* (the first Zagreb index is the sum of the squared degrees, which in our setting is obviously constant). In this case, one can give a very precise description of all extremal trees, discussed in [5] as the *weight* of a tree and later in [21] as a special case of the generalized *Randić index* of trees. As described in [5], trees that maximize $p_3(T)$ can be obtained by the following greedy algorithm:

- Sort the prescribed vertex degrees in decreasing order: $d_1 \geq d_2 \geq d_3 \geq \cdots$.
- Start with a single vertex of degree d_1.
- At step k, a vertex of degree d_k is attached to one of the vertices of highest degree for which this is still possible.

If the degrees of the non-leaves are pairwise distinct, this algorithm yields a unique tree (the greedy tree), but generally there is more than one optimal solution. It is obvious that the greedy tree can always be obtained by the above algorithm, in agreement with Theorem 2.1.

3 Caterpillars

In this section we deal with the maximization problem analogous to the minimization problem of Section 2. It is no longer possible to fully characterize the solution, as explained in the introduction, but the problem can be reduced to the study of caterpillars:

Proposition 3.1. *Let $f(x)$ be a strictly increasing and convex function (i.e. the increments $f(x+1) - f(x)$ are nondecreasing). Furthermore let $T_{\max}$ be a tree that maximizes*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

among all trees with degree sequence $(d_1, \ldots, d_n)$*. Then* $T_{\max}$ *is a caterpillar.*

Proof. Assume (for contradiction) that $T_{\max}$ is not a caterpillar.

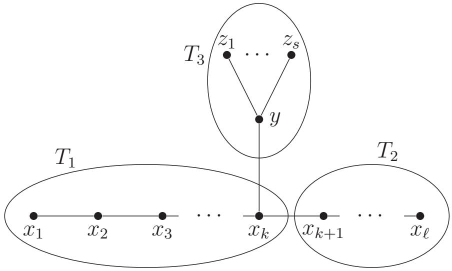

Figure 4: T_1, T_2 and T_3 in an optimal tree $T_{\max}$ that is not a caterpillar.

Let $P = (x_1, x_2, \ldots, x_\ell)$ be a longest path of $T_{\max}$. As $T_{\max}$ is not a caterpillar, we have that $\ell \geq 5$ and there exists an x_k, $2 < k < \ell - 1$, such that x_k has a non-leaf neighbor y that is not on P. Let $N(y) = \{x_k, z_1, \ldots, z_s\}$, $s \geq 1$, be the neighbors of y. Furthermore, after deleting the edges (x_k, x_{k+1}) and (x_k, y), let T_1, T_2 and T_3 denote the components containing x_k, x_{k+1} and y respectively, as illustrated in Figure 4. Without loss of generality we can also assume that $|V(T_1)| \geq |V(T_2)| \geq 2$.

Let T' be obtained from $T_{\max}$ by replacing each edge (y, z_i) of $T_{\max}$ by the new edge (x_ℓ, z_i), $1 \leq i \leq s$. Then T' and $T_{\max}$ have the same degree sequence.

Now we consider the distance between two vertices u and v. Note that $d_{T'}(u, v) \neq d_{T_{\max}}(u, v)$ only when $u \in V(T_3) \setminus \{y\}$ and $v \in V(T_1) \cup V(T_2) \cup \{y\}$ (or vice versa). The contributions of y and x_ℓ cancel, so it suffices to consider $v \in V(T_1)$ and $v \in V(T_2) \setminus \{x_\ell\}$. Then we obtain

$$
\begin{aligned}
W_f(T')-&W_f(T_{\max}) \\
&= \sum_{u \in V(T_3)\setminus\{y\}} \Bigg[\sum_{v \in V(T_1)} \big(f(d_{T'}(u,v)) - f(d_{T_{\max}}(u,v)) \big) \\
&\quad + \sum_{v \in V(T_2)\setminus\{x_\ell\}} \big(f(d_{T'}(u,v)) - f(d_{T_{\max}}(u,v)) \big) \Bigg] \\
&= \sum_{u \in V(T_3)\setminus\{y\}} \Bigg[\sum_{v \in V(T_1)} \big(f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k,x_\ell) + d_{T_{\max}}(x_k,v)) \\
&\quad - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k,v) + 1) \big) \\
&\quad + \sum_{v \in V(T_2)\setminus\{x_\ell\}} \big(f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_\ell,v)) \\
&\quad - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k,v) + 1) \big) \Bigg].
\end{aligned}
$$

