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Altered Wiener Indices

Damir Vukičević[a] and Janez Žerovnik[b]

[a] *Department of Mathematics, University of Split, Croatia*
[b] *Faculty of Mechanical Engineering, University of Maribor, Smetanova 17, SI-2000 Maribor, Slovenia and IMFM, Jadranska 19, SI-1000 Ljubljana, Slovenia E-mail: janez.zerovnik@imfm.uni-lj.si*

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Abstract

Recently Nikolić, Trinajstić and Randić put forward a novel modification $^{m}W(G)$ of the Wiener number $W(G)$, called modified Wiener index , which definition was generalized later by Gutman and the present authors. Here we study another class of modified indices defined as $W_{\min,\lambda}(G)=\sum(V(G)^{\lambda}m_{G}(u,v)^{\lambda}-m_{G}(u,v)^{2\lambda})$ and show that some of the important properties of $W(G)$, $^{m}W(G)$ and $^{\lambda}W(G)$ are also properties of $W_{\min,\lambda}(G)$, valid for most values of the parameter λ. 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 $\lambda\geq1$ or $\lambda<0$, $W_{\min,\lambda}(P_n)>W_{\min,\lambda}(T_n)>W_{\min,\lambda}(S_n)$. Thus for these values of the parameter λ, $W_{\min,\lambda}(G)$ 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 $W_{\min,\lambda}(G)$ then, in the general case, this ordering is different for different λ.

Key words: Wiener number, modified Wiener indices, branching, chemical graph theory

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 the reviews[14,15] and the recent paper.[16] One of the newest such modifications was put forward by Nikolić, Trinajstić and Randić.[17] This idea was generalized by Gutman and the present authors[18] 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

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

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[19] 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[12,26–31] or are linearly related with it.[32–37] 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[36,38] 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,

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

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[18] are defined as

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

Denoting $n(G)=|V(G)|$, the equality (2) can be also reformulated as

$$W(G)=\sum_{uv\in E(G)}\begin{pmatrix} n(G)\min\{n_G(u,v),n_G(v,u)\}- \\ -\min\{n_G(u,v),n_G(v,u)\}^2\end{pmatrix}.$$

Let us prove this claim. Recalling that,

$n(G)=n_G(u,v)+n_G(v,u)$, we get

$$W(G)=\sum_{uv\in E(G)}\left(n_G(u,v)\cdot n_G(v,u)\right)$$

$$=\sum_{uv\in E(G)}\begin{pmatrix}\min\{n_G(u,v),n_G(v,u)\}\cdot \\ \cdot\max\{n_G(u,v),n_G(v,u)\}\end{pmatrix}$$

$$=\sum_{uv\in E(G)}\begin{pmatrix}\min\{n_G(u,v),n_G(v,u)\}\cdot \\ \cdot\left(n(G)-\min\{n_G(u,v),n_G(v,u)\}\right)\end{pmatrix}$$

$$=\sum_{uv\in E(G)}\begin{pmatrix}n(G)\cdot\min\{n_G(u,v),n_G(v,u)\} \\ -\min\{n_G(u,v),n_G(v,u)\}^2\end{pmatrix}$$

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

$$W_{\min,\lambda}(G)=\sum_{uv\in E(G)}\left(n(G)^{\lambda}\, m_G(u,v)^{\lambda}-m_G(u,v)^{2\lambda}\right). \quad (3)$$

which we initiate in this paper. Of course, these indices generalize the Wiener index for the trees and not for general graphs. These indices allow small modifications of the Wiener index, hence since Wiener index is of great use in the large number of QSPR and QSAR studies, these indices may improve the results obtained in such studies. For brevity, we denote:

$$m_G(u,v)=\min\{n_G(u,v),n_G(v,u)\}$$

We first prove that the indices $W_{\min,\lambda}(G)$ for $\lambda < 0$ and for $\lambda \geq 1$ obey the inequalities (1) and can therefore be viewed as "branching indices".

Theorem 1. *For real number λ ($\lambda \geq 1$ or $\lambda < 0$), the modified Wiener index $W_{\min,\lambda}(G)$ satisfies the inequality*

$$W_{\min,\lambda}(P_n) > W_{\min,\lambda}(T_n) > W_{\min,\lambda}(S_n)$$

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.

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 $W_{\min,\lambda}(G)$. We also prove that the statement of Theorem 3 does not hold for, $\lambda\in[0,1)$ and therefore the corresponding indices fail to properly measure branching.

