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New Indices Based on the Modified Wiener Indices

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The Wiener index of a tree T obeys the relation $W(T) = \sum_e n_1(e) \cdot n_2(e)$ where $n_1(e)$ and $n_2(e)$ are the numbers of vertices on the two sides of the edge e, and where the summation goes over all edges of T. Recently, a class of modified Wiener indices ${}^mW_\lambda(T) = \sum_e [n_1(e) \cdot n_2(e)]^\lambda$, was put forward and it has been shown that some of the main properties of W are, in fact, properties of ${}^mW_\lambda$. Here we show that any nontrivial linear combination of the indices ${}^mW_\lambda$ gives rise to an index TI which is suitable for modeling branching-dependent properties of organic compounds. We also demonstrate that if trees are ordered with regard to TI then, in the general case, this ordering is different from any of orderings based on any ${}^mW_\lambda$.

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1 Introduction

The molecular-graph-based quantity W, nowadays known under the name *Wiener index* or *Wiener number*, is one of the most thoroughly studied molecular-structure-descriptors [2, 3] and it is still a topic of current research. For example, the fiftieth anniversary of the appearence of the Wiener's seminal paper [1] was celebrated by a special issues of MATCH [4].

A large number of modifications and extensions of the Wiener index was considered in the chemical literature; an extensive bibliography on this matter can be found in the reviews [5, 6]. Some recent modifications are based on the following formula for the calculation of the Wiener number of acyclic (molecular) graphs:

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

where T denotes a tree (= connected and acyclic graph) [2, 7], $n_1(e)$ 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. [Recall that formula (1) is *not* the definition of the Wiener index, but a mathematical theorem[1]; the Wiener index is *defined* as the sum of distances between all pairs of vertices.] One of the newest such modifications was put forward by Nikolić, Trinajstić and Randić [8]. They introduced the "*modified Wiener index*" ${}^mW$, defined as ${}^mW(T) = \sum_e [n_1(e) \cdot n_2(e)]^{-1}$ in analogy to formula (1). More recently, Gutman et al.[9] have defined "*a class of modified Wiener indices*" ${}^mW_\lambda$, defined as

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

where λ is a parameter that may assume different values. Clearly, for $\lambda = +1$ and $\lambda = -1$, the modified Wiener index ${}^mW_\lambda$ reduces to the ordinary Wiener index W and the Nikolić–Trinajstić–Randić index ${}^mW$, respectively.

Eq. (2) may be understood as a sum of increments, each associated with a particular edge of the molecular graph. Clearly, the contribution of the edge e, denoted by ${}^mW_e = {}^mW_e(G)$, is equal to $[n_1(e) \cdot n_2(e)]^\lambda$. The quantities $n_1(e)$ and $n_2(e)$ may be defined in a somewhat more formal manner: Let G be an arbitrary graph and let its edge e connect

the vertices u and v. Then $n_1(e)$ is the number of vertices of G whose distance to u is smaller than the distance to v. Similarly, $n_2(e)$ is the number of vertices of G whose distance to u is greater than the distance to v. If so, then any of the modified Wiener indices ${}^mW_\lambda$, Eq. (2), is a well-defined quantity for all graphs G. [Note that in the case $\lambda = +1$ (i.e. the original Wiener index) this definition on general graphs is known as the Szeged index [10, 11], which is in general different from the sum of all distances.]
An important property of the Wiener index are the inequalities

$$W(P_n) > W(T_n) > W(S_n) \tag{3}$$

where P_n, S_n, and T_n denote respectively the n-vertex path, the n-vertex star (cf. Figure 1), and any n-vertex tree different from P_n and S_n, and n is any integer greater than 4. Because of the relation (3), the Wiener index may be viewed as a "*branching index*", namely a topological index capable of measuring the extent of branching of the carbon-atom skeleton of molecules and capable of ordering isomers according to the extent of branching. (Branching is an important structural concept which is difficult to define in a rigorous way that would satisfactory reflect the intuition. For more references on the problem of measuring branching see the paper [12].)
It is known [12, 9] that the Wiener index and its modifications, i.e. the class of modified Wiener indices ${}^mW_\lambda$ (as defined in [9]) have the following two properties, which are clearly needed for any descriptor which may be used for measuring branching.
First, in order that a topological index TI be acceptable as a measure of branching it must satisfy the inequalities

