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Note

Altered Wiener Indices of Thorn Trees*

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Three modifications of the Wiener index $W(\mathrm{G})$ of a structure G have been recently proposed: the λ-modified Wiener index ${}^{\lambda}W(\mathrm{G}) = \sum_{uv\in \mathrm{E(G)}} n_{\mathrm{G}}(u,v)^{\lambda} n_{\mathrm{G}}(v,u)^{\lambda}$, the λ-variable Wiener index ${}_{\lambda}W(\mathrm{G}) = \frac{1}{2}\sum_{uv\in \mathrm{E(G)}} (n(\mathrm{G})^{\lambda} - n_{\mathrm{G}}(u,v)^{\lambda} - n_{\mathrm{G}}(v,u)^{\lambda})$ and the λ-altered Wiener index $W_{\min,\lambda}(\mathrm{G}) = \frac{1}{2}\sum_{uv\in \mathrm{E(G)}} (n(\mathrm{G})^{\lambda} m_{\mathrm{G}}(u,v)^{\lambda} - m_{\mathrm{G}}(u,v)^{2\lambda})$ where $n(\mathrm{G})$ is the number of vertices of G, and $m_{\mathrm{G}} = \min\{n_{\mathrm{G}}(u,v), n_{\mathrm{G}}(v,u)\}$. For a given positive integer k, explicit formulae are available for calculating the k-modified Wiener index and the k-variable Wiener index of a thorn tree by means of the i-modified Wiener indices and the i-variable Wiener indices, respectively, of the parent tree for integers i and k with $0 \le i \le k$. It is pointed out in the present report that this is not the case of the k-altered Wiener index.

Keywords
Wiener index
altered Wiener index
modified Wiener index
variable Wiener index
thorn tree

INTRODUCTION

The molecular-graph-based quantity, introduced by Wiener[1] in 1947 and formalized *via* the distance matrix by Hosoya,[2] nowadays known under the name Wiener index (*e.g.*, Ref. 3) or Wiener number (*e.g.*, Ref. 4), is one of the oldest and the most thoroughly studied topological indices,[5] and it is still a topic of current research interest (*e.g.*, Ref. 6). Its computational and mathematical properties and its usefulness in the structure-property-activity modeling are continuously discussed.[7–13] In the present report, we discuss altered Wiener indices of thorn trees.

Let G be a connected graph with vertex set V(G) and edge set E(G). Recall that the Wiener index of G is defined as the sum of all distances in G. It was already known to Wiener that for a tree, the Wiener index can be also computed by summing up the edge contributions, where the contribution of each edge uv is the product of the number of vertices closer to the vertex u and the number of vertices closer to the vertex v. Formally:

$$W(\mathrm{G}) = \sum_{uv\in \mathrm{E(G)}} n_{\mathrm{G}}(u,v)\, n_{\mathrm{G}}(v,u) \qquad (1)$$

where $n_{\mathrm{G}}(u,v)$ is the number of vertices closer to the vertex u than vertex v and $n_{\mathrm{G}}(v,u)$ is the number of vertices closer to the vertex v than vertex u.

A large number of modifications and extensions of the Wiener index have been considered in the chemical

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literature [*e.g.*, Ref. 14]. Motivated by formula (1), the λ-modified Wiener indices ${}^{\lambda}W$,[15] the λ-variable Wiener indices ${}_{\lambda}W$,[16,17] and the λ-altered Wiener indices $W_{\min,\lambda}$[18] are defined as:

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

$$_{\lambda}W(\mathrm{G}) = \frac{1}{2}\sum_{uv\in \mathrm{E(G)}} (n(\mathrm{G})^{\lambda} - n_{\mathrm{G}}(u,v)^{\lambda} - n_{\mathrm{G}}(v,u)^{\lambda})$$

