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On Subtrees of Fan Graphs, Wheel Graphs, and "Partitions" of Wheel Graphs Under Dynamic Evolution

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Abstract: The number of subtrees, or simply the subtree number, is one of the most studied counting-based graph invariants that has applications in many interdisciplinary fields such as phylogenetic reconstruction. Motivated from the study of graph surgeries on evolutionary dynamics, we consider the subtree problems of fan graphs, wheel graphs, and the class of graphs obtained from "partitioning" wheel graphs under dynamic evolution. The enumeration of these subtree numbers is done through the so-called subtree generation functions of graphs. With the enumerative result, we briefly explore the extremal problems in the corresponding class of graphs. Some interesting observations on the behavior of the subtree number are also presented.

Keywords: subtree; generating function; fan graph; wheel graph; "partitions" of wheel graph

1. Introduction

The study of graph invariants or topological indices has been proven to be of crucial importance in various interdisciplinary topics. Generally, the existing known topological indices could be divided into distance-based, degree-based, or structure-based ones; some of the studies on these three categories are referred to in [1–4] and the references therein. The number of subtrees, or simply the subtree number, is one of the counting-based graph invariants.

Finding and/or enumerating special topological structures or graph patterns has become an important problem due to their applications including, to name a few, frequent subgraphs mining [5], network optimization design [6,7], and local network reliability [8,9]. In particular, the subtree number has also been shown to be correlated to phylogenetic reconstruction [10] and various chemical indices such as the Wiener index (closely correlated with the boiling point of paraffin [3]), the Merrifield–Simmons index, and the Hosoya index [11]. Research results also show that there exists an amazing "negative correlation" between the number of subtrees and the Wiener index [12–17]. Therefore, the subtree number index can indirectly characterize the physical–chemical characteristics of molecules.

Various topics related to the subtree number have been explored over the past years, such as extremal problems [12,18,19], the subtree density problem [20–22], generic chemical structures storage problems [23,24], fault tolerant computing and parallel scheduling [25,26], recognition of substructure [27], simplification of the flow networks [28], Markovian queuing systems decomposition [29], and matching problems [30,31].

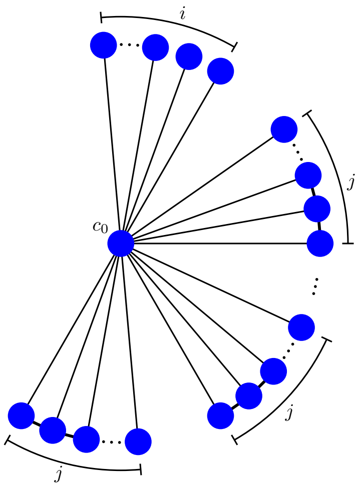
By using "generating functions", Yan and Yeh [4] presented a linear-time algorithm to evaluate the subtree weight sum of a tree, leading to an algorithmic approach to compute the subtree number of a tree. Following this approach and more recently, Yang et al. [32,33] proposed enumerating algorithms for BC-subtrees of trees, unicyclic, and edge-disjoint bicyclic graphs and computed the subtree number on spiro and polyphenyl hexagonal chains [17]. With structure mapping and weights transferring of cycles, Yang et al. [34] also presented enumerating algorithms for subtrees of hexagonal and phenylene chains. More recently, Chin et al. [35] presented the subtree number of complete graphs, complete bipartite graphs, and theta graphs, as well as the ratio of spanning trees to all subtrees of the above graphs.

Let $K_{1,n} = (V(K_{1,n}), E(K_{1,n}); f, g)$ be a weighted star on $n+1$ vertices with center c_0, vertex weight function $f(v) = y$ for all $v \in V(K_{1,n})$, and edge weight function $g(e) = z$ for all $e \in E(K_{1,n})$. Suppose the n leaves are labeled, in counterclockwise order, $c_1, c_2, \ldots, c_n$, then the wheel graph W_n is obtained from $K_{1,n}$ by adding the edges (c_i, c_{i+1}) for $i = 1, \ldots, n$ (here we let $c_{n+1} = c_1$).

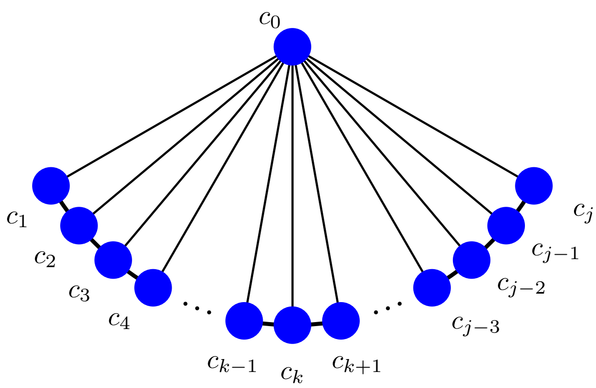
As is well known, star $K_{1,n}$ and wheel graphs W_n are very typical network topologies used in designing and implementing communication networks. The wheel graph W_n is the planar graph with a chromatic number not greater than 4. Specifically, the chromatic number of W_n is 3 for odd n and 4 for even n. Some researchers have tried to apply this property of W_n to prove the famous Four Color Theorem [36]. Moreover, W_n can also be used in wireless ad hoc networks [37]. Therefore, it is worth studying the new structural characteristics of these two graphs, especially from new perspectives.

Inspired by the significant effect of graph surgeries on evolutionary dynamics in [38], we are motivated to study the subtree number in graphs resulting from graph surgeries. In particular, we will consider a class of graphs that "lie in between" the fan and wheel graphs, called the "partitions" (explanation will be given later) of wheel graphs.

Definition 1. *Given the star $K_{1,n}$ on $n+1$ vertices defined above with center vertex c_0 and $0 \le j \le n$, the graph $K^j_{1,n}$ is obtained from $K_{1,n}$ by adding the edges (c_s, c_{s+1}) for all $1 \le s \le n-1$ except for $s = j, 2j, 3j, \ldots$ (see Figure 1a). If $n = j > 0$, we call $K^j_{1,j}$ the fan graph on $j+1$ vertices. It is also easy to see that $K^0_{1,0}$ is the single vertex c_0, and $K^1_{1,n}$ is the star $K_{1,n}$.*



(**a**) The graph $K^j_{1,n}$.



(**b**) The fan graph $K^j_{1,j}$.

Figure 1. The graph $K^j_{1,n}$ and the fan graph $K^j_{1,j}$.

From the definitions of the graph $K_{1,n}^{j}$ and the wheel graph W_n, we see that the graph $K_{1,n}^{j}$ can be vividly described in terms of W_n through "partitions" (and deletion of edges $\{(c_s, c_{s+1})|s = j, 2j, 3j, \ldots\}$) perspective.

The reason that we consider our graphs as vertex and edge weighted is to use the so-called subtree generating functions. We assume a graph $G = (V(G), E(G); f, g)$ to be a weighted graph and define the vertex-weight function $f : V(G) \to \Re$ and edge-weight function $g : E(G) \to \Re$, where $\Re$ is the real number. Unless otherwise noted, for a graph G, we initialize its vertex weight function $f(v) = y$ for each $v \in V(G)$ and its edge weight function $g(e) = z$ for each $e \in E(G)$ throughout this paper.

The following notations need to be listed before introducing the main tool:

- $G - X$ denotes the graph obtained from G by removing all elements of X;
- $S(G)$ (resp. $S(G; v)$) denotes the set of subtrees of G (resp. containing v);
- $S(G; (a, b))$ denotes the set of subtrees of G containing the edge (a, b);
- $\omega(T_1)$ denotes the weight of subtree $T_1 \in S(G)$;
- $F(\cdot)$ is the sum of weights of subtrees in $S(\cdot)$;
- $\eta(\cdot)$ is the cardinality (namely the number) of the corresponding $S(\cdot)$ set of subtrees.