Furthermore, we prove that the indices 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 $W_{\min,\lambda_1}(G)$ and $W_{\min,\lambda_2}(G)$. More formally, let the set of all trees be denoted by T. Denote the set of some topological indices (e. g. the set of the modified Wiener indices $W_{\min,\lambda}(G)$ for all values of λ) by $\Im$. We can define an equivalence relation $\equiv$ on the set $\Im$ as

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

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 $\lambda \neq \eta$, the modified Wiener indices $W_{\min,\lambda}(G)$ and $W_{\min,\eta}(G)$ are not equivalent.*

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 descriptor. However, continuing along the research avenue initiated by recent papers[16–25] we show that there are additional new interesting ways of generalizations 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) $W_{\min,\lambda}(G)$ are in contrast to W not integer valued, (2) $W_{\min,\lambda}(G)$ is an additive function of edge contributions, and, as shown here (3) $W_{\min,\lambda}(G)$ correctly reflects the extent of branching of the molecular graph for many values of the parameter λ.

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'' have $n = n_R + a + b + 1$ 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 $n_R \geq 2$.

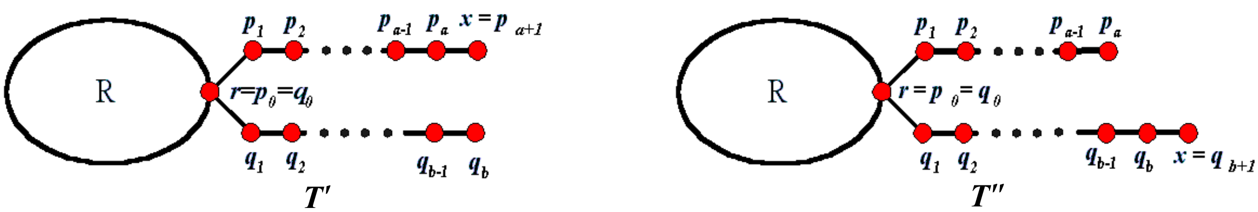

Figure 1. Graphs T' and T''.

Theorem 3. *Let T' and T'' be trees the structure of which is shown in Figure 1. Then the transformation $T' \to T''$ increases $W_{\min,\lambda}(G)$ if $\lambda \geq 1$ and if $\lambda < 0$.*

First, suppose that $\lambda \geq 1$. We shall prove that $W_{\min,\lambda}(T') < W_{\min,\lambda}(T'')$. 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 simplicity, we shall denote $r = p_0 = q_0$. We have:

$$W_{\lambda,\min}(T'') - W_{\lambda,\min}(T') =$$

$$= \sum_{uv \in E(T'')} \left((n \cdot m_{T''}(u,v))^{\lambda} - m_{T''}(u,v)^{2\lambda} \right) - \sum_{uv \in E(T')} \left((n \cdot m_{T'}(u,v))^{\lambda} - m_{T'}(u,v)^{2\lambda} \right) =$$

$$= \sum_{uv \in E(T)} \left[\left((n \cdot m_{T''}(u,v))^{\lambda} - m_{T''}(u,v)^{2\lambda} \right) - \left((n \cdot m_{T'}(u,v))^{\lambda} - m_{T'}(u,v)^{2\lambda} \right) \right] +$$

$$+ \sum_{i=1}^{a} \left[\left((n \cdot m_{T''}(p_{i-1},p_i))^{\lambda} - m_{T''}(p_{i-1},p_i)^{2\lambda} \right) - \left((n \cdot m_{T'}(p_i,p_{i+1}))^{\lambda} - m_{T'}(p_i,p_{i+1})^{2\lambda} \right) \right] +$$

$$+ \sum_{i=1}^{b} \left[\left((n \cdot m_{T''}(q_i,q_{i+1}))^{\lambda} - m_{T''}(q_i,q_{i+1})^{2\lambda} \right) - \left((n \cdot m_{T'}(q_{i-1},q_i))^{\lambda} - m_{T'}(q_{i-1},q_i)^{2\lambda} \right) \right] +$$

$$+ \left[\left((n \cdot m_{T''}(v,q_1))^{\lambda} - m_{T''}(v,q_1)^{2\lambda} \right) - \left((n \cdot m_{T'}(v,p_1))^{\lambda} - m_{T'}(v,p_1)^{2\lambda} \right) \right] \tag{4}$$

Note that:

