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Reciprocal Complementary Wiener Numbers of Non-Caterpillars

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Abstract

The reciprocal complementary Wiener number of a connected graph G is defined as

$$RCW(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d+1-d(u,v\mid G)}$$

where $V(G)$ is the vertex set. $d(u,v\mid G)$ is the distance between vertices u and v, and d is the diameter of G. A tree is known as a caterpillar if the removal of all pendant vertices makes it as a path. Otherwise, it is called a non-caterpillar. Among all n-vertex non-caterpillars with given diameter d, we obtain the unique tree with minimum reciprocal complementary Wiener number, where $4\le d\le n-3$. We also determine the n-vertex non-caterpillars with the smallest, the second smallest and the third smallest reciprocal complementary Wiener numbers.

Keywords

Reciprocal Complementary Wiener Number, Wiener Number, Caterpillar

1. Introduction

The Wiener number was one of the oldest topological indices, which was introduced by Harry Wiener in 1947. About the recent reviews on matrices and topological indices related to Wiener number, refer to [1]-[4]. The RCW number is one of the hotest additions in the family of such descriptors. The notion of RCW number was first put forward by Ivanciuc and its applications were discussed in [5]-[8].

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Let G be a simple connected graph with vertex set $V(G)$. For two vertices $u,v\in V(G)$, let $d(u,v\,|\,G)$ denote the distance between u and v in G. Then, the RCW number of G is defined by

$$RCW(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d+1-d(u,v\,|\,G)}$$

where d is the diameter and the summation goes over all unordered pairs of distinct vertices of G. Some properties of the RCW number have been obtained in [9] [10].

A tree is called a caterpillar if the removal of all pendant vertices makes it as a path. Otherwise, it is called a non-caterpillar.

For integers n and d satisfying $4\le d\le n-3$, let $N_{n,d,i}$ be the tree obtained from the path P_{d+1} labelled as $v_0,v_1,\cdots,v_d$ by attaching the path P_2 and $n-d-3$ pendant vertices to vertex v_i for $2\le i\le\left\lfloor\frac{d}{2}\right\rfloor$ (see **Figure 1**). Let $N_{n,d}=N_{n,d,\left\lfloor\frac{d}{2}\right\rfloor}$.

In this paper, we show that among all n-vertex non-caterpillars with given diameter d, $N_{n,d}$ is the unique tree with minimum RCW number where $4\le d\le n-3$. Furthermore, we determine the non-caterpillars with the smallest, the second smallest and the third smallest RCW numbers.

2. RCW Numbers of Non-Caterpillars

All n-vertex trees with diameter 2, 3, $n-2$ and $n-1$ are caterpillars. Let n and d be integers with $n\ge 7$ and $4\le d\le n-3$. Let $\mathbf{NC}(n,d)$ be the class of non-caterpillars with n vertices and diameter d. Let $\mathcal{NC}(n,d)$ be the class of non-caterpillars obtained by attaching the stars $s_{n_1},\cdots,s_{n_t}$ at their centers and $s=n-d-1-\sum_{i=1}^{t}n_i$ pendant vertices to one center (fixed if it is bicentral) of the path P_{d+1}, where $t\ge 1$, $s\ge 0$ and $n_i\ge 2$ for $i=1,2,\cdots,t$ (see **Figure 2**). Recall that $N_{n,d}=N_{n,d,\left\lfloor\frac{d}{2}\right\rfloor}$. Obviously, $N_{n,d}\in\mathcal{NC}(n,d)\subseteq\mathbf{NC}(n,d)$ and $\mathcal{NC}(n,n-3)=\{N_{n,n-3}\}$.

Let T be a tree. For $u\in V(T)$ and $A\subseteq V(T)$, let $\delta_T(u)$ be the degree of u in T and $d_T(u,A)$ be the sum of all distances from u to the vertices in A, *i.e.*, $d_T(u,A)=\sum_{v\in A}d_T(u,v)$. Here and in the following $d_T(u,v)$ denotes the distance between vertices u and v in T.

