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Variable Wiener Indices*

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Abstract. Recently Nikolić, Trinajstić and Randić put forward a novel modification ${}^{m}W(G)$ of the Wiener index $W(G)$, defined as ${}^{m}W(G) = \sum_{uv\in E(G)} n_G(u,v)^{-1} n_G(v,u)^{-1}$. This definition was generalized to ${}^{\lambda}W(G) = \sum_{uv\in E(G)} n_G(u,v)^{\lambda} n_G(v,u)^{\lambda}$ by Gutman and the present authors. Another class of modified indices ${}_{\lambda}W(G) = \frac{1}{2}\sum_{uv\in E(G)} \left(v(G)^{\lambda} - n_G(u,v)^{\lambda} - n_G(v,u)^{\lambda}\right)$ is studied here. It is shown that some of the main properties of $W(G)$, ${}^{m}W(G)$ and ${}^{\lambda}W(G)$ are also properties of ${}_{\lambda}W(G)$, valid for all values of the parameter $\lambda \neq 0$. In particular, if T_n is any n-vertex tree, different from the n-vertex path P_n and the n-vertex star S_n, then for any $\lambda > 1$, ${}_{\lambda}W(P_n) > {}_{\lambda}W(T_n) > {}_{\lambda}W(S_n)$, whereas for any $\lambda < 1$, ${}_{\lambda}W(P_n) < {}_{\lambda}W(T_n) < {}_{\lambda}W(S_n)$. Thus ${}_{\lambda}W(G)$ provides a novel class of structure-descriptors, suitable for modeling branching-dependent properties of organic compounds, applicable in QSPR and QSAR studies. We also demonstrate that if trees are ordered with regard to ${}_{\lambda}W(G)$ then, in the general case, this ordering is different for different λ.

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INTRODUCTION

The molecular-graph-based quantity, introduced [1] by Wiener in 1947, nowadays known under the name *Wiener number* or *Wiener index*, is one of the most thoroughly studied topological indices [2,3]. Its chemical applications [4-8] and mathematical properties [9,10] are well documented. Of the several review articles on the Wiener number we mention just a few [11-13].

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 papers [14,15]. One of the newest such modifications was put forward by Nikolić, Trinajstić and Randić [16]. This idea was generalized by Gutman and the present authors [17] where a class of modified Wiener indices was defined, with the original Wiener number and the Nikolić-Trinajstić-Randić index as special cases.

An important property of a topological index *TI* are the inequalities

$$TI(P_n) > TI(T_n) > TI(S_n) \qquad \text{or} \qquad TI(P_n) < TI(T_n) < TI(S_n) \qquad (1)$$

where P_n, S_n, and T_n denote respectively the n-vertex path, the n-vertex star, and any n-vertex tree different from P_n and S_n, and n is any integer greater than 4. Such topological 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. (For more details on the problem of measuring branching see the paper [18] and the references quoted therein.)

Among a remarkably large number of modifications and extensions of the Wiener number put forward recently, there are many which on trees (i.e. acyclic systems) concide [19-25] or are linearly related with it [26-30]. Therefore an interesting property of a class of newly defined indices is that they provide distinct indices in the sense that they order the trees differently.

More precisely, the Wiener number of a chemical graph is defined to be the sum of all distances in the graph.

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v).$$

In the papers [31,29] by Gutman et al., the following modification is proposed:

$$W_\lambda(G) = \sum_{u,v \in V(G)} d_G(u,v)^\lambda, \ \lambda \neq 0.$$

It was already known to Wiener that on a tree, the Wiener number can also be computed by summing up the edge contributions, where the contribution of each edge uv is the number of vertices closer to the vertex u times the number of vertices closer to the vertex v. Formally,

$$W(G)=\sum_{uv\in E(G)} n_G(u,v)\, n_G(v,u). \tag{2}$$

where $n_G(u,v)$ is the number of vertices closer to the vertex u than vertex v and $n_G(v,u)$ is the number of vertices closer to the vertex v than vertex u. The modified Wiener indices [17,31-37] are defined as

$${}^{\lambda}W(G)=\sum_{uv\in E(G)} n_G(u,v)^{\lambda}\, n_G(v,u)^{\lambda}.$$

Equality (2) can be also reformulated as

$$W(G)=\frac{1}{2}\sum_{uv\in E(G)}\left(V(G)^2-n_G(u,v)^2-n_G(v,u)^2\right).$$

Let us prove this claim. Recalling that $V(G)=n_G(u,v)+n_G(v,u)$, we get

$$W(G)=\sum_{uv\in E(G)}\left(\frac{1}{2}n_G(u,v)\cdot\left(V(G)-n_G(u,v)\right)+\frac{1}{2}n_G(v,u)\cdot\left(V(G)-n_G(v,u)\right)\right)$$
$$=\frac{1}{2}\sum_{uv\in E(G)}\left(\left(n_G(u,v)+n_G(v,u)\right)V(G)-n_G(u,v)^2-n_G(v,u)^2\right)=$$
$$=\frac{1}{2}\sum_{uv\in E(G)}\left(V(G)^2-n_G(u,v)^2-n_G(v,u)^2\right).$$

Therefore it is natural to study the following possible class of indices

$${}_{\lambda}W(G)=\frac{1}{2}\sum_{uv\in E(G)}\left(V(G)^{\lambda}-n_G(u,v)^{\lambda}-n_G(v,u)^{\lambda}\right). \tag{3}$$

which we initiate in this paper. We first prove that the indices ${}_{\lambda}W, \lambda\neq 0,1,$ obey the inequalities (1) and can therefore be viewed as ``*branching indices* ''. We call indices ${}_{\lambda}W$ *variable Wiener indices* to distinguish them from modified Wiener indices W_{λ}. (The name variable Wiener indices is given in analogy with the name variable Zagreb indices proposed by Trinajstić et al.)

