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Research Article

Steiner Wiener index and line graphs of trees*

Matjaž Kovše[1], Valisoa Razanajatovo Misanantenaina[2], Stephan Wagner[3,4†]

[1] *GoStudent, Ernst-Melchior-Gasse 20, 1020 Vienna, Austria*
[2] *Department of Logistics, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa*
[3] *Department of Mathematics, Uppsala Universitet, Box 480, 751 06 Uppsala, Sweden*
[4] *Department of Mathematical Sciences, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa*

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Abstract

A classical theorem due to Buckley [*Congr. Numer.* **32** (1981) 153–162] relates the Wiener index of a tree with the Wiener index of its line graph by a simple identity. We generalise this identity to the Steiner Wiener index and also use related ideas to resolve a problem due to Kovše, Rasila and Vijayakumar [*AKCE Int. J. Graphs Comb.* **17** (2020) 833–840] on the minimum value of the Steiner Wiener index of line graphs of trees.

Keywords: Steiner distance; Wiener index; k-Steiner Wiener index; trees; line graphs; block graphs.

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1. Introduction

The Wiener index of a graph, defined as the sum of all distances between vertices, is one of the most famous examples of a topological index in chemical graph theory. Its history goes back to the 1947 paper by Wiener [20], and many of its properties have been thoroughly studied. Books on mathematical chemistry and specifically chemical graph theory such as [6, 16, 17] all have a section devoted to the Wiener index. Trees have been of particular interest throughout the history of the Wiener index, see [5] for a topical survey.

Many different variants of the Wiener index have been considered in the literature, for example the hyper-Wiener index [8]

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

and the generalised Wiener index [7]

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

The classical Wiener index $W(G)$ is the special case $\alpha = 1$, the Harary index [13, 21] is obtained as the special case $\alpha = -1$:

$$H(G) = \sum_{\{v,w\}\subseteq V(G)} \frac{1}{d(v,w)}.$$

A relatively recent generalisation of the Wiener index is known as the k-Steiner Wiener index, see [11]. For a graph G and a subset U of k vertices, a k-Steiner tree is a tree of minimum size that contains all vertices of U and is a (not necessarily induced) subgraph of G. The number of edges of such a Steiner tree is called the Steiner distance of U, see [4]. Note that a 2-Steiner tree is simply a shortest path between two vertices, so this notion reduces to the classical graph distance for $k = 2$.

The k-Steiner Wiener index $SW_k(G)$ is now defined as the sum of the Steiner distances over all vertex subsets of cardinality k. The classical Wiener index $W(G)$ is the special case where $k = 2$. Note also that trivially $SW_1(G) = 0$, since 1-Steiner trees are just single vertices.

A line graph $L(G)$ of a graph G is obtained by associating a vertex with each edge of the graph and connecting two vertices with an edge if and only if the corresponding edges of G have a vertex in common. An important property of line graphs is the fact that they are claw-free: no induced subgraph is a claw (a complete bipartite graph $K_{1,3}$).

*Dedicated to the memory of Nenad Trinajstić.
†Corresponding author (stephan.wagner@math.uu.se).

Line graphs of trees are always block graphs, i.e., graphs where each block (maximal 2-connected subgraph) is complete. The blocks of the line graph correspond to the vertices of the tree. In fact, a graph is a line graph of a tree if and only if it is a connected claw-free block graph, or equivalently a connected block graph in which each cut vertex belongs to exactly two blocks. Figure 1 shows an example of a tree and its line graph.