Lemma 1 *Let T be a tree with minimum RCW number in* $\mathbf{NC}(n,d)$, *where* $4\le d\le n-3$. *Then,* $T\in\mathcal{NC}(n,d)$.

Proof. Suppose that $T\in\mathbf{NC}(n,d)\setminus\mathcal{NC}(n,d)$. Let $P(T)=v_0v_1\cdots v_d$ be a diametral path of T. If d is odd, we require that $\delta_T\left(v_{\left\lfloor\frac{d}{2}\right\rfloor}\right)\ge\delta_T\left(v_{\left\lceil\frac{d}{2}\right\rceil}\right)$. Then at least one of $v_2,\cdots,v_{d-2}$ has degree at least three. There are two cases.

Case 1. One of $v_2,\cdots,v_{d-2}$ different from $v_{\left\lfloor\frac{d}{2}\right\rfloor}$ has degree at least three. Let $w_1,w_2,\cdots,w_k$ be all the neighbors outside $P(T)$ except those of $v_{\left\lfloor\frac{d}{2}\right\rfloor}$, where w_i is a neighbor of $v_{i'}\in V(P(T))$. Let T_i be the subtree of $T-v_{i'}$ containing w_i. T^* be the tree formed from T by deleting edges $w_iv_{i'}$ and adding edges $w_iv_{\left\lfloor\frac{d}{2}\right\rfloor}$ for

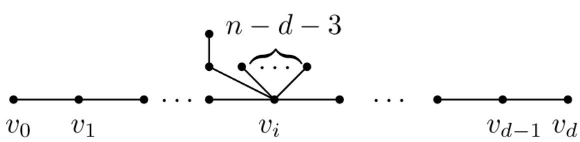

Figure 1. The tree $N_{n,d,i}$.

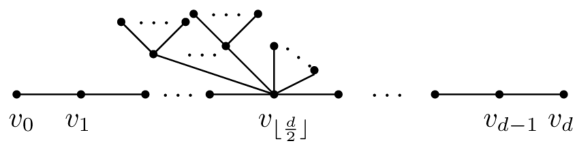

Figure 2. The tree *NC* (*n*,*d*).

all $i = 1, 2, \cdots, k$. Obviously, $T^* \in \mathbf{NC}(n,d)$. Let $A = V(P(T))$ and $B = V(T) \setminus A$. It is easily seen that

$$\begin{aligned} RCW(T) - RCW(T^*) &= \sum_{u \in B, v \in A}\left[\frac{1}{d+1-d_T(u,v)} - \frac{1}{d+1-d_{T^*}(u,v)}\right] \\ &\quad + \sum_{\{u,v\} \subseteq B}\left[\frac{1}{d+1-d_T(u,v)} - \frac{1}{d+1-d_{T^*}(u,v)}\right] \\ &\geq \sum_{\substack{u \in V(T_i) \\ 1 \leq i \leq k}} \sum_{v \in A}\left[\frac{1}{d+1-d_T(u,v)} - \frac{1}{d+1-d_{T^*}(u,v)}\right] \\ &\quad + \sum_{\substack{u \in V(T_i), v \in V(T_j) \\ 1 \leq i < j \leq k}}\left[\frac{1}{d+1-d_T(u,v)} - \frac{1}{d+1-d_{T^*}(u,v)}\right] \end{aligned}$$

with equality if and only if $\delta_T\left(v_{\left\lfloor \frac{d}{2} \right\rfloor}\right) = 2$. Since $i' \neq \left\lfloor \frac{d}{2} \right\rfloor$, $d_T(u, v_{i'}) = d_{T^*}\left(u, v_{\left\lfloor \frac{d}{2} \right\rfloor}\right)$ for $u \in V(T_i)$ and $v_{i'} \in A$ with $1 \leq i \leq k$. We get