Since P is a longest path in $T_{\max}$, we obtain that $d_{T_{\max}}(x_k, v) \le d_{T_{\max}}(x_k, x_\ell)$ for all $v \in V(T_2) \setminus \{x_\ell\}$ and $d_{T_{\max}}(x_k, x_\ell) \ge 2$. We are also going to use the fact that $d_{T_{\max}}(x_\ell, x_{\ell-1}) = 1$ and $d_{T_{\max}}(x_\ell, v) \ge 2$ for all $v \in V(T_2) \setminus \{x_\ell, x_{\ell-1}\}$.

With this we obtain that the contribution from each $u \in V(T_3) \setminus \{y\}$ to $W_f(T') - W_f(T_{\max})$ is at least

$$
\begin{aligned}
&\sum_{v \in V(T_1)} \big[f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + d_{T_{\max}}(x_k, v)) \\
&\quad - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, v) + 1)\big] \\
&\quad + \sum_{v \in V(T_2) \setminus \{x_{\ell-1}, x_\ell\}} \big[f(d_{T_{\max}}(u,y) + 2) \\
&\quad - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + 1)\big] \\
&\quad + f(d_{T_{\max}}(u,y) + 1) - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell)) \\
\ge &\sum_{v \in V(T_1) \setminus \{x_k\}} \big[f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + 1) \\
&\quad - f(d_{T_{\max}}(u,y) + 2)\big] \\
&\quad + f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell)) - f(d_{T_{\max}}(u,y) + 1) \\
&\quad + \sum_{v \in V(T_2) \setminus \{x_{\ell-1}, x_\ell\}} \big[f(d_{T_{\max}}(u,y) + 2) \\
&\quad - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + 1)\big] \\
&\quad + f(d_{T_{\max}}(u,y) + 1) - f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell)) \\
= &\big[f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + 1) - f(d_{T_{\max}}(u,y) + 2)\big] \\
&\quad \cdot \big(|V(T_1)| - 1 - |V(T_2)| + 2\big) \\
\ge &\, f(d_{T_{\max}}(u,y) + d_{T_{\max}}(x_k, x_\ell) + 1) - f(d_{T_{\max}}(u,y) + 2) > 0.
\end{aligned}
$$

Thus $W_f(T') > W_f(T_{\max})$, contradicting the optimality of $T_{\max}$. ■

Remark 3. If the function f in Proposition 3.1 is not strictly increasing, but only non-decreasing, we obtain the weaker result that there always exists a caterpillar that is an optimal solution.

Remark 4. Proposition 3.1 is wrong if f is not convex, and it is not hard to construct counterexamples. Consider for instance $f(x) = \sqrt{x}$ and the degree sequence $(20, 20, 20, 3, 1, 1, \ldots, 1)$. There are only two non-isomorphic caterpillars in this case, and the value of W_f for these two caterpillars is $858 + 573\sqrt{2} + 760\sqrt{3} + 38\sqrt{5} \approx 3069.67$ and $858 + 573\sqrt{2} + 437\sqrt{3} + 361\sqrt{5} \approx 3232.47$ respectively. However, it turns out that a tree with a center of degree 3 whose neighbors all have degree 20 (the other vertices being leaves) is optimal in this case: for this tree, W_f attains a value of $2226 + 573\sqrt{2} + 114\sqrt{3} \approx$

3233.8. The difference is very small in this example, but it increases if 20 is replaced by a larger value.

Remark 5. Note that the Wiener index as well as the hyper-Wiener index and the generalized Wiener index with $\alpha > 1$ form strictly increasing and convex functions, and thus Proposition 3.1 holds.

