The Wiener index of cacti given matching number

Shang-wang Tan, Qi-long Wang
Department of Mathematics
China University of Petroleum
Qingdao 266580, China

Abstract

The Wiener index is the sum of distances between all pairs of vertices in a connected graph. A cactus is a connected graph in which any two of its cycles have at most one common vertex. In this article, we present some graphic transformations and derive the formulas for calculating the Wiener index of new graphs. With these transformations, we characterize the graphs having the smallest Wiener index among all cacti given matching number and cycle number.
Key words: Wiener index, cactus, cycle, matching

1. Introduction

All graphs considered in this paper will be finite, simple and undirected. Undefined notations and terminologies can be found in [1]. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$ (so the vertex number $|V(G)|$ is its *order*). The *cycle number* of G is $|E(G)|-|V(G)|+1$. A *pendent vertex* of G is a vertex of degree one and a *pendent edge* of G is an edge incident to a pendent vertex. Two distinct edges of G are independent if they are not adjacent in G. A *matching* of G is a set of pairwise independent edges, while a *maximum matching* of G is a matching of maximum cardinality and the cardinality of a maximum matching of G is its *matching number*. The *distance* $d_G(u,v)$ between two distinct vertices u and v of G is the number of edges on a shortest path connecting these vertices in G. For convenience, set $d_G(u,u)=0$. The distance $W(G,v)$ of a vertex $v \in V(G)$ is the sum of distances between v and all other vertices of G. Let $deg_G(v)$ be the degree of vertex v and let $N_G(v)$ be the set of all adjacent vertices of v in G.

The *Wiener index* $W(G)$ of a connected graph G is a graph invariant based on distances [2,3]. It is defined as the sum of distances between all pairs of vertices of G:

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v) = \frac{1}{2}\sum_{v\in V(G)} W(G,v).$$

The Wiener index is the oldest topological index related to molecular branching [4].

A quantity closely related to $W(G)$ is the *average distance* $\mu(G)$ defined by

$$\mu(G) = \frac{W(G)}{\binom{|V(G)|}{2}}.$$

When G represents a network (e.g., an interconnection network connecting many processors), $\mu(G)$ is the average distance between the nodes (or processors) of the network. Hence it is a measure of the average delay of messages for traversing from one node to another (see, for example, [5]). It is obvious that studying $\mu(G)$ is equivalent to studying $W(G)$.

There are two groups of closely related problems of the Wiener index which have attracted the attention of researchers for a long time:

(a) how Wiener index depends on the structure of a graph;

(b) how Wiener index can be efficiently calculated, especially without the aid of a computer (by so-called *paper-and-pencil* methods).

Many chemical applications of the Wiener index deal with acyclic organic molecules, whose molecular graphs are trees. Therefore, for trees and hexagonal systems, the greatest progress in solving the above problems was made (see two recent surveys [6,7]). It is worth indicating that many scholars have investigated the relations of Wiener index and some isomorphic invariants of graphs, such as order, maximum degree, diameter, degree sequence, matching number, et al. (see, for example, [8-18]).

Except trees, many results of the other graphs in solving the above problems were also made. For example, Tang and Deng [19] characterized the graphs having the first three smallest and largest Wiener indices among all unicyclic graphs. Du and Zhou [18] determined the graphs having the minimal Wiener index among all unicyclic graphs given order and matching number. Balakrishnan et al. [5] presented an expression of $W(G)$ for a connected graph G with at least two cut vertices.

A connected graph is a *cactus* if any two of its cycles have at most one common vertex. It is obvious that both trees and unicyclic graphs are special cacti. For eigenvalues on some matrices associated cacti such as adjacency (Laplacian or signless Laplacian) matrix, for example, see [20-26]. Motivated by the results above, in this article we give some graphic transformations and derive the formulas for calculating the Wiener index of new graphs, then we characterize the graphs having the smallest Wiener index among all cacti given matching number and cycle number.

The rest of the article is organized as follows. In Section 2, we present some graphic transformations and derive the formulas for calculating the Wiener index of new graphs. In Section 3, we determine the graphs having the smallest Wiener index among all cacti given matching number and cycle number. In Section 4, we summarize our conclusions and indicate some directions for future work.

2. Some transformations changing the Wiener index

In this section we present three graphic transformations and derive the formulas for calculating the Wiener index of new graphs (see Theorems 2.4, 2.8 and 2.9), which have not been studied before and will be used in the next section.

Definition 2.1. Let G, H be two connected graphs and let uv be a nonpendent edge of G such that it is not contained in triangles. Let A be the graph obtained from G and H by identifying u and a vertex $\tilde{u}$ of H (still denote the new vertex by u). Let A_{uv} be the graph obtained from G and H in the following way: delete uv, identify u and v, and denote the new vertex by w; add an edge wz and identifying z and $\tilde{u}$ (still denote the new vertex by z). We call the procedure from A to A_{uv} an α_1 transformation of A at uv if $|V(H)| = 1$ and the produce from A to A_{uv} an α_2 transformation of A at uv if $|V(H)| = 2$. Diagrams from A to A_{uv} are shown in Fig. 1 for a cut edge uv of G.

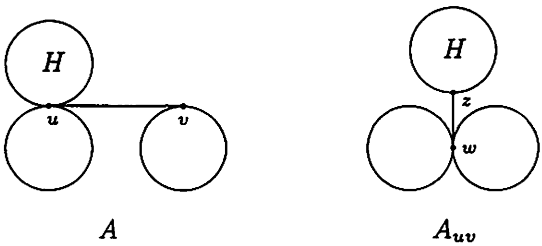


Fig. 1 Diagrams for a cut edge uv from A to A_{uv}

Remark 2.2. Let $M(B)$ be a maximum matching of a graph B and let $\eta(B)$ be the matching number of B. By the definitions of A and A_{uv}, it is not difficult to see the following facts.

(1) If $|V(H)| = 1$, namely $H \cong P_1$, then $\eta(A) = \eta(A_{uv})$ when $uv \in M(A)$ or one of u and v is not saturated by $M(A)$.

(2) If $|V(H)| = 2$, namely $H \cong P_2$, then $\eta(A) \leq \eta(A_{uv}) \leq \eta(A)+1$. In particular, $\eta(A) = \eta(A_{uv})$ when v is saturated by $M(A)$.

Let G be a connected graph and let uv be a nonpendent edge of G such that it is not contained in triangles. For convenience, we define some fixed notations as follows:

$V_u = \{x : x \in V(G)$ and uv is not in each shortest path from u to $x\}$.

$V_v = \{x : x \in V(G)$ and uv is in some shortest path from u to $x\}$.

$N(a, V_v) = \{y : y \in V_v - \{v\}$ and uv is in some shortest path from a to $y\}$, where $a \in V_u$.

$N(V_u, b) = \{x : x \in V_u - \{u\}$ and uv is in some shortest path from b to $x\}$, where $b \in V_v$.

$\Omega(u, v) = \{(x, y) : x \in V_u - \{u\}, y \in V_v - \{v\}$ and uv is in some shortest path from x to $y\}$.

$\Theta(u, v) = \{x : x \in V(G),\ d_G(x, u) = d_G(x, v)\}$.

Lemma 2.3. *Let A and A_{uv} be the two graphs presented in Definition 2.1. Then*

(1) $d_A(a, b) = d_{A_{uv}}(a, b)$ *if $a \neq b$ and $a, b \in V_u$ or $a, b \in V_v$.*

(2) $d_A(a, b) = d_{A_{uv}}(a, b)$ *If $a \neq b$ and $a, b \in V(H)$.*

(3) $V_u - (N(V_u, v) \bigcup \{u\}) = \Theta(u, v)$.