$$\begin{aligned} \sum_{v \in A} \frac{1}{d+1-d_T(u,v)} &= \sum_{v \in A} \frac{1}{d+1-d_T(u,v_{i'}) - d_T(v_{i'},v)} \\ &= \sum_{k=1}^{i'} \frac{1}{d+1-d_T(u,v_{i'}) - k} + \sum_{k=1}^{d-i'} \frac{1}{d+1-d_T(u,v_{i'}) - k} \\ &\geq \sum_{k=1}^{\left\lfloor \frac{d}{2} \right\rfloor} \frac{1}{d+1-d_{T^*}\left(u, v_{\left\lfloor \frac{d}{2} \right\rfloor}\right) - k} + \sum_{k=1}^{\left\lceil \frac{d}{2} \right\rceil} \frac{1}{d+1-d_{T^*}\left(u, v_{\left\lfloor \frac{d}{2} \right\rfloor}\right) - k} \\ &= \sum_{v \in A} \frac{1}{d+1-d_{T^*}\left(u, v_{\left\lfloor \frac{d}{2} \right\rfloor}\right) - d_{T^*}\left(v_{\left\lfloor \frac{d}{2} \right\rfloor}, v\right)} = \sum_{v \in A} \frac{1}{d+1-d_{T^*}(u,v)}. \end{aligned}$$

Then

$$\begin{aligned} &\sum_{\substack{u \in V(T_i) \\ 1 \leq i \leq k}} \sum_{v \in A}\left[\frac{1}{d+1-d_T(u,v)} - \frac{1}{d+1-d_{T^*}(u,v)}\right] \\ &= \sum_{\substack{u \in V(T_i) \\ 1 \leq i \leq k}}\left[\sum_{v \in A} \frac{1}{d+1-d_T(u,v)} - \sum_{v \in A} \frac{1}{d+1-d_{T^*}(u,v)}\right] \geq 0 \end{aligned}$$

with equality if and only if $i' = \left\lceil \frac{d}{2} \right\rceil$ (which is only possible for odd number *d*). But $\delta_T\left(v_{\left\lfloor \frac{d}{2} \right\rfloor}\right) \geq \delta_T\left(v_{\left\lceil \frac{d}{2} \right\rceil}\right)$, and thus if $\delta_T\left(v_{\lfloor \frac{d}{2} \rfloor}\right)=2$ then $\delta_T\left(v_{\lceil \frac{d}{2} \rceil}\right)=2$. So $i' \neq \left\lceil \frac{d}{2} \right\rceil$ for $i=1,2,\cdots,k$. Thus

$$\begin{aligned} &RCW(T)-RCW(T^*) \\ &> \sum_{\substack{u\in V(T_i),v\in V(T_j)\\ 1\le i<j\le k}} \left[\frac{1}{d+1-d_T(u,v)}-\frac{1}{d+1-d_{T^*}(u,v)}\right] \ge 0, \end{aligned}$$

since $d_T(u,v) \ge d_{T^*}(u,v)$ for $u\in V(T_i), v\in V(T_j)$ $(1\le i<j\le k)$. It follows that $RCW(T) > RCW(T^*)$. This is a contradiction.

Case 2. Any verter v_i with $i=2,3,\cdots,d-2$ and $i\neq \left\lfloor \frac{d}{2} \right\rfloor$ has degree two. Obviously, $\delta_T\left(v_{\lfloor \frac{d}{2} \rfloor}\right) \ge 3$. Let $xyz\cdots v_{\lfloor \frac{d}{2} \rfloor}$ be the (unique) path from *x* to $v_{\lfloor \frac{d}{2} \rfloor}$ in *T* such that $d_T\left(x, v_{\lfloor \frac{d}{2} \rfloor}\right) = \max_{u\in V(T)\setminus V(P(T))} d_T\left(u, v_{\lfloor \frac{d}{2} \rfloor}\right)$. Since $T \notin \mathcal{NC}(n,d)$, we have $d_T\left(x, v_{\lfloor \frac{d}{2} \rfloor}\right) \ge 3$. Let $x_1,\cdots,x_r,z$ be the neighbors of *y* in *T*, where $x_1 = x$ and $r\ge 1$. Let T^{**} be the tree obtained from *T* by deleting edges yx_i and adding edges zx_i for all $i=1,2,\cdots,r$. Then $T^{**}\in \mathbf{NC}(n,d)$. Let $N_y=\{x_1,\cdots,x_r\}$, $C=V(T)\setminus N_y$. Since $d_T(u,v)=d_{T^{**}}(u,v)+1$ for $u\in N_y, v\in C\setminus\{y,z\}$, we get