Unlike in Section 2, the optimal tree differs for different functions f. For instance, let $(d_1, \ldots, d_7) = (80, 76, 60, 30, 11, 6, 2)$ be the degree sequence of the internal vertices. Then the unique optimal tree with respect to the Wiener index is the caterpillar T_1 with $(d_{1,1}, \ldots, d_{1,7}) = (d_1, d_4, d_5, d_6, d_7, d_3, d_2)$, whereas the unique optimal tree with respect to the hyper-Wiener index is the caterpillar T_2 with $(d_{2,1}, \ldots, d_{2,7}) = (d_1, d_4, d_5, d_7, d_6, d_3, d_2)$. Here $d_{i,j}$ is the degree of the j-th vertex on the backbone of T_i.

Under the assumption that T is a caterpillar, $W_f(T)$ can be directly calculated from its degree sequence. We skip the details.

Lemma 3.2. *Let T be a caterpillar on n vertices and $v_1, \ldots, v_k$ the vertices on the backbone of T in this order. Then*

$$\begin{aligned} W_f(T) = {} & \frac{1}{2} \sum_{i=1}^{k} \sum_{j=1}^{k} f(|j-i|+2)(d_i-2)(d_j-2) \\ & + \sum_{i=1}^{k} \sum_{j=0}^{k+1} f(|j-i|+1)(d_i-2) \\ & + \sum_{i=0}^{k} \sum_{j=i+1}^{k+1} f(j-i) - \frac{1}{2} f(2)(n-k-2) \end{aligned} \tag{4}$$

for $d_\ell = \deg(v_\ell)$ and $f(x)$ an arbitrary function.

Maximizing (4) is essentially a quadratic assignment problem (QAP), which is known to be NP-hard even in rather special cases [3]. For the Wiener index, there is an efficient algorithm [4], but it seems unlikely that such an algorithm exists for more general functions f. However, we can further characterize the structure of the caterpillars maximizing (4).

Theorem 3.3. *Let $x_1 \geq x_2 \geq \cdots \geq x_k \geq 0$ be integers with $k \geq 3$ and let $f(x)$ be a strictly increasing and convex function. Further let S_k be the set of all permutations of $\{1, \ldots, k\}$ and suppose that $(y_1, \ldots, y_k)$ is a permutation of $(x_1, \ldots, x_k)$ such that w.l.o.g. $y_1 \geq y_k$ and*

$$\begin{aligned} & \frac{1}{2} \sum_{i=1}^{k} \sum_{j=1}^{k} f(|j-i|+2) y_i y_j + \sum_{i=1}^{k} \sum_{j=0}^{k+1} f(|j-i|+1) y_i \\ & \quad = \max_{\pi \in S_k} \left(\frac{1}{2} \sum_{i=1}^{k} \sum_{j=1}^{k} f(|j-i|+2) x_{\pi(i)} x_{\pi(j)} + \sum_{i=1}^{k} \sum_{j=0}^{k+1} f(|j-i|+1) x_{\pi(i)} \right). \end{aligned}$$

Then there exists a $2 \le t \le k-1$ *such that*

$$y_1 \ge y_2 \ge \cdots \ge y_{t-1} \ge y_t \le y_{t+1} \le \cdots \le y_k.$$

Moreover, if $k \ge 4$*, then* $t \ne k-1$.

Proof. Let us consider the permutation

$$(z_1, \dots, z_k) = (y_1, \dots, y_{\ell-1}, y_{\ell+1}, y_\ell, y_{\ell+2}, \dots, y_k)$$

of $(x_1, \dots, x_k)$. Since $(y_1, \dots, y_k)$ is optimal, we get

$$\begin{aligned} 0 &\le \frac{1}{2}\sum_{i=1}^{k}\sum_{j=1}^{k} f(|j-i|+2)(y_i y_j - z_i z_j) + \sum_{i=1}^{k}\sum_{j=0}^{k+1} f(|j-i|+1)(y_i - z_i) \\ &= (y_{\ell+1} - y_\ell)\Bigg(\sum_{i=1}^{\ell-1}(f(\ell-i+3) - f(\ell-i+2))y_i \\ &\quad - \sum_{i=\ell+2}^{k}(f(i-\ell+2) - f(i-\ell+1))y_i + f(\ell+2) - f(k-\ell+2)\Bigg). \end{aligned} \tag{5}$$

Now let us define the function

$$\begin{aligned} g(\ell) := &\sum_{i=1}^{\ell-1}(f(\ell-i+3) - f(\ell-i+2))y_i - \sum_{i=\ell+2}^{k}(f(i-\ell+2) - f(i-\ell+1))y_i \\ &+ f(\ell+2) - f(k-\ell+2) \end{aligned}$$

for $1 \le \ell \le k-1$. Obviously $g(1) < 0$, $g(k-1) > 0$ and $g(\ell) < g(\ell+1)$.