Proof. **(1)** We only prove the case of $a, b \in V_u$. Assume, for a contradiction, that the result does not hold. Then

$$J = \{(x, y) : x, y \in V_u, x \neq y \text{ and } d_A(x, y) \neq d_{A_{uv}}(x, y)\} \neq \emptyset.$$

Assume that $(a, b) \in J$ such that $d_A(a, b) = \min\{d_A(x, y) : (x, y) \in J\}$. Then by the definition of A_{uv} we have that $d_A(a, b) = d_{A_{uv}}(a, b) + 1$. This indicates that there is a shortest path containing uv from a to b in A. Denote such a shortest path by

$$P_{a,b} = a_0 a_1 a_2 \cdots a_r,$$

where $a_0 = a$, $a_r = b$ and $r \geq 2$. From the assumption of (a, b) we have $a_1, a_{r-1} \in V_v$. Since $P_{a,b}$ contains uv, assume, without loss of generality, that $u = a_i$ and $v = a_{i+1}$. Then $a_i a_{i+1} \cdots a_{r-1} a_r$ is a shortest path containing uv from $u = a_i$ to $b = a_r$. So by the definition of V_v we get that $b \in V_v$, a contradiction to the choice of $b \in V_u$.

(2) By the definitions of A and A_{uv} it is obvious that the result holds.

(3) Assume that $x \in \Theta(u, v)$, namely $d_G(x, u) = d_G(x, v)$. It is easy to see that all shortest paths in A from x to u and from x to v do not contain the edge uv. Hence $x \in V_u$ and $x \notin N(V_u, v) \bigcup \{u\}$. It follows that $x \in V_u - (N(V_u, v) \bigcup \{u\})$. So we get

$$\Theta(u, v) \subseteq V_u - (N(V_u, v) \bigcup \{u\}). \tag{2.1}$$

Next assume that $x \in V_u - (N(V_u, v) \bigcup \{u\})$. Denote the length of a path P by $l(P)$. Let P and $\tilde{P}$ be two shortest paths in A from u to x and from v to x, respectively. Then $u\tilde{P}$ is a path in A from u to x. Since $u\tilde{P}$ contains uv, by the definition of V_u and $x \in V_u$ we see that $u\tilde{P}$ is not a shortest path in A from u to x. Thus, $l(P) < l(u\tilde{P})$, namely $l(P) \leq l(\tilde{P})$. Analogously, since vP is a path in A from v to x and contains uv, by the definition of $N(V_u, v)$ and $x \notin N(V_u, v)$ we also see that vP is not a shortest path in A from v to x. It follows that $l(\tilde{P}) < l(vP)$, namely $l(\tilde{P}) \leq l(P)$. Therefore, $d_G(x, u) = l(P) = l(\tilde{P}) = d_G(x, v)$. This indicates that $x \in \Theta(u, v)$. So

$$V_u - (N(V_u, v) \bigcup \{u\}) \subseteq \Theta(u, v). \tag{2.2}$$

By Eqs. (2.1) and (2.2) we complete the proof of (3). □

Theorem 2.4. *Let A and A_{uv} be the two graphs presented in Definition 2.1. Then*

$$W(A) - W(A_{uv}) = |\Omega(u, v)| - |\Theta(u, v)| - (|V(H)| - 1)(|V_u| - 1). \tag{2.3}$$

Proof. It is obvious that $u \in V_u$ and $v \in V_v$. Set

$$g(a, b, x, y) = d_A(a, b) - d_{A_{uv}}(x, y), \quad f(a, b) = W(A, a) - W(A_{uv}, b).$$

By Lemma 2.3 (1)-(2) we have

$$g(x, y, x, y) = 0, \quad x, y \in V_u. \tag{2.4}$$

$$g(x, y, x, y) = 0, \quad x, y \in V(H). \tag{2.5}$$

$$g(x, y, x, y) = 0, \quad x, y \in V_v. \tag{2.6}$$

For $a \in V_u - \{u\}$, $x \in N(a, V_v) - \{v\}$, $y \in V_v - (N(a, V_v) \bigcup \{v\})$, by the definition of $N(a, V_v)$ it follows that $d_A(a, x) = d_{A_{uv}}(a, x) + 1$, $d_A(a, y) = d_{A_{uv}}(a, y)$. So we have

$$g(a, x, a, x) = 1, \quad a \in V_u - \{u\}, \quad x \in N(a, V_v) - \{v\}. \tag{2.7}$$

$$g(a, x, a, x) = 0, \quad a \in V_u - \{u\}, \quad x \in V_v - (N(a, V_v) \bigcup \{v\}). \tag{2.8}$$

In a similar way to obtain Eqs. (2.7) and (2.8) we also get

$$g(b, x, b, x) = 1, \quad b \in V_v - \{v\}, \quad x \in N(V_u, b) - \{u\}. \tag{2.9}$$

$$g(b, x, b, x) = 0, \quad b \in V_v - \{v\}, \quad x \in V_u - (N(V_u, b) \bigcup \{u\}). \tag{2.10}$$

For arbitrary $a \in V(H)$ and $x \in V_v$, it is easy to see that there must exist a shortest path containing uv in A from a to x. So we get

$$g(a, x, a, x) = 0, \quad a \in V(H) - \{u\}, \quad x \in V_v - \{v\}. \tag{2.11}$$

Also it is easy to see that

$$g(u,x,w,x)=0, \qquad x\in V_u-\{u\}. \tag{2.12}$$

$$g(u,x,w,x)=1, \qquad x\in V_v-\{v\}. \tag{2.13}$$

$$g(u,x,w,x)=-1, \quad x\in V(H)-\{u\}. \tag{2.14}$$

$$g(v,x,z,x)=-1, \quad x\in V_v-\{v\}. \tag{2.15}$$

$$g(v,x,z,x)=0, \qquad x\in N(V_u,v). \tag{2.16}$$

$$g(v,x,z,x)=1, \qquad x\in V(H)-\{u\}. \tag{2.17}$$

$$g(a,x,a,x)=-1, \quad a\in V_u-\{u\},\ \ x\in V(H)-\{u\}. \tag{2.18}$$

For arbitrary $a\in V_u$, $b\in V_v$ and $q\in V(A)-\{u,v\}$, we also have

$$V_u-\{u\}=N(V_u,b)\bigcup[V_u-(N(V_u,b)\bigcup\{u\})], \tag{2.19}$$

$$V_v-\{v\}=N(a,V_v)\bigcup[V_v-(N(a,V_v)\bigcup\{v\})], \tag{2.20}$$

$$f(q,q)=\sum_{x\in V_u-\{u\}} g(q,x,q,x)+\sum_{x\in V_v-\{v\}} g(q,x,q,x)$$

$$+\sum_{x\in V(H)-\{u\}} g(q,x,q,x)+g(q,u,q,w)+g(q,v,q,z). \tag{2.21}$$

Now let $a\in V_u-\{u\}$, $b\in V_v-\{v\}$ and $c\in V(H)-\{u\}$. By applying Eqs. (2.21), (2.4), (2.20), (2.8), (2.18), (2.12) and (2.7), we get

$$f(a,a)=0+\sum_{x\in N(a,V_v)} g(a,x,a,x)+\sum_{x\in V(H)-\{u\}}(-1)+0+g(a,v,a,z)$$

$$=|N(a,V_v)|-(|V(H)|-1)+g(a,v,a,z). \tag{2.22}$$

By applying Eqs. (2.21), (2.19), (2.10), (2.6), (2.11), (2.13), (2.15) and (2.9), we get