$$TI(P_n) < TI(T_n) < TI(S_n) \quad , \quad n = 5, 6, \ldots \tag{4}$$

where P_n and S_n are the n-vertex path graph and star, respectively (see Figure 1), and where T_n is any n-vertex tree, different from P_n and S_n. Indeed, among n-vertex trees P_n is the least branched and S_n the most branched species.
Second, if T and T^* are graphs whose structure is depicted in Figure 1, then one requires that the inequality

$$TI(T^*) < TI(T) \tag{5}$$

holds irrespective of the actual form of the fragment R. This is because the vertex v_0 in T^* is more branched (has greater degree) than the vertex v_0 in T whereas the other structural details in T and T^* are the same.

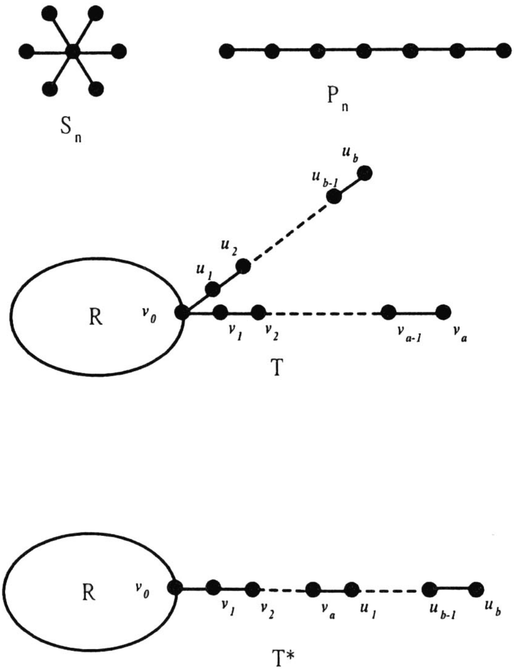

Figure 1: T^* is less branched than T.

Clearly, if instead of (4) and (5), the reversed inequalitites (6) and (7) are obeyed, TI also satisfies minimal requirements for being suitable for measuring branching.

$$TI(P_n) > TI(T_n) > TI(S_n) \quad , \quad n = 5, 6, \dots \tag{6}$$

$$TI(T^*) > TI(T) \tag{7}$$

We shall analyze the set of topological indices, linear combinations of two different generalized modified Wiener indices ${}^{m}W_{\lambda}$, given by the following formula:

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G) = \alpha_1 \cdot {}^{m}W_{\lambda_1}(G) + \alpha_2 \cdot {}^{m}W_{\lambda_2}(G)\,, \ \alpha_1,\alpha_2 > 0, \ \lambda_1,\lambda_2 \in \langle -1,0\rangle\,. \quad (8)$$

In the next section we first prove that any linear combination of modified Wiener indices has the above two properties (**Theorem 1**).

In Section 3 we also show (**Theorem 4**) that any nontrivial linear combination of modified Wiener indices gives rise to a quantity which is essentially different from any ${}^{m}W_{\lambda}$. In other words, we prove that if trees are ordered with regard to TI then, in the general case, this ordering is different from any of orderings based on any ${}^{m}W_{\lambda}$.

In Section 4 we discuss a couple of open questions.

