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Modified terminal Wiener index of a type of dendrimer nanostars

LIHUI YANG, HONGBO HUA[a]
Department of mathematics, Hunan City University Yiyang City, Hunan 413000, P. R. China
[a]*Faculty of Mathematics and Physics, Huaiyin Institute of Technology, Huai'an City, Jiangsu 223003, P. R. China*

The *terminal wiener index (TW)* of a tree *T* was defined recently by Gutman et al [1] as $TW(T)=\sum_{e=uv\in E(T)} n(e;u)n(e;v)$, where *n(e;u)* is the number of pendent vetices in *T* lying closer to *u* than to *v*. In this paper, we first introduce a new topological index, named *modified terminal wiener index (MTW),* by extending the definition of terminal wiener index to any connected graph. Then we investigate the mathematical property of *MTW* and compute the *MTW* for a type of dendrimer nanostars.

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1. Introduction

Let *G* be a graph with edge set *E(G)*. For an edge *e=uv* in *E(G),* we let *n(e;u)* and *n(e;v)* be the number of pendent vetices in *G* lying closer to *u* than to *v* and the number of pendent vertices in *G* lying closer to *v* than to *u*, respectively. The *terminal wiener index (TW)* of a tree *T* was defined recently by Gutman et al [1] as the sum

$$\mathrm{TW}(T)=\sum_{e=uv\in E(\mathrm{T})} n(e;u)n(e;v).$$

This index has been investigated in [2] for thorn graphs and in [3] for equiseperability. The problem of computing topological indices of nanostructures is introduced firstly by Diudea and his coauthors [4-8]. After that, there are many papers dealing with computing topological indices of various nanostrutures, see [9-25] and the references cited therien. Obviously, the above definition for *TW* is invalid for graph without pendent vertices. Suppose that $\delta(\mathrm{e};u)$ and $\delta(\mathrm{e};v)$ are the number of vetices of minimum degree in *G* lying closer to u than to v and the number of vertices of minimum degree in *G* lying closer to *v* than to *u*, respectively. Now, we extend the definition of *TW* to any connected graph by replacing in the above formula $n(e;u)$ and $n(e;v)$ by $\delta(\mathrm{e};u)$ and $\delta(\mathrm{e};v)$, respectively, and we call this new index *modified terminal wiener index (MTW),* that is,

$$MTW(\mathrm{G})=\sum_{e\in E(G)} \delta(e;u)\delta(e;v).$$

From the definition above, it is evident that if the graph under consideration is a tree, then *MTW* coincides with *TW*.

A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers, see Figs. 1 and 2 for instance.

In this paper, we first investigate the mathematical property of *MTW* index, and then we give explicit computing formulas of *MTW* index for a type of dendrimer nanostars.

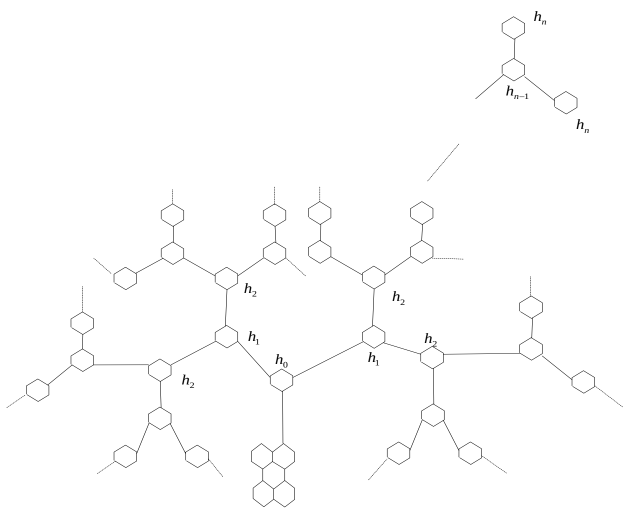

Fig. 1. The dendrimer nanostar NS[n].

2. Main results

We first investigate the mathematical properties of the modified terminal wiener index *(MTW)*.

Proposition 1. *Let G be a nontrival connected graph on* $n \geq 4$ *vertices. Then*

$$MTW(G) \geq 0,$$

where the equality holds if and only if G is a graph with exactly one vertex of minimum degree.