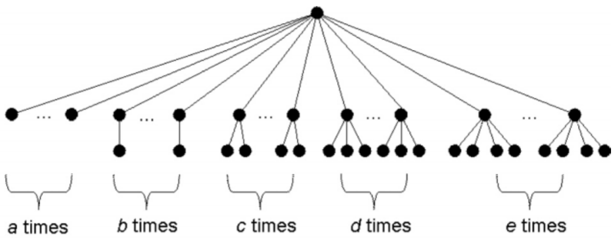
$$W_{\min,\lambda}(\mathrm{G}) = \sum_{uv\in \mathrm{E(G)}} (n(\mathrm{G})^{\lambda} m_{\mathrm{G}}(u,v)^{\lambda} - m_{\mathrm{G}}(u,v)^{2\lambda})$$

where n(G) is the number of vertices of G and $m_{\mathrm{G}}(u,v) = \min\{n_{\mathrm{G}}(u,v),\ n_{\mathrm{G}}(v,u)\}$. All the three types of modifications of the Wiener index may be viewed as 'branching indices' and structural descriptors, suitable for modeling branching-dependent properties of organic compounds and applicable in the quantitative structure-property-activity studies.[19]

For a graph G with n vertices $v_1,\ldots, v_n$, the thorn graph $\mathrm{G}^* = \mathrm{G}^*(p_1,\ldots, p_n)$ of G is obtained by attaching p_i thorns (pendant edges) to each vertex v_i for $i = 1,\ldots, n$. If G is a tree, then G* is called a thorn tree. In Refs. 20 and 21, formulae are reported for the Wiener index of several classes of thorn graphs. Let $\deg_{\mathrm{G}}(v)$ be the degree of the vertex v in G. When $p_i = r \deg_{\mathrm{G}}(v_i) + s$ for $i = 1,\ldots, n$, there is a closed formula for calculating the k-modified Wiener index (or the k-variable Wiener index) of the thorn tree T* in terms of the i-modified Wiener indices (or the i-variable Wiener indices) of the tree T for integers i and k with $0 \le i \le k$).[22–24] In this report, we point out that such a relation does not hold for the k-altered Wiener index.

RESULTS

Let $\mathrm{G}_{a,b,c,d,e}$ be graph depicted by the following figure:



It is easily seen that the number of vertices of $\mathrm{G}_{a,b,c,d,e}$ is equal to:

$$n = n(\mathrm{G}_{a,b,c,d,e}) = 1 + a + 2b + 3c + 4d + 5e \quad (2)$$

and that if $n \ge 10$, then:

$$\begin{aligned} W_{\min,1}(\mathrm{G}_{a,b,c,d,e}) &= 1\cdot(n-1)\cdot(a+b+2c+3d+4e)+ \\ &+2\cdot(n-2)\cdot b+3\cdot(n-3)\cdot c+ \\ &+4\cdot(n-4)\cdot d+5\cdot(n-5)\cdot e; \end{aligned}$$

and

$$\begin{aligned} W_{\min,2}(\mathrm{G}_{a,b,c,d,e}) &= 1\cdot(n^2-1)\cdot(a+b+2c+3d+4e)+ \\ &+4\cdot(n^2-4)\cdot b+9\cdot(n^2-9)\cdot c+ \\ &+16\cdot(n^2-16)\cdot d+25\cdot(n^2-25)\cdot e. \end{aligned}$$

Let us consider graphs: $\mathrm{G}_{7,0,36,0,5}$ and $\mathrm{G}_{0,26,0,22,0}$. Note that:

$$n(\mathrm{G}_{7,0,36,0,5}) = n(\mathrm{G}_{0,26,0,22,0}) = 141;$$

$$W_{\min,1}(\mathrm{G}_{7,0,36,0,5}) = W_{\min,1}(\mathrm{G}_{0,26,0,22,0}) = 32164;$$

$$W_{\min,2}(\mathrm{G}_{7,0,36,0,5}) = W_{\min,2}(\mathrm{G}_{0,26,0,22,0}) = 10888648.$$