2 Theorem 1 and its proof

Theorem 1 *Let* $\alpha_1,\alpha_2 > 0$, $\lambda_1,\lambda_2 \in \langle -1,0\rangle$. *Then*

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(P_n) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T_n) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(S_n) \quad , \quad n = 5,6,\ldots \quad (9)$$

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T^*) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T) \quad , \quad (10)$$

where P_n *and* S_n *are the* n*-vertex path graph and star, and* T *and* T^* *are graphs whose structure is depicted in Figure 1.*

In other words, $W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}$ satisfies (4) and (5), and can be called a "branching index".

Proof. Recall that

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G) = \alpha_1 \cdot {}^{m}W_{\lambda_1}(G) + \alpha_2 \cdot {}^{m}W_{\lambda_2}(G) \quad (11)$$

and let us prove that (4) holds for $W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}$, i.e.

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(P_n) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T_n) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(S_n)\,, \ n = 5,6,\ldots \quad (12)$$

We have, by Theorem 1 of [9],

$${}^{m}W_{\lambda_1}(P_n) \ < \ {}^{m}W_{\lambda_1}(T_n) \ < \ {}^{m}W_{\lambda_1}(S_n)\,, \ n = 5,6,\ldots \quad (13)$$

$${}^{m}W_{\lambda_2}(P_n) \ < \ {}^{m}W_{\lambda_2}(T_n) \ < \ {}^{m}W_{\lambda_2}(S_n)\,, \ n = 5,6,\ldots \quad (14)$$

Multiplying (13) with α_1 and (14) with α_2 and summarizing the resulting inequalities, the claim follows.

Along the same lines it can be proved

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T^*) < W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(T)\,. \tag{15}$$

In order to obtain ${}^mW_{\lambda_1}(T^*) < {}^mW_{\lambda_1}(T)$ and ${}^mW_{\lambda_2}(T^*) < {}^mW_{\lambda_2}(T)$ we can use:

Theorem 2 (Theorem 2 of [9]) *Let T' and T'' be trees the structure of which is shown in Figure 2. Then the transformation $T' \to T''$ increases ${}^mW_\lambda$ if $\lambda > 0$ and decreases ${}^mW_\lambda$ if $\lambda < 0$.*

Theorem 2 for $\lambda < 0$ clearly implies ${}^mW_\lambda(T^*) < {}^mW_\lambda(T)$.

Summing up ${}^mW_{\lambda_1}(T^*) < {}^mW_{\lambda_1}(T)$ multiplied by α_1 and ${}^mW_{\lambda_2}(T^*) < {}^mW_{\lambda_2}(T)$ multiplied by α_2 gives (15).

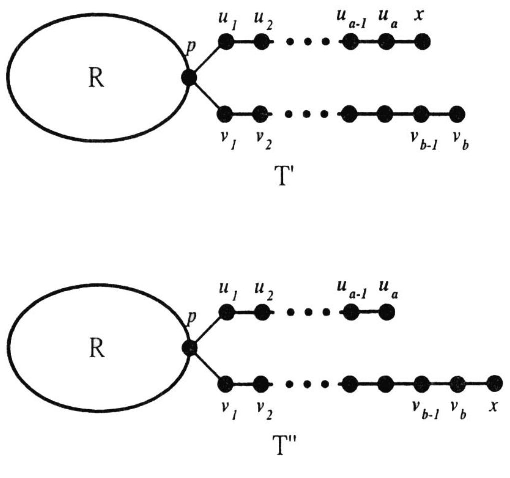

Figure 2: T' is less branched than T''.

□

3 Theorem 4 and its proof

Before proving the main results we recall the following lemma that is proved in [9]:

Lemma 3 *Let* $\lambda_1, \lambda_2 \in \langle -\infty, 0\rangle \setminus \{-1\}$, $\lambda_1 \neq \lambda_2$. *There is a rational number* $q \in \langle 1, \infty\rangle$ *such that*

$$\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}} \neq \sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}. \tag{16}$$

Now, we shall prove that the indices (8) are really a generalization of the modified Wiener indices, i.e. we shall prove that for each $\alpha_1, \alpha_2 > 0$ and each $\lambda_1, \lambda_2 \in \langle -1, 0\rangle$ such that $\lambda_1 \neq \lambda_2$, there is no $\lambda_3 < 0$ such that