For $k = 3$, we immediately obtain by using (5) that $y_1 \ge y_2 \le y_3$.

For $k \ge 4$, we have that there exists a $t' \in \{2, 3, \dots, k-2\}$ such that

$$g(t'-1) < 0, \qquad g(t'+1) > 0.$$

Together with (5) we obtain

$$\begin{aligned} y_{\ell+1} - y_\ell &\le 0 \qquad \text{for } 1 \le \ell \le t'-1, \\ y_{\ell+1} - y_\ell &\ge 0 \qquad \text{for } t'+1 \le \ell \le k-1, \end{aligned}$$

which means

$$y_1 \ge y_2 \ge \cdots \ge y_{t'-1} \ge y_{t'} \qquad \text{and} \qquad y_{t'+1} \le y_{t'+2} \le \cdots \le y_k.$$

Since $y_1 \geq y_k$, we have $g(k-2) > 0$ and thus for $k = 4$, the theorem holds. To choose t properly for $k \geq 5$, we have to distinguish the following two cases.

- If $y_{t'} \leq y_{t'+1}$, then $t = t'$ fulfills the theorem.
- If $y_{t'} \geq y_{t'+1}$, then $t = t'+1$. Since $g(k-2) > 0$ and $k \geq 5$, we obtain that $t' \neq k-2$ and thus $t \neq k-1$ in this case.

∎

In terms of our maximization problem, this means that the degrees of the vertices on the backbone of an optimal caterpillar have to be unimodular (decreasing up to a certain point, then increasing). Note, however, that the optimal tree is not necessarily unique: for example, for $k = 6$ and $(d_1, \ldots, d_6) = (81, 77, 30, 25, 18, 9)$, the two caterpillars T_1 and T_2 with $(d_{1,1}, \ldots, d_{1,6}) = (d_1, d_4, d_6, d_5, d_3, d_2)$ and $(d_{2,1}, \ldots, d_{2,6}) = (d_1, d_4, d_5, d_6, d_3, d_2)$, where $d_{i,j}$ is the degree of the j-th vertex on the backbone of T_i, both maximize the Hyper-Wiener index.

4 Terminal Wiener index

In this final section, we consider the problem of finding the tree with prescribed degree sequence $(d_1, \ldots, d_n)$ that maximizes the terminal Wiener index (as mentioned earlier, the minimization problem has been solved in [20]). The techniques are very similar to the previous section.

Lemma 4.1. *Let $(d_1, d_2, \ldots, d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_i = 2(n-1)$. Then there always exists a caterpillar with maximum terminal Wiener index among all trees that have this particular degree sequence.*

Proof. Let $T_{\max}$ be a tree with maximum terminal Wiener index. We assume that $T_{\max}$ is not a caterpillar. Similar to the proof of Proposition 3.1, there exists a longest path $P = (x_1, x_2, \ldots, x_\ell)$ in $T_{\max}$ with $\ell \geq 5$ and an x_k, $2 < k < \ell - 1$, such that x_k has a neighbor $y \notin P$ and $\deg_{T_{\max}}(y) \geq 2$. We define T_1, T_2 and T_3 as shown in Figure 4 and $N(y) = \{x_k, z_1, \ldots, z_s\}$, $s \geq 1$, to be the neighbors of y. Without loss of generality we can assume that $|L(T_1)| \geq |L(T_2)|$, where $L(T_i)$ is the set of leaves of $T_{\max}$ in T_i.

