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COMPARATIVE RESULTS BETWEEN THE NUMBER OF SUBTREES AND WIENER INDEX OF GRAPHS

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Abstract. For a graph G, we denote by $N(G)$ the number of non-empty subtrees of G. If G is connected, its Wiener index $W(G)$ is the sum of distances between all unordered pairs of vertices of G. In this paper we establish some comparative results between N and W. It is shown that $N(G) > W(G)$ if G is a graph of order $n \geq 7$ and diameter 2 or 3. Also some graphs are constructed with large diameters and $N > W$. Moreover, for a tree $T \ncong S_n$ of order n, we prove that $W(T) > N(T)$ if T is a starlike tree with maximum degree 3 or a tree with exactly two vertices of maximum degrees 3 one of which has two leaf neighbors, or a broom with $k \log_2 n$ leaves. And a method is provided for constructing the graphs with $N < W$. Finally several related open problems are proposed to the comparison between N and W.

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1. Introduction

Throughout this paper we only consider undirected, finite and simple graphs. For a graph $G = (V(G), E(G))$ with vertex set $V(G)$ and edge set $E(G)$, the degree of vertex $v \in V(G)$ is denoted by $\deg_G(v)$, that is, $\deg_G(v) = |N_G(v)|$ where $N_G(v)$ is the open neighborhood. Here $N_G[v] = N_G(v) \cup \{v\}$ is the closed neighborhood of v. For any graph G, we denote by $L(G)$ the *line graph* of G. Denote by C_n and K_n the cycle and the complete graph on n vertices, respectively. Similarly, P_n and S_n are the path and the star on n vertices, respectively. Other undefined notations and terminology on graph theory can be found in [4].

The number of subtrees was first studied for trees [29] in 2005. For any connected graph G, we denote by $N(G)$ the number of non-empty subtrees in G. The properties of $N(T)$ of various classes of trees T have been studied [1, 2, 17, 23, 27, 30, 31, 38, 39]. However, there are few results on $N(G)$ for general graphs G. Recently, Andriantiana and Wang [3] considered the extremal unicyclic graphs with respect to N. Furthermore, two of present authors and Wang [35] characterized the extremal graphs with respect to N among all connected graphs of order n with k cut edges. For a graph G with $S \subseteq V(G)$, we denote by $N(S, G)$ the number of subtrees of G that contain at least one vertex of S. In particular, if $S = \{v\}$, then $N(S, G)$ can also be simplified into $N(v, G)$, which is called the *subtree number of vertex* v in G. More generally, for any connected subgraph H of a graph

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G with $v \in V(H)$, we denote by $N_G(v, H)$ the number of subtrees of H in G that contain v. Similarly, for a set $V = \{v_1, v_2, \ldots, v_t\} \subseteq V(G)$ with $t \geq 2$, $N(v_1, v_2, \ldots, v_t; G)$ is the number of non-empty subtrees of G that contain the vertices $v_1, v_2, \ldots, v_t$, while $N(\overline{v_1}, \overline{v_2}, \ldots, \overline{v_k}, v_{k+1}, \ldots, v_t; G)$ denotes the number of subtrees of G that do not contain the vertices $v_1, v_2, \ldots, v_k$ but contain the remaining vertices $v_{k+1}, \ldots, v_t$. Here, relevant to the number of subtrees, we define a novel invariant $LN(G)$ called *local sum of subtrees* of a graph G:

$$LN(G) = \sum_{v \in V(G)} N(v, G).$$

For any tree T, the subtree polynomial of T was introduced [16] as follows:

$$\Phi_T(x) = \sum_{k=1}^{n} N_k(T) x^k$$

where $N_k(T)$ denotes the number of subtrees in T of order k. The concept of subtree polynomial of trees can be extended to general graphs. Clearly, $N(G) = \Phi_G(1)$ holds for any graph G. Moreover, for any subtree T of order k in a graph G, T is counted once in $N(v, G)$ for any vertex $v \in V(T) \subseteq V(G)$, that is, T is counted k times in $LN(G)$. Therefore it follows that

$$LN(G) = \sum_{k=1}^{n} k N_k(G) \tag{1.1}$$

for any graph of order n. Equivalently, we have $LN(G) = \Phi'_G(1)$ for any graph G.

If P is a path connecting two vertices u and v in a graph G, then we call P as a u,v-path and denote it by uPv. In particular, a shortest u,v-path is called a u,v-*geodesic* in G, whose length is just the distance $d_G(u, v)$ between u and v in G. As one of the most well-studied topological indices in chemical graph theory, the Wiener index [32] of a connected graph G is defined as

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

For more results on the Wiener index, please refer to [7, 8, 11–13, 18–22, 28, 34, 36, 37]. In particular, the chemical applications of W are reported for acyclic molecules [9] and benzenoid hydrocarbons [10]. Other distance-related topics of graphs can be found in [15, 25]. Moreover,

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} Tr_G(v) \tag{1.2}$$

where $Tr_G(v)$ is the *transmission* of vertex v, that is the sum of distances from v to other vertices, in graph G. As a special distance, the *eccentricity*, denoted by $\varepsilon_G(v)$, of vertex v in a graph G is the maximum distance from v to any other vertex in G.

An interesting "negative" correlation has been observed between the number of subtrees and the Wiener index of general graphs. It was shown that, in some given collection of connected graphs, the extremal graphs minimizing (maximizing, resp.) the number of subtrees are identical to the extremal ones maximizing (minimizing, resp.) the Wiener index. Such classes of graphs include various trees [29, 33] and unicyclic graphs [3, 33]. Other related works are reported in [27, 30, 35, 36]. Note that in [24] the extremal graphs are determined with respect to N and W among all cacti and block graphs, respectively, which strengthen this "negative" correlation between them.

For any positive integer k, we write $[k] = \{1, 2, \ldots, k\}$. A vertex v in a tree T is a *branching vertex* if $\deg_T(v) \geq 3$. A tree T is a *starlike tree* if T contains only one branching vertex. For a starlike tree T with branching vertex $v \in V(T)$, we write $T = T(n_1, n_2, \ldots, n_k)$ if $T - v = \bigcup_{i=1}^{k} P_{n_i}$ where the pendant path P_{n_i} is called an n_i-*arm* of T. A tree $H(n_1, n_2, n_3, n_4, n_5)$ is obtained by attaching at the leaf of the n_3-arm in $T(n_1, n_2, n_3)$ two pendant paths of lengths n_4 and n_5, respectively.

Note that $W(P_n) = \binom{n+1}{3} > \binom{n+1}{2} = N(P_n)$ and $N(S_n) = 2^{n-1} + n - 1 > (n-1)^2 = W(S_n)$ for $n > 4$. Therefore N and W are incomparable even for the trees. In this paper we focus on the comparison between N and W of graphs. The paper is organized as follows. In Section 2 some lemmas will be provided for proving the subsequent results. In Section 3, we prove that $N(G) > W(G)$ for any graph G of order $n \geq 7$ and diameter 2 or 3 and provide a method for constructing more graphs with $N > W$. In Section 4 it is shown that $N(G) < W(G)$ for some graphs G, including starlike trees with maximum degree 3, special trees with two vertices of maximum degrees 3, brooms with not many leaves and some special unicyclic graphs. Moreover, a method is provided for getting some new graphs with $N < W$. We conclude the paper in Section 5 by proposing several problems related to comparison relation between N and W.

2. Preliminaries

In this section we will list or prove some lemmas for the use of subsequent proofs.

If G is a disconnected graph with t components $G_1, G_2, \ldots, G_t$, then we have

$$N(G) = \sum_{i=1}^{t} N(G_i). \tag{2.1}$$

Also, for any subset $S \subseteq V(G)$, we have

$$N(G) = N(S, G) + N(G \setminus S) \tag{2.2}$$

where $G \setminus S$ denote the induced subgraph of G by $V(G) \setminus S$. In particular, we have

$$N(G) = N(v, G) + N(G - v) \tag{2.3}$$

for any vertex $v \in V(G)$ where $G - v$ is a short form of $G \setminus \{v\}$.