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2} \equiv {}^{m}W_{\lambda_3}. \tag{17}$$

where $\equiv$ is the equivalence relation, defined formally as

$$(TI_1 \equiv TI_2) \Leftrightarrow [(\forall T_a, T_b \in \mathcal{T})(TI_1(T_a) \leq TI_1(T_b)) \Leftrightarrow (TI_2(T_a) \leq TI_2(T_b))].$$

In words: for two topological indices TI_1 and TI_2, $TI_1 \equiv TI_2$ if and only if they define exactly the same order among the set of all trees T.

Theorem 4 *Let* $\lambda_1, \lambda_2 \in \langle -1, 0\rangle$, $\lambda_3 < 0$, $\alpha_1, \alpha_2 > 0$ *and* $\lambda_1 \neq \lambda_2$. *Then*

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2} \not\equiv {}^{m}W_{\lambda_3}. \tag{18}$$

Before proving the theorem let us define a family of graphs $G_3(x,y)$, see Figure 3. For later reference note that

$${}^{m}W_{\lambda}(G_3(a,b)) = (a+b)(a+2b)^{\lambda} + b[2(a+2b-1)]^{\lambda} \tag{19}$$

and

$${}^{m}W_{\lambda}(S_n) = (n-1)(n-1)^{\lambda} = (n-1)^{\lambda+1}. \tag{20}$$

Proof. We have to find two graphs G and H such that

$$\begin{aligned} W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G) &\leq W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(H) \\ {}^{m}W_{\lambda_3}(H) &> {}^{m}W_{\lambda_3}(G) \end{aligned}$$

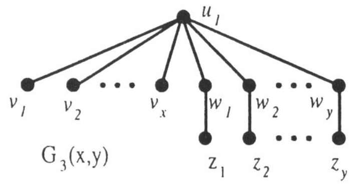

Figure 3: The graphs $G_3(x,y)$.

or graphs G and H such that

$$\begin{aligned} W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G) &\geq W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(H) \\ {}^{m}W_{\lambda_3}(H) &< {}^{m}W_{\lambda_3}(G). \end{aligned}$$

We will distinguish three cases:

1) $\lambda_3 < -1$.

Consider the path P_2 and the star S_4.

$$\begin{aligned} {}^{m}W_{\lambda_3}(P_2) &= 1 \\ W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(P_2) &= \alpha_1 + \alpha_2 \\ {}^{m}W_{\lambda_3}(S_4) &= 3 \cdot 3^{\lambda_3} < 1 \\ W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(S_4) &= \alpha_1 \cdot {}^{m}W_{\lambda_1}(S_4) + \alpha_2 \cdot {}^{m}W_{\lambda_2}(S_4) > \alpha_1 + \alpha_2 \end{aligned}$$

2) $\lambda_3 = -1$.

Let a be the smallest natural number such that

$$a^{\lambda_2+1}\left[4 \cdot 7^{\lambda_2} + 3 \cdot \left(14 - \frac{2}{a}\right)^{\lambda_2}\right] \cdot \alpha_2 > \alpha_1 + \alpha_2. \tag{21}$$