$$f(b,b)=\sum_{x\in N(V_u,b)} g(b,x,b,x)+0+0+1+(-1)=|N(V_u,b)|. \tag{2.23}$$

By applying Eqs. (2.21), (2.18), (2.11), (2.5), (2.14) and (2.17), we get

$$f(c,c)=\sum_{x\in V_u-\{u\}}(-1)+0+0+(-1)+1=-(|V_u|-1). \tag{2.24}$$

By applying Eqs. (2.4), (2.13) and (2.14), we get

$$f(u,w) = \sum_{x\in V_u-\{u\}} g(u,x,w,x) + \sum_{x\in V_v-\{v\}} g(u,x,w,x)$$

$$+ \sum_{x\in V(H)-\{u\}} g(u,x,w,x) + g(u,v,w,z)$$

$$= 0 + (|V_v|-1) - (|V(H)|-1) + 0 = |V_v| - |V(H)|. \qquad (2.25)$$

By applying Eqs. (2.19), (2.16), (2.15) and (2.17), we get

$$f(v,z) = \sum_{x\in V_u-\{u\}} g(v,x,z,x) + \sum_{x\in V_v-\{v\}} g(v,x,z,x)$$

$$+ \sum_{x\in V(H)-\{u\}} g(v,x,z,x) + g(v,u,z,w)$$

$$= \sum_{x\in V_u-(N(V_u,v)\bigcup\{u\})} g(v,x,z,x) + \sum_{x\in V_v-\{v\}} (-1) + \sum_{x\in V(H)-\{u\}} 1+0$$

$$= -|V_u - (N(V_u,v)\bigcup\{u\})| - (|V_v|-1) + (|V(H)|-1). \qquad (2.26)$$

Therefore, from Eqs. (2.22)-(2.26) we get

$$2[W(A) - W(A_{uv})] = \sum_{a\in V_u-\{u\}} f(a,a) + f(u,w) + f(v,z)$$

$$+ \sum_{b\in V_v-\{v\}} f(b,b) + \sum_{c\in V(H)-\{u\}} f(c,c)$$

$$= \sum_{a\in V_u-\{u\}} [|N(a,V_v)| + g(a,v,a,z)] + \sum_{b\in V_v-\{v\}} |N(V_u,b)|$$

$$-2(|V_u|-1)(|V(H)|-1) - |V_u - (N(V_u,v)\bigcup\{u\})|.$$

Note that

$$\bigcup_{a\in V_u-\{u\}} \{(a,y) : y\in N(a,V_v)\} = \Omega(u,v) = \bigcup_{b\in V_u-\{v\}} \{(x,b) : x\in N(V_u,b)\},$$

$$\sum_{a\in V_u-\{u\}} g(a,v,a,z) = \sum_{x\in V_u-(N(V_u,v)\bigcup\{u\})} g(a,v,a,z)$$

$$= -|V_u - (N(V_u,v)\bigcup\{u\})|.$$

So we get

$$W(A)-W(A_{uv}) = |\Omega(u,v)|-|V_u-(N(V_u,v)\bigcup\{u\})|-(|V(H)|-1)(|V_u|-1).$$

Therefore, by combining Lemma 2.3 (3) we arrive at Eq. (2.3). □

Corollary 2.5. *Let A and A_{uv} be the two graphs given in Definition 2.1 in which uv is a nonpendent cut edge of G.*

(1) *If $|V(H)| = 1$, then we have that $W(A_{uv}) < W(A)$.*

(2) *If $|V(H)| = 2$, $deg_A(u) \geq 3$ and $deg_A(v) \geq 3$, then we have that $W(A_{uv}) < W(A)$.*

Proof. Now $\Theta(u,v) = \emptyset$. Let G_u and G_v be the two components of $G-uv$ containing u and v, respectively. Then

$$V_u = V(G_u), \quad V_v = V(G_v).$$

$$\Omega(u,v) = \{(x,y) : x \in V_u - \{u\}, \ y \in V_v - \{v\}\}.$$

(1) Since uv is a nonpendent edge of G, we have $|V_u| \geq 2$ and $|V_v| \geq 2$. Therefore, $\Omega(u,v) \neq \emptyset$. From Eq. (2.3) it follows that

$$W(A_{uv}) = W(A) - |\Omega(u,v)| < W(A).$$

(2) Since $deg_A(u) \geq 3$ and $deg_A(v) \geq 3$, we have $|V_u| \geq 2$ and $|V_v| \geq 3$. Hence

$$|\Omega(u,v)| = (|V_u|-1)(|V_v|-1) \geq 2(|V_u|-1).$$

From Eq. (2.3) it follows that

$$W(A_{uv}) = W(A) - |\Omega(u,v)| + (|V_u|-1) \leq W(A) - (|V_u|-1) < W(A).$$

This proof is complete. □

Corollary 2.6. *Let G be a cactus and let $C = b_1b_2\cdots b_kb_1$ be a cycle of G with $k \geq 6$. Let C^i be the component containing the vertex b_i in $G-E(C)$ $(i = 1,2,\cdots,k)$. Assume that A and $A_{b_1b_2}$ are the two graphs presented in Definition 2.1.*

(1) *Assume that k is an even number. If $|V(H)| = 1$, or $|V(H)| = 2$ and $deg_G(b_2) \geq 3$, then we have $W(A_{b_1b_2}) < W(A)$.*

(2) *Assume that k is an odd number. If $|V(H)| = 1$ and $|V(C^1)| + |V(C^2)| \geq \frac{|V(C^{\lfloor \frac{k}{2} \rfloor+2})|+3}{2}$, then we have $W(A_{b_1b_2}) \leq W(A)$.*

Proof. Write $l = \lfloor \frac{k}{2} \rfloor$. By the structure of C and $k \geq 6$, it follows that $\Theta(b_1,b_2) = \emptyset$ if k is an even number, $\Theta(b_1,b_2) = V(C^{l+2})$ if k is an odd number, and

$$V_{b_1} = V(C^1)\bigcup(\bigcup_{i=l+2}^{k} V(C^i)), \quad V_{b_2} = \bigcup_{i=2}^{l+1} V(C^i).$$

Therefore, again by the structure of C and $k \geq 6$ we get

$$\Omega(b_1, b_2) \supseteq \{(x, y) : x \in V_{b_1} - (\{b_1\} \bigcup \Theta(b_1, b_2)),\ y \in V(C^2) - \{b_2\}\}$$
$$\bigcup \{(x, y) : x \in V(C^1) - \{b_1\},\ y \in V(C^3) \bigcup V(C^4)\}$$
$$\bigcup \{(x, y) : x \in V(C^k),\ y \in V(C^3)\}.$$

So we deduce

$$|\Omega(b_1, b_2)| \geq (|V_{b_1}| - |\Theta(b_1, b_2)| - 1)(|V(C^2)| - 1) + 2|V(C^1)| - 1. \quad (2.27)$$

(1) At present $\Theta(b_1, b_2) = \emptyset$.

Assume that $|V(H)| = 1$. Note that $|\Omega(b_1, b_2)| \geq 2|V(C^1)| - 1 \geq 1$ by Eq. (2.27). So from Eq. (2.3) we immediately deduce $W(A_{b_1, b_2}) < W(A)$.