Again we consider the tree T' arising from $T_{\max}$ by replacing each edge (y, z_i) by the edge (x_ℓ, z_i), $1 \leq i \leq s$. The contributions to the terminal Wiener index of $T_{\max}$ and T' differ only in the following four cases:

(1) $u \in L(T_3)$ and $v \in L(T_1)$: we obtain

$$d_{T_{\max}}(u, v) = d_{T_{\max}}(u, y) + 1 + d_{T_{\max}}(x_k, v),$$

$$d_{T'}(u,v) = d_{T_{\max}}(u,y) + d_{T_{\max}}(x_\ell, x_k) + d_{T_{\max}}(x_k, v).$$

(2) $u \in L(T_3)$ and $v \in L(T_2) \setminus \{x_\ell\}$: we get

$$d_{T_{\max}}(u,v) = d_{T_{\max}}(u,y) + 1 + d_{T_{\max}}(x_k, v),$$
$$d_{T'}(u,v) = d_{T_{\max}}(u,y) + d_{T_{\max}}(x_\ell, v).$$

(3) y and $v \in L(T_1) \cup L(T_2) \setminus \{x_\ell\}$: since y is an inner vertex of $T_{\max}$, there is no contribution to the terminal Wiener index of $T_{\max}$; for T' we get

$$d_{T'}(y,v) = 1 + d_{T_{\max}}(x_k, v).$$

(4) x_ℓ and $v \in L(T_1) \cup L(T_2) \setminus \{x_\ell\}$: as x_ℓ is an inner vertex of T', we get no contribution in this case; for $T_{\max}$ we have a contribution of

$$d_{T_{\max}}(x_\ell, v) = d_{T_{\max}}(x_\ell, x_k) + d_{T_{\max}}(x_k, v)$$

if $v \in L(T_1)$ and

$$d_{T_{\max}}(x_\ell, v)$$

if $v \in L(T_2) \setminus \{x_\ell\}$.

Thus we have

$$\begin{aligned}
TW(T') - TW(T_{\max}) = & \sum_{u \in L(T_3)} \Bigg(\sum_{v \in L(T_1)} (d_{T_{\max}}(x_\ell, x_k) - 1) \\
& + \sum_{v \in L(T_2) \setminus \{x_\ell\}} (d_{T_{\max}}(x_\ell, v) - d_{T_{\max}}(x_k, v) - 1) \Bigg) \\
& + \sum_{v \in L(T_1)} (1 - d_{T_{\max}}(x_\ell, x_k)) \\
& + \sum_{v \in L(T_2) \setminus \{x_\ell\}} (d_{T_{\max}}(x_k, v) - d_{T_{\max}}(x_\ell, v) + 1) \\
= & \, (d_{T_{\max}}(x_\ell, x_k) - 1) \, |L(T_1)| \, (|L(T_3)| - 1) \\
& + \sum_{v \in L(T_2) \setminus \{x_\ell\}} (d_{T_{\max}}(x_\ell, v) - d_{T_{\max}}(x_k, v) - 1)(|L(T_3)| - 1) \\
\geq & \, (|L(T_3)| - 1)(d_{T_{\max}}(x_\ell, x_k) - 1)(|L(T_1)| - |L(T_2)| + 1),
\end{aligned}$$

where the last inequality holds since $d_{T_{\max}}(x_\ell, v) \geq 2$ and $d_{T_{\max}}(x_k, v) \leq d_{T_{\max}}(x_k, x_\ell)$ for all $v \in L(T_2) \setminus \{x_\ell\}$. Hence together with $d_{T_{\max}}(x_\ell, x_k) \geq 2$ we arrive at

$$TW(T') \geq TW(T_{\max}).$$

Repeatedly applying this operation of transforming $T_{\max}$ to T' whenever $T_{\max}$ is not a caterpillar, we can always find a caterpillar tree with maximum terminal Wiener index (the process terminates since the diameter increases with every step). ■

Lemma 4.1 guarantees the existence of a caterpillar tree that maximizes the terminal Wiener index. But in contrast to the results of the previous section, not all optimal solutions have to be caterpillar trees. The following definition and proposition describe all possible optimal solutions.

Definition 5. A tree is called starlike if there is at most one vertex with degree greater than 2.