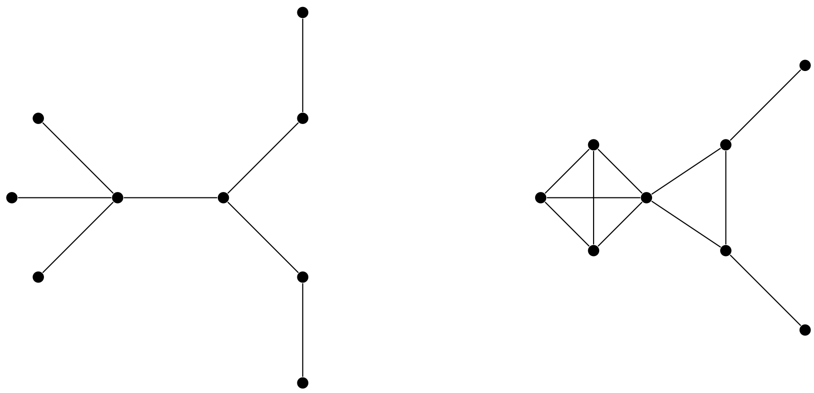

Figure 1: A tree (left) and its line graph (right).

Buckley [2] proved the following elegant relation between the Wiener index of a tree and its line graph.

Theorem 1.1. *For every tree T on n vertices, we have $W(L(T)) = W(T) - \binom{n}{2}$.*

Thus the difference of the Wiener indices of a tree T and its line graph $L(T)$ only depends on the size of T, but not its structure. Among other things, this result led to research into the Wiener index of iterated line graphs of trees, see for instance [9] and the references therein. In the following section, we present a generalisation of Theorem 1.1 to the k-Steiner Wiener index. Its proof is based on a representation of the k-Steiner Wiener index of a tree or its line graph as a sum over all edges.

There are several recent papers dealing with bounds and inequalities for the k-Steiner Wiener index as well as extremal problems, in particular concerning different classes of trees, see [12, 15, 19, 22, 23]. As part of their study of the Steiner Wiener index of block graphs, Kovše, Rasila and Vijayakumar [10] applied Buckley's theorem to determine the claw-free block graphs (equivalently, line graphs of trees) with given block sizes $b_1, b_2, \ldots, b_t$ that minimise the Wiener index. The analogous question for the k-Steiner Wiener index was left as an open problem [10, Problem 1]. In Section 3, we resolve this problem. Further results on the Steiner Wiener index of line graphs, in particular various bounds and inequalities, can be found in [14].

2. A generalisation of Buckley's theorem

The most classical result on the Wiener index of trees, which already appears in Wiener's original paper [20], states that it can be calculated by summing the contributions of all edges. For an edge uv in T, let $n_{uv}(T)$ denote the number of vertices of T that lie closer to u than to v. We have

$$W(T) = \sum_{uv \in E(T)} n_{uv}(T) n_{vu}(T), \tag{1}$$

since the edge uv belongs to the path between two vertices if and only if they lie on different sides of uv. More generally, uv belongs to the Steiner tree of a vertex set U if and only if U contains vertices on both sides of uv; or equivalently, if it does not only consist of vertices on one side of uv. The number of such vertex sets is $\binom{n}{k} - \binom{n_{uv}(T)}{k} - \binom{n_{vu}(T)}{k} = \sum_{j=1}^{k-1} \binom{n_{uv}(T)}{j}\binom{n_{vu}(T)}{k-j}$, where n is the total number of vertices. Summing over all edges of T, we obtain the following (known) generalisation of (1), see [11, Theorem 4.3] and [1, Proposition 21]:

Lemma 2.1. *For every positive integer k and every tree T on n vertices, we have*

$$SW_k(T) = (n-1)\binom{n}{k} - \sum_{uv \in E(T)} \left(\binom{n_{uv}(T)}{k} + \binom{n_{vu}(T)}{k} \right).$$

Our next goal is an analogous formula for the k-Steiner Wiener index of the line graph:

Lemma 2.2. *For every positive integer k and every tree T on n vertices, we have*

$$SW_k(L(T)) = (n-2)\binom{n-1}{k} - \sum_{uv \in E(T)} \left(\binom{n_{uv}(T)-1}{k} + \binom{n_{vu}(T)-1}{k} \right).$$