Next assume that $|V(H)| = 2$ and $deg_G(b_2) \geq 3$. It is obvious that

$$|V(C^2)| \geq (deg_G(b_2) - 2) + 1 \geq 2.$$

So by Eq. (2.27) we have

$$|\Omega(b_1, b_2)| \geq (|V_{b_1}| - 1) + 2|V(C^1)| - 1 \geq |V_{b_1}|.$$

Therefore, from Eq. (2.3) we deduce

$$W(A_{b_1 b_2}) = W(A) - |\Omega(b_1, b_2)| + (|V_{b_1}| - 1) < W(A).$$

(2) At present $\Theta(b_1, b_2) = V(C^{l+2})$. Note that

$$|V_{b_1}| \geq |V(C^1)| + |V(C^k)| + |V(C^{k-1})| + |V(C^{l+2})| \geq |\Theta(b_1, b_2)| + 3,$$

so from $|V(C^1)| + |V(C^2)| \geq \frac{1}{2}[|V(C^{l+2})| + 3]$ and Eq. (2.27) we deduce

$$|\Omega(b_1, b_2)| \geq 2(|V(C^2)| - 1) + 2|V(C^1)| - 1 \geq |\Theta(b_1, b_2)|.$$

Hence by Eq. (2.3) we get

$$W(A_{b_1 b_2}) = W(A) - |\Omega(b_1, b_2)| + |\Theta(b_1, b_2)| \leq W(A). \quad \square$$

Lemma 2.7 [5,6]. *Let G be a connected graph with a cut-vertex u and let G_1 and G_2 be two connected subgraphs of G with $V(G_1) \bigcap V(G_2) = \{u\}$, $G_1 \bigcup G_2 = G$, $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$. Then*

$$W(G) = W(G_1) + W(G_2) + (n_1 - 1)W(G_2, u) + (n_2 - 1)W(G_1, u).$$

Theorem 2.8. *Let G be a connected graph and let u and v be two distinct vertices of G in which u is a cut-vertex of G. Assume that G_1 and G_2 are* *two non-trivial connected subgraphs of* G *such that* $V(G_1)\bigcap V(G_2)=\{u\}$, $G_1\bigcup G_2=G$ *and* $v\in V(G_2)$. *Write*

$$n_1=|V(G_1)|,\quad N_{G_1}(u)=\{u_1,u_2,\cdots,u_s\},$$

$$G'=G-\{uu_1,uu_2,\cdots,uu_s\}+\{vu_1,vu_2,\cdots,vu_s\}.$$

Then

$$W(G)-W(G')=(n_1-1)\{[W(G,u)-W(G,v)]+(n_1-1)d_G(u,v)\}. \quad (2.28)$$

In particular, if $W(G,u)\geq W(G,v)$, *then* $W(G)>W(G')$.

Proof. Denote the vertex u of G_1 by w. By Lemma 2.6 we get

$$W(G)=W(G_1)+W(G_2)+(|V(G_2)|-1)W(G_1,w)+(n_1-1)W(G_2,u).$$

$$W(G')=W(G_1)+W(G_2)+(|V(G_2)|-1)W(G_1,w)+(n_1-1)W(G_2,v).$$

Therefore, we have

$$W(G)-W(G')=(n_1-1)[W(G_2,u)-W(G_2,v)]. \quad (2.29)$$

It is easy to see that

$$W(G,u)=\sum_{a\in V(G_1)}d_G(a,u)+\sum_{b\in V(G_2)}d_G(b,u)=W(G_1,u)+W(G_2,u).$$

$$\begin{aligned}W(G,v)&=\sum_{a\in V(G_1)-\{u\}}d_G(a,v)+\sum_{b\in V(G_2)}d_G(b,v)\\&=W(G_1,u)+(n_1-1)d_{G_2}(u,v)+W(G_2,v).\end{aligned}$$

So it follows that

$$W(G,u)-W(G,v)=[W(G_2,u)-W(G_2,v)]-(n_1-1)d_{G_2}(u,v). \quad (2.30)$$

Since $d_{G_2}(u,v)=d_G(u,v)$, by Eqs. (2.29) and (2.30) we get Eq. (2.28). It is obvious that the additional assertion holds from Eq. (2.28). □

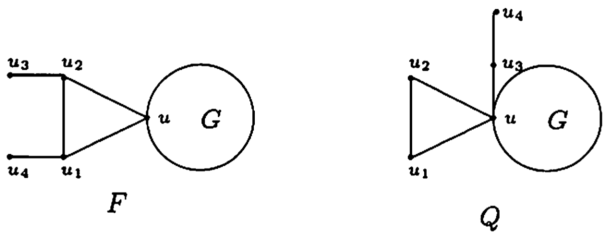


Fig. 2 Diagrams from F to Q

Theorem 2.9. *Let G be a connected graph with at least two vertices, including a vertex u, and let F, Q be the two graphs shown in Fig. 2. Then*

$$W(F) - W(Q) = |V(G)| - 2. \tag{2.31}$$

In particular, if $|V(G)| \geq 3$, then $W(Q) < W(F)$.

Proof. Write $U = \{u, u_1, u_2, u_3, u_4\}$. Let H and N be the vertex-induced subgraphs of U in F and Q, respectively. It is easy to see that

$$W(H) = 16, \quad W(H, u) = 6, \quad W(N) = 17, \quad W(N, u) = 5.$$

By Lemma 2.7 we have

$$\begin{aligned} W(F) &= W(H) + W(G) + (|V(H)| - 1)W(G, u) + (|V(G)| - 1)W(H, u) \\ &= 16 + W(G) + 4W(G, u) + 6(|V(G)| - 1). \\ W(Q) &= W(N) + W(G) + (|V(N)| - 1)W(G, u) + (|V(G)| - 1)W(N, u) \\ &= 17 + W(G) + 4W(G, u) + 5(|V(G)| - 1). \end{aligned}$$

Therefore, we easily get Eq. (2.31). If $|V(G)| \geq 3$, then from Eq. (2.31) we immediately deduce $W(Q) < W(F)$. □

3. On the minimal Wiener index of cacti

In this section we use the transformations given in Section 2 to determine the graphs having the smallest Wiener index in some types of cacti (see Theorem 3.8, Corollaries 3.10 and 3.11), which have not been studied before.

Let G be a connected graph. For two vertex-disjoint connected subgraphs G_1 and G_2 of G, we call $\min\{d_G(a, b) : a \in V(G_1), b \in V(G_2)\}$ the distance of G_1 and G_2. Let $P = u_0u_1u_2 \cdots u_k$ be a path of G with distinct vertices $u_0, u_1, \cdots, u_k$. If

$$deg_G(u_0) \geq 3, deg_G(u_1) = \cdots = deg_G(u_{k-1}) = 2, deg_G(u_k) = 1,$$

then we call P a *pendent path* of length k at u_0 in G.

A cactus with at least two cycles is called a *bundle* if all of its cycles have exactly one common vertex, which is called the *center* of the bundle. Let G be a cactus. The *base* of G, denoted by $\hat{G}$, is such a unique connected subgraph of G that it has the same cycles as G and has not pendent edges. A vertex v of $\hat{G}$ is called a *branch vertex* of $\hat{G}$ if $deg_{\hat{G}}(v) \geq 3$.

Let $C(n, m, r)$ be the set of all cacti with order n, matching number m and cycle number r. Assume that Z is a cactus having the smallest Wiener index in $C(n, m, r)$. We assume that $n \geq 10$, $m \geq 3$ and also assume that

$r \geq 2$ (otherwise, Z is a tree or unicyclic graph and Z has been determined in [15,18]). Let $M(Z)$ be a maximum matching of Z containing pendent edges as most as possible. For a cycle $C = b_1 b_2 \cdots b_k b_1$ of Z, from now we always denote the component containing the vertex b_i in $Z - E(C)$ by C^i $(i = 1, 2, \cdots, k)$. In the next few lemmas we investigate the structural properties of Z.

Lemma 3.1. *Each vertex of Z not in $\hat{Z}$ is on some pendent path of length at most* 2.

Proof. In order to prove the result, we only need to show the two following claims.

Claim 1. Each pendent path of Z has length at most 2.

Suppose, for a contradiction, that there exists a pendent path $v_0 v_1 \cdots v_k$ of Z at v_0 with length $k \geq 3$. Then $e = v_{k-3}v_{k-2}$ is a nonpendent cut edge of Z. By an α_1 transformation of Z at e, we obtain a cactus Z_e with n vertices and r cycles. From the assumption of $M(Z)$, it is easy to see that $e \in M(Z)$ or v_{k-2} is not saturated by $M(Z)$. So by Remark 2.2 (1) we have $\eta(Z_e) = \eta(Z)$. Therefore, $Z_e \in C(n, m, r)$. But by Corollary 2.5 (1) we have $W(Z_e) < W(Z)$, a contradiction to the choice of Z.

Claim 2. Each vertex of Z not in $\hat{Z}$ is on some pendent path.