From definitions of W, N we can get easily the following result and skip the proof.

Lemma 2.1. *Let G be a connected graph with two non-adjacent vertices $u, v \in V(G)$. Then*

(i) $W(G + uv) < W(G)$;
(ii) $N(G + uv) > N(G)$.

Based on Lemma 2.1, the following result holds clearly.

Lemma 2.2. *Let G be a connected non-complete graph with two non-adjacent vertices $u, v \in V(G)$. If $N(G) > W(G)$, then $N(G + uv) > W(G + uv)$.*

For any integer $n \geq 4$, we denote by $\mathcal{G}_n^2$ and $\mathcal{G}_n^3$ the set of graphs of order n with diameter 2 and the set of n-vertex graphs with diameter 3, respectively. Below is a result on the Wiener index of graphs from $\mathcal{G}_n^2$.

Lemma 2.3 ([34])**.** *If $G \in \mathcal{G}_n^2$ has m edges, then $W(G) = n(n-1) - m$.*

Lemma 2.4 ([29])**.** *Let T be a tree of order $n \geq 4$. Then we have*

$$\binom{n+1}{2} \leq N(T) \leq 2^{n-1} + n - 1$$

with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$.

Lemma 2.5 ([14]). *Let T be a tree of order $n > 4$ with all branching vertices $u_1, u_2, \ldots, u_k$. If $T - u_i = \bigcup_{t=1}^{m_i} T_{it}$ with $\deg_T(u_i) = m_i$ and $n(T_{ij}) = n_{ij}$ where $i \in [k]$ and $j \in [m_i]$, then*

$$W(T) = \binom{n+1}{3} - \sum_{i=1}^{k} \sum_{1 \le p < q < r \le m_i} n_{ip} n_{iq} n_{ir}.$$

Lemma 2.6 ([5]). *For any tree T of order n, we have $W(L(T)) = W(T) - \binom{n}{2}$.*

In the following we provide a lower bound on $N(v, G)$ in terms of the degree of v.

Lemma 2.7. *Let G be a connected graph of order n with an arbitrary vertex $v \in V(G)$ of degree $k \ge 2$. Then*

(i) $N(v, G) \ge 2^{k-1}(n - k + 1)$;
(ii) $Tr_G(v) \le k - 1 + \binom{n-k+1}{2}$.

Proof. Assume that $N_G(v) = \{v_1, v_2, \ldots, v_k\}$. Choose any vertex $v_i \in N_G(v)$, set $V_1 = N_G[v] \setminus \{v_i\}$ and $V_2 = (V(G) \setminus N_G(v)) \cup \{v_i\}$, then $V(G) = V_1 \cup V_2$ with $|V_1| = k$, $|V_2| = n - k + 1$ and $V_1 \cap V_2 = \{v\}$.

Since $H = G[V_1]$ contains a subgraph S_k with v as the center, $N_G(v, H) \ge 2^{k-1}$ holds from the fact $N(v, S_k) = 2^{k-1}$. Denote by $\mathcal{T}_1$ the set of above subtrees containing v in H. Note that $N(v, u; G) \ge 1$, that is, there is at least one path connecting v and u in G, for any vertex $u \in V_2 \setminus \{v\}$ and the single vertex v is also a subtree containing v in V_2. There are at least $n-k+1$ subtrees that contain v in V_2. These above subtrees form a set $\mathcal{T}_2$. Note that the unification at v of two subtrees (including a single-vertex subtree v as a trivial one) from $\mathcal{T}_1$ and $\mathcal{T}_2$, respectively, forms a subtree containing v in G. Therefore, $N(v, G) \ge 2^{k-1}(n - k + 1)$ follows immediately.

Next we turn to prove the upper bound on $Tr_G(v)$. From definition, we have

$$\begin{aligned} Tr_G(v) &\le k + \sum_{u \in V(G) \setminus N_G(v)} d_G(v, u) \\ &= k + 2 + \ldots + n - k \\ &= k - 1 + \binom{n-k+1}{2}, \end{aligned}$$

completing the proof. □

For two vertex-disjoint graphs G_1, G_2 with $v_i \in V(G_i)$ for $i \in [2]$, we denote by $G_1 v_1 \smile v_2 G_2$ a new graph obtained by inserting an edge connecting the vertices v_1 of G_1 and v_2 of G_2. Here $G_1 v_1 \smile v_2 G_2$ is called the v_1v_2-*link graph* of graphs G_1 and G_2.

Lemma 2.8. *Let $G = G_1 v_1 \smile v_2 G_2$ be the v_1v_2-link graph of two vertex-disjoint graphs G_1 and G_2 of orders n_1 and n_2, respectively, with $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Then*

(i) $W(G) = W(G_1) + W(G_2) + n_1 Tr_{G_2}(v_2) + n_2 Tr_{G_1}(v_1) + n_1 n_2$;
(ii) $N(G) = N(G_1) + N(G_2) + N(v_1, G_1) N(v_2, G_2)$.

Proof. From the structure of G, we have

$$\begin{aligned} W(G) &= W(G_1) + W(G_2) + \sum_{x \in V(G_1), y \in V(G_2)} \Big[d_{G_1}(x, v_1) + 1 + d_{G_2}(v_2, y) \Big] \\ &= W(G_1) + W(G_2) + n_2 Tr_{G_1}(v_1) + n_1 Tr_{G_2}(v_2) + n_1 n_2. \end{aligned}$$

And any subtree in G is fallen into the following classes: (A). the subtrees only in G_1; (B). the subtrees only in G_2; (C). the subtrees containing the vertices of G_1 and G_2. So we get $N(G) = N(G_1) + N(G_2) + N(v_1, G_1) N(v_2, G_2)$, completing the proof. □

3. Graphs with $N > W$

In this section we prove some results on the graphs with $N > W$. Note that $\mathcal{G}_n^2$ contains a single graph P_n if $n = 3$. So in the following we always assume that $n \geq 4$ in $\mathcal{G}_n^2$.

3.1. Graphs with small diameters

Any graph with diameter 1 is a complete graph and *vice versa*. In K_n, any edge is corresponding with a subtree P_2 and any vertex is a single-vertex subtree. Therefore

$$N(K_n) \geq n + \binom{n}{2} > \binom{n}{2} = W(K_n).$$

We first prove the result for the graphs in $\mathcal{G}_n^2$ with $n \geq 4$. Before doing it, we need the following preliminary results.

Lemma 3.1 ([35]). *Let G be a connected graph of order n without any cut edge. Then $N(G) \geq n^2$ with equality holding if and only if $G \cong C_n$.*

Theorem 3.2. *For any graph $G \in \mathcal{G}_n^2$ with $n \geq 5$, we have $N(G) > W(G)$.*

Proof. Assume that G has m edges and $v \in V(G)$ with maximum degree $\Delta(G)$. Based on the value of $\Delta(G)$, we divide into the following cases.

Case 1. $\Delta(G) = n - 1$.

In this case $G[N_G[v]]$ contains S_Δ as a subgraph. By Lemma 2.1, we have

$$\begin{aligned} N(G) - W(G) &\geq N(S_n) - W(S_n) \\ &= 2^{n-1} + n - 1 - (n-1)^2 > 0. \end{aligned}$$

The last inequality holds because the function $h(x) = 2^x + x - x^2 > 0$ with $x \geq 4$.

Case 2. $\Delta(G) < n - 1$.