Proof. Let ϕ be the canonical map from edges of T to vertices of $L(T)$. In a block graph, the edges of a Steiner tree are not always unique, but the vertices are: given a set U of vertices, the Steiner tree of U needs to contain (in addition to U) precisely all those vertices that lie on shortest paths between vertices of U, since all of them are cut vertices. For a given edge $e = uv$ of T, let us determine the number of vertex subsets U of cardinality k in $L(T)$ for which the image $\phi(e)$ is contained in a Steiner tree of U. Clearly, this is the case if and only if either

- $\phi(e) \in U$: there are $\binom{n-2}{k-1}$ such sets, or
- $\phi(e) \notin U$, but U contains elements $\phi(f_1), \phi(f_2)$ where f_1 and f_2 lie on different sides of e in T. The number of these sets is
$$\binom{n-2}{k} - \binom{n_{uv}(T)-1}{k} - \binom{n_{vu}(T)-1}{k}.$$

Summing over all edges e, we obtain $SW_k(L(T)) + \binom{n-1}{k}$ (note that we have an overcount of 1 for each of the $\binom{n-1}{k}$ sets, since every Steiner tree has one vertex more than it has edges), thus:

$$\begin{aligned} SW_k(L(T)) &= -\binom{n-1}{k} + (n-1)\left(\binom{n-2}{k-1} + \binom{n-2}{k}\right) - \sum_{uv\in E(T)}\left(\binom{n_{uv}(T)-1}{k} + \binom{n_{vu}(T)-1}{k}\right) \\ &= (n-2)\binom{n-1}{k} - \sum_{uv\in E(T)}\left(\binom{n_{uv}(T)-1}{k} + \binom{n_{vu}(T)-1}{k}\right). \end{aligned} \tag{2}$$

□

Now we can easily relate the Steiner Wiener indices of trees and their line graphs, thereby generalising Buckley's theorem.

Theorem 2.1. *For every tree T on n vertices and every $k \geq 2$, we have*

$$SW_k(L(T)) + SW_{k-1}(L(T)) = SW_k(T) - \binom{n}{k}. \tag{3}$$

Equivalently,

$$SW_k(L(T)) = SW_k(T) - SW_{k-1}(T) + SW_{k-2}(T) - \cdots + (-1)^k SW_2(T) - \binom{n-1}{k} - (-1)^k(n-1) \tag{4}$$

for all $k \geq 2$.

Proof. Lemma 2.2, combined with the standard recursion for binomial coefficients, readily yields

$$\begin{aligned} SW_k(L(T)) + SW_{k-1}(L(T)) &= (n-2)\left(\binom{n-1}{k} + \binom{n-1}{k-1}\right) \\ &\quad - \sum_{uv\in E(T)}\left(\binom{n_{uv}(T)-1}{k} + \binom{n_{uv}(T)-1}{k-1} + \binom{n_{vu}(T)-1}{k} + \binom{n_{vu}(T)-1}{k-1}\right) \\ &= (n-2)\binom{n}{k} - \sum_{uv\in E(T)}\left(\binom{n_{uv}(T)}{k} + \binom{n_{vu}(T)}{k}\right). \end{aligned}$$

This proves the first identity in view of Lemma 2.1, the second follows easily by induction on k: for $k = 2$, the statement becomes

$$W(L(T)) = W(T) - \binom{n-1}{2} - (n-1) = W(T) - \binom{n}{2},$$

which is exactly (3) for $k = 2$ (i.e., Buckley's theorem), since $SW_1(G) = 0$ for all graphs G. For the induction step, we assume that the identity holds for $SW_{k-1}(L(T))$. The first part of the theorem now yields

$$\begin{aligned} SW_k(L(T)) &= SW_k(T) - SW_{k-1}(L(T)) - \binom{n}{k} \\ &= SW_k(T) - SW_{k-1}(T) + SW_{k-2}(T) - \cdots + (-1)^k SW_2(T) + \binom{n-1}{k-1} + (-1)^{k-1}(n-1) - \binom{n}{k} \\ &= SW_k(T) - SW_{k-1}(T) + SW_{k-2}(T) - \cdots + (-1)^k SW_2(T) - \binom{n-1}{k} - (-1)^k(n-1), \end{aligned}$$

completing the proof of (4). □

As mentioned before, the special case $k = 2$ is precisely Buckley's theorem. For $k = 3$, we can simplify the relation further to obtain an identity involving the Wiener index.

