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A Remark on Modified Wiener Indices

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For any λ, ${}^{m}W_{\lambda}(T) = \sum_{e} [n_1(e) \cdot n_2(e)]^{\lambda}$, is the modified Wiener number of tree T. A question was asked in Ref. [6] whether each pair of indices ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$ differs in the sense that there are two trees T_1 and T_2 ordered differently by ${}^{m}W_{\lambda_1}$ and ${}^{m}W_{\lambda_2}$. In this paper we complete the answer to this question in positive.

Key words: Wiener number, modified Wiener number, Nikolić–Trinajstić–Randić index, a class of modified Wiener numbers.

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1 Introduction

The molecular-graph based quantity W, introduced [8] by Harold Wiener in 1947, nowadays known under the name *Wiener number* or *Wiener index*, is one of the most studied molecular-structure-descriptors [4].

Already in Wiener's seminal paper [8] the following formula for the calculation of the Wiener number of acyclic (molecular) graphs was reported:

$$W(T) = \sum_e n_1(e) \cdot n_2(e) \tag{1}$$

where T denotes a tree (= connected and acyclic graph), $n_1(e)$ and $n_2(e)$ are the number of vertices of T lying on the two sides of the edge e, and where the summation goes over all edges of T.

A large number of modifications and extensions of the Wiener number was considered in the chemical literature; an extensive bibliography on this matter can be found in the reviews [1]. One of such modification, generalizing the idea of Nikolić, Trinajstić and Randić [3], was put forward by Gutman, Vukičević and Žerovnik [2]. The modified Wiener indices of a tree T are defined by

$$^{m}W_\lambda(T) = \sum_e [n_1(e) \cdot n_2(e)]^\lambda \ . \tag{2}$$

Clearly, for $\lambda = +1$ and $\lambda = -1$, the modified Wiener number $^{m}W_\lambda$ reduces to the ordinary Wiener number W and the Nikolić–Trinajstić–Randić index ^{m}W, respectively.

Properties of $^{m}W_\lambda$ and some related indices were studied in [2, 5, 6, 7]. In particular, it has been shown in [2] that if trees are ordered with regard to $^{m}W_{\lambda_1}$ and $^{m}W_{\lambda_2}$ for distinct $\lambda_1, \lambda_2 < 0$, then the two orderings are different. Analogous result was proved by Vukičević for $\lambda_1, \lambda_2 > 0$ [7].

In the proof of [2], the graphs used are not necessarily of the same order, i.e. may have different numbers of vertices. In this paper we will show

Theorem 1. *For arbitrary different λ_1, $\lambda_2 \in \mathbb{R}$ there are graphs G_1 and G_2 of the same order such that*

$$^{m}W_{\lambda_1}(G_1) - {}^{m}W_{\lambda_1}(G_2) < 0 \tag{3}$$

and

$$^{m}W_{\lambda_2}(G_1) - {}^{m}W_{\lambda_2}(G_2) > 0\,. \tag{4}$$

This theorem summarizes Theorem 2 and Theorem 3 of this paper and the result of Vukičević in [7].

The rest of paper is organized as follows. In the next section we give some definitions and claims which are used in Section 3, where the two theorems are proved. In Section 4, we give some examples illustrating Theorem 2.

2 Preliminaries

For arbitrary $\lambda \in \mathbb{R}$ we define a function:

$$f_\lambda(a,b,c) = (a+b+c)(a+2b+3c)^\lambda + (b+c)\cdot 2^\lambda(a+2b+3c-1)^\lambda + c\cdot 3^\lambda(a+2b+3c-2)^\lambda .$$

For a later reference note that for $m > 4$ and $\lambda \in \mathbb{R}$ we have:

$$2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda > 0 \tag{5}$$

(because $m > 4 \Rightarrow 3m-6 > 2m-2 \Rightarrow (2m-2)^\lambda > (3m-6)^\lambda$) and

$$m^\lambda - 2^\lambda(m-1)^\lambda > 0 \tag{6}$$

(since $m > 2 \Rightarrow 2m-2 > m \Rightarrow m^\lambda > (2m-2)^\lambda$).