Such a certainly exists, because $\lambda_2 + 1 > 0$. Let $b = 3a$. We have

$${}^{m}W_{\lambda_3}(P_2) = 1$$

$$
\begin{aligned}
{}^{m}W_{\lambda_3}(G_3(a,b)) &= (a+b)(a+2b)^{-1} + b\left[2(a+2b-1)\right]^{-1} < \frac{4}{7} + \frac{1}{4} < 1 \\
W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(P_2) &= \alpha_1 \cdot {}^{m}W_{\lambda_1}(P_2) + \alpha_2 \cdot {}^{m}W_{\lambda_2}(P_2) = \alpha_1 \cdot 1 + \alpha_2 \cdot 1 = \alpha_1 + \alpha_2 \\
W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G_3(a,b)) &> \alpha_2 \cdot {}^{m}W_{\lambda_2}(G_3(a,b)) \\
&= \left\{(a+b)(a+2b)^{\lambda_2} + b\left[2(a+2b-1)\right]^{\lambda_2}\right\} \cdot \alpha_2 \\
&= a^{\lambda_2+1}\left[4 \cdot 7^{\lambda_2} + 3 \cdot \left(14 - \frac{2}{a}\right)^{\lambda_2}\right] \cdot \alpha_2 > \alpha_1 + \alpha_2,
\end{aligned}
$$

so

$$
\begin{aligned}
{}^{m}W_{\lambda_3}(P_2) &> {}^{m}W_{\lambda_3}(G_3(a,b)) \\
W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(P_2) &< W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G_3(a,b)).
\end{aligned}
$$

3) $\lambda_3 > -1$.

Without loss of generality, we may assume that $\lambda_1 < \lambda_2$. Furthermore, we will assume $\alpha_2 = 1$. This follows from observation that, for any constant $C > 0$, $C \cdot {}^{m}W_{\lambda}$ gives the same order as ${}^{m}W_{\lambda}$ (See Lemma 5) and transitivity of the relation $\equiv$.

We will consider two subcases:

3.1) $\lambda_2 \neq \lambda_3$.

From Lemma 3, it follows that there is a rational number $q \in \langle 1, \infty \rangle$ such that

$$
\sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}} \neq \sqrt[\lambda_3+1]{\frac{q+1+2^{\lambda_3}}{q+2}}. \tag{22}
$$

Distinguish two subsubcases:

3.1.1) . $\sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}} < \sqrt[\lambda_3+1]{\frac{q+1+2^{\lambda_3}}{q+2}}$

Analogously as in the paper [9], after a tedious computation, we get that there are natural numbers a, b and c such that

$$
\begin{aligned}
\frac{(a+b)(a+2b)^{\lambda_2} + b\left(2^{\lambda_2}(a+2b)^{\lambda_2}\right)}{c \cdot c^{\lambda_2}} &< 1 \\
\frac{(a+b)(a+2b)^{\lambda_3} + b\left(2^{\lambda_3}(a+2b)^{\lambda_3}\right)}{c \cdot c^{\lambda_3}} &> 1.
\end{aligned}
$$

It follows that

$$
\lim_{m \to \infty} \frac{\begin{pmatrix} \alpha_1 \cdot \left[(ma+mb)(ma+2mb)^{\lambda_1} + mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_1}\right)\right] \\ + (ma+mb)(ma+2mb)^{\lambda_2} + mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right) \end{pmatrix}}{\alpha_1 \cdot mc \cdot (mc)^{\lambda_1} + mc \cdot (mc)^{\lambda_2}} < 1
$$

$$\lim_{m\to\infty} \frac{(ma+mb)(ma+2mb)^{\lambda_3} + mb\left(2^{\lambda_3}(ma+2mb-1)^{\lambda_3}\right)}{mc\cdot(mc)^{\lambda_3}} > 1.$$

So, there is sufficiently large integer m, such that

$$\begin{pmatrix} \alpha_1 \cdot \begin{bmatrix} (ma+mb)(ma+2mb)^{\lambda_1} + \\ +mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_1}\right) \end{bmatrix} \\ +(ma+mb)(ma+2mb)^{\lambda_2} + \\ +mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right) \end{pmatrix} < \begin{pmatrix} \alpha_1\cdot mc\cdot(mc)^{\lambda_1} + \\ +mc\cdot(mc)^{\lambda_2} \end{pmatrix}$$

$$(ma+mb)(ma+2mb)^{\lambda_3} + mb\left(2^{\lambda_3}(ma+2mb-1)^{\lambda_3}\right) > mc\cdot(mc)^{\lambda_3}.$$