Suppose, for a contradiction, that there are vertices of Z not in $\hat{Z}$ with degree at least 3. Let u be such a vertex with the largest distance from $\hat{Z}$ and let $uvv' \cdots$ be the unique shortest path from u to $\hat{Z}$. By Claim 1 we know that all other vertices adjacent to u except v are on pendent paths of lengths at most 2.

Case 1 Suppose that Z has a pendent edge $H = uu'$ at u.

First assume that $deg_Z(v) \geq 3$. By an α_2 transformation of Z at uv, we obtain a cactus Z_{uv} with n vertices and r cycles. By Remark 2.2 (2) we have $\eta(Z_{uv}) = m, m + 1$.

If $\eta(Z_{uv}) = m$, then $Z_{uv} \in C(n, m, r)$, and from Corollary 2.5 (2) it follows that $W(Z_{uv}) < W(Z)$, a contradiction to the choice of Z.

If $\eta(Z_{uv}) = m + 1$, then by an α_1 transformation of Z_{uv} at wz, we can get a cactus $N \in C(n, m, r)$. But by Corollary 2.5 we have that $W(N) < W(Z_{uv}) < W(Z)$, a contradiction to the choice of Z.

Next assume that $deg_Z(v) = 2$. From $deg_Z(v) = 2$ we know that vv' is a cut edge of Z not in $\hat{Z}$. By an α_1 transformation of Z at vv', we get a cactus $Z_{vv'}$ with n vertices and r cycles. By the assumption of $M(Z)$ we may assume that $uu' \in M(Z)$. Then $vv' \in M(Z)$ or v is not saturated by $M(Z)$. It follows that $\eta(Z_{vv'}) = \eta(Z)$ by Remark 2.2 (1). Therefore, $Z_{vv'} \in C(n, m, r)$. But by Corollary 2.5 (1) we have $W(Z_{vv'}) < W(Z)$, a contradiction to the choice of Z.

Case 2 Suppose that Z has not pendent edges at u.

From the assumption of u we see that uv is a cut edge of Z not in $\hat{Z}$. By an α_1 transformation of Z at uv, we get a cactus Z_{uv} with n vertices and r

cycles. From the assumption of $M(Z)$ we also see that $uv \in M(Z)$ or u is not saturated by $M(Z)$. It follows that $\eta(Z_{uv}) = \eta(Z)$ from Remark 2.2 (1). Thus, $Z_{uv} \in C(n,m,r)$. But by Corollary 2.5 (1) we have $W(Z_{uv}) < W(Z)$, a contradiction to the choice of Z. □

For each $v \in V(\hat{Z})$, let $\psi(v)$ and $\phi(v)$ be the numbers of pendent edges and pendent paths of length 2 at v in Z, respectively.

Lemma 3.2. **(1)** *There exists at most a vertex u of $\hat{Z}$ such that $\phi(u) \neq 0$ or $\psi(u) \geq 2$.*

(2) *The vertex u with $\phi(u) \neq 0$ or $\psi(u) \geq 2$ is a branch vertex of $\hat{Z}$.*

Proof. **(1)** Suppose, for a contradiction, that there exist two distinct vertices u and v of $\hat{Z}$ with $\phi(u) \neq 0$ or $\psi(u) \geq 2$ and $\phi(v) \neq 0$ or $\psi(v) \geq 2$. Also assume, without loss of generality, that $W(Z,u) \geq W(Z,v)$.

First assume that $\phi(u) \neq 0$. Let $uu'u''$ be a pendent path of length 2 at u and put $Z' = Z - uu' + vu'$. Then $Z' \in C(n,m,r)$ and by Theorem 2.8 we have $W(Z') < W(Z)$, a contradiction to the choice of Z.

Next assume that $\psi(u) \geq 2$. Let $uu_1, uu_2, \cdots, uu_{\psi(u)}$ be all pendent edges at u. If v is saturated by $M(Z)$, then write $Z' = Z - uu_1 + vu_1$, otherwise set

$$Z' = Z - \{uu_1, uu_2, \cdots, uu_{\psi(u)}\} + \{vu_1, vu_2, \cdots, vu_{\psi(u)}\}.$$

Then $Z' \in C(n,m,r)$ and by Theorem 2.8 we have that $W(Z') < W(Z)$, a contradiction to the choice of Z.

(2) Suppose, for a contradiction, that the vertex u with $\phi(u) \neq 0$ or $\psi(u) \geq 2$ is not a branch vertex of $\hat{Z}$. From $r \geq 2$ and the assumption above we see that there is a cycle not containing u. Let C be a cycle not containing u and having the largest distance from u. Denote a shortest path connecting u and C by $uxy \cdots v$, where $v \in V(C)$. Write $C = b_1 b_2 \cdots b_k b_1$ in which $b_1 = v$. From $u \in V(\hat{Z})$ and $r \geq 2$ we deduce $|V(C^1)| \geq 5$. By the assumption of C it is not difficult to see that all of $b_2, b_3, \cdots, b_k$ are not branch vertices of $\hat{Z}$. So by the result of (1) we have $|V(C^i)| \leq 2$ for $i = 2, 3, \cdots, k$.

If $W(Z,u) \geq W(Z,v)$, then in a similar way to prove (1) we can get contradictions.

Next assume that $W(Z,v) > W(Z,u)$. If $vb_2, vb_k \notin M(Z)$, then set

$$G' = Z - \{vb_2, vb_k\} + \{ub_2, ub_k\}.$$

Clearly $Z' \in C(n,m,r)$ and by Theorem 2.8 we have that $W(Z') < W(Z)$, a contradiction to the choice of Z. Hence now assume, without loss of generality, that $vb_2 \in M(Z)$. Then by the assumption of $M(Z)$ and $vb_2 \in M(Z)$ it follows that there are not pendent edges at v and b_2.

Let $k \geq 4$. By an α_1 transformation of Z at vb_2, we get a cactus Z_{vb_2} with n vertices and r cycles. Since $vb_2 \in M(Z)$, from Remark 2.2 (1) it follows that $\eta(Z_{vb_2}) = \eta(Z)$. So $Z_{vb_2} \in C(n, m, r)$. It is easy to see that

$$|\Omega(v, b_2)| \geq |\{(x, y) : x \in V(C^1) - \{v\}, y \in V(C^3)\}| \geq 4.$$

On the other hand, $\Theta(v, b_2) = V(C^{l+2})$ if $k = 2l + 1$ is an odd number and $\Theta(v, b_2) = \emptyset$ if k is an even number. So by Theorem 2.4 we have

$$W(Z_{vb_2}) = W(Z) - |\Omega(v, b_2)| + |\Theta(v, b_2)| < W(Z),$$

a contradiction to the choice of Z.

Let $k = 3$. If b_3 has not pendent edges, set $M' = M(Z) - \{vb_2\} + \{b_2b_3\}$, then M' is a maximum matching of Z containing the same pendent edges as $M(Z)$ and $vb_2, vb_k \notin M'$. This becomes a case proved above. Now assume that b_3 has a pendent edge b_3b'. Write $Z' = Z - b_3b' + vb'$. Form the assumption of $M(Z)$ we deduce $b_3b' \in M(Z)$. Therefore, $M' = M(Z) - \{vb_2, b_3b'\} + \{b_2b_3, vb'\}$ is a matching of Z' with $|M'| = m$. It follows that $Z' \in C(n, m, r)$. It is easy to see that

$$W(Z, b_3) = 2 + |V(C^1)| + W(C^1, v), \quad W(Z, v) = 4 + W(C^1, v).$$

It is obvious that $W(Z, b_3) > W(Z, v)$. So by Theorem 2.8 we have that $W(Z') < W(Z)$, a contradiction to the choice of Z. □