In this case G is a 2-self-centered graph, that is, any vertex in G has eccentricity 2. We first claim that $\delta(G) \geq 2$. Otherwise, G has a pendant vertex v with $vu \in E(G)$. Then $\varepsilon_G(v) = \varepsilon_G(u) + 1$ as a clear contradiction. Next we prove that G contains no cut edge. Otherwise, assume that $e = v_1v_2$ is a cut edge of G with $G - v_1v_2 = G_1 \cup G_2$ such that $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Considering that $\delta(G) \geq 2$, we have $V(G_1) \setminus \{v_1\} \neq \emptyset$ and $V(G_2) \setminus \{v_2\} \neq \emptyset$. Moreover, $\varepsilon_G(v_1) = 2 = \varepsilon_G(v_2)$ since $G \in \mathcal{G}_n^2$. Then the distance is 3 between any vertex in $V(G_1) \setminus \{v_1\}$ and any vertex in $V(G_2) \setminus \{v_2\}$, which is a clear contradiction. Therefore there does not exist any cut edge in G. From Lemma 3.1, we have $N(G) \geq n^2$. By Lemma 2.3, we have

$$\begin{aligned} N(G) - W(G) &\geq n^2 - n(n-1) + m \\ &= n + m > 0, \end{aligned}$$

completing the proof. ∎

Remark 3.3. A classical result from random graph theory asserts that almost every graph has diameter 2, *cf.* [6], p. 312, Exercise 7. From Theorem 3.2, $N(G) > W(G)$ holds for almost all graphs G.

A double star DS_{n_1,n_2} with $n_1 \leq n_2$ is a tree obtained by adding an edge at the central vertices of two stars S_{n_1+1} and S_{n_2+1}, respectively. Let $\mathcal{G}_n^{3(1)}$ and $\mathcal{G}_n^{3(0)}$ be the sets of n-vertex graphs with diameter 3 and at least one cut edge and the set of n-vertex ones with diameter 3 without any cut edge, respectively. Then $\mathcal{G}_n^3 = \mathcal{G}_n^{3(1)} \cup \mathcal{G}_n^{3(0)}$. By definitions, we have $W(\mathrm{DS}_{2,2}) = 29 > 28 = N(\mathrm{DS}_{2,2})$. We now turn to the comparison results of graphs in $\mathcal{G}_n^3$ with $n \geq 7$. Let $\mathcal{A}_n^0$ be the set connected of graphs of order n without any cut edge. Below we first prove a result on N.

Lemma 3.4. *Let $G \in \mathcal{A}_n^0 \setminus \{C_n\}$ with $n \geq 7$. Then $N(G) \geq \frac{3n^2}{2} - \frac{n}{2}$.*

Proof. Let $G \in \mathcal{A}_n^0 \setminus \{C_n\}$ with $u, v \in V(G)$ and denote by $\mathcal{T}(u,v)$ the set of three distinct subtrees containing vertices u and v in G. The set $\mathcal{T}(u,v)$ is *uniquely determined* by the pair $\{u,v\}$ or $\{u,v\}$-UD for short, if $\mathcal{T}(u,v) \cap \mathcal{T}(x,y) = \emptyset$ for two distinct vertex pairs $\{u,v\}$ and $\{x,y\}$ in $V(G)$. We first prove the existence of $\mathcal{T}(u,v)$ for any $\{u,v\} \subseteq V(G)$.

Let $\mathcal{V}_c$ be the set of cut vertices of G. Based on the value of $|\mathcal{V}_c|$, we divide the argument into the following two cases.

Case 1. $|\mathcal{V}_c| = 0$.

In this case, G is a 2-connected graph. For any two vertices $u, v \in V(G)$, there exist two internally vertex-disjoint paths, say P' and P'', that connect u and v in G. Since $G \ncong C_n$, there must be a vertex $x \in v(G)$ with $\deg_G(x) \geq 3$. Let $V_0 = V(P') \cup V(P'')$. Now we distinguish the following two subcases based on the position of x in G.

Subcase 1.1. $x \in V_0 \setminus \{u,v\}$.

In this subcase we assume, without loss of generality, that $x \in V(P')$ with a different vertex $y \in N_G(x)$ from two neighbors of x on P'. If $y \in V(P')$, we assume, w.l.o.g., that $y \in uP'x$. Then we select $\mathcal{T}(u,v) = \{P', P'', uP'yxP'v\}$. If $y \notin V(P')$, there is a y,v-path, say P^*, since $G - x$ is connected. Let z be the first vertex of P^* lying on P'. Then $\mathcal{T}(u,v) = \{P', P'', uP_1zP^*yxP'v\}$ if $z \in uP'x$ and $\mathcal{T}(u,v) = \{P', P'', uP_1xyP^*zP'v\}$ if $z \in xP'v$.

Subcase 1.2. $x \in \{u,v\}$.

In this subcase we assume, w.l.o.g., that $x = u$, that is, $\deg_G(u) \geq 3$ with a different vertex $u' \in N_G(u)$ from its two neighbors on P' and P'', respectively. If $u' \notin V_0$, then there is a u',v-path, say P^*, in G since $G-u$ is still connected. Then we select $\mathcal{T}(u,v) = \{P', P'', uu'P^*v\}$. While $u' \in V_0$, similar as Subcase 1.1, other than P' and P'', there is still another u,v-path P^{**} in G. Therefore we get $\mathcal{T}(u,v) = \{P', P'', P^{**}\}$.

Case 2. $|\mathcal{V}_c| \geq 1$.

In this case G contains at least two blocks that are maximal 2-connected subgraphs of G. Based on the positions of u and v in G, we divide into the following subcases.

Subcase 2.1. u and v lie on two distinct blocks of G.

Suppose that $u \in V(B_1)$ and $v \in V(B_2)$ where B_1 and B_2 are two distinct blocks of G. Then there must be $x \in \mathcal{V}_c \cap V(B_1)$ and $y \in \mathcal{V}_c \cap V(B_2)$ (possibly $x = y$) such that x and y lie on a u,v-geodesic of G. Note that B_1 and B_2 are blocks in G, that is, there are two distinct u,x-paths, say $P^{1,1}$, $P^{1,2}$, and another two distinct y,v-ones, say $P^{2,1}$, $P^{2,2}$, in G. Also there exists at least one x,y-path, say P^*, in G (P^* is just a single vertex if $x = y$). Then there are at least 4 distinct u,v-paths in G. Thus $\mathcal{T}(u,v)$ can be at least 4 choices by removing one u,v-path from these above 4 ones.

Subcase 2.2. u and v lie on a same block of G.

In this subcase we assume that u and v belong to a block B of G. Based on the property of B, we consider the following subcases.

Subcase 2.2.1. B is not a cycle.

Note that B is a 2-connected subgraph of G. By a similar reasoning as that in Case 1, we can get $\mathcal{T}(u,v) = \{P', P'', P^\dagger\}$ composed of three distinct u,v-paths in B.

Subcase 2.2.2. B is a cycle.

In this case $V(B)$ can be partitioned into $V(P')$ and $V(P'')$ where P' and P'' are two u,v-paths in B. According with the statuses of u and v, we only need to consider the following subcases.

Subcase 2.2.2.1. At least one vertex of u and v is a cut vertex in B.

We assume, w.l.o.g., that v is a cut vertex in B with $vz \in E(G)$ such that $z \in V(B')$ where B' is a different block of G from B. Then $\mathcal{T}(u,v) = \{P', P'', uP'vz\}$.

Subcase 2.2.2.2. Neither u and v is a cut vertex in B.

In this subcase there must be a cut vertex, say y, lying on one path, say P', of P' and P''. Assume that $z \in V(B')$ is a neighbor of y where $B' \neq B$ is a block of G. Denote by T^* a tree obtained from P' by attaching a pendant vertex z at y. Then $\mathcal{T}(u,v)=\{P',P'',T^*\}$. This completes the proof of existence $\mathcal{T}(u,v)$ consisting of three distinct subtrees for any $\{u,v\}\subseteq V(G)$.

Next we prove the $\{u,v\}$-UD property of $\mathcal{T}(u,v)$ for any $\{u,v\}\subseteq V(G)$.