$$\begin{aligned} &RCW(T)-RCW(T^{**}) \\ &= \sum_{u\in N_y, v\in C}\left[\frac{1}{d+1-d_T(u,v)}-\frac{1}{d+1-d_{T^*}(u,v)}\right] \\ &= \frac{r-1}{d+1-1}+\frac{r-1}{d+1-2}+\sum_{u\in N_y,v\in C\setminus\{y,z\}}\frac{1}{d+1-d_T(u,v)} \\ &\quad -\frac{r-1}{d+1-1}-\frac{r-1}{d+1-2}-\sum_{u\in N_y,v\in C\setminus\{y,z\}}\frac{1}{d+1-d_{T^*}(u,v)} \\ &> 0. \end{aligned}$$

This is a contradiction.

By combining Cases 1 and 2, we find that $T\in \mathbf{NC}(n,d)\setminus \mathcal{NC}(n,d)$ is impossible. The result follows.

Lemma 2 *Let* $T\in \mathcal{NC}(n,d)$ *with* $4\le d\le n-3$. *Then*

$$RCW(T) \ge RCW(N_{n,d}),$$

with equality if and only if $T = N_{n,d}$.

Proof. Let *T* be a tree with the minimum RCW number in $\mathcal{NC}(n,d)$. Let $P(T)=v_0v_1\cdots v_d$ be a diametral path of *T*.

Suppose that there is a vertex $u\in V(T)\setminus V(P(T))$ with $\delta_T(u)\ge 3$. Let $u_1,u_2,\cdots,u_s$ be the neighbors of *u* different from $v_{\lfloor \frac{d}{2} \rfloor}$ in *T*, where $s\ge 2$. Clearly, u_i are pendant vertices for $i=1,2,\cdots,s$. Let T' be the tree obtained from *T* by deleting edges uu_i and adding edges $v_{\lfloor \frac{d}{2} \rfloor}u_i$ for $i=2,\cdots,s$. Obviously, $T'\in \mathcal{NC}(n,d)$. Let $N_u=\{u_2,\cdots,u_s\}$, $D=V(T)\setminus N_u$, and $K=\left\{u,u_1,v_{\lfloor \frac{d}{2} \rfloor},v_{\lfloor \frac{d}{2} \rfloor -1}\right\}$. Since $d_T(u,v)=d_{T'}(u,v)+1$ for $u\in N_u, v\in D\setminus K$, we get

$$
\begin{aligned}
&RCW(T)-RCW(T')\\
&=\sum_{u\in N_u,v\in D}\left[\frac{1}{d+1-d_T(u,v)}-\frac{1}{d+1-d_{T^*}(u,v)}\right]\\
&=\frac{s-1}{d+1-1}+\frac{s-1}{d+1-2}+\frac{s-1}{d+1-2}+\frac{s-1}{d+1-3}+\sum_{u\in N_u,v\in D\setminus K}\frac{1}{d+1-d_T(u,v)}\\
&\quad-\frac{s-1}{d+1-2}-\frac{s-1}{d+1-1}-\frac{s-1}{d+1-3}-\frac{s-1}{d+1-2}-\sum_{u\in N_u,v\in D\setminus K}\frac{1}{d+1-d_{T'}(u,v)}\\
&>0,
\end{aligned}
$$

and then $RCW(T)>RCW(T')$, this is a contradiction. Thus any vertex of T outside $P(T)$ has degree at most two.

