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MODIFIED WIENER INDICES OF THORN TREES

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Abstract. The λ-modified Wiener index ${}^{m}W_{\lambda}$ provides a class of structure–descriptors to measure the branching of the carbon-atom skeleton molecules. A thorn tree is formed by attaching some new vertices of degree one to each vertex of the parent tree. An explicit expression is deduced enabling the calculation of the k-modified Wiener index of a type of thorn tree in terms of the i-modified Wiener indices of the parent tree for any natural number k with $0 \le i \le k$.

1. INTRODUCTION

The Wiener index (W) is one of the oldest molecular–graph–based structure–descriptors [1, 2]. It is the the sum of distances between all unordered pairs of vertices in the graph. Let T be a tree on n vertices and let e be one of its edges. Let $n_{T,1}(e)$ and $n_{T,2}(e)$ be the numbers of vertices of T lying on the two sides of the edge e. Then [1]

$$W(T) = \sum_{e} n_{T,1}(e) \cdot n_{T,2}(e)$$

where the summation goes over all edges of T.

Recently, Gutman et al. [3] put forward the λ-modified Wiener index ${}^{m}W_{\lambda}$, defined as

$$ {}^{m}W_{\lambda}(T) = \sum_{e} [n_{T,1}(e) \cdot n_{T,2}(e)]^{\lambda} $$

where λ is a real number. Clearly, 1-modified Wiener index ${}^{m}W_{1}$ is just the ordinary Wiener index W. Note that -1-modified Wiener index ${}^{m}W_{-1}$ has been studied in [4, 5]. If T is a tree on n vertices, different from the n–vertex path P_n and the n–vertex star S_n, it has been proven that [3]

$$ {}^{m}W_{\lambda}(P_n) > {}^{m}W_{\lambda}(T) > {}^{m}W_{\lambda}(S_n) $$

when $\lambda > 0$, and

$$ {}^{m}W_{\lambda}(P_n) < {}^{m}W_{\lambda}(T) < {}^{m}W_{\lambda}(S_n) $$

when $\lambda < 0$. Hence for different $\lambda \neq 0$, ${}^{m}W_{\lambda}$ measures the extent of branching of the molecular carbon–atom skeleton, and can thus be viewed as a class of structure–descriptors [2].

The thorn graph $G^{\star} = G^{\star}(p_1, p_2, \ldots, p_n)$ of a graph G on n vertices $v_1, v_2, \ldots, v_n$ is formed by attaching $p_i \geq 0$ new vertices of degree one to each vertex v_i of G [6, 7]. For G being a tree T, $T^{\star}$ is called a thorn tree. Special cases of thorn graphs have been already considered by Cayley [8] and later by Pólya [9]. Gutman [6] established relations between $W(G^{\star})$ and $W(G)$ for a connected graph G.

Let T be a tree on n vertices $v_1, v_2, \ldots, v_n$. In this paper, we consider the thorn tree $T^{\star}_{a,b} = T^{\star}(p_1, p_2, \ldots, p_n)$ with $p_i = ad_i + b$, $i = 1, 2, \ldots, n$ where d_i is the degree of vertex v_i, and a and b are real numbers such that each $p_i \geq 0$ is an integer. For three special classes of thorn trees $T^{\star}_{a,b}$ with $a = 0$, or $a = 1$ and $b = 0$, or $a = -1$, Vukičević and Graovac [10] have recently found explicit formulae for ${}^{m}W_{\lambda}(T^{\star}_{a,b})$ in terms of μ-modified Wiener indices of T, where λ, μ are natural numbers with $0 \leq \mu \leq \lambda$ if $a = 1$ and $b = 0$, or if $a = -1$, and $\lambda = \mu$ is a real number if $a = 0$.

We present an explicit formula to calculate ${}^{m}W_{k}(T^{\star}_{a,b})$ in terms of i-modified Wiener indices of T for any natural number k with $0 \leq i \leq k$, and thus generalize the results in [10].

2. THE RESULT

Theorem 1. *If $T^\star = T^\star_{a,b}$ is the thorn graph of a tree T on n vertices and k is a natural number, then*

$$\begin{aligned} {}^{m}W_k(T^\star) &= \sum_{i=0}^{k} \left[\binom{k}{i}\left(-a(2a+b+1)n+a^2\right)^{k-i} \cdot (2a+b+1)^{2i} \cdot {}^{m}W_i(T)\right] \\ &\quad + [(2a+b)n-2a] \cdot [(2a+b+1)n-2a-1]^k \,. \end{aligned} \tag{1}$$

In particular,

$$W(T^\star) = (2a+b+1)^2 W(T) + (a+b)(2a+b+1)n^2 - (5a^2+3ab+3a+b)n + 3a^2 + 2a\,. \tag{2}$$

Proof. Let $V(T)$ and $E(T)$ be the vertex set and edge set of T, respectively. We have

$${}^{m}W_k(T^\star) = \sum_{e \in E(T)} [n_{T^\star,1}(e) \cdot n_{T^\star,2}(e)]^k + \sum_{e \in E(T^\star) \setminus E(T)} [n_{T^\star,1}(e) \cdot n_{T^\star,2}(e)]^k \,.$$