We define the weight of a subtree T_s of G, denoted by $\omega(T_s)$, as the product of the weights of the vertices and edges in T_s. The generating function of subtrees of G, denoted by $F(G; f, g)$, is the sum of weights of subtrees of G. Namely, $F(G; f, g) = \sum\limits_{T_1 \in S(G)} \omega(T_1)$. Similarly, we define $F(G; f, g; v_i) = \sum\limits_{T_1 \in S(G; v_i)} \omega(T_1), F(G; f, g; (u, v)) = \sum\limits_{T_1 \in S(G;(u,v))} \omega(T_1)$.

By substituting each vertex weight $y = 1$ and edge weight $z = 1$ in these generating functions, we have the corresponding numbers of subtrees under various constraints, i.e., $\eta(T) = F(T; 1, 1), \eta(T; v_i) = F(T; 1, 1; v_i)$, and $\eta(T; (u, v)) = F(T; 1, 1; (u, v))$.

We introduce the following lemma, which will frequently be used in our work.

Lemma 1. *[4] Let P_n be a path on n vertices, with vertex weight function $f(v) = y$ for all $v \in V(P_n)$ and edge weight function $g(e) = z$ for all $e \in E(P_n)$, then $F(P_n; f, g) = \sum\limits_{t=0}^{n-1} (n - t) y^{t+1} z^t$.*

In Section 2, we will present the subtree generating functions of $K_{1,n}^{j} (1 \le j \le n)$ and the wheel graph W_n. Through using these generating functions and theoretical analysis, we study the extremal graphs, subtree fitting problems, and subtree density behaviors of these graphs in Section 3. Lastly, in Section 4, we summarize our results and comment on potential topics for future work.

2. Subtree Generating Functions of $K_{1,N}^{J} (1 \le J \le N)$ and Wheel Graph W_n

In this section, we will establish the subtree generating functions of $K_{1,n}^{j} (1 \le j \le n)$ and wheel graph W_n and provide the theoretical background for our computational analysis. We start by studying the subtree problem of $K_{1,n}^{j} (1 \le j \le n)$.

2.1. Subtree Generating Functions and Subtree Numbers of $K_{1,N}^{J}$

Theorem 1. *Let $K_{1,n}^{j}$ be the weighted graph defined as above, and n, j be non-negative integers with $0 \le j \le n$ and $n \equiv i \ (mod\ j)$. Then*

$$F(K_{1,n}^{j}; f, g) = F(K_{1,j}^{j}; f, g; c_0)^{\frac{n-i}{j}} * y(1 + yz)^i * y^{-\frac{n-i}{j}} + iy + \frac{n - i}{j} \sum_{t=0}^{j-1} (j - t) y^{t+1} z^t, \quad (1)$$

with $F(K_{1,j}^{j}; f, g; c_0) = F(K_{1,j-1}^{j-1}; f, g; c_0) + \sum_{r=1}^{j} r(yz)^r F(K_{1,j-r}^{j-r}; f, g; c_0)$, *and* $F(K_{1,0}^{0}; f, g; c_0) = y$, $F(K_{1,1}^{1}; f, g; c_0) = y + y^2 z$.

Proof. We consider the subtrees of $K_{1,n}^{j}$ by cases

(i) not containing the center c_0,
(ii) containing the center c_0.

From Lemma 1, we have the subtree generating function of case (i) as

$$\frac{n-i}{j}\sum_{t=0}^{j-1}(j-t)y^{t+1}z^t + iy. \tag{2}$$

With the contraction method of [4] and structure analysis, we have the subtree generating function of case (ii) as

$$F(K_{1,j}^{j}; f, g; c_0)^{\frac{n-i}{j}} * y(1+yz)^i * y^{-\frac{n-i}{j}}. \tag{3}$$

Denote $e_j = (c_0, c_j)$ and $\widetilde{e_j} = (c_{j-1}, c_j)$, and divide all subtrees for $S(K_{1,j}^{j}; c_0)$ (see Figure 1b) into four cases $S(K_{1,j}^{j}; c_0) = \mathcal{S}_1 \bigcup \mathcal{S}_2 \bigcup \mathcal{S}_3 \bigcup \mathcal{S}_4$ where

- $\mathcal{S}_1$ is the collection of subtrees that contain neither e_j nor $\widetilde{e_j}$;
- $\mathcal{S}_2$ is the collection of subtrees that contain e_j, but not $\widetilde{e_j}$;
- $\mathcal{S}_3$ is the collection of subtrees that contain $\widetilde{e_j}$, but not e_j;
- $\mathcal{S}_4$ is the collection of subtrees that contain both e_j and $\widetilde{e_j}$.

From the definitions of subtree weight and subtree generating function, we know that:
(a) $\mathcal{S}_1 = S(K_{1,j-1}^{j-1}; c_0)$;
(b) $\mathcal{S}_2 = \{T_1 + e_j | T_1 \in \mathcal{S}_1\}$, where $T_1 + e_j$ are the trees obtained from T_1 by attaching an edge e_j at vertex c_0;
(c) We can write $\mathcal{S}_3$ as

$$\mathcal{S}_3 = \{T + (c_0, c_{j-k}) + \bigcup_{h=2-k}^{r} (c_{j-k-h+1}, c_{j-k-h+2}) | T \in S(K_{1,j-k-r}^{j-k-r}; c_0)\} \tag{4}$$

for $k = 1, 2, \ldots, j-1$ and $r = 1, 2, \ldots, j-k$;
(d) For each subtree $T_4 \in \mathcal{S}_4$, we know that T_4 must not contain the edge (c_0, c_{j-1}). Consequently, we can further consider the subtrees that contain edges $(c_0, c_j) \bigcup_{r=1}^{k} (c_{j-r}, c_{j-r+1})$ but not (c_{j-k-1}, c_{j-k}) recursively for $k = 1, 2, \ldots, j-1$.
With (a)–(d),we have

$$\sum_{T_1 \in \mathcal{S}_1} \omega(T_1) = F(K_{1,j-1}^{j-1}; f, g; c_0), \tag{5}$$

$$\sum_{T_2 \in \mathcal{S}_2} \omega(T_2) = \sum_{T_1 \in \mathcal{S}_1} f(c_j) g(e_j) \omega(T_1) = yzF(K_{1,j-1}^{j-1}; f, g; c_0), \tag{6}$$

$$\begin{aligned}\sum_{T_3 \in \mathcal{S}_3} \omega(T_3) &= \sum_{k=1}^{j-1}\left(\sum_{r=1}^{j-k}\left[\prod_{h=2-k}^{r}\Big(f(c_{j-k-h+1}) g((c_{j-k-h+1}, c_{j-k-h+2}))\Big) f(c_j) g(c_0, c_{j-k}) F(K_{1,j-k-r}^{j-k-r}; f, g; c_0)\right]\right) \\ &= \sum_{k=1}^{j-1}\left(\sum_{r=1}^{j-k}(yz)^{r+k} F(K_{1,j-k-r}^{j-k-r}; f, g; c_0)\right),\end{aligned} \tag{7}$$

$$\begin{aligned}\sum_{T_4\in\mathcal{S}_4}\omega(T_4)&=f(c_j)g(e_j)\sum_{k=1}^{j-1}\left(\prod_{r=1}^{k}f(c_{j-r})g((c_{j-r},c_{j-r+1}))\right)F(K_{1,j-k-1}^{j-k-1};f,g;c_0)\\&=\sum_{k=1}^{j-1}(yz)^{k+1}F(K_{1,j-k-1}^{j-k-1};f,g;c_0).\end{aligned}\tag{8}$$

Hence, by Equations (5)–(8), we have

$$\begin{aligned}F(K_{1,j}^{j};f,g;c_0)&=\sum_{T_1\in\mathcal{S}_1}\omega(T_1)+\sum_{T_2\in\mathcal{S}_2}\omega(T_2)+\sum_{T_3\in\mathcal{S}_3}\omega(T_3)+\sum_{T_4\in\mathcal{S}_4}\omega(T_4)\\&=F(K_{1,j-1}^{j-1};f,g;c_0)+\sum_{r=1}^{j}r(yz)^rF(K_{1,j-r}^{j-r};f,g;c_0)\end{aligned}\tag{9}$$

with $F(K_{1,0}^{0};f,g;c_0)=y$, $F(K_{1,1}^{1};f,g;c_0)=y+y^2z$.