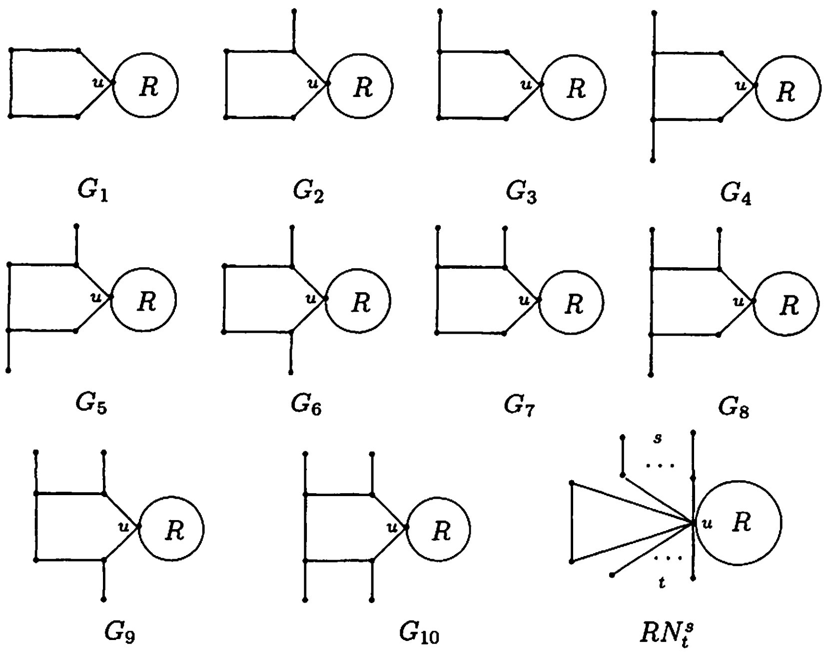


Fig. 3 Diagrams in Lemma 3.3

Lemma 3.3. *Let G_i and RN_t^s be the graphs shown in Fig. 3 in which R is a connected graph (including the vertex u) and each G_i has at least* 10 *vertices ($i = 1, 2, \cdots, 10$). Then*

$$W(G_1) > W(RN_0^1); \quad W(G_{10}) > W(RN_0^3);$$

$$W(G_i) > W(RN_1^1), \ i = 2, 3;$$

$$W(G_i) > W(RN_2^1), \ i = 4, 5;$$

$$W(G_i) > W(RN_2^1) \ \text{or} \ W(G_i) > W(RN_0^2), \ i = 6, 7;$$

$$W(G_i) > W(RN_1^2), \ i = 8, 9.$$

Proof. Put $W(R, u) = \mu$, $|V(R)| = \nu$ and $k = 2s + t$. Applying Lemma 2.6, by direct calculations we get

$$W(RN_t^s) = k(k + s + 4) + 3 + W(R) + (k + 2)\mu + (k + s + 2)(\nu - 1).$$

$$W(G_1) = 9 + W(R) + 4\mu + 6\nu, \qquad W(G_2) = 18 + W(R) + 5\mu + 8\nu,$$

$$W(G_3) = 17 + W(R) + 5\mu + 9\nu, \qquad W(G_4) = 28 + W(R) + 6\mu + 12\nu,$$

$$W(G_5) = 30 + W(R) + 6\mu + 11\nu, \qquad W(G_6) = 31 + W(R) + 6\mu + 10\nu,$$

$$W(G_7) = 29 + W(R) + 6\mu + 11\nu, \qquad W(G_8) = 44 + W(R) + 7\mu + 14\nu,$$

$$W(G_9) = 46 + W(R) + 7\mu + 13\nu, \qquad W(G_{10}) = 64 + W(R) + 8\mu + 16\nu.$$

Therefore, the results easily follow. □

Lemma 3.4. *Let $C = b_1 b_2 \cdots b_k b_1$ be a cycle of Z such that $|V(C^1)| \geq 2$ and $|V(C^i)| \leq 2$ ($i = 2, 3, \cdots, k$). Then C is a triangle and there exists a maximum matching M' of Z such that $b_1 b_2, b_1 b_k \notin M'$.*

Proof. Suppose, for a contradiction, that $k \geq 4$. We distinguish two cases.

Case 1 Assume that k is an even number and set $k = 2l$.

Case 1.1 Assume that $l \geq 3$. If b_1 or b_2 are not saturated by $M(Z)$, then write $e = b_1 b_2$. If some edge of C belongs to $M(Z)$, then we also denote such an edge by e. By an α_1 transformation of Z at e we obtain a cactus Z_e with n vertices and r cycles, and by Remark 2.2 (1) we also have $\eta(Z_e) = \eta(Z)$. Hence, $Z_e \in C(n, m, r)$. But by Corollary 2.6 (1) we have $W(Z_e) < W(Z)$, a contradiction to the choice of Z. Therefore, now assume that both b_1 and b_2 are saturated by $M(Z)$ and all edges of C do not belong to $M(Z)$. At present by the assumptions of C we see that there exists a unique pendent edge at b_2. Taking $u = b_2$, $v = b_1$ and $H = C^2$ in Theorem 2.4, then by an α_2 transformation of Z at $b_2 b_1$ we obtain a cactus $Z_{b_2 b_1}$ with n vertices and r cycles. Since b_1 is saturated by $M(Z)$, by Remark 2.2 (2) it follows that $\eta(Z_{b_2 b_1}) = \eta(Z)$. Hence, $Z_{b_2 b_1} \in C(n, m, r)$. Note that $deg_Z(b_1) \geq 3$ from $|V(C^1)| \geq 2$, so by Corollary 2.6 (1) we have that $W(Z_{b_2b_1}) < W(Z)$, a contradiction to the choice of Z.

Case 1.2 Assume that $l = 2$. By $n \geq 10$, we get that $|V(C^1)| \geq 4$. By the symmetry of vertices b_2 and b_4, assume, without loss of generality, that $|V(C^2)| \geq |V(C^4)|$.

Assume that $b_1b_2 \in M(Z)$ or one of b_1 and b_2 is not saturated by $M(Z)$. By an α_1 transformation of Z at b_1b_2 we obtain a cactus $Z_{b_1b_2}$ with n vertices and r cycles. From Remark 2.2 (1) we see that $\eta(Z_{b_1b_2}) = \eta(Z)$. Thus, $Z_{b_1b_2} \in C(n, m, r)$. Note that

$$\Theta(b_1, b_2) = \emptyset, \;\; \Omega(b_1, b_2) \supseteq \{(x, y) : x \in V(C^1) - \{b_1\}, y \in V(C^3)\} \neq \emptyset,$$

so from Theorem 2.4 we deduce $W(Z_{b_1b_2}) = W(Z) - |\Omega(b_1, b_2)| < W(Z)$, a contradiction to the choice of Z. Analogously, if $b_1b_4 \in M(Z)$ or b_4 is not saturated by $M(Z)$, then we can also get a contradiction.

Next assume that $b_1b_2, b_1b_4 \notin M(Z)$ and all of b_1, b_2, b_4 are saturated by $M(Z)$. It is obvious that at most one of b_2b_3 and b_3b_4 belongs to $M(Z)$. So from $|V(C^2)| \geq |V(C^4)|$ we deduce $|V(C^2)| = 2$, i.e., there is a unique pendent edge at b_2. Taking $u = b_2$, $v = b_1$ and $H = C^2$ in Theorem 2.4, then by an α_2 transformation of Z at b_2b_1, we obtain a cactus $Z_{b_2b_1}$ with n vertices and r cycles. Since b_1 is saturated by $M(Z)$, by Remark 2.2 (2) we have $\eta(Z_{b_2b_1}) = \eta(Z)$. Therefore, $Z_{b_2b_1} \in C(n, m, r)$. From $|V(C^1)| \geq 3$ it follows that

$$|\Omega(b_2, b_1)| = |\{(x, y) : x \in V_{b_2} - \{b_2\}, y \in V(C^1) - \{b_1\}\}| \geq 2(|V_{b_2}| - 1).$$

Note that $|V_{b_2}| \geq |\{b_2\} \bigcup V(G^3)| \geq 2$ and $\Theta(b_2, b_1) = \emptyset$, so by Theorem 2.4 we deduce

$$W(Z_{b_2b_1}) = W(Z) - |\Omega(b_1, b_2)| + |V_{b_2}| - 1 \leq W(Z) - (|V_{b_2}| - 1) < W(Z),$$

a contradiction to the choice of Z.