Suppose that there are at least two vertices of T outside $P(T)$ with degree two. Let $y\in V(T)\setminus V(P(T))$ with $\delta_T(y)=2$ and let x be the neighbor of y which is different from $v_{\lfloor \frac{d}{2}\rfloor}$ in T. Let T'' be the tree formed from T by deleting edge yx and adding edge $v_{\lfloor \frac{d}{2}\rfloor}x$. Obviously, $T''\in\mathcal{NC}(n,d)$. Let $F=\left\{x,y,v_{\lfloor \frac{d}{2}\rfloor}\right\}$. Since $RCW(T)>RCW(T'')$ and $d_T(x,v)=d_{T''}(x,v)+1$ for $v\in V(T)\setminus F$, we get

$$
\begin{aligned}
&RCW(T)-RCW(T'')\\
&=\frac{1}{d+1-1}+\frac{1}{d+1-2}+\sum_{v\in V(T)\setminus F}\frac{1}{d+1-d_T(x,v)}\\
&\quad-\frac{1}{d+1-1}-\frac{1}{d+1-2}-\sum_{v\in V(T)\setminus F}\frac{1}{d+1-d_{T''}(x,v)}\\
&>0.
\end{aligned}
$$

This is a contradiction. Thus there is exactly one vertex outside $P(T)$ with degree two and all other vertices of T outside $P(T)$ are pendant vertices. Then, $T=N_{n,d}$.

By a direct calculation, we get

$$
RCW\left(N_{n,d,\lfloor \frac{d}{2}\rfloor}\right)=d+\frac{n-d+1}{d-2}+\frac{(n-d-2)(n-d-3)-2}{2(d-1)}+(n-d-1)\left(\sum_{k=1}^{\frac{d}{2}}\frac{2}{d-k}+\frac{1}{d}\right).\quad \text{where } d \text{ is even;}
$$

$$
RCW\left(N_{n,d,\lfloor \frac{d}{2}\rfloor}\right)=d+\frac{n-d-3}{d-2}+\frac{2}{d-3}+\frac{(n-d-2)(n-d-3)+4(n-d)-2}{2(d-1)}+(n-d-1)\left(\sum_{k=1}^{\frac{d-1}{2}}\frac{2}{d-k}+\frac{1}{d}\right).\quad \text{where } d \text{ is odd.}
$$

Combining Lemmas 1 and 2, we get

Theorem 1 *Let* $T\in\mathbf{NC}(n,d)$, *and* $4\le d\le n-3$. *Then*

$$
RCW(T)\ge RCW(N_{n,d})
$$

with equality if and only if $T=N_{n,d}$.

Lemma 3 *For* $4 \le d \le n-3$, *there is* $RCW\left(N_{n,d,\left\lfloor \frac{d}{2} \right\rfloor}\right) > RCW\left(N_{n,d+1,\left\lfloor \frac{d+1}{2} \right\rfloor}\right)$.

Proof. If *d* is even, then

$$\begin{aligned} & RCW\left(N_{n,d,\frac{d}{2}}\right) - RCW\left(N_{n,d+1,\frac{d}{2}}\right) \\ & = \left(-1 + \sum_{k=1}^{\frac{d}{2}-1} \frac{2}{d-k}\right) + \frac{5(n-d-1)}{d} - \frac{n-d-2}{d+1} - \frac{4(n-d-2)+1}{d} + \frac{n-d-1}{d-2} \\ & \quad - \frac{n-d-3}{d-1} + \frac{(n-d-2)(n-d-3)}{2(d-1)} - \frac{(n-d-3)(n-d-4)}{2d} \\ & > \left(-1 + \sum_{k=1}^{\frac{d}{2}-1} \frac{2}{d-k}\right) > 0. \end{aligned}$$

If *d* is odd, then

$$\begin{aligned} & RCW\left(N_{n,d,\frac{d-1}{2}}\right) - RCW\left(N_{n,d+1,\frac{d+1}{2}}\right) \\ & = \left(-1 + \sum_{k=1}^{\frac{d-1}{2}} \frac{2}{d-k}\right) + \frac{n-d-3}{d-2} - \frac{n-d-4}{d} + \frac{(n-d-2)(n-d-3)}{2(d-1)} \\ & \quad - \frac{(n-d-3)(n-d-4)}{2d} + \frac{n-d-1}{d-1} - \frac{n-d-2}{d+1} + \frac{2}{d-3} \\ & > \left(-1 + \sum_{k=1}^{\frac{d-1}{2}} \frac{2}{d-k}\right) > 0. \end{aligned}$$

The result follows.