Combining Equations (2), (3), and (9), we have Equation (1) and the theorem follows. □

Following similar arguments to Theorem 1, we can also obtain the subtree generating functions of the graphs obtained from identifying the centers of different fan graphs $K_{1,j_t}^{j_t}$ $(t=1,2,\ldots,l)$. We skip the tedious details for the sake of space.

Theorem 2. *Let $K_{1,j_1}^{j_1},K_{1,j_2}^{j_2},\ldots,K_{1,j_l}^{j_l}$ be different weighted fan graphs, and suppose there are n_{j_t} copies of $K_{1,j_t}^{j_t}$ for $t=1,2,\ldots,l$. Let $G=\bigcup_{t=1}^{l}(K_{1,j_t}^{j_t})^{n_{j_t}}$ be the graph that is constructed by identifying the centers of these $\sum_{t=1}^{l}n_{j_t}$ fan graphs with c_0. Then*

$$F(G;f,g)=y^{1-\sum_{t=1}^{l}n_{j_t}}\prod_{t=1}^{l}F(K_{1,j_t}^{j_t};f,g;c_0)^{n_{j_t}}+\sum_{t=1}^{l}\left(n_{j_t}\sum_{r=0}^{j_t-1}(j_t-r)y^{r+1}z^r\right),\tag{10}$$

with $F(K_{1,j_t}^{j_t};f,g;c_0)=F(K_{1,j_t-1}^{j_t-1};f,g;c_0)+\sum_{r=1}^{j_t}r(yz)^rF(K_{1,j_t-r}^{j_t-r};f,g;c_0)$ and $F(K_{1,0}^{0};f,g;c_0)=y$, $F(K_{1,1}^{1};f,g;c_0)=y+y^2z$.

Actually, a single fan graph is a special case of the above discussion, so we can further obtain the subtree generating function for the subtrees containing a particular vertex. Again, we skip the similar but technical details.

Theorem 3. *Let $K_{1,j}^{j}$ be a weighted fan graph with vertex weigh f and edge weigh g (see Figure 1b), then*

$$F(K_{1,j}^{j};f,g;c_1)=F(K_{1,j}^{j};f,g;c_0)-F(K_{1,j-1}^{j-1};f,g;c_0)+\sum_{t=0}^{j-1}y^{t+1}z^t\,,\tag{11}$$

with $F(K_{1,j}^{j};f,g;c_0)=F(K_{1,j-1}^{j-1};f,g;c_0)+\sum_{r=1}^{j}r(yz)^rF(K_{1,j-r}^{j-r};f,g;c_0)$ and $F(K_{1,0}^{0};f,g;c_0)=y$, $F(K_{1,1}^{1};f,g;c_0)=y+y^2z$.

Adding an edge between any two fan graphs (to construct a bigger fan) of a graph will also increase the number of subtrees. Let G be the weighted graph as defined in Theorem 2, and suppose $K_{1,j_r}^{j_r}$ (with non-center vertices labeled counterclockwise as $c_{j_1}^1,c_{j_2}^1,\ldots,c_{j_r}^1$) and $K_{1,j_s}^{j_s}$ (with non-center vertices labelled clockwise as $c_{j_1}^2,c_{j_2}^2,\ldots,c_{j_s}^2$) are the two sub-fan graphs of G with $j_r\geq 1$. Define $G'=G+(c_{j_r}^1,c_{j_s}^2)$ to be the graph obtained from G by adding one edge $(c_{j_r}^1,c_{j_s}^2)$. Meanwhile, denote $\overline{G}$ the graph of

$G - \left(\bigcup_{t=1}^{r} (c_0, c_{j_t}^1) \cup \bigcup_{t=1}^{s} (c_0, c_{j_t}^2) \right)$ that contains c_0, and denote $\overline{S}$ the collection of subtrees in $S(K_{1,j_r+j_s}^{j_r+j_s}; c_0)$ that contain $(c_{j_r}^1, c_{j_s}^2)$. By dividing the subtrees of G and G' into two cases of containing center c_0 or not, with Lemma 1, definitions of subtree weight and subtree generating function, and combining structure analysis, we have the following theorem:

Theorem 4. *Let G and G' be the weighted graphs defined above. Then,*

$$F(G'; f, g) = F(G; f, g) + y^{-1}F(\overline{G}; f, g; c_0) \sum_{T \in \overline{S}} \omega(T) + \sum_{t=0}^{j_s} t y^{t+1} z^t + j_s \sum_{t=j_s+1}^{j_r} y^{t+1} z^t + \sum_{t=j_r+1}^{j_r+j_s-1} (j_r + j_s - t) y^{t+1} z^t. \quad (12)$$

By letting $y = z = 1$ in the subtree generating functions from the above theorems, we have the corresponding subtree numbers of the various related graphs above.

Corollary 1. *The subtree number of $S(K_{1,j}^j, c_0)$ is*

$$\eta(K_{1,j}^j; c_0) = \eta(K_{1,j-1}^{j-1}; c_0) + \sum_{r=1}^{j} r\eta(K_{1,j-r}^{j-r}; c_0), \quad (13)$$

with $\eta(K_{1,0}^0; c_0) = 1, \eta(K_{1,1}^1; c_0) = 2$.

With Corollary 1, we have the number of subtrees of $K_{1,j}^j$ that contain central vertex c_0 as illustrated in Figure 2.

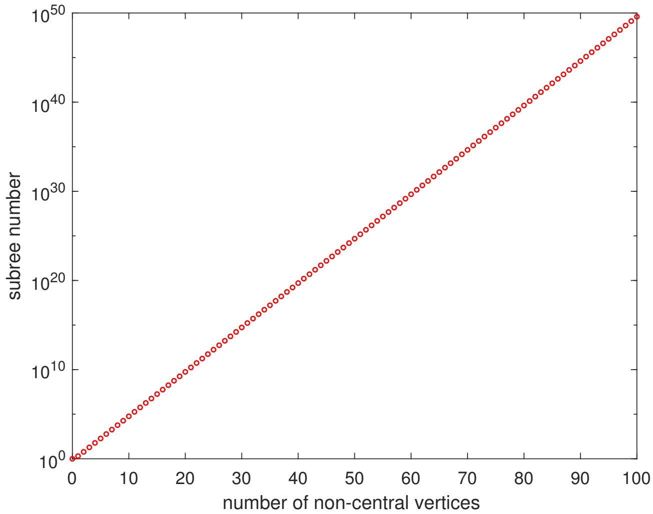


Figure 2. Number of subtrees of $K_{1,j}^j$ that contain central vertex c_0, in semi-log(Log-Y) coordinates.