Corollary 2.1. *For every tree T on n vertices,*

$$SW_3(L(T)) = \frac{n-4}{2}W(T) - \frac{n(n-1)(n-5)}{6}.$$

Proof. Simply combine the second identity of Theorem 2.1 for $k = 3$ with the fact that $SW_3(T) = \frac{n-2}{2}W(T)$, see [11, Corollary 4.5]. □

3. An extremal problem

In [10], it was shown that the minimum value of the k-Steiner Wiener index among block graphs with given block sizes $b_1, b_2, \ldots, b_t$ is attained by the star-like block graph, which has the property that all blocks share a common cut vertex. For claw-free block graphs, which are precisely line graphs of trees, the authors of [10] made use of Buckley's theorem and a result on the Wiener index of trees with given degree sequence [18, 24] to prove that the minimum Wiener index is always attained by the line graph of a so-called greedy tree. The analogous question for the k-Steiner Wiener index was left as an open problem. Our goal in this section is to settle this open problem.

Let us first explain the notion of a greedy tree. Given a degree sequence $(d_1, d_2, \ldots, d_r)$ of a tree (without loss of generality non-decreasing), the greedy tree $\mathcal{G}(D)$ is a tree obtained by starting with the highest degree at the root, and then assigning the degrees in order to the vertices from top to bottom and left to right, see Figure 2.

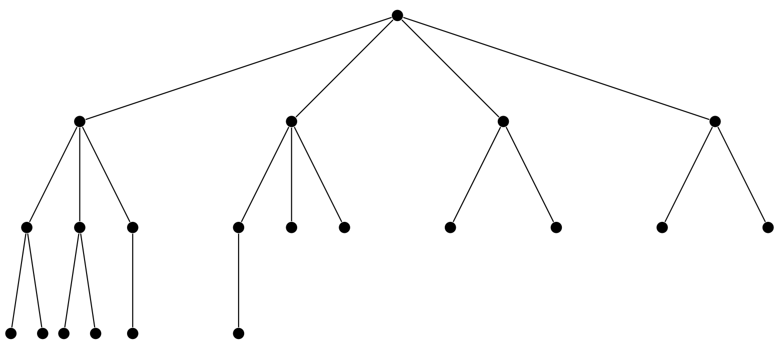

Figure 2: A greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 2, 2, 1, 1, \ldots, 1)$.

Note that a claw-free block graph with block sizes $b_1, b_2, \ldots, b_t$ is precisely the line graph of a tree with degree sequence $(b_1, b_2, \ldots, b_t, 1, 1, \ldots, 1)$. So we can reformulate the problem as: given the degree sequence $(b_1, b_2, \ldots, b_t, 1, 1, \ldots, 1)$ of a tree T, is it true that $SW_k(L(T))$ attains its minimum when T is a greedy tree?

For $k = 2$ and $k = 3$, we find that $SW_k(L(T))$ is minimal precisely when $W(T)$ is, by Buckley's theorem and Corollary 2.1, respectively. For other values of k, however, we cannot reduce the problem to a question about the Wiener index of T in this way. Nevertheless, we will prove that the answer is still affirmative for arbitrary $k \geq 2$, even though the greedy tree is not necessarily the unique tree that yields the minimum (see Remark 3.1 below).

We first need a few definitions. By a complete branch of a tree T, we mean a subtree S such that there is only one edge between S and $T \setminus S$. Such a complete branch has a natural root (the only vertex with an edge to $T \setminus S$) to which smaller complete branches $S_1, S_2, \ldots, S_r$ are attached. We write $S = [S_1, S_2, \ldots, S_r]$ for short. We also need an auxiliary invariant, defined as $SW_k^\varepsilon(L(T)) = SW_k(L(T)) + \varepsilon W(T)$, where $\varepsilon > 0$. The following lemma is the key to resolving the aforementioned problem, as it allows us to apply a general result from [1].