Assume that $\{x_1,y_1\}\subseteq V(G)$ and $\{x_2,y_2\}\subseteq V(G)$ with $\{x_1,y_1\}\neq\{x_2,y_2\}$. Next it suffices to prove that $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$. Note that all subtrees in $\mathcal{T}(u,v)$ are u,v-paths listed in Case 1, or Subcase 2.1, or Subcase 2.2.1. Then $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$ holds if both $\{x_1,y_1\}$ and $\{x_2,y_2\}$ satisfy the assumptions in one of (sub)cases: Case 1, Subcase 2.1 and Subcase 2.2.1. Note that $\mathcal{T}(u,v)$ in Subcase 2.2.2.1 consists of two u,v-paths and another u,x-path with a cut vertex v as a neighbor of x, and, in Subcase 2.2.2.2, it consists of two u,v-paths and another starlike tree obtained by attaching a pendant vertex at a cut vertex of one of these u,v-paths. Similarly as above, $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$ if both $\{x_1,y_1\}$ and $\{x_2,y_2\}$ satisfy the assumptions in Subcase 2.2.2.1 or 2.2.2.2.

Assume that $\{x_1,y_1\}$ satisfies the assumptions in one of subcases: Subcase 2.1 and Subcase 2.2.1. Now we consider the position of the pair $\{x_2,y_2\}$. If $\{x_2,y_2\}$ satisfies the assumptions in Subcase 2.2.2.1, we can assume that $\{x_2,y_2\}\subseteq V(B)$ and y_2 is a cut vertex with a neighbor $z\in V(B')$ where B, B' are two distinct blocks in G. The only worst possibility that $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)\neq\emptyset$ is that $x_1=x_2$ and $y_1=z$ where $\{x_1,y_1\}$ satisfies the assumptions in Subcase 2.1. But, from the selecting rule of $\mathcal{T}(x_1,y_1)$ (with 4 choices), we can select one $\mathcal{T}(x_1,y_1)$ such that $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$. If $\{x_2,y_2\}$ satisfies the assumptions in Subcase 2.2.2.2, then $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$ from the selecting rules of $\mathcal{T}(x_1,y_1)$ and $\mathcal{T}(x_2,y_2)$. Finally we suppose that $\{x_1,y_1\}$ and $\{x_2,y_2\}$ satisfy the assumptions of Subcases 2.2.2.1 and 2.2.2.2, respectively. Then $\mathcal{T}(x_1,y_1)\cap\mathcal{T}(x_2,y_2)=\emptyset$ from the selecting rules of $\mathcal{T}(x_1,y_1)$ and $\mathcal{T}(x_2,y_2)$. This completes the proof of $\{u,v\}$-UD property of $\mathcal{T}(u,v)$ for any $\{u,v\}\subseteq V(G)$.

Therefore, the number of subtrees containing two distinct vertices of G is at least $3\binom{n}{2}=\frac{3n^2-3n}{2}$. Moreover, each single vertex is also a subtree in G. Therefore, we have

$$\begin{aligned}N(G)&\geq n+\frac{3n^2-3n}{2}\\&=\frac{3n^2}{2}-\frac{n}{2},\end{aligned}$$

completing the proof. ∎

Since $\mathcal{G}_n^{3(0)}\setminus\{C_6,C_7\}\subseteq\mathcal{A}_n^0\setminus\{C_n\}$, from Lemma 3.4, we have the following result.

Corollary 3.5. *For any graph $G\in\mathcal{G}_n^{3(0)}\setminus\{C_6,C_7\}$, we have $N(G)\geq\frac{3n^2}{2}-\frac{n}{2}$.*

Theorem 3.6. *Let $G\in\mathcal{G}_n^{3(0)}$ with $n\geq 7$. Then $N(G)>W(G)$.*

Proof. For any vertex $v\in V(G)$, we have $\varepsilon_G(v)\in\{2,3\}$ and $Tr_G(v)=2n-2-\deg_G(v)$ if $\varepsilon_G(v)=2$ or

$$\begin{aligned}Tr_G(v)&\leq\deg_G(v)+2\times 1+3\Big[n-2-\deg_G(v)\Big]\\&=3n-4-2\deg_G(v)\end{aligned}$$

if $\varepsilon_G(v)=3$. Therefore $Tr_G(v)\leq 3n-4-2\deg_G(v)$ for any vertex $v\in V(G)$ since $2n-2-\deg_G(v)\leq 3n-4-2\deg_G(v)$ from the fact $\deg_G(v)\leq n-2$. Assume that $m(G)=m$. Then, from Equality (1.2), we have

$$\begin{aligned}W(G)&\leq\frac{1}{2}(3n-4)n-\sum_{v\in V(G)}\deg_G(v)\\&=\frac{3n^2}{2}-2(n+m).\end{aligned}$$

By Corollary 3.5, we have $N(G)-W(G)\geq 2m+\frac{3n}{2}>0$ for any $G\in\mathcal{G}_n^{3(0)}\setminus\{C_7\}$ with $n\geq 7$. Moreover, we have $N(C_7)=49>42=W(C_7)$, completing the proof. ∎

Before doing it, we list the following elementary results, omitting the proofs.

Lemma 3.7. *Let $f(x) = 2^x - x^2$ with $x \geq 4$. Then $f(x) \geq 0$ for any $x \geq 4$.*

Lemma 3.8. *Let $g(x,y) = 2^x + 2^y - 2xy$ with $x > 0$ and $y > 0$. If $x+y = n \geq 7$, then $g(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor) \geq 0$.*

In the following we provide a lower bound on the number of subtrees of graphs with diameter 2 or 3 containing a specific vertex.

Lemma 3.9. *Let $G \in \mathcal{G}_n^2 \cup \mathcal{G}_n^3$ without any non-pendant cut edge and $v \in V(G)$ of degree 2 with $\varepsilon_G(v) = 2$. Then $N(v,G) \geq 2^{n-3} + 2\sqrt{2}^{n-3} + 3$.*

Proof. Assume that $N_G(v) = \{x, y\}$. Since $\varepsilon_G(v) = 2$, $N_G[x] \cup N_G[y] = V(G)$. Denote by $P = xvy$ a subtree of G which is just a path of order 3. Therefore, we have $N(P,G) \geq 2^{n-3}$ where P is viewed as a single part with the remaining $n-3$ vertices attached at x or/and y in G. Note that $N_G(x) \setminus \{v\} \neq \emptyset$ and $N_G(y) \setminus \{v\} \neq \emptyset$ since G contains no non-pendant cut edge. Thus the edges vx and vy lie on a common cycle, say C, in G. Then there are at least two subtrees containing v that are obtained by removing the edges vx and vy, respectively, from a spanning unicyclic subgraph of G including C. Therefore $N(v,x,y;G) \geq 2^{n-3} + 2$.

Assume that $|N_G(x) \setminus \{v,y\}| = n_1$ and $|N_G(y) \setminus \{v,x\}| = n_2$. Then $n_1 + n_2 \geq n-3$. Similarly as above, we have $N(\overline{y}, v, x; G) \geq 2^{n_1}$ and $N(\overline{x}, v, y; G) \geq 2^{n_2}$. It follows that

$$\begin{aligned} N(v,G) &= N(v,x,y;G) + N(\overline{y},v,x;G) + N(\overline{x},v,y;G) + N(\overline{x},\overline{y},v;G) \\ &\geq 2^{n-3} + 2 + 2^{n_1} + 2^{n_2} + 1 \\ &\geq 2^{n-3} + 2\sqrt{2}^{n-3} + 3, \end{aligned}$$

completing the proof. □

Theorem 3.10. *Let $G \in \mathcal{G}_n^{3(1)}$ with $n \geq 7$. Then $N(G) > W(G)$.*

Proof. Based on the statuses of cut edges in $G \in \mathcal{G}_n^{3(1)}$, we divide into the following cases.

Case 1. There is a non-pendant cut edge, say v_1v_2, in G.