Corollary 2. *Let n, j be positive integers with $1 \leq j \leq n$, and $i \equiv n \ (mod\ j)$, then*

$$\eta(K_{1,n}^j) = \frac{(j+1)(n-i)}{2} + i + 2^i b_j^{\frac{n-i}{j}}, \quad (14)$$

with $b_j = b_{j-1} + \sum_{r=1}^{j} r b_{j-r}$ and $b_0 = 1, b_1 = 2$.

With Corollary 2, we have the subtree number of $K_{1,n}^j$, see details in subsection 3.1.

Corollary 3. *Let* $G = \bigcup_{t=1}^{l} (K_{1,j_t}^{j_t})^{n_{j_t}}$, j_t, n_{j_t} *and* l *be defined in Theorem 2, then*

$$\eta(G) = \prod_{t=1}^{l} \eta(K_{1,j_t}^{j_t}; c_0)^{n_{j_t}} + \frac{1}{2}\sum_{t=1}^{l} n_{j_t} \times j_t(j_t+1), \tag{15}$$

with $\eta(K_{1,j_t}^{j_t}; c_0) = \eta(K_{1,j_t-1}^{j_t-1}; c_0) + \sum_{r=1}^{j_t} r\eta(K_{1,j_t-r}^{j_t-r}; c_0)$ *and* $\eta(K_{1,0}^{0}; c_0) = 1$, $\eta(K_{1,1}^{1}; c_0) = 2$.

Let G_1 be the graph defined in Theorem 2 with $l = 4, j_1 = 2, n_{j_1} = 4; j_2 = 3, n_{j_2} = 3; j_3 = 4, n_{j_3} = 2; j_4 = 5, n_{j_4} = 1$, with Corollary 1 and Corollary 3, we have $\eta(G_1) = 6,048,255,225,665$.

Corollary 4. *The number of subtrees of the fan graph* $K_{1,j}^{j}$ *containing* c_1 *is*

$$\eta(K_{1,j}^{j}; c_1) = \eta(K_{1,j}^{j}; c_0) - \eta(K_{1,j-1}^{j-1}; c_0) + j, \tag{16}$$

with $\eta(K_{1,j}^{j}; c_0) = \eta(K_{1,j-1}^{j-1}; c_0) + \sum_{r=1}^{j} r\eta(K_{1,j-r}^{j-r}; c_0)$ *and* $\eta(K_{1,0}^{0}; c_0) = 1$, $\eta(K_{1,1}^{1}; c_0) = 2$.

Similarly, the number of subtrees of $K_{1,j}^{j}$ that contain central vertex c_1 (see Figure 3) can be obtained from Corollary 4.

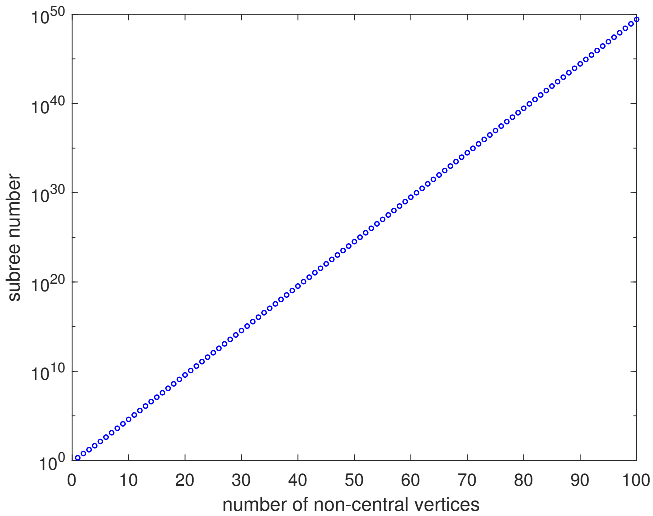


Figure 3. Number of subtrees of $K_{1,j}^{j}$ that contain the vertex c_1, in semi-log(Log-Y) coordinates.

Corollary 5. *Let* G *be the graph defined in Theorem 2, and* G' *be a merged graph from* G *with* $j_r \geq 1$ *and* $j_s \geq 1$ *(Theorem 4), then*

$$\eta(G') = \eta(G) + \eta(\overline{G}; c_0)\eta(K_{1,j_r+j_s}^{j_r+j_s}; c_0, (c_{j_r}^1, c_{j_s}^2)) + j_r j_s, \tag{17}$$

where $\eta(K_{1,j_r+j_s}^{j_r+j_s}; c_0, (c_{j_r}^1, c_{j_s}^2))$ *is the number of subtrees containing both vertex* c_0 *and edge* $(c_{j_r}^1, c_{j_s}^2)$.

Let G, $\overline{G}$, and G' be the graphs defined in Corollary 5 with $l = 2, j_1 = 2, n_{j_1} = 3; j_2 = 3, n_{j_2} = 2$, $j_r = 2$ and $j_s = 3$, with Corollary 1, Corollary 5, and structural analysis, we have $\eta(G)$ = 77,997, $\eta(\overline{G}; c_0) = 684$ $\eta(K_{1,j_r+j_s}^{j_r+j_s}; c_0, (c_{j_r}^1, c_{j_s}^2)) = 75$, and $\eta(G')$ = 129,303.

2.2. Subtree Generating Function and Subtree Number of Wheel Graph W_n

Next we consider the subtree generating function of the weighted wheel graph W_n.

Theorem 5. *Let W_n $(n \geq 3)$ be the weighted wheel graph on $n+1$ vertices with vertex weight function $f \equiv y$ and edge weight function $g \equiv z$. Then*

$$\begin{aligned} F(W_n; f, g) =& y + yzF(W_{n-1}; f, g) + (1+2yz)F(K_{1,n-1}^{n-1}; f, g; c_0) - 2yzF(K_{1,n-2}^{n-2}; f, g; c_0) \\ &+ \sum_{t=1}^{n-1} \Big((1-yz)(n-t) + 2yz \Big) y^t z^{t-1} + 2\sum_{k=1}^{n-1} (yz)^{k+1} F(K_{1,n-1-k}^{n-1-k}; f, g; c_0) \\ &+ \sum_{l=0}^{n-3} \sum_{r=0}^{n-3-l} (yz)^{l+r+3} F(K_{1,n-l-r-3}^{n-l-r-3}; f, g; c_0), \end{aligned} \tag{18}$$

with $F(W_3; f, g) = 4y + 6y^2z + 12y^3z^2 + 16y^4z^3$, $F(K_{1,j}^{j}; f, g; c_0) = F(K_{1,j-1}^{j-1}; f, g; c_0) + \sum_{r=1}^{j} r(yz)^r F(K_{1,j-r}^{j-r}; f, g; c_0)$, $F(K_{1,0}^{0}; f, g; c_0) = y$, *and* $F(K_{1,1}^{1}; f, g; c_0) = y + y^2z$.

Proof. For convenience, we let $e_t^* = (c_0, c_t)$ for $t = 1, 2, \ldots, n$, $e_n = (c_1, c_n)$ and $e_{n-r} = (c_{n-r}, c_{n-r+1})$ for $r = 1, 2, \ldots, n-1$. We also follow the convention that $\bigcup_{r=i}^{j} (c_r, c_{r+1}) = \emptyset$ if $j < i$, and $\sum_{t=i}^{j} b_t = 0$, if $j < i$.