Theorem 1. *For any real number $\lambda>1$, the variable Wiener index $_{\lambda}W$ satisfies the inequalities*

$$_{\lambda}W(P_n) > {}_{\lambda}W(T_n) > {}_{\lambda}W(S_n)$$

where P_n, S_n, and T_n denote respectively the n-vertex path, the n-vertex star, and any n-vertex tree different from P_n and S_n, and n is any integer greater than 4. For any real number $\lambda<1$, the variable Wiener index $_{\lambda}W$ satisfies the inequalities

$$_{\lambda}W(P_n) < {}_{\lambda}W(T_n) < {}_{\lambda}W(S_n).$$

Instead of proving Theorem 1 we prove a stronger statement (Theorem 3), which may be of independent interest because it shades some light on the partial ordering induced by $_{\lambda}W$.

Furthermore, we prove that the indices $_{\lambda}W, \lambda \neq 0,1,$ studied here provide classes of distinct indices in the sense that they order the trees differently. More precisely, no matter what the values of λ_1 and λ_2 are, there always exist trees that are oppositely ordered with regard to $_{\lambda_1}W$ and $_{\lambda_2}W$. More formally, let the set of all trees be denoted by $\mathcal{T}$. Denote the set of some topological indices (e. g. the set of the modified Wiener indices $_{\lambda}W$ for all values of λ) by $\mathfrak{I}$. We can define an equivalence relation $\equiv$ on the set $\mathfrak{I}$ as

$$(i_1 \equiv i_2) \Leftrightarrow [(\forall T_a, T_b \in \mathcal{T}) (i_1(T_a) \leq i_1(T_b)) \Leftrightarrow (i_2(T_a) \leq i_2(T_b))].$$

In words: two topological indices i_1 and i_2 are considered to be *equivalent* if they order all trees in the exactly same manner. We will prove

Theorem 2. *For each two distinct real numbers λ_1, λ_2 ($\lambda_1, \lambda_2 \neq 0,1$), the modified Wiener indices $_{\lambda_1}W$ and $_{\lambda_2}W$ are not equivalent.*

The Wiener number is used in many QSAR and QSPR studies. It is known that it is well correlated with many important chemical properties of chemical compunds. Therefore, it may be very useful to investigate the Wiener-like indices. Namely, some modifications may have better prediction capabilities (for some chemical properties) than the original Wiener number. Small alternations of good predicting indices can result in indices with the better predicting abbilities. For a very recent positive example let us recall that very shortly after the first paper on modified Wiener indices appeared, their applicability in QSPR/QSAR studies has been demonstrated [37].

It is beyond scope of this paper to provide further motivation and/or possible chemical interpretation of the new indices, which is necessary for proposing it as a practically useful topological descriptors. However, continuing along the research avenue initiated by recent papers [16-18,29,31-36] we show that there are additional new interesting ways of generalization of the Wiener number which posses certain important properties of W and may provide interesting choices for topological descriptors. Let us in conclusion resume some noteworthy properties of the type of indices defined here: (1) ${}_{\lambda}W$ are in contrast to W not integer valued, (2) ${}_{\lambda}W$ is an additive function of edge contributions, and, as shown here (3) ${}_{\lambda}W$ reflects the extent of branching of the molecular graph.

PROOF OF THEOREM 1

Instead of directly proving Theorem 1 we prove a somewhat more general statement, namely Theorem 3. For this, consider the trees T' and T'', depicted in Figure 1. By R we denote an arbitrary fragment with n_R vertices, and $a \geq 0$, $b \geq 1$. Hence both T' and T'' possess $n_R+a+b+1$ vertices. Note that the vertex r belongs to the fragment R. If r would be the only vertex of R, then it would be $T'=T''$. Therefore, the only interesting case is when $n_R \geq 2$.

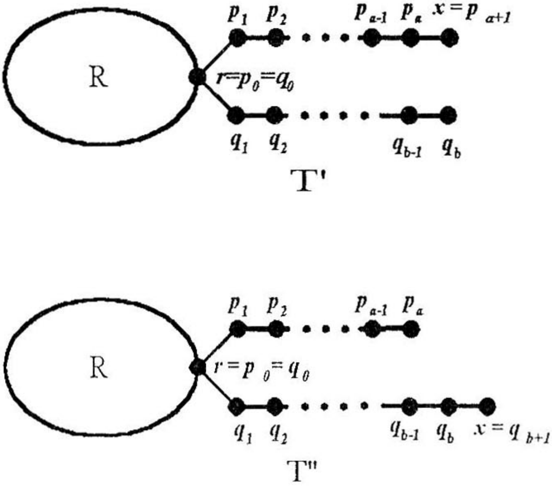


Figure 1

Theorem 3. *Let T' and T'' be trees the structure of which is shown in Figure 1. Then the transformation $T' \rightarrow T''$ increases ${}_{\lambda}W$ if $\lambda > 1$ and decreases ${}_{\lambda}W$ if $\lambda < 1$.*

First, suppose that $\lambda > 1$. We shall prove that ${}_{\lambda}W(T') < {}_{\lambda}W(T'')$.