Lemma 1. *For arbitrary $m \in \mathbb{N}$ greater than 4 and arbitrary $\lambda \in \mathbb{R}^-$ there exists an $\varepsilon = \varepsilon(\lambda) \in [-\frac{m}{12}, \frac{m}{4}]$ such that*

$$f_\lambda(0, \frac{m}{2}, 0) - f_\lambda(\frac{m}{4} + 3\varepsilon, 0, \frac{m}{4} - \varepsilon) = 0 . \tag{7}$$

Proof. First note that

$$\begin{aligned} f_\lambda(0,\frac{m}{2},0) - f_\lambda(\frac{m}{4}+3\varepsilon,0,\frac{m}{4}-\varepsilon) &= \frac{m}{2}\cdot m^\lambda + \frac{m}{2}\cdot 2^\lambda(m-1)^\lambda \; - \\ - \; ((\frac{m}{2}+2\varepsilon)\cdot m^\lambda + (\frac{m}{4}-\varepsilon)\cdot 2^\lambda(m-1)^\lambda &+ (\frac{m}{4}-\varepsilon)\cdot 3^\lambda(m-2)^\lambda) \; = \\ = \; -\varepsilon(2m^\lambda - 2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda) &+ \frac{m}{4}\cdot(2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda) . \end{aligned} \tag{8}$$

If $\varepsilon = 0$, then from (5) follows

$$f_\lambda(0,\frac{m}{2},0) - f_\lambda(\frac{m}{4}+3\varepsilon,0,\frac{m}{4}-\varepsilon) = \frac{m}{4}\cdot(2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda) > 0 .$$

If $\varepsilon = \frac{m}{4}$, then from (6) follows

$$f_\lambda(0,\frac{m}{2},0) - f_\lambda(\frac{m}{4}+3\varepsilon,0,\frac{m}{4}-\varepsilon) = -\frac{m}{2}\cdot m^\lambda + \frac{m}{2}\cdot 2^\lambda(m-1)^\lambda = -\frac{m}{2}\cdot(m^\lambda - 2^\lambda(m-1)^\lambda) < 0 .$$

The expression on the lefthand side of (7) is a continuous function of ε, therefore there exists $\varepsilon = \varepsilon(\lambda) \in (0, \frac{m}{4})$, such that (7) holds. □

Lemma 2. *For any $\lambda \in \mathbb{R} - \{0\}$,* $\lim_{m\to\infty} \frac{\varepsilon(\lambda)}{m} = \frac{2^\lambda - 3^\lambda}{4(2 - 2^\lambda - 3^\lambda)}$.

Proof. From Lemma 1, inserting $\varepsilon(\lambda)$ into (7) using (8) we have

$$\varepsilon(\lambda) = \frac{m(2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda)}{4(2m^\lambda - 2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda)}\,, \tag{9}$$

therefore

$$\lim_{m\to\infty} \frac{\varepsilon(\lambda)}{m} = \lim_{m\to\infty} \frac{2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda}{4(2m^\lambda - 2^\lambda(m-1)^\lambda - 3^\lambda(m-2)^\lambda)} =$$

$$= \lim_{m\to\infty} \frac{2^\lambda(1-\frac{1}{m})^\lambda - 3^\lambda(1-\frac{2}{m})^\lambda}{4(2-2^\lambda(1-\frac{1}{m})^\lambda - 3^\lambda(1-\frac{2}{m})^\lambda)} = \frac{2^\lambda - 3^\lambda}{4(2-2^\lambda-3^\lambda)}\,. \quad \square$$

Lemma 3. *Let* $\lambda_1\,,\ \lambda_2 < 0\,.$ $\lambda_1 \neq \lambda_2$ *implies* $\varepsilon(\lambda_1) \neq \varepsilon(\lambda_2)\,.$

Proof. Hint: for $\lambda < 0\,,\ \varepsilon(\lambda)$ is an increasing function, because its derivative is positive. $\square$

3 Theorems

Let $G(a,b,c)$ be a tree, depicted on Fig. 1.