We first consider the subtrees of $W_n (n \geq 3)$ in different cases:
(i) not containing the edge e_n^*,
(ii) containing the edge e_n^*.
The subtrees in case (i) can be further partitioned into four categories. As a result, we have

$$S(W_n - e_n^*) = \overline{\mathcal{S}_1} \bigcup \overline{\mathcal{S}_2} \bigcup \overline{\mathcal{S}_3} \bigcup \overline{\mathcal{S}_4}\,,$$

where

- $\overline{\mathcal{S}_1}$ is the set of subtrees of $S(W_n - e_n^*)$ that contain neither e_n nor e_{n-1};
- $\overline{\mathcal{S}_2}$ is the set of subtrees of $S(W_n - e_n^*)$ that contain e_{n-1}, but not e_n;
- $\overline{\mathcal{S}_3}$ is the set of subtrees of $S(W_n - e_n^*)$ that contain e_n but not e_{n-1};
- $\overline{\mathcal{S}_4}$ is the set of subtrees of $S(W_n - e_n^*)$ that contain both e_n and e_{n-1}.

From the definition of subtree weight and with structure analysis, we have

$$\sum_{T \in \overline{\mathcal{S}_1}} \omega(T) = y + F(K_{1,n-1}^{n-1}; f, g), \tag{19}$$

$$\sum_{T \in \overline{\mathcal{S}_2}} \omega(T) = \sum_{T \in \overline{\mathcal{S}_3}} \omega(T) = yzF(K_{1,n-1}^{n-1}; f, g; c_1), \tag{20}$$

and

$$\sum_{T \in \overline{\mathcal{S}_4}} \omega(T) = yz\Big(F(W_{n-1}; f, g) - F(K_{1,n-1}^{n-1}; f, g) \Big). \tag{21}$$

Thus, we have

$$\begin{aligned} \sum_{T \in S(W_n - e_n^*)} \omega(T) =& \sum_{T \in \overline{\mathcal{S}_1}} \omega(T) + \sum_{T \in \overline{\mathcal{S}_2}} \omega(T) + \sum_{T \in \overline{\mathcal{S}_3}} \omega(T) + \sum_{T \in \overline{\mathcal{S}_4}} \omega(T) \\ =& y + F(K_{1,n-1}^{n-1}; f, g) + yz\Big(2F(K_{1,n-1}^{n-1}; f, g; c_1) + F(W_{n-1}; f, g) - F(K_{1,n-1}^{n-1}; f, g) \Big). \end{aligned} \tag{22}$$

Similarly, for case (ii), we have

$$S(W_n; e_n^*) = \mathcal{S}_1 \bigcup \mathcal{S}_2 \bigcup \mathcal{S}_3 \bigcup \mathcal{S}_4\,,$$

where

- $\mathcal{S}_1$ is the set of subtrees in $S(W_n; e_n^*)$ that contain neither e_n nor e_{n-1};
- $\mathcal{S}_2$ is the set of subtrees in $S(W_n; e_n^*)$ that contain e_n, but not e_{n-1};
- $\mathcal{S}_3$ is the set of subtrees in $S(W_n; e_n^*)$ that contain e_{n-1} but not e_n;
- $\mathcal{S}_4$ is the set of subtrees in $S(W_n; e_n^*)$ that contain both e_n and e_{n-1}.

Analyzing each case, we have:

(a) $\mathcal{S}_1 = \{T + (c_0, c_n) | T \in S(K_{1,n-1}^{n-1}; c_0)\}$, where $T + (c_0, c_n)$ are the trees obtained from $T(\in S(K_{1,n-1}^{n-1}; c_0))$ by attaching the edge (c_n, c_0) at vertex c_0;

(b) $\mathcal{S}_2 = \{T + e_n^* + (c_1, c_n) + \bigcup_{r=1}^{k-1} (c_r, c_{r+1}) | T \in S(\widetilde{K}_{1,n-1-k}^{n-1-k} c_0)\}$, where $\widetilde{K}_{1,n-1-k}^{n-1-k} (k = 1, 2, \ldots, n-1)$ is the graph of $W_n - \left(e_k \bigcup e_{n-1} \bigcup e_n^* \bigcup_{r=1}^{k} e_r^*\right)$ that contains c_0, and obviously, $\widetilde{K}_{1,n-1-k}^{n-1-k} \cong K_{1,n-1-k}^{n-1-k}$;

(c) $\mathcal{S}_3 = \{T + e_n^* + \bigcup_{r=1}^{k} (c_{n-r}, c_{n-r+1}) | T \in S(K_{1,n-1-k}^{n-1-k}; c_0)\}$ for $k = 1, 2, \ldots, n-1$;

(d) In a similar manner as (b) and (c), use variables l and r to count the number of edges trailing off (c_{n-1}, c_n) and (c_1, c_n), respectively, then the subtrees in $\mathcal{S}_4$ are indexed by these two variables, which count extra edges that are on the two sides of the T shape containing the 3 edges required by $\mathcal{S}_4$. With (a)–(d), we have

$$\sum_{T_1 \in \mathcal{S}_1} \omega(T_1) = \sum_{T \in S(K_{1,n-1}^{n-1}; c_0)} f(c_n) g(e_n^*) \omega(T) = yzF(K_{1,n-1}^{n-1}; f, g; c_0), \tag{23}$$

$$\begin{aligned} \sum_{T_2 \in \mathcal{S}_2} \omega(T_2) = \sum_{T_3 \in \mathcal{S}_3} \omega(T_3) =& f(c_n) g(e_n^*) \sum_{k=1}^{n-1} \prod_{r=1}^{k} (g(e_{n-r}) f(c_{n-r})) F(K_{1,n-1-k}^{n-1-k}; f, g; c_0) \\ =& yz \sum_{k=1}^{n-1} (yz)^k F(K_{1,n-1-k}^{n-1-k}; f, g; c_0), \end{aligned} \tag{24}$$

$$\sum_{T_4 \in \mathcal{S}_4} \omega(T_4) = \sum_{l=0}^{n-3} \sum_{r=0}^{n-3-l} (yz)^{l+r+3} F(K_{1,n-l-r-3}^{n-l-r-3}; f, g; c_0). \tag{25}$$

Now with Equations (23)–(25), we have

$$\begin{aligned} \sum_{T \in S(W_n; (c_0, c_n))} \omega(T) =& \sum_{T_1 \in \mathcal{S}_1} \omega(T_1) + \sum_{T_2 \in \mathcal{S}_2} \omega(T_2) + \sum_{T_3 \in \mathcal{S}_3} \omega(T_3) + \sum_{T_4 \in \mathcal{S}_4} \omega(T_4) \\ =& yzF(K_{1,n-1}^{n-1}; f, g; c_0) + 2 \sum_{k=1}^{n-1} (yz)^{k+1} F(K_{1,n-1-k}^{n-1-k}; f, g; c_0) \\ &+ \sum_{l=0}^{n-3} \sum_{r=0}^{n-3-l} (yz)^{l+r+3} F(K_{1,n-l-r-3}^{n-l-r-3}; f, g; c_0). \end{aligned} \tag{26}$$

By Theorem 1, Theorem 3, and Equations (22) and (26), we have

$$\begin{aligned} F(W_n; f, g) =& y + yzF(W_{n-1}; f, g) + (1 + 2yz) F(K_{1,n-1}^{n-1}; f, g; c_0) - 2yzF(K_{1,n-2}^{n-2}; f, g; c_0) \\ &+ \sum_{t=1}^{n-1} \left((1 - yz)(n - t) + 2yz\right) y^t z^{t-1} + 2 \sum_{k=1}^{n-1} (yz)^{k+1} F(K_{1,n-1-k}^{n-1-k}; f, g; c_0) \\ &+ \sum_{l=0}^{n-3} \sum_{r=0}^{n-3-l} (yz)^{l+r+3} F(K_{1,n-l-r-3}^{n-l-r-3}; f, g; c_0). \end{aligned} \tag{27}$$

Note that W_2 is not a wheel graph. With Theorem 1 and Lemma 1, we have

$$\sum_{T \in S(W_2)} \omega(T) = 3y + 4y^2 z + 5y^3 z^2. \tag{28}$$

Now from Equations (27) and (28), we have

$$F(W_3; f, g) = 4y + 6y^2z + 12y^3z^2 + 16y^4z^3. \tag{29}$$

The subtree generating function of W_n now follows from Equations (27) and (29). □

Letting $y = z = 1$ in Equation (18), we have the following corollary.