Let T be any acyclic molecular graph with at least one edge, $v \in V(R)$ and $a \geq 0$, $b \geq 1$. For the sake of the simplicity, we shall denote $r = p_0 = q_0$. We have:

$$
\begin{aligned}
&{}_{\lambda}W(T') - {}_{\lambda}W(T'') = \\
&= \frac{1}{2}\sum_{uv \in E(T')} \left(V(T')^{\lambda} - n_{T'}(u,v)^{\lambda} - n_{T'}(v,u)^{\lambda} \right) - \frac{1}{2}\sum_{uv \in E(T'')} \left(v(T'')^{\lambda} - n_{T''}(u,v)^{\lambda} - n_{T''}(v,u)^{\lambda} \right) \\
&= \frac{1}{2}\sum_{uv \in E(T'')} \left(n_{T''}(u,v)^{\lambda} + n_{T''}(v,u)^{\lambda} \right) - \frac{1}{2}\sum_{uv \in E(T')} \left(n_{T'}(u,v)^{\lambda} + n_{T'}(v,u)^{\lambda} \right) \\
&= \frac{1}{2}\sum_{uv \in E(R)} \left[\left(n_{T''}(u,v)^{\lambda} + n_{T''}(v,u)^{\lambda} \right) - \left(n_{T'}(u,v)^{\lambda} + n_{T'}(v,u)^{\lambda} \right) \right] + \\
&+ \frac{1}{2}\sum_{i=1}^{a} \left[\left(n_{T''}(p_{i-1},p_i)^{\lambda} + n_{T''}(p_i,p_{i-1})^{\lambda} \right) - \left(n_{T'}(p_i,p_{i+1})^{\lambda} + n_{T'}(p_{i+1},p_i)^{\lambda} \right) \right] + \\
&+ \frac{1}{2}\sum_{i=1}^{b} \left[\left(n_{T''}(q_{i-1},q_i)^{\lambda} + n_{T''}(q_i,q_{i-1})^{\lambda} \right) - \left(n_{T'}(q_i,q_{i+1})^{\lambda} + n_{T'}(q_{i+1},q_i)^{\lambda} \right) \right] + \\
&+ \frac{1}{2}\left[\left(n_{T''}(v,q_1)^{\lambda} + n_{T''}(q_1,v)^{\lambda} \right) - \left(n_{T'}(v,p_1)^{\lambda} + n_{T'}(p_1,v)^{\lambda} \right) \right]
\end{aligned} \tag{4}
$$

Note that, for each $uv \in E(R)$,

$$n_{T''}(u,v)^{\lambda} = n_{T'}(u,v)^{\lambda} \qquad \text{and} \qquad n_{T''}(v,u)^{\lambda} = n_{T'}(v,u)^{\lambda},$$

that, for each $i = 1,\dots,a$

$$n_{T''}(p_{i-1},p_i)^{\lambda} + n_{T''}(p_i,p_{i-1})^{\lambda} = n_{T'}(p_i,p_{i+1})^{\lambda} + n_{T'}(p_{i+1},p_i)^{\lambda},$$

and that for each $i = 1,\dots,b$

$$n_{T''}(q_{i-1},q_i)^{\lambda} + n_{T''}(q_i,q_{i-1})^{\lambda} = n_{T'}(q_i,q_{i+1})^{\lambda} + n_{T'}(q_{i+1},q_i)^{\lambda}.$$

Therefore (4) reduces to

$$
\begin{aligned}
&{}_{\lambda}W(T') - {}_{\lambda}W(T'') = \\
&= \frac{1}{2}\left[\left(n_{T''}(v,q_1)^{\lambda} + n_{T''}(q_1,v)^{\lambda} \right) - \left(n_{T'}(v,q_1)^{\lambda} + n_{T'}(q_1,v)^{\lambda} \right) \right] = \\
&= \frac{1}{2}\left[\left((b+1)^{\lambda} + (V(R)+a)^{\lambda} \right) - \left((V(R)+b)^{\lambda} + (a+1)^{\lambda} \right) \right].
\end{aligned}
$$

Let $f_{\lambda}(x) = x^{\lambda}$. Note that:

1) $f_{\lambda}''(x) > 0$, for $x>0$, $\lambda>1$;

2) $a+1 < b+1$, $V(R)+a < V(R)+b$;

3) $(b+1)+(V(R)+a)=(a+1)+(V(R)+b)$.

From basic properties of convex functions (see, for example calculus textbook [38]) one can easily verify that from $f''(x)>0$ for $a \le x \le b$ and for $a < x_1 = b-d \le x_2 = a+d < b$ it follows that $f(x_1)+f(x_2) < f(a)+f(b)$. Namely, from the Lagrange's theorem, it follows that there is $y_2 \in [x_2, b]$ such that $f(b)-f(x_2)=(b-x_2)\cdot f'(y_2)$. Analogously, there is $y_1 \in [a, x_1]$ such that $f(x_1)-f(a)=f'(y_1)\cdot(x_1-a)$. Hence, it is sufficient to prove that $(b-x_2)\cdot f'(y_2) > (x_1-a)\cdot f'(y_1)$, i.e. that $f'(y_2) > f'(y_1)$, but this follows from $f''(x)>0$ on the interval. Using the last observation on $f_\lambda(x)$, we get

$$_\lambda W(T') - {}_\lambda W(T'') = \frac{1}{2}\Big[\big((b+1)^\lambda + (V(R)+a)^\lambda\big) - \big((V(R)+b)^\lambda + (a+1)^\lambda\big)\Big] < 0.$$

This proves the theorem when $\lambda > 1$.

Suppose that $\lambda < 1$, $\lambda \ne 0$. Now $_\lambda W(T') > {}_\lambda W(T'')$ can be shown analogously as in the proof of the previous case. In this case

$$_\lambda W(T') - {}_\lambda W(T'') = \frac{1}{2}\Big[\big((b+1)^\lambda + (v(T)+a)^\lambda\big) - \big((v(T)+b)^\lambda + (a+1)^\lambda\big)\Big] > 0$$

follows from concavity of $f_\lambda(x) = x^\lambda$.
This completes the proof of Theorem 3.

As the path P_n and the star S_n can be obtained from any tree by repeated application of the transformation $T' \to T''$ or its inverse, Theorem 1 follows from Theorem 3.

PROOF OF THEOREM 2

We will distinguish five cases:

CASE 1: $\lambda < 1 < \mu$ or $\lambda > 1 > \mu$.
Note that from the proof of Theorem 3 we know that these indices order differently graphs T' and T''.