Proposition 4.2. *Let $T_{\max}$ be a tree that maximizes the terminal Wiener index among all trees with the same degree sequence. Then $T_{\max}$ is either a caterpillar or a starlike tree.*

Proof. Assume that $T_{\max}$ is not a caterpillar as presented in Figure 4 with $P = (x_1, x_2, \ldots, x_\ell)$, $\ell \geq 5$, being a longest path in $T_{\max}$ and $y \in N(x_k) \setminus \{x_{k-1}, x_{k+1}\}$.

If $|L(T_3)| > 1$, then the proof of Lemma 4.1 leads to a contradiction.

Thus let us consider the case $|L(T_3)| = 1$. This implies that $s = 1$ and, for the sake of simplicity, we denote z_1 by z. Furthermore we define $L(x_k)$ to be the set of leaves of $T_{\max}$ in the connected subgraph of $T_{\max}$ containing x_k after deleting the edges (x_{k-1}, x_k), (x_k, x_{k+1}) and (x_k, y). Without loss of generality we assume $|L(T_1) \setminus L(x_k)| \geq |L(T_2)|$. Now let T' be the tree arising from $T_{\max}$ by deleting the edges (y, z), (x_{k-1}, x_k) and adding the edges (x_k, z), (x_{k-1}, y). Then we obtain

$$d_{T'}(u, v) = d_{T_{\max}}(u, v) + 1$$

for $u \in L(T_1) \setminus L(x_k)$ and $v \in L(T_2) \cup L(x_k)$ and

$$d_{T'}(u, v) = d_{T_{\max}}(u, v) - 1$$

for $u \in L(T_3)$ and $v \in L(T_2) \cup L(x_k)$. For all other pairs of leaves the distances in $T_{\max}$ and T' are the same. Hence we get

$$\begin{aligned} TW(T') - TW(T_{\max}) &= \sum_{v \in L(T_2) \cup L(x_k)} \left(\sum_{u \in L(T_1) \setminus L(x_k)} 1 - \sum_{u \in L(T_3)} 1 \right) \\ &= (|L(T_2)| + |L(x_k)|)\,(|L(T_1) \setminus L(x_k)| - |L(T_3)|). \end{aligned}$$

If $|L(T_1)\setminus L(x_k)| > 1$, we have $TW(T') > TW(T_{\max})$ and thus $T_{\max}$ has to be a caterpillar. Otherwise we have $|L(T_1) \setminus L(x_k)| = |L(T_2)| = |L(T_3)| = 1$. We can repeat this argument to show that indeed every component of $T_{\max} \setminus \{x_k\}$ contains only a single leaf of $T_{\max}$. Thus $T_{\max}$ has to be a starlike tree. ∎

Remark 6. If the prescribed degree sequence only contains a single value > 2, then all possible trees are starlike, and it is easy to see that they all have the same terminal Wiener index. If this is not the case, then the above proposition shows that every optimal tree is indeed a caterpillar.

Again, one can give a simple formula for the terminal Wiener index of a caterpillar. We skip the details.

Lemma 4.3. *Let T be a caterpillar on n vertices and $v_1, v_2, \ldots, v_k$ be the k non-leaves that form the backbone of T in this order. Furthermore let d_i be the degree of vertex v_i, $1 \le i \le k$. Then*

$$TW(T) = (n-1)(n-k-1) + \frac{1}{2}\sum_{i=1}^{k}\sum_{j=1}^{k} |j-i|\,(d_i-2)(d_j-2).$$

Combining Lemmas 4.1 and 4.3, we obtain the following theorem:

Theorem 4.4. *Let T be a caterpillar and $(d_1, d_2, \ldots, d_n)$ be its degree sequence with $d_i \ge 2$ for $1 \le i \le k$ and $d_{k+1} = \cdots = d_n = 1$. Furthermore let d'_i be the degree of the i-th vertex on the backbone of T. If*

$$\sum_{i=1}^{k}\sum_{j=1}^{k} |j-i|\,(d'_i-2)(d'_j-2) = \max_{\pi\in S_k}\sum_{i=1}^{k}\sum_{j=1}^{k} |j-i|\,(d_{\pi(i)}-2)(d_{\pi(j)}-2)$$

with S_k the set of all permutations of $\{1,\ldots,k\}$, then T has maximum terminal Wiener index among all trees with the same degree sequence.