Corollary 6. *The subtree number of $W_n (n \geq 3)$ is*

$$\eta(W_n) = \eta(W_{n-1}) + 3\eta(K^{n-1}_{1,n-1}; c_0) + 2n - 1 + 2\sum_{k=2}^{n-1}\eta(K^{n-1-k}_{1,n-1-k}; c_0) + \sum_{l=0}^{n-3}\sum_{r=0}^{n-3-l}\eta(K^{n-l-r-3}_{1,n-l-r-3}; c_0), \tag{30}$$

with $\eta(W_3) = 38$, $\eta(K^j_{1,j}; c_0) = \eta(K^{j-1}_{1,j-1}; c_0) + \sum_{r=1}^{j} r\eta(K^{j-r}_{1,j-r}; c_0)$, $\eta(K^0_{1,0}; c_0) = 1$ *and* $\eta(K^1_{1,1}; c_0) = 2$.

With Corollary 6, the subtree numbers of W_n $(n = 3, 4, \ldots, 50)$ are shown in Table 1.

Table 1. The subtree numbers of wheel graph W_n $(n = 3, 4, \ldots, 50)$.

n	$\eta(W_n)$	n	$\eta(W_n)$	n	$\eta(W_n)$
3	38	19	2,899,980,984	35	269,604,917,347,967,886
4	112	20	9,128,846,611	36	848,689,059,340,934,448
5	332	21	28,736,686,630	37	2,671,587,471,512,527,895
6	1007	22	90,460,187,232	38	8,409,887,625,375,274,755
7	3110	23	284,759,535,167	39	26,473,477,146,304,448,341
8	9704	24	896,394,265,075	40	83,335,833,180,604,495,475
9	30,431	25	2,821,758,641,457	41	262,332,788,908,879,910,034
10	95,643	26	8,882,611,305,147	42	825,797,133,240,010,600,373
11	300,885	27	27,961,563,560,618	43	2,599,525,999,414,007,165,103
12	946,923	28	88,020,178,967,761	44	8,183,045,386,844,876,767,480
13	2,980,538	29	277,078,636,493,555	45	25,759,400,682,377,496,173,050
14	9,382,101	30	872,215,572,630,716	46	81,087,992,568,389,361,552,840
15	29,533,519	31	2,745,646,560,009,062	47	255,256,813,613,269,834,457,576
16	92,968,088	32	8,643,018,158,636,696	48	803,522,677,430,288,749,342,627
17	292,653,642	33	27,207,348,527,149,292	49	2,529,408,261,449,734,855,548,318
18	921,243,536	34	85,645,986,192,695,055	50	7,962,321,827,121,343,008,620,568

As a matter of fact, with the generating function and further structural and theoretical analysis, we can also solve the subtree generation computing problems for the following more generalized types of graphs; here we skip the similar but technical details.

(i) Graph $G = \bigcup_{i=1}^{l} F^{t_i}_{i,n_i}$ is constructed by identifying the center c^i_0 of l graphs $F^{t_i}_{i,n_i} (i = 1, 2, \ldots, l)$ to c_0, where $\overline{F^{t_i}_{i,n_i}} (n_i \geq 1, 2 \leq t_i \leq n_i)$ is the graph constructed from a vertex c^i_0 and a path $P_{c^i_1 c^i_{n_i}} = c^i_1 c^i_2 \cdots c^i_{n_i}$ by connecting c^i_0 with c^i_1, $c^i_{n_i}$, and any other arbitrary $t_i - 2$ vertices on the path $P_{c^i_1 c^i_{n_i}}$; for the special case $n_i = 1$, the graph $F^{t_i}_{i,n_i}$ is a path $c^i_0 c^i_1$ on vertices c^i_0 and c^i_1.

(ii) Graph $G = W_n - \bigcup_{t=1}^{l} (c_0, c_{j_t}) (1 \leq l, j_t \leq n)$, namely the graph obtained from wheel W_n by deleting random l different edges $(c_0, c_{j_t}) (t = 1, 2, \ldots, l)$ (each j_t is different the others).

3. Behaviors of $K^J_{1,N} (1 \leq J \leq N)$ and W_n in Terms of Subtrees

With the subtree generating functions established, we can now analyze the behaviors of the graphs $K^j_{1,n} (1 \leq j \leq n)$ and W_n in terms their subtree numbers and other related properties.

3.1. Subtree Numbers and $K_{1,N}^{J}$

We start with the subtree numbers of the graphs $K_{1,n}^{j}$ for different n and j. First, we take a quick look at the extremal problems.

Proposition 1. *Among all* $K_{1,n}^{j}$ $(1 \leq j \leq n)$:

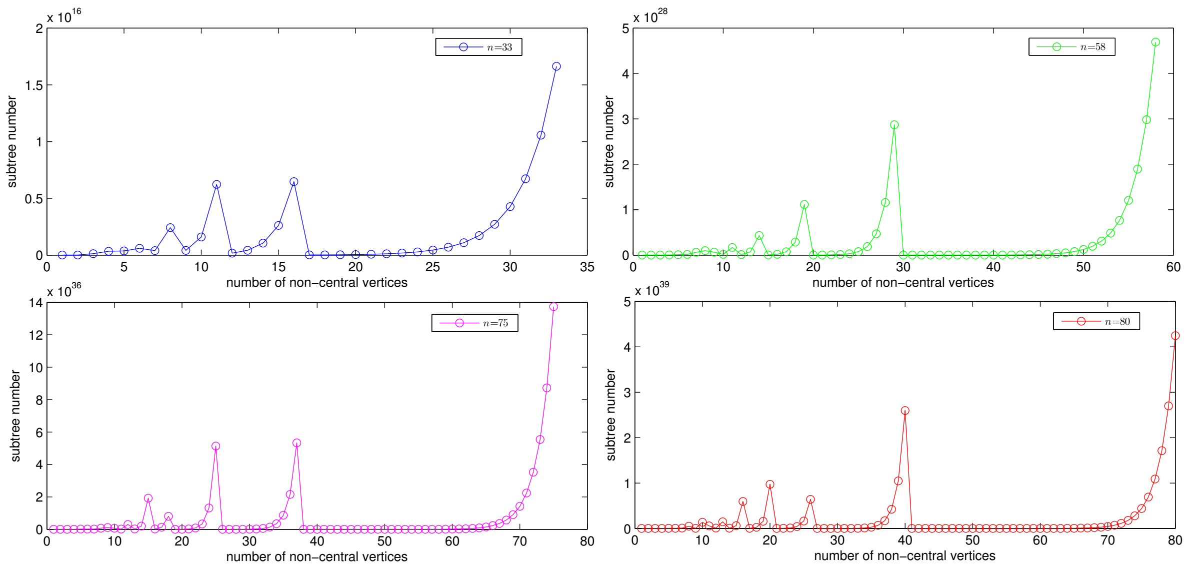
- *the graph* $K_{1,n}^{1}$ *has* $2^n + n$ *subtrees, fewer than any other* $K_{1,n}^{j}(j \neq 1)$; *and*
- *the graph* $K_{1,n}^{n}$ *has* $\frac{n(n+1)}{2} + b_n$ *subtrees (where* $b_n = b_{n-1} + \sum_{r=1}^{n} r b_{n-r}$ *and* $b_0 = 1, b_1 = 2$*), more than any other* $K_{1,n}^{j}(j \neq n)$.