$(n \cdot m_{T''}(u,v))^{\lambda} - m_{T''}(u,v)^{2\lambda} = (n \cdot m_{T'}(u,v))^{\lambda} - m_{T'}(u,v)^{2\lambda}$, for each $uv \in E(R)$, that

$(n \cdot m_{T''}(p_{i-1},p_i))^{\lambda} - m_{T''}(p_{i-1},p_i)^{2\lambda} = (n \cdot m_{T'}(p_i,p_{i+1}))^{\lambda} - m_{T'}(p_i,p_{i+1})^{2\lambda}$ for each $i=1,\ldots,a$, and that

$(n \cdot m_{T''}(q_i,q_{i+1}))^{\lambda} - m_{T''}(q_i,q_{i+1})^{2\lambda} = (n \cdot m_{T'}(q_{i-1},q_i))^{\lambda} - m_{T'}(q_{i-1},q_i)^{2\lambda}$ for each $i=1,\ldots,b$.

Therefore (4) reduces to

$$W_{\min,\lambda}(T'') - W_{\min,\lambda}(T') = \left((n \cdot m_{T''}(v,q_1))^{\lambda} - m_{T''}(v,q_1)^{2\lambda} \right) - \left((n \cdot m_{T'}(v,p_1))^{\lambda} - m_{T'}(v,p_1)^{2\lambda} \right) =$$

$$= n^{2\lambda} \cdot \left[\left(\left(\frac{m_{T''}(v,q_1)}{n} \right)^{\lambda} - \left(\frac{m_{T''}(v,q_1)}{n} \right)^{2\lambda} \right) - \left(\left(\frac{m_{T'}(v,p_1)}{n} \right)^{\lambda} - \left(\frac{m_{T'}(v,p_1)}{n} \right)^{2\lambda} \right) \right].$$

Let $f_\lambda : \left(0, \frac{1}{2}\right) \to \mathbb{R}$ be defined by $f_\lambda(x) = x^\lambda - x^{2\lambda}$. As $\lambda \geq 1$,

$f_\lambda'(x) = \lambda x^{\lambda-1} - 2\lambda x^{2\lambda-1} = \lambda \cdot x^{\lambda-1} \cdot \left(1 - 2x^\lambda\right) > 0$ and the limits (as $x \to \frac{1}{2}$) are >0 for λ>1 and =0 for λ=1.

From definition of m_G we have $\frac{m_G(v,u)}{n(G)} \leq \frac{1}{2}$ and because of $m_{T'}(v,p_1) < m_{T''}(v,q_1)$ it follows that

$$W_{\min,\lambda}(T'') - W_{\min,\lambda}(T') = n^{2\lambda} \cdot \left(f_\lambda\left(\frac{m_{T''}(v,q_1)}{n}\right) - f_\lambda\left(\frac{m_{T'}(v,p_1)}{n}\right)\right) > 0.$$

This proves the first part of Theorem 3. When λ<0, analogous reasoning gives

$$W_{\min,\lambda}(T'') - W_{\min,\lambda}(T') = n^{2\lambda} \cdot \left(f_\lambda\left(\frac{m_{T''}(v,q_1)}{n}\right) - f_\lambda\left(\frac{m_{T'}(v,p_1)}{n}\right)\right) > 0,$$

because $f_\lambda'(x) = \lambda \cdot x^{\lambda-1} \cdot \left(1 - 2x^\lambda\right) > 0$ for λ < 0, concluding the proof of Theorem 3.

Note that the statement Theorem 1 follows from Theorem 3, because 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. We now show that statement Theorem 3 does not hold for other λ.

Lemma 4. *Let* $\lambda \in [0,1)$ *and G*(*x*,*y*) *stand for the graph given on Figure 2. There are numbers* $a', a'', b', b'' \in \mathbb{N}$ *such that*

$$\begin{aligned} &a' < b'; \\ &W_{\min,\lambda}\left(G(a'+1,b')\right) < \\ &< W_{\min,\lambda}\left(G(a',b'+1)\right) \end{aligned} \qquad (5)$$

$$\begin{aligned} &a'' < b''; \\ &W_{\min,\lambda}\left(G(a''+1,b'')\right) > \\ &> W_{\min,\lambda}\left(G(a'',b''+1)\right) \end{aligned} \qquad (6)$$

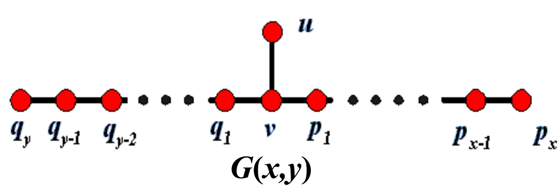

Figure 2. Graph *G*(*x*,*y*).