Therefore we have to solve the following maximization problem:

$$\max_{\pi\in S_k}\sum_{i=1}^{k}\sum_{j=1}^{k} |j-i|\,\alpha_{\pi(i)}\alpha_{\pi(j)}$$

with $\alpha_\ell \ge 0$, where S_k is the set of all permutations of $\{1,\ldots,k\}$. Maximizing the Wiener index leads to the exact same problem, and a solution can be found in quadratic time by means of an algorithm described in [4].

References

[1] T. Bıyıkoğlu, J. Leydold, Graphs with given degree sequence and maximal spectral radius, *El. J. Combin.* **15** (2008) R119.

[2] R. E. Burkard, E. Çela, G. Rote, G. J. Woeginger, The quadratic assignment problem with a monotone anti-Monge and a symmetric Toeplitz matrix: Easy and hard cases, *Math. Programming* **82** (1998) 125–158.

[3] E. Çela, *The Quadratic Assignment Problem: Theory and Algorithms*, Kluwer, Dordrecht, 1998.

[4] E. Çela, N. S. Schmuck, S. Wimer, G. J. Woeginger, The Wiener maximum quadratic assignment problem, *Discr. Optim.* **8** (2011) 411–416.

[5] C. Delorme, O. Favaron, D. Rautenbach, Closed formulas for the numbers of small independent sets and matchings and an extremal problem for trees, *Discr. Appl. Math.* **130** (2003) 503–512.

[6] H. Deng, The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 393–402.

[7] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[8] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Discr. Appl. Math.* **122** (2002) 127–137.

[9] I. Gutman, B. Furtula, M. Petrović, Terminal Wiener index, *J. Math. Chem.* **46** (2009) 522–531.

[10] A. Iranmanesh, A. S. Kafrani, O. Khormali, A new version of hyper–Wiener index, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 113–122.

[11] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, S. G. Wagner, Some new results on distance-based graph invariants, *Eur. J. Comb.* **30** (2009) 1149–1163.

[12] R. Kirk, H. Wang, The hyper-Wiener index of trees, *Congr. Numer.* **187** (2007) 40–54.

[13] D. J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper–Wiener index for cycle–containing structures, *J. Chem. Inf. Comput. Sci.* **35** (1995) 50–52.

[14] H. Liu, X. F. Pan, On the Wiener index of trees with fixed diameter, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 85–94.

[15] M. Liu, B. Liu, On the kth smallest and kth greatest modified Wiener indices of trees, *Discr. Appl. Math.* **158** (2010) 699–705.

[16] M. Liu, B. Liu, On the variable Wiener indices of trees with given maximum degree, *Math. Comput. Model.* **52** (2010) 1651–1659.

[17] M. Liu, B. Liu, Trees with the seven smallest and fifteen greatest hyper–Wiener indices, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 151–170.

[18] M. Liu, B. Liu, Q. Li, Erratum to 'The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees'. *MATCH Commun. Math. Comput. Chem.* **64** (2010) 743–756.

[19] R. Shi, The average distance of trees, *Systems Sci. Math. Sci.* **6** (1993) 18–24.

[20] L. Székely, H. Wang, T. Wu, The sum of the distances between leaves of a tree and the 'semi-regular' property, *Discr. Math.* **311** (2011) 1197–1203.

[21] H. Wang, Extremal trees with given degree sequence for the Randić index, *Discr. Math.* **308** (2008) 3407–3411.

[22] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **156** (2008) 2647–2654.

[23] H. Wang, Corrigendum: The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **157** (2009) 3754–3754.

[24] S. Wang, X. Guo, Trees with extremal Wiener indices, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 609–622.

[25] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[26] G. Yu, L. Feng, A. Ilić, The hyper–Wiener index of trees with given parameters. *Ars Combin.* **96** (2010) 395–404.

[27] X.-D. Zhang, Y. Liu, M.-X. Han, Maximum Wiener index of trees with given degree sequence, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 661–682.

[28] X. D. Zhang, Q. Y. Xiang, L. Q. Xu, R. Y. Pan, The Wiener index of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 623–644.