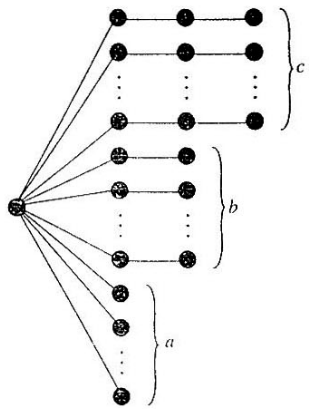

Figure 1: The graph $G(a,b,c)$.

Lemma 4. *For arbitrary $\lambda \in \mathbb{R}$ and $a, b, c \in \mathbb{N}_0$, ${}^{m}W_{\lambda}(G(a,b,c)) = f_{\lambda}(a,b,c)$.*

Proof. Clear. □

Theorem 2. *For arbitrary different λ_1, $\lambda_2 \in \mathbb{R}^-$ there are graphs G_1 and G_2 of the same order such that*

$$ {}^{m}W_{\lambda_1}(G_1) - {}^{m}W_{\lambda_1}(G_2) < 0 \quad \textit{and} \quad {}^{m}W_{\lambda_2}(G_1) - {}^{m}W_{\lambda_2}(G_2) > 0 . $$

Proof. Let $\varepsilon(\lambda_1)$ be such that $f_{\lambda_1}(0, \frac{m}{2}, 0) - f_{\lambda_1}(\frac{m}{4} + 3\varepsilon(\lambda_1), 0, \frac{m}{4} - \varepsilon(\lambda_1)) = 0$ and $\varepsilon(\lambda_2)$ such that $f_{\lambda_2}(0, \frac{m}{2}, 0) - f_{\lambda_2}(\frac{m}{4} + 3\varepsilon(\lambda_2), 0, \frac{m}{4} - \varepsilon(\lambda_2)) = 0$. From $\lambda_1 \neq \lambda_2$ it follows that $\varepsilon(\lambda_1) \neq \varepsilon(\lambda_2)$. Without loss of generality we can assume that $\varepsilon(\lambda_1) < \varepsilon(\lambda_2)$. Because of (5) and (6) we have, for each $j \in \{1,2\}$:
(i) if $\varepsilon < \varepsilon(\lambda_j)$, then $f_{\lambda_j}(0, \frac{m}{2}, 0) - f_{\lambda_j}(\frac{m}{4} + 3\varepsilon, 0, \frac{m}{4} - \varepsilon) > 0$ and
(ii) if $\varepsilon > \varepsilon(\lambda_j)$, then $f_{\lambda_j}(0, \frac{m}{2}, 0) - f_{\lambda_j}(\frac{m}{4} + 3\varepsilon, 0, \frac{m}{4} - \varepsilon) < 0$.
Therefore, for each $\varepsilon \in (\varepsilon(\lambda_1), \varepsilon(\lambda_2))$

$$ f_{\lambda_1}(0, \frac{m}{2}, 0) - f_{\lambda_1}(\frac{m}{4} + 3\varepsilon, 0, \frac{m}{4} - \varepsilon) < 0 \tag{10} $$

and

$$ f_{\lambda_2}(0, \frac{m}{2}, 0) - f_{\lambda_2}(\frac{m}{4} + 3\varepsilon, 0, \frac{m}{4} - \varepsilon) > 0 . \tag{11} $$