Note that *G*(*x*,*y*) has *x*+*y*+*2* vertices. Similarly as in the previous section, we will compare graphs *G*(*a*,*b*+1) and *G*(*a*+1,*b*). Let *n*=|*G*(*a*+1,*b*)| =|*G*(*a*,*b*+1)|=*a*+*b*+3.

$$W_{\min,\lambda}\left(G(a,b+1)\right) - W_{\min,\lambda}\left(G(a+1,b)\right) =$$

$$= n^{2\lambda} \cdot \left[\begin{array}{l} \left(\left(\frac{m_{G(a,b+1)}(v,q_1)}{n}\right)^\lambda - \left(\frac{m_{G(a,b+1)}(v,q_1)}{n}\right)^{2\lambda} \right) - \\ \left(\left(\frac{m_{G(a+1,b)}(v,p_1)}{n}\right)^\lambda - \left(\frac{m_{G(a+1,b)}(v,p_1)}{n}\right)^{2\lambda} \right) \end{array} \right] = (a+b+3)^{2\lambda} \left[\begin{array}{l} \left(\left(\frac{a+2}{a+b+3}\right)^\lambda - \left(\frac{a+2}{a+b+3}\right)^{2\lambda} \right) - \\ \left(\left(\frac{a+1}{a+b+3}\right)^\lambda - \left(\frac{a+1}{a+b+3}\right)^{2\lambda} \right) \end{array} \right]$$

From the Lagrange's theorem, it follows that there are numbers $r, s \in (0,1)$ such that

$$W_{\min,\lambda}\left(G(a,b+1)\right) - W_{\min,\lambda}\left(G(a+1,b)\right) = (a+b+3)^{2\lambda} \cdot \left(\lambda\left(\frac{a+1+r}{a+b+3}\right)^{\lambda-1} - 2\lambda\left(\frac{a+1+s}{a+b+3}\right)^{2\lambda-1} \right). \qquad (7)$$

Therefore,

$$W_{\min,\lambda}\left(G(a,b+1)\right)-W_{\min,\lambda}\left(G(a+1,b)\right)>(a+b+3)^{2\lambda}\cdot\left(\lambda\left(\frac{a+1}{a+b+3}\right)^{\lambda-1}-2\lambda\left(\frac{a+2}{a+b+3}\right)^{2\lambda-1}\right)$$

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

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

Therefore, if we take $a'=a$ and sufficiently large $b'=b'(a')$ we have

$$W_{\min,\lambda}\left(G(a',b'+1)\right)-W_{\min,\lambda}\left(G(a'+1,b')\right)>0.$$

This proves (5). Let us return to the relation (7). We have

$$W_{\min,\lambda}\left(G(a,b+1)\right)-W_{\min,\lambda}\left(G(a+1,b)\right)=(a+b+3)^{2\lambda}\cdot\left(\lambda\left(\frac{a+1+r}{a+b+3}\right)^{\lambda-1}-2\lambda\left(\frac{a+1+s}{a+b+3}\right)^{2\lambda-1}\right).$$

It follows that

$$W_{\min,\lambda}\left(G(a,b+1)\right)-W_{\min,\lambda}\left(G(a+1,b)\right)<(a+b+3)^{2\lambda}\cdot\left(\lambda\left(\frac{a+2}{a+b+3}\right)^{\lambda-1}-2\lambda\left(\frac{a+1}{a+b+3}\right)^{2\lambda-1}\right).$$

For $b=a+1$ the last inequality reads

$$W_{\min,\lambda}\left(G(a,a+2)\right)-W_{\min,\lambda}\left(G(a+1,a+1)\right)<(2a+4)^{2\lambda}\cdot\lambda\cdot\left(\left(\frac{a+2}{2a+4}\right)^{\lambda-1}-2\left(\frac{a+1}{2a+4}\right)^{2\lambda-1}\right).$$

Note that

$$\lim_{a\to\infty}\left(\left(\frac{a+2}{2a+4}\right)^{\lambda-1}-2\left(\frac{a+1}{2a+4}\right)^{2\lambda-1}\right)=\left(\frac{1}{2}\right)^{\lambda-1}-2\cdot\left(\frac{1}{2}\right)^{2\lambda-1}=\left(\frac{1}{2}\right)^{\lambda-1}\cdot\left[1-2\left(\frac{1}{2}\right)^{\lambda}\right]=\left(\frac{1}{2}\right)^{\lambda-1}\cdot\left[1-2^{1-\lambda}\right]<0.$$

Therefore, for the sufficiently large a'' and $b''=a''+1$, we have $W_{\min,\lambda}\left(G(a'',b''+1)\right)-W_{\min,\lambda}\left(G(a''+1,b'')\right)<0.$ This proves the relation (6) and Lemma 4.