CASE 2: $\lambda, \mu > 1$.
Without loss of generality, we may assume that $\lambda < \mu$. Let $f : \left[0, \frac{1}{2}\right] \times (1, +\infty) \to \mathbf{R}$ be the function of two variables defined by

$$f(x,\alpha) = (1-x)^{\alpha-1} - x^{\alpha-1}.$$

Note that the partial derivative on the first variable is negative,

$$\frac{\partial}{\partial x} f(x,\alpha) = (\alpha-1)\cdot\left(-(1-x)^{\alpha-2} - x^{\alpha-2}\right) < 0. \tag{5}$$

Since $f(0,\alpha)=1$ and $f\left(\frac{1}{2},\alpha\right)=0$, there is, for each $\alpha \in (1,+\infty)$, a unique $x_\alpha \in \left(0,\frac{1}{2}\right)$ such that $f(x_\alpha,\alpha)=\frac{1}{2}$. This allows us to define the function $\phi:(1,+\infty)\to \mathbf{R}$ with $\phi(\alpha)=x_\alpha$. Hence $\phi(\alpha)=x \Leftrightarrow f(x,\alpha)=\frac{1}{2}$. We have, for each $x>0, \alpha\in(1,+\infty)$

$$\frac{\partial}{\partial \alpha} f(x,\alpha) = (1-x)^{\alpha-1}\ln(1-x) - x^{\alpha-1}\ln x > 0, \tag{6}$$

From (5) and (6), it follows that the function ϕ is a strictly increasing function. Therefore, there is a rational number $q \in \left(0,\frac{1}{2}\right)$ such that $\phi(\lambda) < q < \phi(\mu)$, or

$$f(q,\lambda) = (1-q)^{\lambda-1} - q^{\lambda-1} < \frac{1}{2};$$
$$f(q,\mu) = (1-q)^{\mu-1} - q^{\mu-1} > \frac{1}{2}.$$

Denote by k denominator of the number q. Of course, $kq \in \mathbf{N}$. Let us first prove a lemma.

Lemma 4.

$$\lim_{n\to\infty} \frac{-1^\lambda - (nk+1)^\lambda + 2^\lambda + (nk)^\lambda - (nkq+2)^\lambda - (nk-nkq)^\lambda + (nkq)^\lambda + (nk-nkq+2)^\lambda}{(nk)^{\lambda-1}} =$$
$$= 2\lambda\left[\left((1-q)^{\lambda-1} - q^{\lambda-1}\right) - \frac{1}{2}\right]$$

Proof.

$$\lim_{n\to\infty} \frac{-1^\lambda - (nk+1)^\lambda + 2^\lambda + (nk)^\lambda - (nkq+2)^\lambda - (nk-nkq)^\lambda + (nkq)^\lambda + (nk-nkq+2)^\lambda}{(nk)^{\lambda-1}} =$$
$$= \lim_{n\to\infty} \frac{-1^\lambda + 2^\lambda - \left[(nk+1)^\lambda - (nk)^\lambda\right] - \left[(nkq+2)^\lambda - (nkq)^\lambda\right] - \left[(nk-nkq)^\lambda - (nk-nkq+2)^\lambda\right]}{(nk)^{\lambda-1}}$$

Using Lagrange's theorem, we get that there are numbers $a_n \in (0,1)$ and $b_n, c_n \in (0,2)$ such that the last expression is equal to

$$\lim_{n\to\infty}\frac{-1^{\lambda}+2^{\lambda}-\lambda\left(nk+a_n\right)^{\lambda-1}-2\lambda\left(nkq+b_n\right)^{\lambda-1}+2\lambda\left(nk-nkq+c_n\right)^{\lambda-1}}{\left(nk\right)^{\lambda-1}}=$$

$$=\lim_{n\to\infty}\left[-\frac{1^{\lambda}}{\left(nk\right)^{\lambda-1}}+\frac{2^{\lambda}}{\left(nk\right)^{\lambda-1}}-\lambda\left(1+\frac{a_n}{nk}\right)^{\lambda-1}-2\lambda\left(q+\frac{b_n}{nk}\right)^{\lambda-1}+2\lambda\left(1-q+\frac{c_n}{nk}\right)^{\lambda-1}\right]=$$

which is, using that $\lim_{n\to\infty}\frac{a_n}{nk}=\lim_{n\to\infty}\frac{b_n}{nk}=\lim_{n\to\infty}\frac{c_n}{nk}=0$, $\lim_{n\to\infty}\left(1+\frac{a_n}{nk}\right)^{\lambda-1}=1$, $\lim_{n\to\infty}\left(q+\frac{b_n}{nk}\right)^{\lambda-1}=q$, and $\lim_{n\to\infty}\left(1-q+\frac{c_n}{nk}\right)^{\lambda-1}=1-q$, equal to

$$=\lambda\left[-1-2q^{\lambda-1}+2\left(1-q\right)^{\lambda-1}\right]=2\lambda\left[\left(\left(1-q\right)^{\lambda-1}-q^{\lambda-1}\right)-\frac{1}{2}\right]$$

as stated in the Lemma.

Hence, because we have chosen q such that $\phi(\lambda)<q<\phi(\mu)$, we have

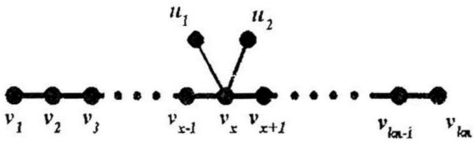
$$\lim_{n\to\infty}\left[-1^{\lambda}-\left(nk+1\right)^{\lambda}+2^{\lambda}+\left(nk\right)^{\lambda}-\left(nkq+2\right)^{\lambda}-\left(nk-nkq\right)^{\lambda}+\left(nkq\right)^{\lambda}+\left(nk-nkq+2\right)^{\lambda}\right]<0$$

and

$$\lim_{n\to\infty}\left[-1^{\mu}-\left(nk+1\right)^{\mu}+2^{\mu}+\left(nk\right)^{\mu}-\left(nkq+2\right)^{\mu}-\left(nk-nkq\right)^{\mu}+\left(nkq\right)^{\mu}+\left(nk-nkq+2\right)^{\mu}\right]>0$$