In this case, we assume that $G - v_1v_2 = G_1 \cup G_2$. Then G can be viewed as the v_1v_2-link graph of graphs G_1 and G_2 of order n_1 and n_2, respectively, with $n_1 + n_2 = n$. Since $G \in \mathcal{G}_n^{3(1)}$, v_1 and v_2 are universal vertices in G_1 and G_2, respectively, with $\varepsilon_G(v_1) = \varepsilon_G(v_2) = 2$. Then $\mathrm{DS}_{n_1-1,n_2-1}$ is the spanning subgraph of G with $n_1 + n_2 = n$. From Lemma 2.2, it suffices to prove $N(\mathrm{DS}_{n_1-1,n_2-1}) > W(\mathrm{DS}_{n_1-1,n_2-1})$. Setting $A = N(\mathrm{DS}_{n_1-1,n_2-1}) - W(\mathrm{DS}_{n_1-1,n_2-1})$, by Lemmas 2.8, 3.7 and 3.8, we have

$$\begin{aligned} A &= 2^{n_1-1} + n_1 - 1 + 2^{n_2-1} + n_2 - 1 + 2^{n_1+n_2-2} - (n_1-1)^2 - (n_2-1)^2 - n_2(n_1-1) - n_1(n_2-1) - n_1n_2 \\ &= 2^{n-2} - (n-2)^2 + \frac{1}{2}(2^{n_1} + 2^{n_2} - 2n_1n_2) > 0. \end{aligned}$$

Case 2. Any cut edge is pendant in G.

In this case, we prove the result by induction on p, the number of pendant cut edges in G. If $p = 1$, without loss of generality, we assume that v_1v_2 is the pendant cut edge with pendant vertex v_2 and $G_1 = G - v_2$. From the structure of G, we have $G_1 \in \mathcal{G}_{n-1}^2 \cup \mathcal{G}_{n-1}^3$ with $\varepsilon_{G_1}(v_1) = 2$. Assume that $\deg_{G_1}(v_1) = k$, which yields $Tr_{G_1}(v_1) = k + 2(n-2-k) = 2n-4-k$ with $k \leq n-3$. By Lemma 2.8, we have

$$\begin{aligned} W(G) &= W(G_1) + n - 1 + Tr_{G_1}(v_1), \\ N(G) &= N(G_1) + 1 + N(v_1, G_1). \end{aligned}$$

Then it follows that

$$N(G) - W(G) = N(G_1) - W(G_1) + N(v_1, G_1) - Tr_{G_1}(v_1) - (n-2). \tag{3.1}$$

Since G has no any non-pendant cut edge, we have $k \geq 2$. If $k = 2$, by Lemma 3.9, we have $N(v_1, G_1) \geq 2^{n-4} + 2\sqrt{2}^{n-4} + 3$. Moreover, $Tr_{G_1}(v_1) = 2n - 6$. Note that $2^{n-4} + 2\sqrt{2}^{n-4} + 3 > 3n - 8$ for $n \geq 4$ since the function $\varphi(x) = 2^x + 2\sqrt{2}^x - 3x - 1 > 0$ for $x \geq 0$. In view of Equality (3.1), we have

$$\begin{aligned} N(G) - W(G) &> N(G_1) - W(G_1) + 2^{n-4} + 2\sqrt{2}^{n-4} + 3 - (3n-8) \\ &> N(G_1) - W(G_1). \end{aligned} \tag{3.2}$$

If $k \geq 3$, combining Equality (3.1), Lemma 2.7 (i) and the fact $Tr_{G_1}(v_1) = 2n - 4 - k$ with $k \leq n - 3$, we have

$$\begin{aligned} N(G) - W(G) &= N(G_1) - W(G_1) + (2^{k-1} - 3)(n-k) - (2k-6) \\ &\geq N(G_1) - W(G_1) + 3(2^{k-1} - 3) - (2k-6) \\ &> N(G_1) - W(G_1). \end{aligned} \tag{3.3}$$

Since $G_1 \in \mathcal{G}_{n-1}^2 \cup \mathcal{G}_{n-1}^3$ without any cut edge, $N(G_1) > W(G_1)$ holds in (3.2) and (3.3) from Lemmas 3.2 and 3.6. Thus $N(G) > W(G)$ for any $G \in \mathcal{G}_n^{3(1)}$ with one pendant cut edge.

Next we assume that $p > 1$ and $N(G') > W(G')$ for any $G' \in \mathcal{G}_n^{3(1)}$ with $p - 1$ pendant cut edge(s). Let $G \in \mathcal{G}_n^{3(1)}$ with p pendant cut edges. As the induction basis, $N(G) > W(G)$ can be routinely checked for any graph $G \in \mathcal{G}_n^{3(1)}$ with $n = 6$ by computer search. By a same reasoning as that in the proof of Inequalities (3.2), (3.3) and the induction hypothesis, we have

$$N(G) - W(G) > N(G') - W(G') > 0,$$

completing the proof. □

Combining Theorems 3.6 and 3.10, we have the following result.

Theorem 3.11. *For any graph $G \in \mathcal{G}_n^3$ with $n \geq 7$, we have $N(G) > W(G)$.*

A *broom* $B_{n,k}$ is a tree obtained by attaching k pendant vertices to a leaf of path P_{n-k}. Note that the property $N(G) > W(G)$ cannot be extended to the graphs with diameter 4. Clearly, $B_{n,n-4}$ has diameter 4. As two examples, we have $N(B_{6,2}) = 24 < 32 = W(B_{6,2})$ and $N(B_{7,3}) = 41 < 46 = W(B_{7,3})$ from some calculations. Other comparison results of general brooms will be presented in Section 4.

3.2. Graphs with large diameters

In this section we provide some graphs with $N > W$ and large diameters.

Let G_0 be a graph of order 5 consisting of two triangles which intersect at one vertex v. Observe that G_0 contains two pairs of non-adjacent vertices v_1, v_1' and v_2, v_2' of degrees 2. Then $L(H(n_1, n_2; 1; n_1, n_2))$ with $n_1 \leq n_2$ can be obtained by attaching at each of v_1 and v_1' in G_0 a pendant path of length $n_1 - 1$ and at each of v_2 and v_2' in it a pendant path of length $n_2 - 1$. Note that $L(H(n_1, n_2; 1; n_1, n_2))$ has order $n = 2(n_1 + n_2) + 1$ and diameter $d = 2n_2 \geq \frac{n-1}{2}$.

Theorem 3.12. *Let $G = L(H(n_1, n_2; 1; n_1, n_2))$ defined as above with $2 \leq n_1 \leq n_2$. If $n_2 \leq n_1 + 19$, then we have $N(G) > W(G)$.*

Proof. Note that $H(n_1,n_2;1;n_1,n_2)$ has order $n=2(n_1+n_2)+2$. Then we have

$$\begin{aligned} W(G) &= W(H(n_1,n_2;1;n_1,n_2)) - \binom{n}{2} \\ &= \binom{2n_1+2n_2+3}{3} - 2(n_1+n_2+1)n_1n_2 - \binom{2n_1+2n_2+2}{2} \\ &= \binom{2n_1+2n_2+2}{3} - 2(n_1+n_2+1)n_1n_2 \end{aligned}$$

from Lemmas 2.6 and 2.5. Note that $N(G-v)=2N(P_{n_1+n_2})=(n_1+n_2+1)(n_1+n_2)$. Since $G-v$ consists of two copies of $P_{n_1+n_2}$, there exist $1+n_1+n_2+3n_1n_2$ subtrees counted in $N(v,G)$ which are formed of v and other vertices in exactly one copy of $P_{n_1+n_2}$. Thus we have $N(v,G)=(1+n_1+n_2+3n_1n_2)^2$. Then it follows from Equality (2.3) that $N(G)=(1+n_1+n_2+3n_1n_2)^2+(n_1+n_2+1)(n_1+n_2)$. Note that $n_1n_2\geq n_1+n_2$ for $2\leq n_1\leq n_2$. Setting $A=N(G)-W(G)$. Therefore,

$$\begin{aligned} A &= (1+n_1+n_2+3n_1n_2)^2+(n_1+n_2+1)(n_1+n_2+2n_1n_2) - \binom{2n_1+2n_2+2}{3} \\ &= 9n_1^2n_2^2+8n_1n_2(n_1+n_2+1)+(n_1+n_2+1)^2-(n_1+n_2+1)(n_1+n_2)\left[1-\frac{2(2n_1+2n_2+1)}{3}\right] \\ &= 9n_1^2n_2^2+8n_1n_2(n_1+n_2+1)+\frac{7(n_1+n_2)}{3}+1-\frac{4(n_1+n_2)^3}{3} \\ &> n_1n_2(9n_1n_2+8)-(n_1+n_2)\left[\frac{4}{3}(n_1+n_2)^2-8n_1n_2-\frac{7}{3}\right] \\ &> \frac{n_1n_2}{3}[-4(n_1-n_2)^2+35n_1n_2+31]. \end{aligned}$$