Proof. Since the contribution of each edge to *MTW* in a connected graph *G* is at least 0, we have $MTW(G) \geq 0$. If *MTW(G)*=0, then the contribution of each edge in *G* to *MTW* is 0. So, for each edge *e=uv* in *G*, we have $\delta(e;u)=0$ or $\delta(e;v)=0$. Suppose that *G* has two vertices, say *x* and *y*, of minimum degree. Assume now that there exists an edge *e=uv* such that $\delta(e;u)=0$. Thus, $\delta(e;v)=2$. Then there exists a path $P_{x,y}$ connecting *x* and *y*. Clearly, there exists an edge $e'=u'v'$ along the path $P_{x,y}$ such that *x* is closer to u' and *y* is closer to v' (here if *x* and *y* are adjacent, then the edge e' is just *xy*). But then, $\delta(e';u')=\delta(e';v')=1$ and thus, *MTW(G)>0,* a contradiction. Conversly, if *G* has exactly one minimum degree vertex, then the contribution of each edge to *MTW* is 0 and then *MTW(G)*=0.

Remark. In Poposition 1, if *n*=2 or 3, then *G* is the paths P_2, P_3 or the cycle C_3. Celarly, each of these graphs has more than one minimum-degree vertex. Thus, we assum that $n \geq 4$ in above proposition.

Proposition 2. *Let G be a connected bipartite graph on* $n \geq 2$ *vertices with n being even. Then*

$$MTW(G) \leq \frac{n^4}{16},$$

where the equality holds if and only if G is a balanced complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Note that the contribution of each edge to *MTW* in a connected graph *G* is at most $\frac{n}{2}\cdot\frac{n}{2}=\frac{n^2}{4}$ and that *G* has at most $\frac{n}{2}\cdot\frac{n}{2}=\frac{n^2}{4}$ edges. So, we have $MTW(G) \leq \frac{n^4}{16}$, with the equality holds only if *G* has exactly $\frac{n}{2}\cdot\frac{n}{2}=\frac{n^2}{4}$ edges and the contribution of each edge to *MTW* is exactly $\frac{n}{2}\cdot\frac{n}{2}=\frac{n^2}{4}$, implying that *G* is isomorphic to $K_{\frac{n}{2},\frac{n}{2}}$. Conversly, if *G* is isomorphic to $K_{\frac{n}{2},\frac{n}{2}}$, we clearly have $MTW(G)=\frac{n^4}{16}$.

We conjecture that among all connected graphs of *n* vertices, the balanced complete bipartite graph $K_{\lfloor\frac{n}{2}\rfloor,\lceil\frac{n}{2}\rceil}$ has the maximum modified terminal wiener index.

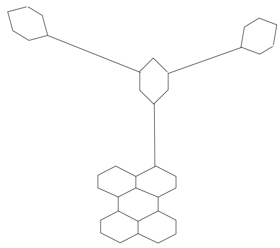

Fig. 2. The dendrimer nanostar NS[1].

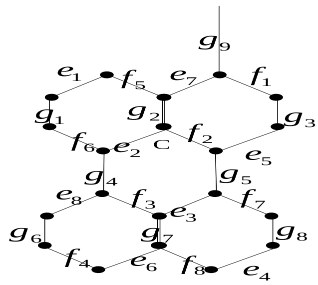

Fig. 3. The nucleus of dendrimer nanostar NS[n].

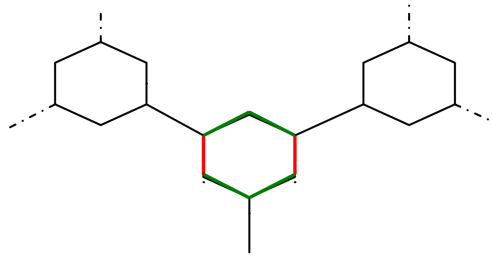

Fig. 4. The red edge denotes edge of Type A and the green edge denotes edge of Type B.

Now, we are in a position to give an explicit computation formula for a type of dendrimer nanostars, as shown in Fig. 1.

By the definition of nanostars, we know that for the nanostar *NS[n]*, there are $3\cdot 2^{n+2}+14$ vertices in total, among which there are $2^{n+3}+8$ vertices of degree 2, and $2^{n+2}+6$ vertices of degree 3, respectively. Firstly, we compute the value $\delta(e;u)e(e;v)$ for any one edge $e=uv$ in *NS[n]*.

For the sake of brevity, if there is an edge whose two ends are of degree *i* and *j*, respectively, then this edge is simply said to be an $(i, j)-$edge in the subsequent part of this paper. We need only to consider the contributions of three types of edges, namely, (2,2)-edge, (2,3)-edge and (3,3)-edge to *MTW*.