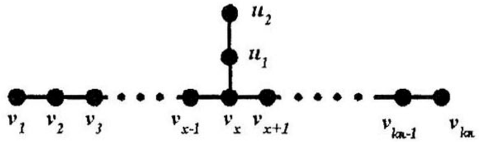
Therefore we can conclude that there is sufficiently large $n\in\mathbf{N}$ such that

$$\begin{aligned}&-1^{\lambda}-\left(nk+1\right)^{\lambda}+2^{\lambda}+\left(nk\right)^{\lambda}-\left(nkq+2\right)^{\lambda}-\left(nk-nkq\right)^{\lambda}+\left(nkq\right)^{\lambda}+\left(nk-nkq+2\right)^{\lambda}<0;\\&-1^{\mu}-\left(nk+1\right)^{\mu}+2^{\mu}+\left(nk\right)^{\mu}-\left(nkq+2\right)^{\mu}-\left(nk-nkq\right)^{\mu}+\left(nkq\right)^{\mu}+\left(nk-nkq+2\right)^{\mu}>0.\end{aligned}\tag{7}$$



G(n,x)

Figure 2



H(n,x)

Figure 3

Denote as $G(n,x)$ and $H(n,x)$ graphs given on the Figure 2 and Figure 3. We have

$$
\begin{aligned}
&{}_{\lambda}W\left(G'(nk,nkq)\right)-{}_{\lambda}W\left(H'(nk,nkq+1)\right)=\\
&=\left\{\begin{array}{l}\sum\limits_{i=1}^{nqk-1}\left[(nk+2)^{\lambda}-i^{\lambda}-(nk+2-i)\right]^{\lambda}+\sum\limits_{i=nkq+3}^{nk+1}\left[(nk+2)^{\lambda}-i^{\lambda}-(nk+2-i)\right]^{\lambda}+\\ +2\cdot\left[(nk+2)^{\lambda}-1^{\lambda}-(nk+1)^{\lambda}\right]+\left[(nk+2)^{\lambda}-(nkq+2)^{\lambda}-(n-nkq)^{\lambda}\right]\end{array}\right\}-\\
&-\left\{\begin{array}{l}\sum\limits_{i=1}^{nqk-1}\left[(nk+2)^{\lambda}-i^{\lambda}-(nk+2-i)\right]^{\lambda}+\sum\limits_{i=nkq+3}^{nk+1}\left[(nk+2)^{\lambda}-i^{\lambda}-(nk+2-i)\right]^{\lambda}+\\ +\left[(nk+2)^{\lambda}-1^{\lambda}-(nk+1)^{\lambda}\right]+\left[(nk+2)^{\lambda}-2^{\lambda}-(nk)^{\lambda}\right]+\\ +\left[(nk+2)^{\lambda}-(nkq)^{\lambda}-(nk+2-nkq)^{\lambda}\right]\end{array}\right\}\\
&=\left\{\left[(nk+2)^{\lambda}-1^{\lambda}-(nk+1)^{\lambda}\right]+\left[(nk+2)^{\lambda}-(nkq+2)^{\lambda}-(nk-nkq)^{\lambda}\right]\right\}-\\
&-\left\{\left[(nk+2)^{\lambda}-2^{\lambda}-(nk)^{\lambda}\right]+\left[(nk+2)^{\lambda}-(nkq)^{\lambda}-(nk+2-nkq)^{\lambda}\right]\right\}\\
&=-1^{\lambda}-(nk+1)^{\lambda}+2^{\lambda}+(nk)^{\lambda}-(nkq+2)^{\lambda}-(nk-nkq)^{\lambda}+(nkq)^{\lambda}+(nk-nkq-2)^{\lambda}.
\end{aligned}
$$

From the relations (7), it directly follows that

$$ {}_{\lambda}W\left(G'(n,nkq)\right)-{}_{\lambda}W\left(H'(n,nkq+1)\right)<0 $$

and, analogously,

$$ {}_{\mu}W\left(G'(n,nkq)\right)-{}_{\mu}W\left(H'(n,nkq+1)\right)>0, $$

which proves the claim in this case.

CASE 3: $0<\lambda,\mu<1$.

Note that $2^{\lambda}+1\neq 2^{\mu}+1$ or equivalently that

$$\frac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}-\frac{2^\lambda+3^\lambda-2}{2^\lambda-1}\neq\frac{2^\mu+3^\mu+4^\mu-3}{2^\mu-1}-\frac{2^\mu+3^\mu-2}{2^\mu-1}.$$

At least one of the following must hold:

SUBCASE 3.1: $\frac{2^\lambda+3^\lambda-2}{2^\lambda-1}\neq\frac{2^\mu+3^\mu-2}{2^\mu-1}$.

Without loss of generality, we may assume that $\frac{2^\lambda+3^\lambda-2}{2^\lambda-1}<\frac{2^\mu+3^\mu-2}{2^\mu-1}$. Hence, there is a rational number q such that $\frac{2^\lambda+3^\lambda-2}{2^\lambda-1}<q<\frac{2^\mu+3^\mu-2}{2^\mu-1}$. Denote $q=\frac{c}{b}, c,b\in\mathbf{N}$. Let us first calculate a useful limit.

Lemma 5.