Assume that $n_2-n_1=t$. It can be routinely checked that $4t^2-70t-171<0$, that is, $4t^2-31<70(2+t)$, if $0\leq t\leq 19$. Equivalently, we have $4(n_1-n_2)^2-31\leq n_1(n_1+t)$, that is, $4(n_1-n_2)^2-35n_1n_2-31<0$ if $0\leq n_2-n_1\leq 9$ with $n_1\geq 2$. Therefore $N(G)>W(G)$ as desired. □

For a graph G with $e\in E(G)$, the *partial subdivision graph* $S_e(G)$ on e is a graph obtained by subdividing the edge e, that is, inserting a vertex of degree 2 adjacent to two ends of e of G. Next we construct more new graphs with $N>W$ from some known ones of this kind.

Theorem 3.13. *Let G_1 and G_2 be two connected graphs of order $n\geq 16$ such that $N(G_i)\geq W(G_i)$ for $i\in\{1,2\}$. Assume that v_1, v_2 are two vertices of degrees $k_1\geq\frac{n}{2}$ and $k_2\geq\frac{n}{2}$ in G_1 and G_2, respectively. Let $G=G_1v_1\smile v_2G_2$. Then $N(G)>W(G)$ and $N(S_e(G))>W(S_e(G))$ where $e=v_1v_2$.*

Proof. Let $V_1\subseteq V(G_1)$ and $V_2\subseteq V(G_2)$ be the sets of vertices of degrees k_1 and k_2 in G_1 and G_2, respectively. Thus $v_i\in V_i$ for $i\in[2]$. By Lemma 2.7, we have, for $i\in[2]$,

$$\begin{aligned} N(v_i,G_i)-Tr_{G_i}(v_i) &\geq \min_{v_p\in V_i}\{N(v_p,G_i)\}-\max_{v_q\in V_i}\{Tr_{G_i}(v_q)\} \\ &\geq 2^{k_i-1}(n-k_i+1)-\left[k_i-1+\frac{(n-k_i)(n-k_i+1)}{2}\right] \\ &= 2^{k_i-1}(n-k_i+1)-\frac{k_i^2}{2}+\frac{2n-1}{2}k_i-\frac{(n-1)(n+2)}{2}. \end{aligned}$$

Define a function $f(x)=2^{x-1}(n-x+1)-\frac{x^2}{2}+\frac{2n-1}{2}x-\frac{(n-1)(n+2)}{2}$ with $x\geq\frac{n}{2}$. Taking the first differential, we have $f'(x)=2^{x-1}\Big[(n-x+1)ln2-1\Big]+n-x-\frac{1}{2}>0$. Therefore $f(x)$ is strictly increasing for $x\geq\frac{n}{2}$. Thus it follows that $f(x)$ attains its minimum $f(\frac{n}{2}) = 2^{\frac{n}{2}-1}(\frac{n}{2}+1) - \frac{n^2+6n-8}{8}$ uniquely at $x = \frac{n}{2}$. Note that

$$\begin{aligned}
f\Big(\frac{n}{2}\Big) - \left[\frac{(n+1)^2}{2} - 1\right] &= 2^{\frac{n}{2}-1}\Big(\frac{n}{2}+1\Big) - \frac{n^2+6n-8}{8} - \frac{(n+1)^2}{2} + 1 \\
&= 2^{\frac{n}{2}-1}\Big(\frac{n}{2}+1\Big) - \frac{5n^2+14n-12}{8} \\
&> \binom{\frac{n}{2}-1}{2}\Big(\frac{n}{2}+1\Big) - \frac{5n^2+14n-12}{8} \\
&= \frac{(n^2-4)(n-4) - 10n^2 - 28n + 24}{16} \\
&= \frac{n^3 - 14n^2 - 32n + 40}{16} \geq 0
\end{aligned}$$

for $n \geq 16$. Therefore we have, for $i \in [2]$,

$$N(v_i, G_i) - Tr_{G_i}(v_i) > \frac{(n+1)^2}{2} - 1. \tag{3.4}$$

Since $\frac{(n+1)^2}{2} - 1 > n$, we have, for $i \in [2]$,

$$N(v_i, G_i) - Tr_{G_i}(v_i) > n. \tag{3.5}$$

From the structure of $G = G_1 v_1 \smile v_2 G_2$ and Lemma 2.8, we have

$$\begin{aligned}
W(G) &= W(G_1) + W(G_2) + n(Tr_{G_1}(v_1) + Tr_{G_2}(v_2)) + n^2, \quad \text{and} \\
N(G) &= N(G_1) + N(G_2) + N(v_1, G_1)N(v_2, G_2).
\end{aligned}$$

Thus, by Inequalities (3.5) for $i \in [2]$ and the assumptions, we get

$$\begin{aligned}
N(G) - W(G) &> N(G_1) - W(G_1) + N(G_1) - W(G_2) + (Tr_{G_1}(v_1) + n)(Tr_{G_2}(v_2) + n) \\
&\quad - n(Tr_{G_1}(v_1) + Tr_{G_2}(v_2)) - n^2 \\
&\geq Tr_{G_1}(v_1)Tr_{G_2}(v_2) > 0.
\end{aligned}$$

Assume that $V(S_e(G)) \setminus V(G) = \{v\}$, that is, v is the newly inserted vertex from G to $S_e(G)$. From the structure of $S_e(G)$, we have

$$\begin{aligned}
W(S_e(G)) &= W(G_1) + W(G_2) + \sum_{x \in V(G_1)} d_G(v, x) + \sum_{y \in V(G_2)} d_G(v, y) \\
&\quad + \sum_{x \in V(G_1), y \in V(G_2)} [d_{G_1}(x, v_1) + 2 + d_{G_2}(v_2, y)] \\
&= \sum_{i=1}^{2} W(G_i) + \sum_{i=1}^{2} Tr_{G_i}(v_i) + 2n + n[Tr_{G_1}(v_1) + Tr_{G_2}(v_2)] + 2n^2 \\
&= W(G) + Tr_{G_1}(v_1) + Tr_{G_2}(v_2) + 2n + n^2, \quad \text{and} \\
N(S_e(G)) &= N(G_1) + N(G_2) + 1 + N(v_1, G_1) + N(v_2, G_2) + N(v_1, G_1)N(v_2, G_2) \\
&= N(G) + 1 + N(v_1, G_1) + N(v_2, G_2).
\end{aligned}$$

Combining Inequalities (3.4) for $i \in [2]$ with the above result $N(G) > W(G)$, we have

$$\begin{aligned}
N(S_e(G)) - W(S_e(G)) &= N(G) - W(G) + 2 + N(v_1, G_1) + N(v_2, G_2) - Tr_{G_1}(v_1) - Tr_{G_2}(v_2) - (n+1)^2 \\
&> 0,
\end{aligned}$$

completing the proof. □

From Theorem 3.13, we arrive at the following remark.