From here, we get

$$\begin{aligned} W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G_3(ma,mb)) &< W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(S_{mc+1}) \\ {}^{m}W_{\lambda_3}(G_3(ma,mb)) &> {}^{m}W_{\lambda_3}(S_{mc+1}). \end{aligned}$$

3.1.2) $\sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}} < \sqrt[\lambda_3+1]{\frac{q+1+2^{\lambda_3}}{q+2}}$

As in the previous case (just reversing the inequality signs) we get

$$\begin{aligned} W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G_3(ma,mb)) &> W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(S_{mc+1}) \\ {}^{m}W_{\lambda_3}(G_3(ma,mb)) &< {}^{m}W_{\lambda_3}(S_{mc+1}). \end{aligned}$$

3.2) $\lambda_2 = \lambda_3$.

We shall use the following claim, which will be proved later:

Claim A. Let $\lambda_1, \lambda_2 \in \langle -1, 0\rangle$, $\lambda_1 < \lambda_2$ and $\beta > 0$. There are graphs G' and H' such that

$$\frac{{}^{m}W_{\lambda_1}(G') - {}^{m}W_{\lambda_1}(H')}{{}^{m}W_{\lambda_2}(H') - {}^{m}W_{\lambda_2}(G')} > \beta. \tag{23}$$

Assume G' and H' are the graphs from the Claim A and let $\beta = \frac{\alpha_2}{\alpha_1}$. Again we distinguish two subsubcases:

3.2.1) ${}^{m}W_{\lambda_2}(H') > {}^{m}W_{\lambda_2}(G')$.

We have

$$\begin{aligned} \frac{{}^{m}W_{\lambda_1}(G') - {}^{m}W_{\lambda_1}(H')}{{}^{m}W_{\lambda_2}(H') - {}^{m}W_{\lambda_2}(G')} &> \frac{\alpha_2}{\alpha_1} \\ \alpha_1\cdot({}^{m}W_{\lambda_1}(G') - {}^{m}W_{\lambda_1}(H')) &> \alpha_2\cdot({}^{m}W_{\lambda_2}(H') - {}^{m}W_{\lambda_2}(G')) \\ W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G') &> W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(H'), \end{aligned}$$

hence ${}^{m}W_{\lambda_3} = {}^{m}W_{\lambda_2}$ and $W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}$ order the graphs G' and H' in different order.

3.2.2) ${}^{m}W_{\lambda_2}(H') < {}^{m}W_{\lambda_2}(G')$.

As in the case 3.2.1, multiplying $\frac{{}^{m}W_{\lambda_1}(G') - {}^{m}W_{\lambda_1}(H')}{{}^{m}W_{\lambda_2}(H') - {}^{m}W_{\lambda_2}(G')} > \frac{\alpha_2}{\alpha_1}$ by $\alpha_1 \cdot ({}^{m}W_{\lambda_2}(H') - {}^{m}W_{\lambda_2}(G'))$ we get

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(G') \quad < \quad W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}(H'),$$

as needed.

All the cases are exhausted and the theorem is proved. □

Proof of Claim A. From Lemma 3, it follows that there is a rational number $q \in \langle 1, \infty \rangle$ such that

$$\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}} \neq \sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}. \tag{24}$$

We distinguish two cases:

1) $\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}} > \sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}$.