Take a rational number (a fraction)

$$ r = \frac{p}{q} \in \left(\lim_{m\to\infty} \frac{\varepsilon(\lambda_1)}{m}, \lim_{m\to\infty} \frac{\varepsilon(\lambda_2)}{m} \right) $$

and define sequences $m_i = 4iq$ and $\varepsilon_i = 4ip$. For large enough i, $r = \frac{p}{q} \in (\frac{\varepsilon_i(\lambda_1)}{m_i}, \frac{\varepsilon_i(\lambda_2)}{m_i})$, where $\varepsilon_i(\lambda)$ is the value of ε, corresponding to m_i and λ (see Lemma 1). Consequently, for the graphs $G_1 = G(0, \frac{m_i}{2}, 0) = G(0, 2iq, 0)$ and $G_2 = G(\frac{m_i}{4} + 3\varepsilon_i, 0, \frac{m_i}{4} - \varepsilon_i) = G(iq + 12ip, 0, iq - 4ip)$, we have ${}^{m}W_{\lambda_1}(G_1) - {}^{m}W_{\lambda_1}(G_2) < 0$ and ${}^{m}W_{\lambda_2}(G_1) - {}^{m}W_{\lambda_2}(G_2) > 0$. □

Theorem 3. *For arbitrary $\lambda_1 \in \mathbb{R}^-$ and $\lambda_2 \in \mathbb{R}^+$ there are graphs G_1 and G_2 such that (3) and (4) hold.*

Proof. Let $m > 2$, $G_1 = G(0, \frac{m}{2}, 0)$ and $G_2 = G(m, 0, 0)$.
As
(i) ${}^{m}W_{\lambda_1}(G_1) - {}^{m}W_{\lambda_1}(G_2) = \frac{m}{2} \cdot m^{\lambda_1} + \frac{m}{2} \cdot 2^{\lambda_1}(m-1)^{\lambda_1} - m \cdot m^{\lambda_1} = \frac{m}{2} \cdot 2^{\lambda_1}(m-1)^{\lambda_1} - \frac{m}{2} \cdot m^{\lambda_1} = \frac{m}{2}(2^{\lambda_1}(m-1)^{\lambda_1} - m^{\lambda_1}) < 0$ (since $m^{\lambda_1} - 2^{\lambda_1}(m-1)^{\lambda_1} > 0$) and
(ii) ${}^{m}W_{\lambda_2}(G_1) - {}^{m}W_{\lambda_2}(G_2) = \frac{m}{2}(2^{\lambda_2}(m-1)^{\lambda_2} - m^{\lambda_2}) > 0$ (since $2^{\lambda_2}(m-1)^{\lambda_2} - m^{\lambda_2} > 0$),
(3) and (4) hold as claimed. □

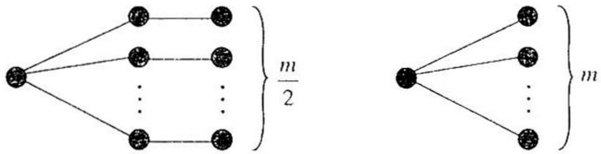

Figure 2: The graphs $G(0, \frac{m}{2}, 0)$ and $G(m, 0, 0)$.

4 Examples

Application of Theorem 2 is illustrated by the following examples.

Example 1. Let be $\lambda_1 = -6$ and $\lambda_2 = -5$. We search for such graphs G_1 and G_2 that ${}^{m}W_{-6}(G_1) - {}^{m}W_{-6}(G_2) < 0$ and ${}^{m}W_{-5}(G_1) - {}^{m}W_{-5}(G_2) > 0$.

Because $\lim\limits_{m\to\infty} \dfrac{\varepsilon(-6)}{m} \approx 0\text{'}001797$ and $\lim\limits_{m\to\infty} \dfrac{\varepsilon(-5)}{m} \approx 0\text{'}003453$, we define the fraction $\frac{\varepsilon}{q} = 0\text{'}002 = \frac{1}{500}$. Therefore, we try with $m_1 = 4q = 2000$ and $\varepsilon_1 = 4p = 4$. So $G_1 = G(0, 2q, 0) = G(0, 1000, 0)$ and $G_2 = G(q + 12p, 0, q - 4p) = G(512, 0, 496)$.