Proof. Note that adding an edge to a graph will strictly increase the subtree number. The extremal structures $K_{1,n}^{1}$ and $K_{1,n}^{n}$ then follow immediately from the fact that the former is a subgraph of any $K_{1,n}^{j}$ and the latter contains any $K_{1,n}^{j}$ as a subgraph. □

We are also interested in knowing which $K_{1,n}^{j}$ $(2 \leq j \leq n-1)$ has the second- or third-largest subtree number. To examine this, we also explore how the subtree numbers of the graphs $K_{1,n}^{j}$ behave. With Corollary 2 and Matlab computing (see Appendix A for more details), we obtain the subtree number behaviors of $K_{1,n}^{j}$ as shown in Figure 4.

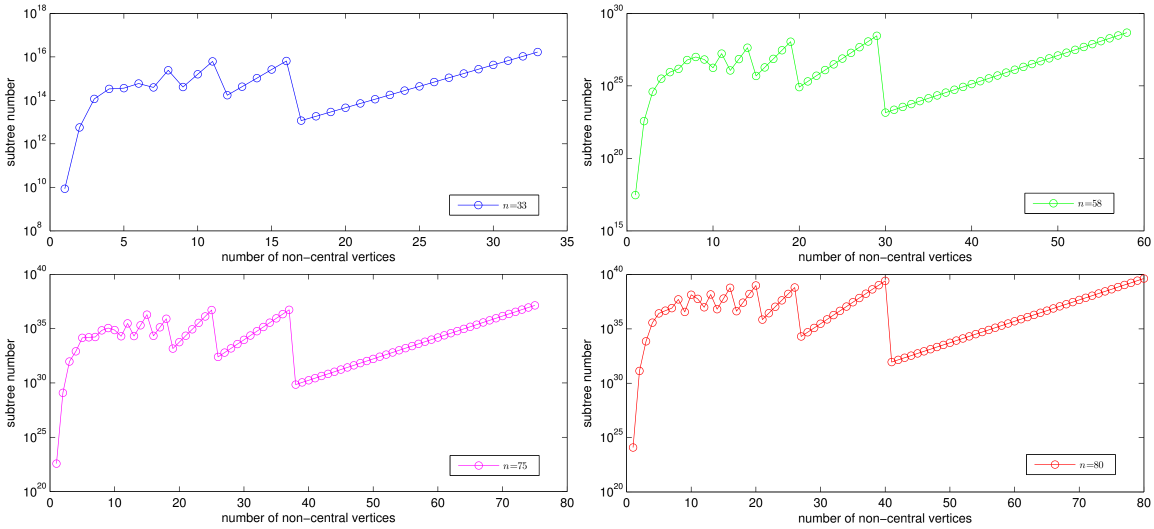
It seems from Figure 4a,b that among all $K_{1,n}^{j}$ $(1 \leq j \leq n-1)$:

- $K_{1,n}^{n-1}$ has the second-largest subtree number; and
- $K_{1,n}^{n-2}$ has the third-largest subtree number for odd (or sufficiently large) n.
- the subtree number $K_{1,n}^{j}$ increment trend meets exponential growth when $j \geq \lceil \frac{n+1}{2} \rceil$.



(a) Subtree numbers of $K_{1,n}^{j}$ with $n = 33, 58, 75, 80$, j from 1 to n, in Cartesian coordinates.

Figure 4. *Cont.*



(b) Subtree numbers of $K_{1,n}^{j}$ with $n = 33, 58, 75, 80$, j from 1 to n, in semi-log(Log-Y) coordinates.

Figure 4. Subtree numbers of $K_{1,n}^{j}$ with $n = 33, 58, 75, 80$, j from 1 to n.

In general, it is not difficult to show the following.

Proposition 2. *Suppose $n >> k$ (i.e., n is much larger than k), then among all $K_{1,n}^{j}$ $(1 \leq j \leq n)$, the graph $K_{1,n}^{n-k}$ has the $(k+1)$-th largest subtree number.*

The proof follows from adjusting the "sizes" of the two sub-fan graphs of $K_{1,n}^{j}$. We skip the details here. The same argument can also show the monotonic behavior for large enough j.

Proposition 3. *If $j > \frac{n}{2}$, then $K_{1,n}^{j+1}$ has a larger subtree number than $K_{1,n}^{j}$.*

Understanding the specific behavior of $K_{1,n}^{j}$ for general j in terms of the subtree number seems to be an interesting and nontrivial problem.

Similarly, from Corollary 6, we can obtain the subtree numbers of wheel graph W_n $(n \geq 3)$, as already shown in Table 1. On the other hand, experimental observation shows that the subtree numbers of W_n $(n \geq 3)$ increase very fast and this growth trend seems to fit the linear regression model after doing the logarithmic transformation. Through implementing the linear regression in the MATLAB software for data of the number of subtrees of W_n from $n = 3$ to 602, the appropriate formula for the subtree number of W_n can be stated as

$$\eta(W_n) \approx exp(0.0126 + 1.1466n). \tag{31}$$

As $exp0.0126 \approx 1$, Equation (31) can be rewritten as

$$\eta(W_n) \approx exp1.1466n. \tag{32}$$

With Corollary 6, Equation (32), and logarithmic transformation for each subtree number of W_n and fitted value, we can obtain the subtree number trend of $W_n (n \geq 3)$, as illustrated in Figure 5 where the original and fitted data are respectively marked in red and blue. We believe Equation (32) can be proved or disproved through traditional analytic combinatorial approaches, but we will not pursue the technical analysis here.

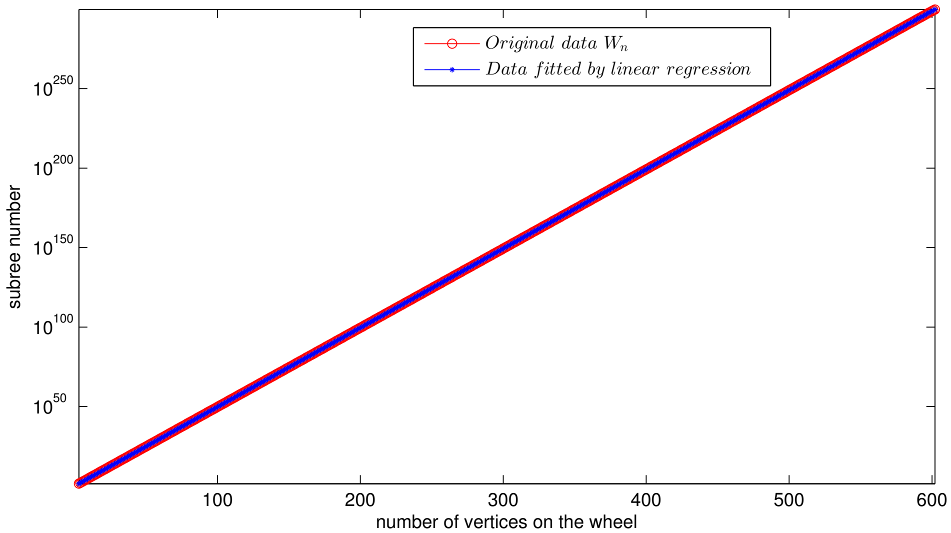


Figure 5. Subtree number trend of wheel graph W_n $(n = 3, 4, \ldots, 602)$, in semi-log(Log-Y) coordinates.