$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left((a+3b+1)^\lambda-1^\lambda-(a+3b)^\lambda\right)+b\cdot\left((a+3b+1)^\lambda-2^\lambda-(a+3b-1)^\lambda\right)+\\ +b\cdot\left((a+3b+1)^\lambda-3^\lambda-(a+3b-2)^\lambda\right)-(a+3b-c)\cdot\left((a+3b+1)^\lambda-1^\lambda-(a+3b)^\lambda\right)-\\ -c\cdot\left((a+3b+1)^\lambda-2^\lambda-(a+3b-1)^\lambda\right)\end{pmatrix}$$
$$=b\left(1-2^\lambda\right)\cdot\left(\frac{2-2^\lambda-3^\lambda}{1-2^\lambda}-q\right)$$

Proof. Using Lagrange's theorem, we get that for each $a\in\mathbf{N}$ there are numbers $x_a\in(0,1)$, $y_a\in(0,2)$ and $z_a\in(0,3)$ such that

$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left((a+3b+1)^\lambda-1^\lambda-(a+3b)^\lambda\right)+b\cdot\left((a+3b+1)^\lambda-2^\lambda-(a+3b-1)^\lambda\right)+\\ +b\cdot\left((a+3b+1)^\lambda-3^\lambda-(a+3b-2)^\lambda\right)-(a+3b-c)\cdot\left((a+3b+1)^\lambda-1^\lambda-(a+3b)^\lambda\right)-\\ -c\cdot\left((a+3b+1)^\lambda-2^\lambda-(a+3b-1)^\lambda\right)\end{pmatrix}=$$
$$=\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left(\lambda\cdot(a+3b+x)^{\lambda-1}-1^\lambda\right)+b\cdot\left(2\lambda\cdot(a+3b-1+y)^{\lambda-1}-2^\lambda\right)+\\ +b\cdot\left(3\lambda\cdot(a+3b-2+z)^{\lambda-1}-3^\lambda\right)-(a+3b-c)\cdot\left(\lambda\cdot(a+3b+x)^{\lambda-1}-1^\lambda\right)-\\ -c\cdot\left(2\lambda\cdot(a+3b-1+y)^{\lambda-1}-2^\lambda\right)\end{pmatrix}$$

which, using that for $\lambda<1$ $\lim_{c\to\infty}(a+3b+x)^{\lambda-1}=0$, $\lim_{a\to\infty}(a+3b+1-y)^{\lambda-1}=0$, and $\lim_{a\to\infty}(a+3b+1-z)^{\lambda-1}=0$, equals

$$=\lim_{a\to\infty}\left(\left(a+b\right)\cdot\left(-1^{\lambda}\right)+b\cdot\left(-2^{\lambda}\right)+b\cdot\left(-3^{\lambda}\right)-\left(a+3b-c\right)\cdot\left(-1^{\lambda}\right)-c\cdot\left(-2^{\lambda}\right)\right)=$$

$$=b\left(2-2^{\lambda}-3^{\lambda}\right)-c\cdot\left(1-2^{\lambda}\right)=b\left(1-2^{\lambda}\right)\cdot\left(\frac{2-2^{\lambda}-3^{\lambda}}{1-2^{\lambda}}-q\right)$$

as claimed in the statement of the Lemma.

For a rational number q such that $\frac{2^{\lambda}+3^{\lambda}-2}{2^{\lambda}-1}<q<\frac{2^{\mu}+3^{\mu}-2}{2^{\mu}-1}$, the limit computed in the Lemma 5 has positive value, and, replacing λ with η, the respective limit is negative

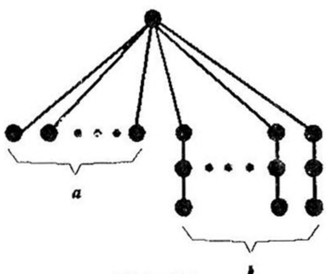
$$\lim_{a\to\infty}\begin{pmatrix}\left(a+b\right)\cdot\left(\left(a+3b+1\right)^{\mu}-1^{\mu}-\left(a+3b\right)^{\mu}\right)+b\cdot\left(\left(a+3b+1\right)^{\mu}-2^{\mu}-\left(a+3b-1\right)^{\mu}\right)+\\ +b\cdot\left(\left(a+3b+1\right)^{\mu}-3^{\mu}-\left(a+3b-2\right)^{\mu}\right)-\left(a+3b-c\right)\cdot\left(\left(a+3b+1\right)^{\mu}-1^{\mu}-\left(a+3b\right)^{\mu}\right)-\\ -c\cdot\left(\left(a+3b+1\right)^{\mu}-2^{\mu}-\left(a+3b-1\right)^{\mu}\right)\end{pmatrix}<0.$$

Hence, there is sufficiently large $a\in\mathbf{N}$ such that

$$\begin{pmatrix}\left(a+b\right)\cdot\left(\left(a+3b+1\right)^{\lambda}-1^{\lambda}-\left(a+3b\right)^{\lambda}\right)+b\cdot\left(\left(a+3b+1\right)^{\lambda}-2^{\lambda}-\left(a+3b-1\right)^{\lambda}\right)+\\ +b\cdot\left(\left(a+3b+1\right)^{\lambda}-3^{\lambda}-\left(a+3b-2\right)^{\lambda}\right)-\left(a+3b-c\right)\cdot\left(\left(a+3b+1\right)^{\lambda}-1^{\lambda}-\left(a+3b\right)^{\lambda}\right)-\\ -c\cdot\left(\left(a+3b+1\right)^{\lambda}-2^{\lambda}-\left(a+3b-1\right)^{\lambda}\right)\end{pmatrix}>0;$$

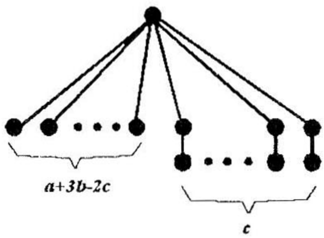
$$\begin{pmatrix}\left(a+b\right)\cdot\left(\left(a+3b+1\right)^{\mu}-1^{\mu}-\left(a+3b\right)^{\mu}\right)+b\cdot\left(\left(a+3b+1\right)^{\mu}-2^{\mu}-\left(a+3b-1\right)^{\mu}\right)+\\ +b\cdot\left(\left(a+3b+1\right)^{\mu}-3^{\mu}-\left(a+3b-2\right)^{\mu}\right)-\left(a+3b-c\right)\cdot\left(\left(a+3b+1\right)^{\mu}-1^{\mu}-\left(a+3b\right)^{\mu}\right)-\\ -c\cdot\left(\left(a+3b+1\right)^{\mu}-2^{\mu}-\left(a+3b-1\right)^{\mu}\right)\end{pmatrix}<0.$$

Denote by $G'(a,b)$ and $H'(a,b,c)$ graphs on $a+3b+1$ vertices depicted on Figure 4 and Figure 5.