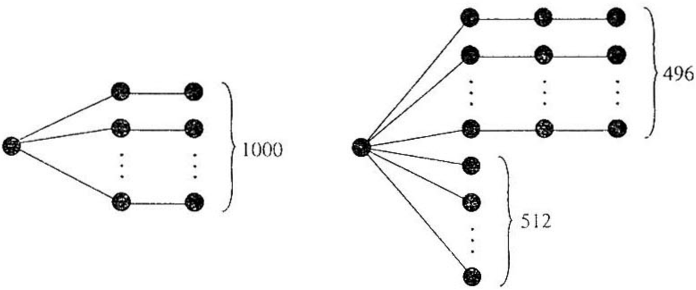

Figure 3: The graphs $G(0, 1000, 0)$ and $G(512, 0, 496)$.

Let us check:

${}^{m}W_{-6}(G_1) = 1000 \cdot 2000^{-6} + 1000 \cdot 2^{-6} \cdot 1999^{-6} \approx 1\text{'}5870 \cdot 10^{-17}$ and ${}^{m}W_{\lambda}(G_2) = 1008 \cdot 2000^{-6} + 496 \cdot 2^{-6} \cdot 1999^{-6} + 496 \cdot 3^{-6} \cdot 1998^{-6} \approx 1\text{'}5882 \cdot 10^{-17}$. Thus ${}^{m}W_{-6}(G_1) < {}^{m}W_{-6}(G_2)$.

${}^{m}W_{-5}(G_1) = 1000 \cdot 2000^{-5} + 1000 \cdot 2^{-5} \cdot 1999^{-5} \approx 3\text{'}2229 \cdot 10^{-14}$ and ${}^{m}W_{\lambda}(G_2) = 1008 \cdot 2000^{-5} + 496 \cdot 2^{-5} \cdot 1999^{-5} + 496 \cdot 3^{-5} \cdot 1998^{-5} \approx 3\text{'}2050 \cdot 10^{-14}$. Thus ${}^{m}W_{-5}(G_1) > {}^{m}W_{-5}(G_2)$.

□

Example 2. Let be $\lambda_1 = -5\text{'}1$ and $\lambda_2 = -5$. Because $\lim\limits_{m\to\infty} \dfrac{\varepsilon(-5\text{'}1)}{m} \approx 0\text{'}003237$ and

$\lim_{m\to\infty} \frac{\varepsilon(-5)}{m} \approx 0'003453$, we take $\frac{p}{q} = 0'0033 = \frac{33}{10000}$. Therefore, $G_1 = G(0,2q,0) = G(0,20000,0)$ and $G_2 = G(q+12p,0,q-4p) = G(10396,0,9868)$.
Indeed, ${}^m W_{-5'1}(G_1) < {}^m W_{-5'1}(G_2)$ and ${}^m W_{-5}(G_1) > {}^m W_{-5}(G_2)$. □

Example 3. Let be $\lambda_1 = -5'01$ and $\lambda_2 = -5$. Because $\lim_{m\to\infty} \frac{\varepsilon(-5'01)}{m} \approx 0'003431$ and $\lim_{m\to\infty} \frac{\varepsilon(-5)}{m} \approx 0'003453$, we define the fraction $\frac{p}{q} = 0'00344 = \frac{172}{50000}$. Therefore, $G_1 = G(0,2q,0) = G(0,100000,0)$ and $G_2 = G(q+12p,0,q-4p) = G(52064,0,49312)$.
Again, ${}^m W_{-5'01}(G_1) < {}^m W_{-5'01}(G_2)$ and ${}^m W_{-5}(G_1) > {}^m W_{-5}(G_2)$. □