Remark 3.14. For two connected graphs G_1 and G_2 of order $n \geq 16$ with $N(G_i) \geq W(G_i)$ and $v_i \in V(G_i)$ for $i \in [2]$, if v_1, v_2 are two diametrical vertices of degrees $k_1 \geq \frac{n}{2}$ and $k_2 \geq \frac{n}{2}$ in G_1 and G_2, respectively, then both the graphs $G = G_1 v_1 \smile v_2 G_2$ and $S_e(G)$ have the property $N > W$ with larger diameters where $e = v_1 v_2$.

4. Graphs with $W > N$

In this section we will present some graphs with $N < W$.

Theorem 4.1. *Let $T = T(n_1, n_2, n_3)$ defined as above with $n_1+n_2+n_3 > 3$. Then $W(T)-N(T) > 0$. Moreover, $W(T) - N(T) > \frac{(n_1+n_2)^2-9}{2} - \frac{4(n_1+n_2+3)}{3} > \frac{3}{2}$ if $n_1 + n_2 \geq 6$.*

Proof. Let v be the vertex with $\deg_T(v) = 3$ in T. Then we have $T - v = \bigcup_{i=1}^{3} P_{n_i}$ with $n = n_1 + n_2 + n_3 + 1$. From Equality (2.3) on the vertex v and Lemma 2.4, we have

$$\begin{aligned} N(T) &= N(v,T) + N(T-v) \\ &= (n_1+1)(n_2+1)(n_3+1) + \sum_{i=1}^{3} \binom{n_i+1}{2}. \end{aligned}$$

By Lemma 2.5, we have

$$\begin{aligned} W(T) &= \binom{n+1}{3} - n_1 n_2 n_3 \\ &= \binom{n_1+n_2+n_3+1}{3} + \binom{n_1+n_2+n_3+1}{2} - n_1 n_2 n_3. \end{aligned}$$

Setting $A = W(T) - N(T)$, then we have

$$\begin{aligned} A &= \binom{n_1+n_2+n_3+1}{3} - 2n_1n_2n_3 - (n_1+n_2+n_3) - 1 \\ &= \binom{n}{3} - n - 2n_1n_2n_3 \\ &= \frac{(n-4)n(n+1)}{6} - 2n_1n_2n_3. \end{aligned}$$

Note that $n_1n_2n_3$ reaches its maximum with $n_1 + n_2 + n_3 = n - 1$ if and only if $|n_i - n_j| \leq 1$ for $i, j \in [3]$.
Therefore $n_1n_2n_3 \leq \begin{cases} \frac{(n+1)^2(n-2)}{27}, n \equiv 0 (\bmod\ 3)\,; \\ \frac{(n-1)^3}{27}, n \equiv 1 (\bmod\ 3)\,; \\ \frac{(n+1)(n-2)^2}{27}, n \equiv 2 (\bmod\ 3)\,. \end{cases}$ Then

$$\begin{aligned} A &= \frac{(n-4)n(n+1)}{6} - 2n_1n_2n_3 \\ &\geq \frac{(n-4)n(n+1)}{6} - \frac{2(n+1)^2(n-2)}{27} \\ &= \frac{(n+1)(5n^2-32n+8)}{54} > 0 \end{aligned}$$

for $n \geq 7$. Furthermore, it can be routinely verified that $A > 0$ for $n \in \{5, 6\}$.

Next we turn to prove $W(T)-N(T) > \frac{(n_1+n_2)^2-9}{2} - \frac{4(n_1+n_2+3)}{3} > \frac{3}{2}$ if $n_1+n_2 \geq 6$. To do it, we first define a function $f(x) = \frac{(x+1)(5x^2-32x+8)}{54}$ with $x \geq 4$. Taking the first differential, we have $f'(x) = \frac{(5x+2)(x-4)}{18} \geq 0$. Hence $f(x)$ is increasing when $x \geq 4$. Then we arrive at $A = f(n) \geq f(n_1+n_2+2)$ since $n_3 \geq 1$. Setting $y = n_1+n_2$, then $f(n_1+n_2+2) = \frac{(y+3)(5y^2-12y-36)}{54}$. Define another function $h(y) = \frac{(y+3)(5y^2-12y-36)}{54}$ with $y \geq 2$. Therefore, we have $A \geq h(y)$ with $y \geq 2$. Since $5y^2-39y+117 > 0$ for $y \geq 6$, we have $\frac{5y^2-12y-36}{54} > \frac{y-3}{2} - \frac{4}{3}$ for $y \geq 6$. Then it follows that

$$\begin{aligned} A \geq h(y) &> \frac{y^2-9}{2} - \frac{4(y+3)}{3} \\ &= \frac{3y^2-8y-51}{6} \geq \frac{3}{2} \end{aligned}$$

for $y \geq 6$. This completes the proof. □

Recall that the brrom $B_{n,k}$ is a tree obtained by attaching k pendant vertices to a leaf of path P_{n-k}. Below we present the brooms with $W > N$.

Theorem 4.2. *Let $T = B_{n,k}$ be a broom with $2 \leq k \leq \log_2 n - 1$. Then $W(T) > N(T)$.*

Proof. Since the result holds for $k = 2$ from Theorem 4.1, we assume that $k \geq 3$ in the following. From the structure of T and Lemma 2.5, we have

$$W(T) = \binom{n+1}{3} - \binom{k}{3} - (n-k-1)\binom{k}{2}.$$

Assume that v is the vertex of degree $k+1$ in T. Based on Equality (2.3) and the fact $N(P_n) = \binom{n+1}{2}$, we have

$$\begin{aligned} N(T) &= N(v,T) + N(T-v) \\ &= 2^k(n-k) + k + \binom{n-k}{2}. \end{aligned}$$

From the assumption $2 \leq k \leq \log_2 n - 1$, that is, $2^k \leq \frac{n}{2}$, it follows that

$$\begin{aligned} W(T) - N(T) &= \frac{n(n^2-1)}{6} - \frac{k(k^2-3k+8)}{6} - \frac{n+k^2-2k}{2}(n-1-k) - 2^k(n-k) \\ &= \frac{n(n^2-1)}{6} - \frac{n^2}{2} - 2^k n - \frac{k^2-3k-1}{2}n + \frac{k(k^2-7)}{3} + k2^k \\ &> \frac{n(n^2-1)}{6} - n^2 - \frac{n^2}{4} \quad \text{as } k^2-3k-1 < k^2-1 < 2^k \text{ for } k \geq 3 \\ &= \frac{n(2n^2-15n-2)}{12} > 0. \end{aligned}$$

Note that the last inequality holds for any $n \geq 8$ since $2 \leq \log_2 n - 1$. □

Next we construct a class of chemical trees with $W > N$ with two 3-degree vertices. Before doing it, we need a preliminary result as follows.