$G'(a,b)$

Figure 4



H'(a,b,c)

Figure 5

Note that

$$
\begin{array}{l}
{}_{\lambda}W\left(G'(a,b)\right)-{}_{\lambda}W\left(H'(a,b,c)\right)= \\
=\left(\begin{array}{l}
(a+b)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)+b\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)+ \\
+b\cdot\left((a+3b+1)^{\lambda}-3^{\lambda}-(a+3b-2)^{\lambda}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)- \\
-c\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)
\end{array}\right)>0 \\
{}_{\mu}W\left(G'(a,b)\right)-{}_{\mu}W\left(H'(a,b,c)\right)= \\
=\left(\begin{array}{l}
(a+b)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)+b\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)+ \\
+b\cdot\left((a+3b+1)^{\mu}-3^{\mu}-(a+3b-2)^{\mu}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)- \\
-c\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)
\end{array}\right)<0.
\end{array}
$$

The claim is proved in this subcase.

SUBCASE 3.2: $\dfrac{2^{\lambda}+3^{\lambda}+4^{\lambda}-3}{2^{\lambda}-1}\neq\dfrac{2^{\mu}+3^{\mu}+4^{\mu}-3}{2^{\mu}-1}$.

Without loss of generality, we may assume that $\dfrac{2^{\lambda}+3^{\lambda}+4^{\lambda}-3}{2^{\lambda}-1}<\dfrac{2^{\mu}+3^{\mu}+4^{\mu}-3}{2^{\mu}-1}$. Hence, there is a rational number q such that $\dfrac{2^{\lambda}+3^{\lambda}+4^{\lambda}-3}{2^{\lambda}-1}<q<\dfrac{2^{\mu}+3^{\mu}+4^{\mu}-3}{2^{\mu}-1}$. Denote $q=\dfrac{c}{b}$, $b,c\in\mathbf{N}$. Let us calculate

$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)+\\ +b\cdot\left((a+4b+1)^{\lambda}-3^{\lambda}-(a+4b-2)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-4^{\lambda}-(a+4b-3)^{\lambda}\right)-\\ -(a+4b-c)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)-c\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)\end{pmatrix}$$

Using Lagrange's theorem, we get that there are numbers $x_a\in(0,1)$, $y_a\in(0,2)$, $z_a\in(0,3)$ and $w_a\in(0,4)$ such that the limit is equal to

$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left(\lambda\cdot(a+4b+x)^{\lambda-1}-1^{\lambda}\right)+b\cdot\left(\lambda\cdot(a+4b-1+y)^{\lambda-1}-2^{\lambda}\right)+\\ +b\cdot\left(\lambda\cdot(a+4b-2+z)^{\lambda-1}-3^{\lambda}\right)+b\cdot\left(\lambda\cdot(a+4b-3+w)^{\lambda-1}-4^{\lambda}\right)-\\ -(a+4b-c)\cdot\left(\lambda\cdot(a+4b+x)^{\lambda-1}-1^{\lambda}\right)-c\cdot\left(\lambda\cdot(a+4b-1+y)^{\lambda-1}-2^{\lambda}\right)\end{pmatrix}$$

$$=\lim_{a\to\infty}\left((a+b)\cdot(-1^{\lambda})+b\cdot(-2^{\lambda})+b\cdot(-3^{\lambda})+b\cdot(-4^{\lambda})-(a+4b-c)\cdot(-1^{\lambda})-c\cdot(-2^{\lambda})\right)$$

$$=b\left(1-2^{\lambda}\right)\left(\frac{3-2^{\lambda}-3^{\lambda}-4^{\lambda}}{1-2^{\lambda}}-q\right)>0.$$

Completely analogously, replacing replacing λ with η, it can be shown that

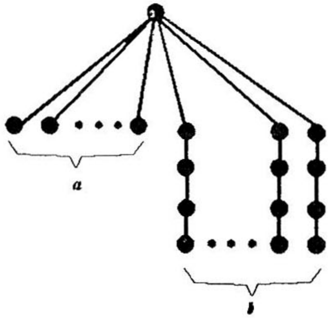
$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)+\\ +b\cdot\left((a+4b+1)^{\mu}-3^{\mu}-(a+4b-2)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-4^{\mu}-(a+4b-3)^{\mu}\right)-\\ -(a+4b-c)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)-c\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)\end{pmatrix}<0.$$

Therefore, there is sufficiently large $a\in\mathbb{N}$ such that

$$\begin{pmatrix}(a+b)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)+\\ +b\cdot\left((a+4b+1)^{\lambda}-3^{\lambda}-(a+4b-2)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-4^{\lambda}-(a+4b-3)^{\lambda}\right)-\\ -(a+4b-c)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)-c\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)\end{pmatrix}>0$$

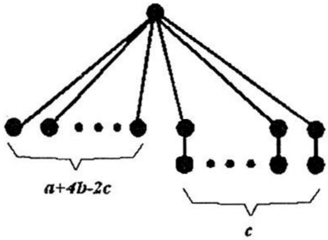
$$\begin{pmatrix}(a+b)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)+\\ +b\cdot\left((a+4b+1)^{\mu}-3^{\mu}-(a+4b-2)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-4^{\mu}-(a+4b-3)^{\mu}\right)-\\ -(a+4b-c)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)-c\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)\end{pmatrix}<0.$$

Denote by $G''(a,b,c)$ and $H''(a,b,c)$ graphs on $a+4b+1$ vertices on Figure 6 and Figure 7.