Case 2 Assume that k is an odd number and set $k = 2l + 1$.

Case 2.1 Assume that $l \geq 3$. If $b_1b_2 \in M(Z)$ or one of b_1 and b_2 is not saturated by $M(Z)$, then by an α_1 transformation of Z at b_1b_2 we obtain a cactus $Z_{b_1b_2}$ with n vertices and r cycles. From Remark 2.2 (1) we have that $\eta(Z_{b_1b_2}) = \eta(Z)$. Therefore, $Z_{b_1b_2} \in C(n, m, r)$. Since

$$|V(C^1)| + |V(C^2)| \geq 3 > 2.5 \geq \frac{1}{2}[|V(G^{l+2})| + 3],$$

by Corollary 2.6 (2) we have $W(Z_{b_1b_2}) \leq W(Z)$. Note that $Z_{b_2b_3}$ is a cactus satisfying the conditions of Case 1.1, so we can get a contradiction by the result of Case 1.1. If $b_1b_k \in M(Z)$ or b_k is not saturated by $M(Z)$, then in a similar way above we can get a contradiction. Hence now assume that $b_1b_2, b_1b_k \notin M(Z)$ and all of b_1, b_2 and b_k are saturated by $M(Z)$.

Assume that b_2 has not pendent edges. Since b_2 is saturated by $M(Z)$, it follows that $b_2b_3 \in M(Z)$. By an α_1 transformation of Z at b_2b_3 we get a cactus $Z_{b_2b_3}$ with n vertices and r cycles. From Remark 2.2 (1) we have that $\eta(Z_{b_2b_3}) = \eta(Z)$. Therefore, $Z_{b_2b_3} \in C(n,m,r)$. It is easy to see that

$$\Theta(b_2,b_3) = C^{l+3}, \quad \Omega(b_2,b_3) \supseteq \{(x,y) : x \in V(C^1),\ y \in V(C^4)\}.$$

Hence by $|V(C^1)| \geq 2 \geq |V(C^{l+3})|$, we get that $|\Omega(b_2,b_3)| \geq |\Theta(b_2,b_3|$. So from Theorem 2.4 we deduce $W(Z_{b_2b_3}) \leq W(Z)$. Note that $Z_{b_2b_3}$ is a cactus satisfying the conditions of Case 1.1, so we can get a contradiction by the result of Case 1.1. Therefore, now assume that b_2 has a pendent edge b_2b_2'. In a similar way above we can prove both b_3 and b_k have a pendent edge. Taking $u = b_2$, $v = b_1$ and $H = C^2$ in Theorem 2.4, then by an α_2 transform of Z at b_2b_1 we get a cactus $Z_{b_2b_1}$ with n vertices and r cycles. From Remark 2.2 (2) we get $\eta(Z_{b_2b_1}) = \eta(Z)$. Thus, $Z_{b_2b_1} \in C(n,m,r)$. Since $\Theta(b_2,b_1) = C^{l+2}$ and

$$\Omega(b_2,b_1) \supseteq \{(x,y) : x \in V_{b_2} - (\{b_2\} \bigcup \Theta(b_2,b_1)),\ y \in V(C^1) - \{b_1\}\}$$

$$\bigcup \{(x,y) : x \in V(C^3),\ y \in V(C^k)\},$$

it follows that

$$|\Omega(b_2,b_1)| \geq (|V_{b_2}| - |\Theta(b_2,b_1)| - 1)(|V(C^1)| - 1) + |V(C^3)| \cdot |V(C^k)|$$

$$\geq (|V_{b_2}| - |V(C^{l+2})| - 1) + 4.$$

Therefore, by Theorem 2.4 we get

$$W(Z_{b_2b_1}) \leq W(Z) + 2(|V(C^{l+2})| - 2) \leq W(Z).$$

Note that $Z_{b_2b_1}$ is a cactus satisfying the conditions of Case 1.1, so we can get a contradiction by the result of Case 1.1.

Case 2.2 Assume that $l = 2$. For $j = 2,3,4,5$, since $|V(C^j)| \leq 2$, there is an integer i $(i = 1,2,\cdots,10)$ such that $Z \cong G_i$ in which $R = C^1$. It is easy to see that $\eta(G_6) = \eta(G_7) = \eta(RN_0^2)$ if u is saturated by $M(Z)$, otherwise $\eta(G_6) = \eta(G_7) = \eta(RN_2^1)$. In addition, we have that

$$\eta(G_1) = \eta(RN_0^1),\ \eta(G_2) = \eta(G_3) = \eta(RN_1^1),\ \eta(G_4) = \eta(G_5) = \eta(RN_2^1),$$

$$\eta(G_8) = \eta(G_9) = \eta(RN_1^2),\ \eta(G_{10}) = \eta(RN_0^3).$$

These indicate that there exist two nonnegative integers s, t such that $RN_t^s \in C(n,m,r)$, and by Lemma 3.3 we have $W(Z) > W(RN_t^s)$, a contradiction to the choice of Z.

From the discussions above we get $k = 3$. Assume, without loss of generality, that $b_1b_2 \in M(Z)$. Then by the assumption of $M(Z)$ it follows that there are not pendent edges at b_2. In a similar way to prove the case on $k = 3$ in Lemma 3.2 (2), we see that b_3 has not pendent edges. Hence $M' = M(Z) - \{b_1b_2\} + \{b_2b_3\}$ is a maximum matching of Z that does not contain b_1b_2 and b_1b_3. □

Lemma 3.5. *Z is a bundle and each cycle of Z is a triangle.*

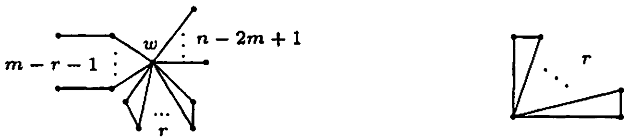
Proof. Assume that Z is not a bundle. Then there exist two cycles of Z that have not common vertices. Let C and $\tilde{C}$ be such two cycles of Z that they have the largest distance among all pairs of cycles without common vertices. Denote a shortest path connecting C and $\tilde{C}$ by $P = ux\cdots v$, where $u \in V(C)$ and $v \in V(\tilde{C})$. Assume, without loss of generality, that $W(Z,u) \geq W(Z,v)$. Let ub and ub' be the two edges incident to u in C. It is obvious that u is a branch vertex of $\hat{Z}$. By Lemmas 3.1 and 3.2 we see that C satisfies the conditions of Lemma 3.4. So C is a triangle and there is a maximum matching M' of Z such that $ub, ub' \notin M'$. Let

$$Z' = Z - \{ub, ub'\} + \{vb, vb'\}.$$

Then $Z' \in C(n,m,r)$ and by Theorem 2.8 we have $W(Z') < W(Z)$, a contradiction to the choice of Z. Therefore, Z is a bundle.