Lemma 4.3. *Let G be a connected graph of order n with a pendant vertex $u \in V(G)$ and G^* be a new graph obtained by attaching two pendant vertices to the vertex u of G. Then $W(G^*) = W(G) + 2Tr_G(u) + 2n + 2$.*

Proof. Assume that $V(G^*) \setminus V(G) = \{v, v'\}$. From the structure of G^*, we have

$$\begin{aligned} W(G^*) &= \sum_{\{x,y\}\subseteq V(G)} d_{G^*}(x,y) + 2\sum_{x\in V(G)} d_{G^*}(v,x) + d_{G^*}(v,v') \\ &= W(G) + 2\sum_{x\in V(G)} (d_G(u,x)+1) + 2 \\ &= W(G) + 2Tr_G(u) + 2n + 2, \end{aligned}$$

finishing the proof. □

Theorem 4.4. *Let $T = H(n_1, n_2, n_3, 1, 1)$ with $n_1 + n_2 + n_3 > 3$. Then $W(T) > N(T)$.*

Proof. Note that T has order $n = n_1 + n_2 + n_3 + 3$. Let u be a vertex of degree 3 in T with two leaf neighbors v and v' where $V_0 = \{v, v'\}$. Then $T \setminus V_0 = T(n_1, n_2, n_3)$ with $N(v, \overline{v'}; T) = N(\overline{v}, v'; T) = n_3 + 1 + (n_1 + 1)(n_2 + 1)$ and $N(v, v'; T) = n_3 + (n_1 + 1)(n_2 + 1)$ from the structure of T, which yield

$$\begin{aligned} N(T) &= N(T \setminus V_0) + N(V_0, T) \\ &= N(T(n_1,n_2,n_3)) + N\big(v, \overline{v'}; T\big) + N(\overline{v}, v'; T) + N(v, v'; T) \\ &= N(T(n_1,n_2,n_3)) + 3[n_3 + (n_1+1)(n_2+1)] + 2. \end{aligned}$$

Let $T_0 = T(n_1, n_2, n_3)$. Then $Tr_{T_0}(u) = \sum_{i=1}^{3} \binom{n_i}{2} + n_3(n_1 + n_2)$. By Lemma 4.3, we have

$$\begin{aligned} W(T) &= W(T_0) + 2n - 2 + 2Tr_{T_0}(u) \\ &= W(T_0) + 2(n_1+n_2+n_3) + 4 + \sum_{i=1}^{3} n_i(n_i+1) + 2n_3(n_1+n_2) \\ &= W(T_0) + (n_1+n_2+n_3+2)^2 - 2n_1n_2 - (n_1+n_2+n_3). \end{aligned}$$

Setting $A = W(T_0) - N(T_0)$ and $B = W(T) - N(T)$. Then we get

$$\begin{aligned} B &= A + (n_1+n_2+n_3+2)^2 - 2n_1n_2 - (n_1+n_2+n_3) - 3[n_3 + (n_1+1)(n_2+1)] - 2 \\ &= A + n_1^2 + n_2^2 - 3n_1n_2 + 2(n_1+n_2)n_3 + n_3^2 - 1 \\ &\geq A + 2(n_1+n_2) - n_1n_2. \end{aligned}$$

If $n_1 + n_2 \leq 5$, then $2(n_1 + n_2) - n_1n_2 > 0$ for $n_1 + n_2 \in \{2, 3, 4, 5\}$. Thus, from Theorem 4.1, $W(T) > N(T)$ follows. While $n_1 + n_2 \geq 6$, by Theorem 4.1, we have $A > n_1n_2 - \frac{4(n_1+n_2+3)}{3}$ since $n_1^2 + n_2^2 > 9$ for $n_1 + n_2 \geq 6$. Then, for $n_1 + n_2 \geq 6$,

$$\begin{aligned} B &> A + 2(n_1+n_2) - n_1n_2 \\ &\geq \frac{2(n_1+n_2)}{3} - 4 \geq 0. \end{aligned}$$

Our result holds from the argument in the two cases above. □

Below we provide a more generalized result than Theorem 4.4.

Theorem 4.5. *Let G be a connected graph of order n with a pendant vertex $u \in V(G)$ and G^* be a new graph obtained by attaching two pendant vertices v and v' to the vertex u of G. If $W(G) > N(G)$ with $2(Tr_G(u)+n) \geq 3N(u,G)$, then $W(G^*) > N(G^*)$.*

Proof. Let $V_0 = \{v, v'\}$. Then, by Equality (2.2), we have

$$\begin{aligned} N(G^*) &= N(G) + 2N(v, v'; G) + N(v, v'; G) \\ &= N(G) + 2(N(v, G) + 1) + N(v, G) \\ &\geq N(G) + 3N(v, G) + 2. \end{aligned}$$

From Lemma 4.3 and the assumptions, it follows that

$$W(G^*) - N(G^*) = W(G) - N(G) + 2(Tr_G(u) + n) \geq 3N(u, G) > 0.$$

□

Let $T = B_{n,k}$ be a broom with $v \in V(T)$ as a leaf farthest from the vertex of maximum degree $k+1$ and $B^*_{n,k}$ be a tree obtained from T by attaching two pendant vertices at v. Then, by elementary calculations, we have $Tr_T(v) = \frac{(n-k)(n+k-1)}{2}$ and $N(v, T) = 2^k(n-k)$. If $k \leq \log_2 \frac{n}{3}$, we have $2(Tr_T(v) + n) \geq 3N(v, T)$. Combining this fact with Theorem 4.2, we have $W(B^*_{n,k}) > N(B^*_{n,k})$ if $k \leq \log_2 \frac{n}{3}$.

Note that $W(C_n) = \frac{n}{2}\lfloor \frac{n^2}{4} \rfloor$ [26] and $N(C_n) = n^2$ [35]. So $W(C_n) > N(C_n)$ for $n > 8$. Next we provide a cycle-containing but non-cycle graph with $W > N$.

Theorem 4.6. *Let $G = L(T(1, n_1, n_2))$ with $n_1 + n_2 \geq 8$. Then $W(G) > N(G)$.*

Proof. By the structure of G, we can assume that v is the unique vertex of degree 2 in C_3 of G. Note that $T(1, n_1, n_2)$ has order $n = n_1 + n_2 + 2$. By Lemma 2.6, we have

$$\begin{aligned} W(G) &= W(T) - \binom{n}{2} \\ &= \binom{n+1}{3} - n_1 n_2 - \binom{n}{2} \\ &= \binom{n_1 + n_2 + 2}{3} - n_1 n_2. \end{aligned}$$

Moreover, we have $N(G - v) = N(P_{n_1+n_2}) = \binom{n_1+n_2+1}{2}$ and

$$\begin{aligned} N(v, G) &= 1 + N(\overline{v_1}, v_2, v; G) + N(\overline{v_2}, v_1, v; G) + N(v_1, v_2, v; G) \\ &= 1 + n_2 + n_1 + 3n_1 n_2. \end{aligned}$$

Then $N(G) = \binom{n_1+n_2+1}{2} + 1 + n_1 + n_2 + 3n_1 n_2$ holds from Equality (2.3). Therefore,

$$\begin{aligned} W(G) - N(G) &= \binom{n_1 + n_2 + 1}{3} - n_1 - n_2 - 1 - 4n_1 n_2 \\ &= \frac{(n_1 + n_2 + 1)(n_1 + n_2 - 3)(n_1 + n_2 + 2)}{6} - 4n_1 n_2 \\ &\geq (n_1 + n_2)^2 + 3(n_1 + n_2) + 2 - 4n_1 n_2 \\ &\geq 3(n_1 + n_2) + 2 > 0 \end{aligned}$$

for $n_1 + n_2 \geq 9$. Moreover, if $n_1 + n_2 = 8$, we have $W(G) - N(G) \geq 75 - 64 > 0$. □

5. Concluding remarks

In this paper we determine some graphs with $N > W$ and $W > N$, respectively. From the results obtained in Sections 3 and 4, we have an intuition that the more is the diameter of graph G, then the more possible is the conclusion $W(G) > N(G)$. Moreover, we have $W(G-e) > N(G-e)$ for any edge e of G if $W(G) > N(G)$. Therefore we pose the following problem.

Problem 5.1. *Determine a constant $d(n)$ such that $W(G) > N(G)$ and $W(T) > N(T)$ for any graph G with diameter at least $d(n)$ where T is a spanning tree of G.*

From Remark 3.3, we find that almost all graphs G satisfy $N(G) > W(G)$. Naturally we have the following problem.

Problem 5.2. *Characterize all the graphs G with $W(G) > N(G)$.*

Maybe the case of trees is a good point for solving Problem 5.2. From definitions, we have $N(P_4) = W(P_4) = 10$ and $N(C_8) = W(C_8) = 64$. Is there any other graph G with $N(G) = W(G)$ than P_4 and C_8? We would like to end up the paper with the following problem.

Problem 5.3. *Characterize all the graphs G with $W(G) = N(G)$.*

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