G''(a,b)

Figure 6



H''(a,b,c)

Figure 7

We have

$$
{}_{\lambda}W\left(G''(a,b)\right)-{}_{\lambda}W\left(H''(a,b,c)\right)=
$$

$$
\begin{pmatrix}
(a+b)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)+\\
+b\cdot\left((a+4b+1)^{\lambda}-3^{\lambda}-(a+4b-2)^{\lambda}\right)+b\cdot\left((a+4b+1)^{\lambda}-4^{\lambda}-(a+4b-3)^{\lambda}\right)-\\
-(a+4b-c)\cdot\left((a+4b+1)^{\lambda}-1^{\lambda}-(a+4b)^{\lambda}\right)-c\cdot\left((a+4b+1)^{\lambda}-2^{\lambda}-(a+4b-1)^{\lambda}\right)
\end{pmatrix}>0
$$

$$
\begin{aligned}
&{}_{\mu}W\left(G''(a,b)\right)-{}_{\mu}W\left(H''(a,b,c)\right)=\\
&\begin{pmatrix}
(a+b)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)+\\
+b\cdot\left((a+4b+1)^{\mu}-3^{\mu}-(a+4b-2)^{\mu}\right)+b\cdot\left((a+4b+1)^{\mu}-4^{\mu}-(a+4b-3)^{\mu}\right)-\\
-(a+4b-c)\cdot\left((a+4b+1)^{\mu}-1^{\mu}-(a+4b)^{\mu}\right)-c\cdot\left((a+4b+1)^{\mu}-2^{\mu}-(a+4b-1)^{\mu}\right)
\end{pmatrix}<0.
\end{aligned}
$$

This proves the Subcase 3.2 and completes proof of the Case 3.

CASE 4: $\lambda,\mu<0$.
This case can be proved analogously as the Case 3.

CASE 5: $(\lambda<0$ and $0<\mu<1)$ or $(\mu<0$ and $0<\lambda<1)$.
Without loss of generality, we may assume that $\lambda<0$ and $0<\mu<1$. Let q be a rational number such that $q>\max\left\{\frac{2^{\lambda}+3^{\lambda}-2}{2^{\lambda}-1},\frac{2^{\mu}+3^{\mu}-2}{2^{\mu}-1}\right\}$. Denote $q=\frac{c}{b}, c,b\in\mathbf{N}$. Let us calculate

$$
\lim_{a\to\infty}\begin{pmatrix}
(a+b)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)+b\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)+\\
+b\cdot\left((a+3b+1)^{\lambda}-3^{\lambda}-(a+3b-2)^{\lambda}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)-\\
-c\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)
\end{pmatrix}
$$

Using Lagrange's theorem, we get that there are numbers $x_{\alpha}\in(0,1)$, $y_{\alpha}\in(0,2)$, and $z_{\alpha}\in(0,3)$ such that the limit is equal to

$$
\begin{aligned}
&\lim_{a\to\infty}\begin{pmatrix}
(a+b)\cdot\left(\lambda\cdot(a+3b+x)^{\lambda-1}-1^{\lambda}\right)+b\cdot\left(2\lambda\cdot(a+3b-1+y)^{\lambda-1}-2^{\lambda}\right)+\\
+b\cdot\left(3\lambda\cdot(a+3b-2+z)^{\lambda}-3^{\lambda}\right)-(a+3b-c)\cdot\left(\lambda\cdot(a+3b+x)^{\lambda-1}-1^{\lambda}\right)-\\
-c\cdot\left(2\lambda\cdot(a+3b-1+y)^{\lambda-1}-2^{\lambda}\right)
\end{pmatrix}=\\
&=\lim_{a\to\infty}\left((a+b)\cdot\left(-1^{\lambda}\right)+b\cdot\left(-2^{\lambda}\right)+b\cdot\left(-3^{\lambda}\right)-(a+3b-c)\cdot\left(-1^{\lambda}\right)-c\cdot\left(-2^{\lambda}\right)\right)=\\
&=b\left(1-2^{\lambda}\right)\cdot\left(\frac{2-2^{\lambda}-3^{\lambda}}{1-2^{\lambda}}-q\right)<0.
\end{aligned}
$$

Completely analogously, it can be shown that

$$\lim_{a\to\infty}\begin{pmatrix}(a+b)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)+b\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)+\\+b\cdot\left((a+3b+1)^{\mu}-3^{\mu}-(a+3b-2)^{\mu}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)-\\-c\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)\end{pmatrix}>0.$$

Hence, there is sufficiently large $a\in\mathbf{N}$ such that

$$\begin{pmatrix}(a+b)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)+b\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)+\\+b\cdot\left((a+3b+1)^{\lambda}-3^{\lambda}-(a+3b-2)^{\lambda}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\lambda}-1^{\lambda}-(a+3b)^{\lambda}\right)-\\-c\cdot\left((a+3b+1)^{\lambda}-2^{\lambda}-(a+3b-1)^{\lambda}\right)\end{pmatrix}<0;$$

$$\begin{pmatrix}(a+b)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)+b\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)+\\+b\cdot\left((a+3b+1)^{\mu}-3^{\mu}-(a+3b-2)^{\mu}\right)-(a+3b-c)\cdot\left((a+3b+1)^{\mu}-1^{\mu}-(a+3b)^{\mu}\right)-\\-c\cdot\left((a+3b+1)^{\mu}-2^{\mu}-(a+3b-1)^{\mu}\right)\end{pmatrix}>0.$$

Let $G'(a,b)$ and $H'(a,b,c)$ be the graphs defined in the Case 3. Note that

$${}_{\lambda}W(G'(a,b))-{}_{\lambda}W(H'(a,b,c))<0 \qquad\text{and}\qquad {}_{\mu}W(G'(a,b))-{}_{\mu}W(H'(a,b,c))>0.$$

This completes the proof of the theorem.

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