Proof of Theorem 2

Let us define

$$P(a,b,c,\eta)=\begin{pmatrix}(a+b)\cdot\left(\left[(a+3b+1)\cdot 1\right]^{\eta}-1^{\eta}\right)+b\cdot\left(\left[(a+3b+1)\cdot 2\right]^{\eta}-2^{\eta}\right)+\\ +b\cdot\left(\left[(a+3b+1)\cdot 3\right]^{\eta}-3^{\eta}\right)-(a+3b-c)\cdot\left(\left[(a+3b+1)\cdot 1\right]^{\eta}-1^{\eta}\right)-\\ -c\cdot\left(\left[(a+3b+1)\cdot 2\right]^{\eta}-2^{\eta}\right)\end{pmatrix}$$

$$Q(a,b,c,\eta)=\begin{pmatrix}(a+b)\cdot\left(\left[(a+4b+1)\cdot 1\right]^{\eta}-1^{\eta}\right)+b\cdot\left(\left[(a+4b+1)\cdot 2\right]^{\eta}-2^{\eta}\right)+\\ +b\cdot\left(\left[(a+4b+1)^{\eta}\cdot 3\right]-3^{\eta}\right)+b\cdot\left(\left[(a+4b+1)^{\eta}\cdot 4\right]-4^{\eta}\right)-\\ (a+4b-c)\cdot\left(\left[(a+4b+1)^{\eta}\cdot 1\right]-1^{\eta}\right)-c\cdot\left(\left[(a+4b+1)\cdot 2\right]^{\eta}-2^{\eta}\right)\end{pmatrix}$$

Furthermore, observe that for the graphs $G'(a,b)$ and $H'(a,b,c)$ with $a+3b+1$ vertices sketched on Figure 3, we get, after straighforward computation using only the definition of $W_{\min,\lambda}$,

$$W_{\min,\eta}\left(G'(a,b)\right)-W_{\min,\eta}\left(H'(a,b,c)\right)=P(a,b,c,\eta)$$

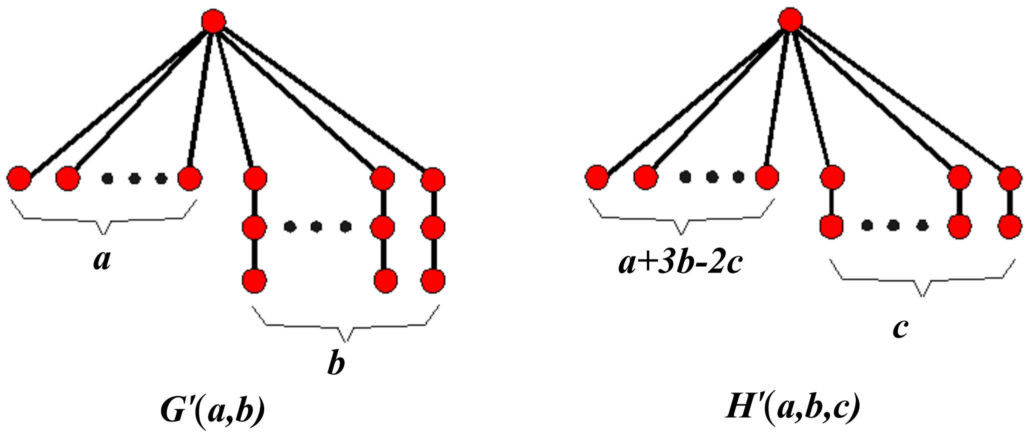

Figure 3. Graphs $G'(a,b)$ and $H'(a,b,c)$.