For any vertex v of T, let d_v be the degree of v in T. It is easy to see that the number of vertices of $T^\star$ is $n + a\sum_{i=1}^{n} d_i + nb = (2a+b+1)n - 2a$, and then $E(T^\star) \setminus E(T)$ contains exactly $(2a+b)n - 2a$ edges. So

$$\sum_{e \in E(T^\star) \setminus E(T)} [n_{T^\star,1}(e) \cdot n_{T^\star,2}(e)]^k = [(2a+b)n-2a] \cdot [(2a+b+1)n-2a-1]^k \,.$$

Let $x = -ayn + a^2$, $y = 2a+b+1$. To prove (1), we only need to show

$$\sum_{e \in E(T)} [n_{T^\star,1}(e) \cdot n_{T^\star,2}(e)]^k = \sum_{i=0}^{k} \binom{k}{i} x^{k-i} y^{2i} \cdot {}^{m}W_i(T)\,. \tag{3}$$

Let $T_1(e)$ be the component of $T - e$ with $n_{T,1}$ vertices. Note that for each $e \in E(T)$,

$$\begin{aligned} n_{T^\star,1}(e) &= n_{T,1}(e) + \sum_{u \in V(T_1(e))} (ad_u + b) \\ &= n_{T,1}(e) + a \sum_{u \in V(T_1(e))} d_u + bn_{T,1}(e) \\ &= n_{T,1}(e) + a\left[2\left(n_{T,1}(e) - 1\right) + 1\right] + bn_{T,1}(e) \\ &= y \cdot n_{T,1}(e) - a\,, \end{aligned}$$

and similarly,

$$n_{T^\star,2}(e) = y \cdot n_{T,2}(e) - a\,.$$

So

$$\begin{aligned} n_{T^\star,1}(e) \cdot n_{T^\star,2}(e) &= y^2 \cdot n_{T,1}(e) \cdot n_{T,2}(e) - ay \cdot [n_{T,1}(e) + n_{T,2}(e)] + a^2 \\ &= y^2 \cdot n_{T,1}(e) \cdot n_{T,2}(e) + x\,, \end{aligned}$$

and it follows that

$$\begin{aligned} \sum_{e\in E(T)} [n_{T^\star,1}(e) \cdot n_{T^\star,2}(e)]^k &= \sum_{e\in E(T)} [y^2 \cdot n_{T,1}(e) \cdot n_{T,2}(e) + x]^k \\ &= \sum_{e\in E(T)} \sum_{i=0}^{k} \binom{k}{i} x^{k-i} [y^2 \cdot n_{T,1}(e) \cdot n_{T,2}(e)]^i \\ &= \sum_{i=0}^{k} \binom{k}{i} x^{k-i} y^{2i} \cdot \sum_{e\in E(T)} [n_{T,1}(e) \cdot n_{T,2}(e)]^i \\ &= \sum_{i=0}^{k} \binom{k}{i} x^{k-i} y^{2i} \cdot {}^{m}W_i(T)\,. \end{aligned}$$

This proves (3). Hence (1) follows. By setting $k = 1$ in (1), we have (2).

Corollary 2. [10] *If T is a tree with n vertices, then for any natural number k,*

$$\begin{aligned} {}^{m}W_k(T^\star_{1,0}) &= \sum_{i=0}^{k} \left[\binom{k}{i}(1-3n)^{k-i} 9^i \cdot {}^{m}W_i(T)\right] + (2n-2)(3n-3)^k\,, \\ {}^{m}W_k(T^\star_{-1,b}) &= \sum_{i=0}^{k} \left[\binom{k}{i}((b-1)n+1)^k - i(b-1)^{2i} \cdot {}^{m}W_i(T)\right] \\ &\quad +[(b-2)n+2][(b-1)n+1]^k\,. \end{aligned}$$

If $a = 0$ and λ is a real number, then replacing the integer k by λ and noting that $x = 0$ in the proof of Theorem 1, we may easily have the following.

Corollary 3. [10] *If T is a tree with n vertices, then for any λ,*

$${}^{m}W_\lambda(T^\star_{0,b}) = (b+1)^{2\lambda} \cdot {}^{m}W_\lambda(T) + bn[(b+1)n-1]^\lambda\,.$$

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References

[1] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947), 17–20.

[2] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[3] I. Gutman, D. Vukičević, J. Žerovnik, *A class of modified Wiener indices*, Croat. Chem. Acta **77** (2004), 103–109.

[4] S. Nikolić, N. Trinajstić, M. Randić, *Wiener index revisited*, Chem. Phys. Lett. **333** (2001), 319–321.

[5] I. Gutman, J. Žerovnik, *Corroborating a modification of the Wiener index*, Croat. Chem. Acta **75** (2002), 603–612.

[6] I. Gutman, *Distance in thorny graphs*, Publ. Inst. Math. (Beograd) **63** (1998), 31–36

[7] D. Bonchev, D. J. Klein, *On the Wiener number of thorn trees, stars, rings, and rods*, Croat. Chem. Acta **75** (2002), 613–620.

[8] A. Cayley, *On the mathematical theory of isomers*, Phil. Magazine **47** (1874), 444–446.

[9] G. Pólya, *Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen*, Acta Math. **68** (1937), 145–254.

[10] D. Vukičević, A. Graovac, *On modified Wiener indices of thorn graphs*, MATCH Commun. Math. Comput. Chem. **50** (2004), 93–108.