Example 4. Let be $\lambda_1 = -5'4$ and $\lambda_2 = -5$. We search for such graphs G_1 and G_2 that ${}^m W_{-5'4}(G_1) - {}^m W_{-5'4}(G_2) < 0$ and ${}^m W_{-5}(G_1) - {}^m W_{-5}(G_2) > 0$.
Because $\lim_{m\to\infty} \frac{\varepsilon(-5'4)}{m} \approx 0'00266398$ and $\lim_{m\to\infty} \frac{\varepsilon(-5)}{m} \approx 0'003453$, we define the fraction $\frac{p}{q} = 0'002664 = \frac{333}{125000}$. Therefore, we try with $m_1 = 4q = 500000$ and $\varepsilon_1 = 4p = 1332$. So $G_1 = G(0,2q,0) = G(0,250000,0)$ and $G_2 = G(q+12p,0,q-4p) = G(128996,0,123668)$.
However,

- ${}^m W_{-5'4}(G_1) \approx 4'30197235\cdot 10^{-26}$ and ${}^m W_{-5'4}(G_2) \approx 4'30197221\cdot 10^{-26}$, thus ${}^m W_{-5'4}(G_1) > {}^m W_{-5'4}(G_2)$;
- ${}^m W_{-5}(G_1) \approx 8'2500\cdot 10^{-24}$ and ${}^m W_{-5}(G_2) \approx 8'2252\cdot 10^{-24}$, thus ${}^m W_{-5}(G_1) > {}^m W_{-5}(G_2)$.

So the graphs G_1 and G_2 are not ordered differently by ${}^m W_{\lambda_1}$ and ${}^m W_{\lambda_2}$.
Therefore, we try with $m_2 = 8q = 1000000$ and $\varepsilon_2 = 8p = 2664$. So $G_1' = G(0,4q,0) = G(0,500000,0)$ and $G_2' = G(2q+24p,0,2q-8p) = G(257992,0,247336)$.
Now:

- ${}^m W_{-5'4}(G_1') \approx 2'03767811\cdot 10^{-27}$ and ${}^m W_{-5'4}(G_2') \approx 2'03767814\cdot 10^{-27}$, thus ${}^m W_{-5'4}(G_1') < {}^m W_{-5'4}(G_2')$;
- ${}^m W_{-5}(G_1') \approx 5'1563\cdot 10^{-25}$ and ${}^m W_{-5}(G_2') \approx 5'1408\cdot 10^{-25}$, thus ${}^m W_{-5}(G_1') > {}^m W_{-5}(G_2')$.

So we have found the graphs needed. □
In general, it may be necessary to try more elements of the sequence before hitting the first m_i, ε_i for which the corresponding graphs would be ordered differently.

References

[1] M. V. Diudea and I. Gutman, Wiener-Type Topological Indices, *Croat. Chem. Acta* **71** (1998) 21–51.

[2] I. Gutman, D. Vukičević and J. Žerovnik, A Class of Modified Wiener Indices, *Croat. Chem. Acta*, to appear.

[3] S. Nikolić, N. Trinajstić and M. Randić, Wiener Index Revisited, *Chem. Phys. Lett.* **333** (2001) 319–321.

[4] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd revised ed. 1992.

[5] D. Vukičević and I. Gutman, Note on a Class of Modified Wiener Indices, *MATCH - Commun. Math. Comput. Chem.* **47** (2003) 107–117.

[6] D. Vukičević and J. Žerovnik, New Indices Based on Modified Wiener Indices, *MATCH - Commun. Math. Comput. Chem.* **47** (2003) 119–132.

[7] D. Vukičević, Distinction Between Modifications of Wiener Indices, *MATCH - Commun. Math. Comput. Chem.* **47** (2003) 87–105.

[8] H. Wiener, Structural Determination of Paraffin Boiling Points, *J. Am. Chem. Soc.* **69** (1947) 17–20.