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

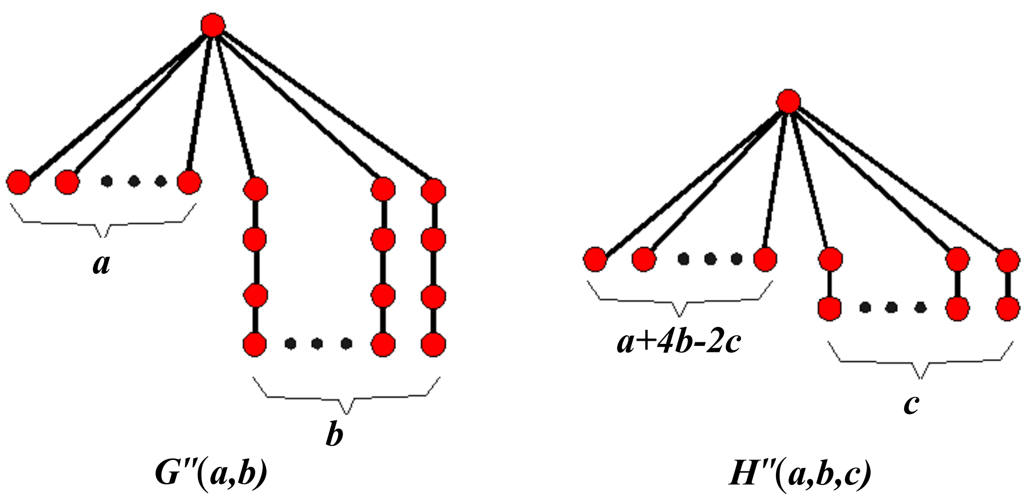

Figure 4. Graphs $G''(a,b)$ and $H''(a,b,c)$.

Note that $W_{\min,\eta}\left(G''(a,b)\right)-W_{\min,\eta}\left(H''(a,b,c)\right)=Q(a,b,c,\eta)$. We will now prove that for each pair of distinct λ and η there are numbers a, b, c such that at least one pair of corresponding graphs is ordered differently by the corresponding indices.

Distinguish three cases:

CASE 1: ($\lambda > 0$ and $\eta < 0$) or ($\lambda < 0$ and $\eta > 0$).

Without loss of generality, we may assume that $\lambda > 0$ and $\eta < 0$. Note that $2^{\lambda}+1 \neq 2^{\eta}+1$ or equivalently that

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

At least one of the following subcases applies:

SUBCASE 2.1: $\dfrac{2^\lambda+3^\lambda-2}{2^\lambda-1}\neq\dfrac{2^\eta+3^\eta-2}{2^\eta-1}$.

Two subsubcases, can be observed, i.e. $\dfrac{2^\lambda+3^\lambda-2}{2^\lambda-1}<\dfrac{2^\eta+3^\eta-2}{2^\eta-1}$ and $\dfrac{2^\lambda+3^\lambda-2}{2^\lambda-1}>\dfrac{2^\eta+3^\eta-2}{2^\eta-1}$.

Since they are solved in similar way, we shall assume that $\dfrac{2^\lambda+3^\lambda-2}{2^\lambda-1}<\dfrac{2^\eta+3^\eta-2}{2^\eta-1}$. Hence, there is a rational number q such that $\dfrac{2^\lambda+3^\lambda-2}{2^\lambda-1}<q<\dfrac{2^\eta+3^\eta-2}{2^\eta-1}$. Denote $q=\dfrac{c}{b}, c,b\in\mathbb{N}$ and let us calculate

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

$$=b\left(2^\lambda+3^\lambda-2\right)-c\cdot\left(2^\lambda-1\right)=b\cdot\left(2^\lambda-1\right)\cdot\left(\frac{2^\lambda+3^\lambda-2}{2^\lambda-1}-q\right)<0$$

Note that $$\lim_{a\to\infty}\frac{P(a,b,c,\eta)}{\left((a+b)\cdot\left(-1^\eta\right)+b\cdot\left(-2^\eta\right)+b\cdot\left(-3^\eta\right)-(a+3b-c)\cdot\left(-1^\eta\right)-c\cdot\left(-2^\eta\right)\right)}=1$$

Hence, for sufficiently large a, the last expression is positive. Let us calculate the denominator of this expression:

$$b\left(2-2^\eta-3^\eta\right)+\left(2^\eta-1\right)c=b\left(2^\eta-1\right)\left(\frac{2-2^\eta-3^\eta}{2^\eta-1}+q\right)=b\left(1-2^\eta\right)\left(\frac{2^\eta+3^\eta-2}{2^\eta-1}-q\right)>0$$

Therefore, there is a sufficiently large $a\in\mathbb{N}$ such that $P(a,b,c,\lambda)<0$ and $P(a,b,c,\eta)>0$ and hence, for the graphs $G'(a,b)$ and $H'(a,b,c)$ graphs depicted on Figure 3,

$$W_{\min,\lambda}\left(G'(a,b)\right)-W_{\min,\lambda}\left(H'(a,b,c)\right)=P(a,b,c,\lambda)<0;$$

$$W_{\min,\eta}\left(G'(a,b)\right)-W_{\min,\eta}\left(H'(a,b,c)\right)=P(a,b,c,\eta)>0$$

The claim is proved in this subcase.