Lemma 3.1. *Let $\varepsilon > 0$ be fixed, and let T be a tree with degree sequence D for which $SW_k^\varepsilon(L(T))$ attains its minimum. Then, for any two disjoint complete branches $A = [A_1, \ldots, A_i]$ and $B = [B_1, \ldots, B_j]$ in T, we have*

- *either $i \geq j$ and $\min\{|A_1|, \ldots, |A_i|\} \geq \max\{|B_1|, \ldots, |B_j|\}$,*
- *or $i \leq j$ and $\max\{|A_1|, \ldots, |A_i|\} \leq \min\{|B_1|, \ldots, |B_j|\}$.*

In other words, T is $|\cdot|$-exchange-extremal in the sense of [1].

Proof. Let a and b be the roots of the complete branches A and B, respectively. Since $SW_k^\varepsilon(L(T))$ is minimal by assumption, it must in particular be minimal under the operations of switching A and B and permuting the $i + j$ branches

$A_1, A_2, \dots, A_i, B_1, B_2, \dots, B_j$ in an arbitrary way (note that neither of these operations affects the degree sequence). When A and B are switched or the branches are permuted, the contribution to the sum in Lemma 2.2 will only change for those edges that lie on the path from a to b. The contribution of any such edge to $SW_k^\varepsilon(L(T))$ is given by

$$-\left(\binom{|A|+x-1}{k}+\binom{|B|+y-1}{k}\right)+\varepsilon(|A|+x-1)(|B|+y-1),$$

where x and y are certain nonnegative integers (depending on the edge). Writing $|A|+|B|=m$ (which is invariant under the aforementioned operations), and summing over all edges on the path from a to b, we obtain a total contribution of the form

$$\sum_{\ell=1}^{L}\left(-\binom{|A|+x_\ell-1}{k}-\binom{m-|A|+y_\ell-1}{k}+\varepsilon(|A|+x_\ell-1)(m-|A|+y_\ell-1)\right). \tag{5}$$

Binomial coefficients are (weakly) convex on the positive integers, and the final term is strictly concave for every fixed $\varepsilon>0$. Therefore, the entire sum represents a strictly concave function of $|A|$, which can only attain its minimum when $|A|$ is either as large or as small as possible (potentially in both cases). Since $|A|=1+|A_1|+\cdots+|A_i|$ and $|B|=1+|B_1|+\cdots+|B_j|$, this happens precisely when one of the two stated conditions holds. □

A tree which minimizes $SW_k^\varepsilon(L(\cdot))$, given the degree sequence, is therefore always $|\cdot|$-exchange-extremal. By Theorem 2.5 of [1], any such tree must be greedy. Therefore, we obtain the following proposition.

Proposition 3.1. *Given $\varepsilon>0$ and a degree sequence D, $SW_k^\varepsilon(L(\cdot))$ is minimized by the greedy tree $\mathcal{G}(D)$, and the greedy tree is the unique tree for which the minimum is attained.*

Theorem 3.1. *The line graph of the greedy tree with degree sequence $(b_1,\dots,b_t,\dots,1)$ minimizes the k-Steiner Wiener index over all claw-free block graphs with block sizes $b_1,\dots,b_t$.*

Proof. Taking the limit $\varepsilon\to 0^+$ in the previous proposition, we find that the greedy tree minimizes $SW_k(L(\cdot))$ among all trees with degree sequence $(b_1,\dots,b_t,\dots,1)$. □