Theorem 2 *For* $n \ge 9$, *there is*

$$RCW\left(N_{n,n-3,\left\lfloor \frac{n-3}{2} \right\rfloor}\right) < RCW\left(N_{n,n-3,\left\lfloor \frac{n-5}{2} \right\rfloor}\right) < RCW\left(N_{n,n-4,\left\lfloor \frac{n-4}{2} \right\rfloor}\right).$$

And $RCW(T) > RCW\left(N_{n,n-4,\left\lfloor \frac{n-4}{2} \right\rfloor}\right)$ for any *n*-vertex non-caterpillar T different from $N_{n,n-3,\left\lfloor \frac{n-3}{2} \right\rfloor}$, $N_{n,n-3,\left\lfloor \frac{n-5}{2} \right\rfloor}$, $N_{n,n-4,\left\lfloor \frac{n-4}{2} \right\rfloor}$.

Proof. Let $T \in \mathbf{NC}(n,d)$, where $4 \le d \le n-3$. If $d = n-3$, then T is a non-caterpillar $N_{n,n-3,i}$ where $1 \le i \le \left\lfloor \frac{n-3}{2} \right\rfloor$. It follows that

$$RCW\left(N_{n,n-3,i}\right) = n-3 + \frac{2}{n-3} + \frac{1}{n-4} + \sum_{k=4}^{i+3} \frac{2}{n-k} + \sum_{k=5}^{n-i} \frac{2}{n-k} + \frac{1}{n-i-4} + \frac{1}{i-1},$$

and hence $RCW\left(N_{n,n-3,i}\right)$ is monotonically decreasing for $1 \le i \le \left\lfloor \frac{n-3}{2} \right\rfloor$. This implies

$$RCW\left(N_{n,n-3,\left\lfloor\frac{n-3}{2}\right\rfloor}\right) < RCW\left(N_{n,n-3,\left\lfloor\frac{n-5}{2}\right\rfloor}\right) < \cdots < RCW\left(N_{n,n-3,2}\right).$$

Now suppose that $d \le n-4$. By Theorem 1 and Lemma 3, there is

$$RCW(T) \ge RCW\left(N_{n,n-4,\left\lfloor\frac{n-4}{2}\right\rfloor}\right)$$

where equality holds if and only if $T \cong N_{n,n-4,\left\lfloor\frac{n-4}{2}\right\rfloor}$. We need only to show

$$RCW\left(N_{n,n-3,\left\lfloor\frac{n-5}{2}\right\rfloor}\right) < RCW\left(N_{n,n-4,\left\lfloor\frac{n-4}{2}\right\rfloor}\right).$$

Case 1. n is odd. Let $i = \left\lfloor\frac{n-5}{2}\right\rfloor = \frac{n-5}{2}$ and $n \ge 9$. Then there is

$$RCW\left(N_{n,n-4,\frac{n-5}{2}}\right) - RCW\left(N_{n,n-3,\frac{n-5}{2}}\right) = \left(-1+\sum_{k=6}^{\frac{n+5}{2}}\frac{2}{n-k}\right)+\frac{2}{n-5}+\frac{1}{n-6} > 0.$$

Case 2. n is even. Let $i = \left\lfloor\frac{n-5}{2}\right\rfloor = \frac{n-6}{2}$. Then there is

$$\begin{aligned}
&RCW\left(N_{n,n-4,\frac{n-4}{2}}\right) - RCW\left(N_{n,n-3,\frac{n-6}{2}}\right) \\
&= \left(-1+\sum_{k=6}^{\frac{n+4}{2}}\frac{2}{n-k}\right)+\frac{2}{n-5}+\frac{1}{n-6}+\frac{2}{n-2}+\frac{4}{n-4}-\frac{2}{n-3}-\frac{2}{n-8} \\
&> \left(-1+\sum_{k=6}^{\frac{n+4}{2}}\frac{2}{n-k}\right)+\frac{5}{n-5}-\frac{2}{n-8} \\
&\ge 0.
\end{aligned}$$

Thus, the proof is finished.

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