Let w be the center of Z. Since $r \geq 2$, it follows that $deg_Z(w) \geq 4$. By Lemmas 3.1 and 3.2 we see that each cycle C of Z satisfies the conditions of Lemma 3.4. Hence C is a triangle. □

Lemma 3.6 [27]. *If $m \leq r$ and $G \in C(n,m,r)$, then $m = r$, $n = 2r+1$, each cycle of G is a triangle and each edge of G is contained in some triangle.*



$C_{n,m,r}$ D_r

Fig. 4 The two extremal cacti

Let $C_{n,m,r}$ and D_r be the two cacti shown in Fig. 4. Then we have

$$W(C_{n,m,r}) = (n+m-r)(n-3) - r + 4, \quad W(D_r) = (2r+1)r.$$

Lemma 3.7. **(1)** *If $m \geq r+1$, then $Z \cong C_{n,m,r}$.*

(2) *If $m \leq r$, then $Z \cong D_r$.*

Proof. By Lemmas 3.1,3.2 and 3.5 we see that Z is such a bundle that all of its cycles are triangles, each vertex not in $\hat{Z}$ (if exist) is on some pendent path of length at most 2 and each vertex v of $\hat{Z}$ except the center has $\phi(v) = 0$ and $\psi(v) \leq 1$.

(1) Suppose, for a contradiction, that $Z \ncong C_{n,m,r}$. Then there must exist a triangle v_1v_2w of Z, where w is the center of Z with $deg_Z(w) \geq 4$ because of $r \geq 2$, such that $\psi(v_1) + \psi(v_2) \neq 0$.

Assume that $\psi(v_1)\psi(v_2) = 0$. Assume, without loss of generality, that $\psi(v_1) = 1$. In a similar way to prove the case on $k = 3$ in Lemma 3.2 (2), we get a contradiction.

Next assume that $\psi(v_1) = \psi(v_2) = 1$. By a transformation descried in Theorem 2.9, Z can be transformed into a cactus $Z' \in C(n,m,r)$, and by Theorem 2.9, we have that $W(Z') < W(Z)$, a contradiction to the choice of Z.

(2) By Lemma 3.6 we see that Z has not pendent edges. Since Z is a bundle whose each cycle is a triangle, it follows that $Z \cong D_r$. □

It has been proved that $C_{n,m,0}$ is the unique graph with the smallest Wiener index in $C(n,m,0)$ [15,18] and $C_{n,m,1}$ is the unique graph with the smallest Wiener index in $C(n,m,1)$ [18]. Hence by Lemma 3.7 and the assumption of Z we obtain the following main result in this section.

Theorem 3.8. *Let $n \geq 10$, $m \geq 3$.*

(1) *If $m \geq r+1$, then $C_{n,m,r}$ is the unique graph having the smallest Wiener index in $C(n,m,r)$.*

(2) *If $m \leq r$, then D_r is the unique graph having the smallest Wiener index in $C(n,m,r)$.*

From now denote the center of $C_{n,m,r}$ by w. Let wu_iv_i and ww_j be all pendent paths of length 2 and pendent edges in $C_{n,m,r}$ $(1 \leq i \leq m-r-1; 1 \leq j \leq n-2m+1)$. It is well known, for a connected graph G, that $W(G) > W(G+uv)$ if $uv \notin E(G)$.

Corollary 3.9. *Let $C(n,m)$ denote the set of all cacti with order $n \geq 10$ and matching number $m \geq 3$.*

(1) *If $n \neq 2m+1$, then $C_{n,m,m-1}$ is the unique graph having the smallest Wiener index in $C(n,m)$.*

(2) *If $n = 2m+1$, then D_m is the unique graph having the smallest Wiener index in $C(n,m)$.*

Proof. Let $G \in C(n,m)$ and let r be the number of cycles in G.

(1) From $n \neq 2m+1$ and Lemma 3.6 we see $m \geq r+1$. So by Theorem 3.8 (1) we have

$$W(G) \geq W(C_{n,m,r}), \tag{3.1}$$

with equality if and only if $G \cong C_{n,m,r}$.

On the other hand, since $C_{n,m,m-1} = C_{n,m,r} + \bigcup_{i=1}^{m-r-1}\{wv_i\} \in C(n,m)$, we have

$$W(C_{n,m,r}) \geq W(C_{n,m,r} + \bigcup_{i=1}^{m-r-1} \{wv_i\}) = W(C_{n,m,m-1}), \tag{3.2}$$

with equality if and only if $m = r + 1$.

By Eqs. (3.1) and (3.2) we get that $W(G) \geq W(C_{n,m,m-1})$, with equality if and only if $G \cong C_{n,m,r}$ and $m = r + 1$, namely $G \cong C_{n,m,m-1}$.

(2) If $m \geq r+1$, then in a similar way to prove **(1)** we can obtain that $W(G) \geq W(C_{n,m,m-1})$. Since

$$C_{n,m,m-1} + w_1w_2 \cong D_m \in C(n,m),$$

$$W(C_{n,m,m-1}) > W(C_{n,m,m-1} + w_1w_2),$$

we have that $W(G) > W(D_m)$.

If $m \leq r$, then by Lemma 3.6 we have $m = r$. So from Theorem 3.8 (2), it follows that D_m is the unique graph having the smallest Wiener index in $C(n,m)$. □

Corollary 3.10. *Let $C(n)$ be the set of all cacti with order $n \geq 10$.*

(1) *If n is an even number and $n = 2k$, then $C_{2k,k,k-1}$ is the unique graph having the smallest Wiener index in $C(n)$.*

(2) *If n is an odd number and $n = 2k+1$, then D_k is the unique graph having the smallest Wiener index in $C(n)$.*

Proof. Let $G \in C(n)$ and let m and r denote the matching number and cycle number of G, respectively.

(1) Since $n = 2k \neq 2m+1$, from Corollary 3.9 (1) we get that $W(G) \geq W(C_{n,m,m-1})$, with equality if and only if $G \cong C_{n,m,m-1}$. On the other hand, since

$$C_{n,m,m-1} + \bigcup_{j=1}^{k-m} \{w_{2j-1}w_{2j}\} \cong C_{2k,k,k-1},$$

it follows that $W(C_{n,m,m-1}) \geq W(C_{2k,k,k-1})$, with equality if and only if $k = m$. Therefore, we deduce $W(G) \geq W(C_{2k,k,k-1})$, with equality if and only if $G \cong C_{n,m,m-1}$ and $k = m$, namely $G \cong C_{2k,k,k-1}$.

(2) If $m \geq r+1$, then by Theorem 3.8 (1) we have $W(G) \geq W(C_{n,m,r})$. On the other hand, from $n \geq 2m+1$ and $n = 2k+1$ we see $k \geq m$. So

$$C_{n,m,r} + (\bigcup_{i=1}^{m-r-1} \{u_iv_i\}) \bigcup (\bigcup_{j=1}^{k-m+1} \{w_{2j-1}w_{2j}\}) \cong D_k,$$

It follows that $W(C_{n,m,r}) > W(D_k)$. Therefore, we have $W(G) > W(D_k)$.

If $m \leq r$, then from Lemma 3.6 and $n = 2k+1$ we deduce $m = k$. So by Corollary 3.9 (2), it follows that $W(G) \geq W(D_k)$, with equality if and only if $G \cong D_k$. □

4. Conclusion and future work

We give three graphic transforms described in Definition 2.1, Theorems 2.8 and 2.9, respectively, and derive the formulas for calculating the Wiener index of new graphs. With the transforms we determine the graphs having the smallest Wiener index among all cacti given order, matching number and cycle number. To the best of our knowledge, the results above have not been studied before. Moreover, the transforms are useful when we investigate the Wiener index of some types of graphs. For example, let $U(n, d)$ be the set of unicyclic graphs with order n and diameter d. For $G \in U(n, d)$, assume that G has a longest path P that does not contain edges of the unique cycle. By applying the two transformations given in Definition 2.1 and Theorems 2.8, it is easy to see that G can be transformed into a unicyclic graph $G' \in U(n, d)$ with $W(G) \geq W(G')$, where G' is the graph obtained from P by adding $n-d-1$ pendent edges to some 2-degree vertex of P and connecting two new pendent vertices with an edge.

Future work: (i) determine the graphs having the smallest or largest Wiener index among all unicyclic graphs with given diameter or number of pendent vertices, (ii) characterize the graphs having the largest Wiener index among all bicyclic graphs with given order.

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