For any (2, 2)-edge $e=uv$ in the hexagon of the n^{th} stage, we have

$\delta(e;u)=3$ and $\delta(e;v)=2^{n+3}+5$ (or

$\delta(e;v)=3$ and $\delta(e;u)=2^{n+3}+5$).

The total number of such edges is 2^{n+2}.

◆ For any (2, 3)-edge $e=uv$ in the hexagon of the n^{th} stage satisfying $d(u)=2$ and $d(v)=3$, we have

$\delta(e;u)=3$ and $\delta(e;v)=2^{n+3}+5$.

The total number of such edges is 2^{n+1}.

◆ For any (2, 3)-edge $e=uv$ of *type A* (see Fig. 4) in the hexagon of the i^{th} ($0\le i\le n-1$) stage satisfying $d(u)=2$ and $d(v)=3$, we have

$$\delta(e;v)=3(2^1+...+2^{n-1-i})+5\cdot 2^{n-i}+1=2^{n-i+3}-5$$

and $\delta(e;u)=2^{n+3}-2^{n-i+3}+13$.

The total number of such edges is 2^{i+1}.

◆ For any (2, 3)-edge $e=uv$ of *type B* (see Fig. 4) in the hexagon of the i^{th} ($0\le i\le n-1$) stage satisfying $d(u)=2$ and $d(v)=3$, we have

$$\delta(e;u)=3(1+2+...+2^{n-i-2})+5\cdot 2^{n-i-1}+2=2^{n-i+2}-1$$

and $\delta(e;v)=2^{n+3}-2^{n-i+2}+9$.

The total number of such edges is 2^{i+2}.

◆ For any (3, 3)-edge $e=uv$, between the vertices in i^{th} layer and vertices in $(i+1)^{th}$ layer ($0\le i\le n-1$), we have

$$\delta(e;u)=3(1+2+...+2^{n-i-2})+5\cdot 2^{n-i-1}=2^{n-i+2}-3$$

and

$$\delta(e;v)=2^{n+3}-2^{n-i+2}+11$$

(or

$$\delta(e;u)=3(1+2+...+2^{n-i-2})+5\cdot 2^{n-i-1}=2^{n-i+2}-3$$

and $\delta(e;v)=2^{n+3}-2^{n-i+2}+11$).

The total number of such edges is 2^{i+1}.

Now, we consider the contributions of the edges in the nucleus, see Fig. 3. In the following, we use $\delta(e)$ to denote the contribution of an edge *e* to *MTW*. By an elementary calculation, we have

$$\delta(e_1)=\delta(e_2)=\delta(e_3)=\delta(e_4)=6(2^{n+3}+2),$$

$$\delta(e_5)=\delta(e_7)=9(2^{n+3}-1),$$

$$\delta(e_6)=\delta(e_8)=3(2^{n+3}+5).$$

$$\delta(f_1)=2^{n+6},$$

$$\delta(f_2)=\delta(f_3)=\delta(f_4)=6(2^{n+3}+2),$$

$$\delta(f_5)=\delta(f_6)=\delta(f_7)=\delta(f_8)=3(2^{n+3}+5).$$

$$\delta(g_1)=\delta(g_2)=\delta(g_3)=2^{n+6},$$

$$\delta(g_4)=\delta(g_5)=6(2^{n+3}+2),$$

$$\delta(g_6)=\delta(g_7)=\delta(g_8)=4(2^{n+3}+4),$$

$$\delta(g_9)=11(2^{n+3}-3).$$

By arguments above, we thus obtain

$$\mathrm{MTW}(\mathrm{NS}[N])=\begin{pmatrix}144.4^n+1330\cdot 2^n+223+\\ \sum_{i=0}^{n-1}2^{i+1}(2^{n-i+3}-5)(2^{n+3}-2^{n-i+3}+13)+\\ \sum_{i=0}^{n-1}2^{i+2}(2^{n-i+2}-1)(2^{n+3}-2^{n-i+2}+9)+\\ \sum_{i=0}^{n-1}2^{i+1}(2^{n-i+2}-3)(2^{n+3}-2^{n-i+2}+11)\end{pmatrix}.$$

3. Conclusion

In this paper, a new topological index, named modified terminal wiener index *(MTW)* is proposed by extending the definition of terminal wiener index to any connected graph. The mathematical properties of *MTW* are investigated and the *MTW* of a type of dendrimer nanostars is obtained.

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*Corresponding author: hongbo.hua@gmail.com