SUBCASE 2.2: $\dfrac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}\neq\dfrac{2^\eta+3^\eta+4^\eta-3}{2^\eta-1}$.

Again, there are two subsubcases: $\dfrac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}<\dfrac{2^\eta+3^\eta+4^\eta-3}{2^\eta-1}$ and $\dfrac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}>\dfrac{2^\eta+3^\eta+4^\eta-3}{2^\eta-1}$

Since both cases can be treated analogously, we assume that $\dfrac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}<\dfrac{2^\eta+3^\eta+4^\eta-3}{2^\eta-1}$. Hence, there is a rational number q such that $\dfrac{2^\lambda+3^\lambda+4^\lambda-3}{2^\lambda-1}<q<\dfrac{2^\eta+3^\eta+4^\eta-3}{2^\eta-1}$. Denote $q=\dfrac{c}{b},\ b,c\in\mathbb{N}$ and

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

$$=b\cdot\left(2^\lambda+3^\lambda+4^\lambda-1\right)-c\left(2^\lambda-1\right)=b\left(2^\lambda-1\right)\left(\frac{2^\lambda+3^\lambda+4^\lambda-1}{2^\lambda-1}-q\right)<0$$

On the other hand, $\lim\limits_{a\to\infty}\dfrac{Q(a,b,c,\eta)}{\left[(a+b)(-1^{\eta})+b\cdot(-2^{\eta})+b(-3^{\eta})+b(-4^{\eta})-(a+4b-c)(-1^{\eta})-c(-2^{\eta})\right]}=1$

Hence, for sufficiently large the last expression is positive. Let us calculate the denominator of this expression:

$$(a+b)(-1^{\eta})+b\cdot(-2^{\eta})+b(-3^{\eta})+b(-4^{\eta})-(a+4b-c)(-1^{\eta})-c(-2^{\eta})=$$
$$=b(3-2^{\eta}-3^{\eta}-4^{\eta})-bq(1-2^{\eta})=b(1-2^{\eta})\left(\frac{2^{\eta}+3^{\eta}+4^{\eta}-3}{2^{\eta}-1}-q\right)>0.$$

Therefore, there is $a\in\mathbb{N}$ such that $Q(a,b,c,\eta)>0$ and $G(a,b,c,\eta)<0$, which implies, for the graphs $G''(a,b)$ and $H''(a,b,c)$ given on Figure 4,

$$W_{\min,\lambda}(G''(a,b))-W_{\min,\lambda}(H''(a,b,c))=Q(a,b,c,\lambda)<0$$
$$W_{\min,\eta}(G''(a,b))-W_{\min,\eta}(H''(a,b,c))=Q(a,b,c,\eta)>0.$$

CASE 2: $\lambda,\mu>0$.

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

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

At least one of the following must hold:

SUBCASE 2.1: $\dfrac{2^{\lambda}+3^{\lambda}-2}{2^{\lambda}-1}\neq\dfrac{2^{\eta}+3^{\eta}-2}{2^{\eta}-1}$.

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

$$\lim_{a\to\infty}\frac{P(a,b,c,\lambda)}{(a+3b+1)^{\lambda}}=\lim_{a\to\infty}\left((a+b)\cdot1^{\lambda}+b\cdot2^{\lambda}+b\cdot3^{\lambda}-(a+3b-c)\cdot1^{\lambda}-c\cdot2^{\lambda}\right)=$$
$$=b(2^{\lambda}+3^{\lambda}-2)-c\cdot(2^{\lambda}-1)=b\cdot(2^{\lambda}-1)\cdot\left(\frac{2^{\lambda}+3^{\lambda}-2}{2^{\lambda}-1}-q\right)<0$$

Completely analogously, we get $\lim\limits_{a\to\infty}\dfrac{P(a,b,c,\mu)}{(a+3b+1)^{\mu}}>0$. Therefore, there is a sufficently large $a\in\mathbb{N}$ such that for graphs $G'(a,b)$ and $H'(a,b,c)$ from Figure 3. The claim is proved in this subcase.