By arguments completely analogous to considerations in the paper [9], it can be proved that there are natural numbers a, b and c such that

$$\begin{aligned}(a+b)(a+2b)^{\lambda_1} + b\left(2^{\lambda_1}(a+2b-1)^{\lambda_1}\right) - c \cdot c^{\lambda_1} &< 0\\ (a+b)(a+2b)^{\lambda_2} + b\left(2^{\lambda_2}(a+2b-1)^{\lambda_2}\right) - c \cdot c^{\lambda_2} &> 0.\end{aligned}$$

Let us introduce an auxiliary quantity

$$t = c \cdot c^{\lambda_1} - \left[(a+b)(a+2b)^{\lambda_1} + b\left(2^{\lambda_1}(a+2b-1)^{\lambda_1}\right)\right] > 0.$$

Note that

$$\lim_{m\to\infty} \frac{mc \cdot (mc)^{\lambda_1} - \left[(ma+mb)(ma+2mb)^{\lambda_1} + mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right)\right]}{m^{\lambda_1+1} \cdot t} = 1,$$

so, for any sufficiently large m, we have

$$mc \cdot (mc)^{\lambda_1} - \left[(ma+mb)(ma+2mb)^{\lambda_1} + mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right)\right] > \frac{1}{2} \cdot m^{\lambda_1+1} \cdot t$$

Let us denote

$$c_m = \left\lceil \left((ma+mb)(ma+2mb)^{\lambda_2} + mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right)\right)^{\frac{1}{\lambda_2+1}} \right\rceil - 1. \tag{25}$$

($\lceil x \rceil$ stands for the minimal integer $\geq x$.) Then

$$mc \leq c_m < m \cdot \left[(a+b)(a+2b)^{\lambda_2} + b\left(2^{\lambda_2}(a+2b-1)^{\lambda_2}\right) \right]^{\frac{1}{\lambda_2+1}},$$

($[x]$ stands for the maximal integer $\leq x$) so

$$c_m^{\lambda_1+1} - \left[(ma+mb)(ma+2mb)^{\lambda_1} + mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right) \right] > \frac{1}{2} t \cdot m^{\lambda_1+1}. \quad (26)$$

From (25) and (26) we obtain

$$\frac{c_m^{\lambda_1+1} - \left[(ma+mb)(ma+2mb)^{\lambda_1} + mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right) \right]}{\left((ma+mb)(ma+2mb)^{\lambda_2} + mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right) \right) - c_m^{\lambda_2+1}} > \frac{\frac{1}{2} \cdot m^{\lambda_1+1} \cdot t}{(c_m+1)^{\lambda_2+1} - c_m^{\lambda_2+1}} \quad (27)$$

Note that the function $(x+1)^{\lambda_2+1} - x^{\lambda_2+1}$ is decreasing, therefore the last expression is at least

$$\frac{\frac{1}{2} \cdot m^{\lambda_1+1} \cdot t}{(cm+1)^{\lambda_2+1} - (cm)^{\lambda_2+1}} \geq \frac{\frac{1}{2} t}{c^{\lambda_2+1}} \cdot \frac{m^{\lambda_1+1}}{(m+1)^{\lambda_2+1} - m^{\lambda_2+1}} \quad (28)$$

Let us prove

$$\lim_{m\to\infty} \frac{m^{\lambda_1+1}}{(m+1)^{\lambda_2+1} - m^{\lambda_2+1}} = \infty. \quad (29)$$

It is sufficient to show that, for sufficiently large m, we have

$$\begin{aligned}
(m+1)^{\lambda_2+1} - m^{\lambda_2+1} &< m^{\frac{\lambda_1}{2}+1} \\
\left(1+\frac{1}{m}\right)^{\lambda_2+1} &< 1 + m^{\frac{\lambda_1}{2}-\lambda_2} \\
\left[\left(1+\frac{1}{m}\right)^m\right]^{\frac{\lambda_2+1}{m}} &< 1 + m^{\frac{\lambda_1}{2}-\lambda_2} \\
\ln\left[\left(1+\frac{1}{m}\right)^m\right] &< \frac{\ln\left(1+m^{\frac{\lambda_1}{2}-\lambda_2}\right)}{\frac{\lambda_2+1}{m}}.
\end{aligned} \quad (30)$$

Note that lefthandside tends to 1 as m tends to infinity, so it is enough to prove that

$$\lim_{m\to\infty} \frac{\ln\left(1+m^{\frac{\lambda_1}{2}-\lambda_2}\right)}{\frac{\lambda_2+1}{m}} > 1.$$