Denote by $\mathrm{G}^*_{a,b,c,d,e}$ the graph obtained from graph $\mathrm{G}_{a,b,c,d,e}$ by adding to each vertex the number of thorns equal to the degree of that vertex in graph $\mathrm{G}_{a,b,c,d,e}$. If $W_{\min,2}(\mathrm{G}^*_{a,b,c,d,e})$ can be expressed in terms of $n(\mathrm{G}_{a,b,c,d,e})$, $W_{\min,1}(\mathrm{G}_{a,b,c,d,e})$ and $W_{\min,2}(\mathrm{G}_{a,b,c,d,e})$, then it necessarily follows that:

$$W_{\min,2}(\mathrm{G}^*_{7,0,36,0,5}) = W_{\min,2}(\mathrm{G}^*_{0,26,0,22,0}). \quad (3)$$

Hence, it is sufficient to prove that relation (3) does not hold. Denote $m = n(\mathrm{G}^*_{a,b,c,d,e}) = 3 \cdot n(\mathrm{G}_{a,b,c,d,e}) - 2 = 3n - 2$ and n as in (2). Then, we have:

$$\begin{aligned} W_{\min,2}(\mathrm{G}^*_{a,b,c,d,e}) &= (2n-2)\cdot 1^2\cdot(m^2-1^2)+ \\ &+(a+b+2c+3d+4e)\cdot 2^2\cdot(m^2-2^2)+ \\ &+b\cdot 5^2\cdot(m^2-5^2)+c\cdot 8^2\cdot(m^2-8^2)+ \\ &+d\cdot 11^2(m^2-11^2)+e\cdot 14^2\cdot(m^2-14^2). \quad (4) \end{aligned}$$

From (4), it follows that:

$$\begin{aligned} W_{\min,2}(\mathrm{G}^*_{7,0,36,0,5}) &= 701\,532\,960, \\ W_{\min,2}(\mathrm{G}^*_{0,26,0,22,0}) &= 701\,534\,256. \quad (5) \end{aligned}$$

Obviously (5) contradicts (3). Therefore, there is indeed no formula for calculating $W_{\min,2}(\mathrm{G}^*_{a,b,c,d,e})$ in terms of $n(\mathrm{G}_{a,b,c,d,e})$, $W_{\min,1}(\mathrm{G}_{a,b,c,d,e})$ and $W_{\min,2}(\mathrm{G}_{a,b,c,d,e})$.

Remark 1. – Since $W_{\min,1}$ coincides with the standard Wiener index, it follows that $W_{\min,1}(\mathrm{G}^*_{7,0,36,0,5}) = W_{\min,1}(\mathrm{G}^*_{0,26,0,22,0})$. Indeed, using formula:

$$\begin{aligned} W_{\min,1}(\mathrm{G}^*_{a,b,c,d,e}) &= (2n-2)\cdot 1\cdot(m-1)+ \\ &+(a+b+2c+3d+4e)\cdot 2\cdot(m-2)+ \\ &+b\cdot 5\cdot(m-5)+c\cdot 8\cdot(m-8)+ \\ &+d\cdot 11(m-11)+e\cdot 14\cdot(m-14), \end{aligned}$$

one gets:

$$W_{\min,1}(G^*_{7,0,36,0,5}) = W_{\min,1}(G^*_{0,26,0,22,0}) = 347996\,.$$

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SAŽETAK

Izmijenjeni Wienerovi indeksi trnovitih stabala

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Nedavno su predložene tri modifikacije Wienerovoga indeksa neke strukture G: λ-modificirani Wienerov indeks ${}^{\lambda}W(\mathrm{G})$, λ-varijabilni Wienerov indeks ${}_{\lambda}W(\mathrm{G})$ i λ-izmijenjeni Wienerov indeks $W_{\min,\lambda}(\mathrm{G})$. Za bilo koji pozitivni cijeli broj k postoje eksplicitne formule za računanje k-modificiranoga Wienerova indeksa i k-varijabilnoga Wienerova indeksa trnovitih stabala pomoću i-modificiranoga Wienerova indeksa i i-varijabilnoga Wienerova indeksa matičnoga stabla za cijele brojeve i s granicama $0 \le i \le k$. U ovome je članku pokazano da to ne vrijedi za k-izmijenjeni Wienerov indeks.