Remark 3.1. *Note that the greedy tree may not be the unique tree minimizing $SW_k(L(\cdot))$ if k is large compared to the size of the tree. Indeed, the expression (5) may no longer be strictly concave when $\epsilon=0$ and attain the minimum for values of $|A|$ other than the maximum and the minimum. This can only happen if the number of vertices n satisfies $n\le 2k-2$ (since $\binom{|A|+x_\ell-1}{k}+\binom{m-|A|+y_\ell-1}{k}$ becomes strictly convex as soon as $(|A|+x_\ell-1)+(m-|A|+y_\ell-1)=n-2>2k-4$). The smallest case of non-uniqueness occurs for $k=4$ and $n=6$, when both trees with degree sequence $(3,2,2,1,1,1)$ yield the same value.*

Remark 3.2. *Let us finally remark that the analogous problem for the maximum is more intricate. It was shown in [10] that the maximum is always attained by a path-like block graph, i.e., a block graph where no block has more than two cut vertices. Equivalently, these are line graphs of caterpillars (trees with the property that removing all leaves yields a path). However, even for the Wiener index, determining the optimal caterpillar given the degree sequence is a nontrivial problem in general (even though an efficient algorithm is available, see [3]).*

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References

[1] E. O. D. Andriantiana, V. Razanajatovo Misanantenaina, S. Wagner, Extremal trees with fixed degree sequence, *Electron. J. Combin.* **28** (2021) #P1.1.
[2] F. Buckley, Mean distance in line graphs, *Congr. Numer.* **32** (1981) 153–162.
[3] E. Çela, N. S. Schmuck, S. Wimer, G. J. Woeginger, The Wiener maximum quadratic assignment problem, *Discrete Optim.* **8** (2011) 411–416.
[4] G. Chartrand, O. R. Oellermann, S. L. Tian, H.-B. Zou, Steiner distance in graphs, *Časopis Pěst. Mat.* **114** (1989) 399–410.
[5] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
[6] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
[7] D. J. Klein, I. Gutman, Wiener-number-related sequences, *J. Chem. Inf. Comput. Sci.* **39** (1999) 534–536.
[8] 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.
[9] M. Knor, M. Mačaj, P. Potočnik, R. Škrekovski, Complete solution of equation $W(L^3(T))=W(T)$ for the Wiener index of iterated line graphs of trees, *Discrete Appl. Math.* **171** (2014) 90–103.
[10] M. Kovše, V. A. Rasila, A. Vijayakumar, Steiner Wiener index of block graphs, *AKCE Int. J. Graphs Comb.* **17** (2020) 833–840.
[11] X. Li, Y. Mao, I. Gutman, The Steiner Wiener index of a graph, *Discuss. Math. Graph Theory* **36** (2016) 455–465.

[12] L. Lu, Q. Huang, J. Hou, X. Chen, A sharp lower bound on Steiner Wiener index for trees with given diameter, *Discrete Math.* **341** (2018) 723–731.
[13] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.
[14] V. A. Rasila, A. Vijayakumar, Steiner Wiener index of line graphs, *Indian J. Pure Appl. Math.*, In press, DOI: 10.1007/s13226-021-00199-1.
[15] V. A. Rasila, A. Vijayakumar, Bounds on the Steiner–Wiener index of graphs, *Discrete Math. Algo. Appl.*, In press, DOI: 10.1142/S1793830922500173.
[16] N. Trinajstić, *Chemical Graph Theory*, 2nd Edition, CRC Press, Boca Raton, 1992.
[17] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2019.
[18] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discrete Appl. Math.* **156** (2008) 2647–2654.
[19] C. Wang, C. Ye, S. Zhang, Z. Wang, H. Li, The Steiner Wiener index of trees with given diameter, *Util. Math.* **108** (2018) 45–52.
[20] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.
[21] K. Xu, K. C. Das, N. Trinajstić, *The Harary index of a graph*, Springer, Heidelberg, 2015.
[22] J. Zhang, H. Wang, X.-D. Zhang, The Steiner Wiener index of trees with a given segment sequence, *Appl. Math. Comput.* **344/345** (2019) 20–29.
[23] J. Zhang, G.-J. Zhang, H. Wang, X.-D. Zhang, Extremal trees with respect to the Steiner Wiener index, *Discrete Math. Algo. Appl.* **11** (2019) #1950067.
[24] 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.