Let us calculate the limit on the lefthandside using L'Hospital's rule

$$\lim_{m\to\infty}\frac{\ln\left(1+m^{\frac{\lambda_1}{2}-\lambda_2}\right)}{\frac{\lambda_2+1}{m}} = \lim_{m\to\infty}\frac{\frac{1}{1+m^{\frac{\lambda_1}{2}-\lambda_2}}\cdot\left(\frac{\lambda_1}{2}-\lambda_2\right)m^{\frac{\lambda_1}{2}-\lambda_2-1}}{(\lambda_2+1)\cdot\left(-\frac{1}{m^2}\right)}$$
$$= \frac{\lambda_2-\frac{\lambda_1}{2}}{\lambda_2+1}\cdot\lim_{m\to\infty}\frac{1}{1+m^{\frac{\lambda_1}{2}-\lambda_2}}\cdot\lim_{m\to\infty}m^{\frac{\lambda_1}{2}-\lambda_2+1}=\infty.$$

Hence (29) is proved. From (27), (28), and (29) it follows that

$$\lim_{m\to\infty}\frac{c_m^{\lambda_1+1}-\left[(ma+mb)(ma+2mb)^{\lambda_1}+mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right)\right]}{\left((ma+mb)(ma+2mb)^{\lambda_2}+mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right)\right)-c_m^{\lambda_2+1}}=\infty,$$

hence for sufficiently large m and any β

$$\frac{c_m^{\lambda_1+1}-\left[(ma+mb)(ma+2mb)^{\lambda_1}+mb\left(2^{\lambda_1}(ma+2mb-1)^{\lambda_1}\right)\right]}{\left((ma+mb)(ma+2mb)^{\lambda_2}+mb\left(2^{\lambda_2}(ma+2mb-1)^{\lambda_2}\right)\right)-c_m^{\lambda_2+1}}>\beta,$$

i.e.

$$\frac{{}^m W_{\lambda_1}(S_{c_m+1})-{}^m W_{\lambda_1}(G_3(ma,mb))}{{}^m W_{\lambda_2}(G_3(ma,mb))-{}^m W_{\lambda_2}(S_{c_m+1})}>\beta,$$

and the claim is proved in this case.

2) $\sqrt[\lambda_1+1]{\frac{q+1+2^{\lambda_1}}{q+2}}<\sqrt[\lambda_2+1]{\frac{q+1+2^{\lambda_2}}{q+2}}$.

The arguments in this case are similar to case 1). Details are ommited for brevity of presentation.

This concludes the proof of Claim A. □

4 Final remark

The following result is obvious:

Lemma 5 *Let $\alpha_1,\alpha_2,\alpha_1',\alpha_2'>0$ be such that $\frac{\alpha_1}{\alpha_1'}=\frac{\alpha_2}{\alpha_2'}$. Then*

$$W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}\equiv W_{\lambda_1,\lambda_2,\alpha_1',\alpha_2'}.$$

Hence all different indices are obtained by considering only $W_{\lambda_1,\lambda_2,\alpha_1,\alpha_2}$ with $\alpha_1+\alpha_2=1$, i.e. the convex combinations of two indices. Equivalently, one can restrict attention to indices with fixed $\alpha_2=1$ as we already did in previous section.

It is natural to ask whether all pairs of indices in this family yield different orders, or are there some more pairs (subfamilies) of indices which give the same order among the set of all trees.

Another question of some interest is the following. In this paper and in [9] it was shown that a large class of indices based on the modified Wiener index are pairwise nonequivalent in the sense that they order the set of all trees in different manner. However, the examples used in the proofs were graphs of different size, i.e. they differed in the number of vertices. It would be interesting to find (not too complicated) proof of Theorem 4 (and Theorem 3 of [9]) based on construction of examples of pairs of graphs on the same number of vertices.

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