SUBCASE 2.2: $\dfrac{2^{\lambda}+3^{\lambda}+4^{\lambda}-3}{2^{\lambda}-1}\neq\dfrac{2^{\eta}+3^{\eta}+4^{\eta}-3}{2^{\eta}-1}$.

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

$$\lim_{a\to\infty}\frac{Q(a,b,c,\lambda)}{(a+4b+1)^{\lambda}}=\lim_{a\to\infty}\left((a+b)\cdot 1^{\lambda}+b\cdot 2^{\lambda}+b\cdot 3^{\lambda}+b\cdot 4^{\lambda}-(a+4b-c)\cdot 1^{\lambda}-c\cdot 2^{\lambda}\right)$$
$$=b\cdot\left(2^{\lambda}+3^{\lambda}+4^{\lambda}-1\right)-c\left(2^{\lambda}-1\right)=b\left(2^{\lambda}-1\right)\left(\frac{2^{\lambda}+3^{\lambda}+4^{\lambda}-1}{2^{\lambda}-1}-q\right)<0$$

whereas $\lim_{a\to\infty}\frac{Q(a,b,c,\mu)}{(a+4b+1)^{\mu}}>0$.

Therefore, there is a sufficiently large $a\in\mathbb{N}$ such that, for graphs $G''(a,b)$ and $H''(a,b,c)$ (see Figure 4),

$$W_{\min,\lambda}\left(G''(a,b)\right)-W_{\min,\lambda}\left(H'(a,b,c)\right)=G(a,b,c,\lambda)<0$$
$$W_{\min,\eta}\left(G''(a,b)\right)-W_{\min,\eta}\left(H''(a,b,c)\right)=G(a,b,c,\eta)>0.$$

CASE 3: $\lambda,\eta<0$.

This case can be solved by a similar techniques to ones used in the proof of the Case 2. We omit the details.

Conclusions

The Wiener number is one of the most useful indices in the QSPR and QSAR studies. It is well correlated with a number of physical and chemical properties of chemical compounds. Therefore it is natural to study the indices that represent small alternations of this index that may give better correlations with specific properties than the original Wiener index. In this paper the family of such alternations is presented as topological index $W_{\min,\lambda}$ (where $W_{\min,1}$ is original Wiener index. The family of these indices generalizes the notion of the Wiener index and may improve results of QSPR and QSAR studies. However, this generalization is valid only for trees and can not be applied to cyclic graphs. On the other hand, the indices studied here can be applied on weighted graphs. A natural generalization to weighted graph would be obtained by replacing the numbers $n_G(u,v)$ and $n(G)=|V(G)|$ with the sums of weights of the corresponding vertices.

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Povzetek

Nedavno so Nikolić, Trinajstić in Randić predlagali modifikacijo Wienerjevega števila $W(G)$, definirano z ${}^{m}W(G) = \sum_{uv \in E(G)} n_G(u,v)^{-1} n_G(u,v)^{-1}$. Invarianto so Gutman in avtorja posplošili na ${}^{\lambda}W(G) = \sum_{uv \in E(G)} n_G(u,v)^{\lambda} n_G(u,v)^{\lambda}$. Tu obravnavamo posplošitev podobnega tipa, $W_{\min,\lambda}(G) = \sum_{uv \in E(G)} (V(G)^{\lambda} m_G(u,v)^{\lambda} - m_G(u,v)^{2\lambda})$ in pokažemo, da nekatere pomembne lastnosti $W(G)$, ${}^{m}W(G)$ and ${}^{\lambda}W(G)$, veljajo tudi za $W_{\min,\lambda}(G)$, za večino vrednosti parametra λ. Dokažemo, da za poljubno drevo (povezan acikličen graf) z n točkami T_n, ki ni pot P_n ali zvezda S_n , velja $W_{\min,\lambda}(P_n) > W_{\min,\lambda}(T_n) > W_{\min,\lambda}(S_n)$, za vse $\lambda \geq 1$ in $\lambda < 0$. Za te vrednosti parametra je torej $W_{\min,\lambda}(G)$ razred topoloških indeksov, ki so lahko uporabni pri obravnavi od razvejanosti odvisnih lastnosti v QSPR in QSAR. Dokažemo tudi, da so vsi novi indeksi različni v naslednjem smislu: če uredimo vsa drevesa glede na $W_{\min,\lambda}(G)$ potem za različne vrednosti parametra λ dobimo različne urejenosti.