Our work can also be easily applied to more general "partitions" of wheel graphs instead of just the $K^j_{1,n}$s. To illustrate the observations, we introduce some simple notations. Given a positive integer n and partition $\pi = (\pi_1, \pi_2, \ldots, \pi_k)$ of n (with $\pi_1 \geq \pi_2 \geq \ldots \geq \pi_k$ and $n = \sum_{i=1}^{k} \pi_i$), the graph K_π is obtained from $K_{1,n}$ by adding edges (c_j, c_{j+1}) for all $1 \leq j \leq n-1$ except for $j = \sum_{i=1}^{s} \pi_i$, for $s = 1, 2, \ldots, k$. It seems that the subtree numbers of K_πs coincide with some sort of ordering of the partitions π of n. In general, larger and fewer parts in π results in more subtrees in K_π. More precise statements along this line requires further study.

3.2. Subtree Densities of $K^J_{1,N}$ and W_n

The subtree generating function can be used to provide more information than just the number of subtrees. For instance, using the subtree generating function, one can easily obtain the total number of vertices in all subtrees, from which we have the average subtree order in a given graph. The ratio of the average subtree order and the order of the original graph is called the subtree density of the graph. We present the formal subtree density definition as follows:

Definition 2 ([20])**.** *Suppose G is a graph with n vertices, then $\mu(G) = \frac{1}{k}\sum\limits_{i=1}^{k} n_i$ is the average order of the subtrees of G, where $n_1, n_2, \ldots, n_k$ are the orders of all of G's k non-empty subtrees, and the subtree density of G is defined as $D(G) = \frac{\mu(G)}{n}$.*

It is essentially the probability that a vertex chosen at random from G will belong to a randomly chosen subtree of G. Some of the work related to subtree densities can be found in [20,21,39].

With Theorem 1, Theorem 5, and substituting $z = 1$, we could obtain the vertex generating function of subtrees of $K^j_{1,n}$ and W_n, respectively, i.e., $F(K^j_{1,n}; y, 1)$ and $F(W_n; y, 1)$). The subtree density of $K^j_{1,n}$ and W_n is simply

$$D(G^*) = \frac{\left.\frac{\partial F(G^*; y, 1)}{\partial y}\right|_{y=1}}{F(G^*; 1, 1) * n(G^*)}, \tag{33}$$

where $n(G^*)$ denotes the vertex number of G^*, and G^* can be $K^j_{1,n}$ or W_n.

We will now apply this to find the subtree densities of $K^j_{1,n}$ and W_n.

Clearly, the vertex number of $K_{1,n}^{j}$ and W_n is $n+1$, namely

$$n(K_{1,n}^{j}) = n(W_n) = n+1. \tag{34}$$

With Theorem 1 and letting $z=1$ in Equation (1), we obtain the vertex generating function of subtrees of $K_{1,n}^{j}(1 \le j \le n)$.

$$F(K_{1,n}^{j}; f, 1) = (1+y)^{i} y^{1-\frac{n-i}{j}} * F(K_{1,j}^{j}; f, 1; c_0)^{\frac{n-i}{j}} + iy + \frac{n-i}{j} \sum_{t=0}^{j-1} (j-t) y^{t+1}, \tag{35}$$

with $i \equiv n \ (mod\ j)$, $F(K_{1,j}^{j}; f, 1; c_0) = F(K_{1,j-1}^{j-1}; f, 1; c_0) + \sum_{r=1}^{j} r y^r F(K_{1,j-r}^{j-r}; f, 1; c_0)$ and $F(K_{1,0}^{0}; f, 1; c_0) = y$, $F(K_{1,1}^{1}; f, 1; c_0) = y + y^2$.

Similarly, letting $z=1$ in Equation (18), we obtain the vertex generating function of subtrees of W_n.

$$\begin{aligned} F(W_n; f, 1) =& y + yF(W_{n-1}; f, 1) + (1+2y)F(K_{1,n-1}^{n-1}; f, 1; c_0) - 2yF(K_{1,n-2}^{n-2};)f, 1; c_0) \\ &+ \sum_{t=1}^{n-1} \Big((1-y)(n-t) + 2y \Big) y^t + 2 \sum_{k=1}^{n-1} y^{k+1} F(K_{1,n-1-k}^{n-1-k}; f, 1; c_0) \\ &+ \sum_{l=0}^{n-3} \sum_{r=0}^{n-3-l} y^{l+r+3} F(K_{1,n-l-r-3}^{n-l-r-3}; f, 1; c_0), \end{aligned} \tag{36}$$

with $F(W_3; f, 1) = 4y + 6y^2 + 12y^3 + 16y^4$, $F(K_{1,j}^{j}; f, 1; c_0) = F(K_{1,j-1}^{j-1}; f, 1; c_0) + \sum_{r=1}^{j} r y^r F(K_{1,j-r}^{j-r}; f, 1; c_0)$ and $F(K_{1,0}^{0}; f, 1; c_0) = y$, $F(K_{1,1}^{1}; f, 1; c_0) = y + y^2$.

From Equations (33)–(35), we can obtain the subtree densities of $K_{1,n}^{j}$ $(1 \le j \le n)$ (plotted in Figure 6); related data can be found in Table 2. Similarly, from Equations (33), (34), and (36), we have subtree densities W_n plotted in Figure 7; related data are listed in Table 3.

From Table 2 and Figure 6, it appears that $K_{1,22}^{1}$ and $K_{1,22}^{12}$ have the smallest and second-smallest subtree densities, respectively. $K_{1,22}^{j}(12 \le j \le 22)$ grows linearly with the increase of j. Moreover, from Table 3 and Figure 7, we see that $W_n(3 \le n \le 24)$ increases first in the interval $[3,8]$ and reaches the maximum value when $n=8$, and then decreases gradually in the interval $[9,24]$ and approximates the limit value of 0.8135.

Similarly, as studied in paper [35], we can also discuss the ratio of spanning trees to all subtrees and spanning tree densities of $K_{1,n}^{j}$ and W_n. We skip the details here.

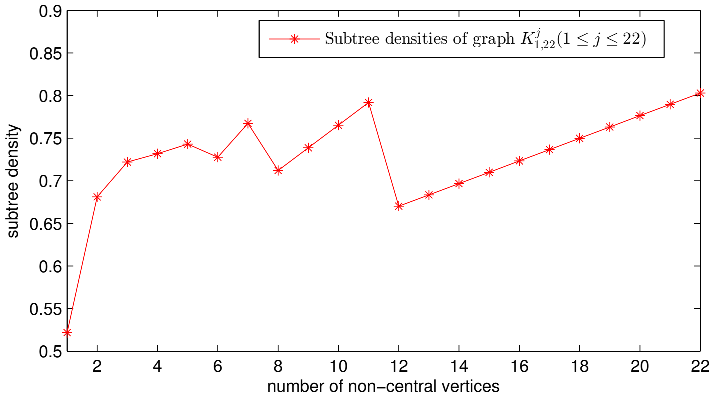


Figure 6. Subtree densities of the graphs $K_{1,22}^{j}$ $(1 \le j \le 22)$.

Table 2. Related data for $K_{1,n}^j$, with $n = 22$ and $j = 1, 2, \ldots, 22$.

j	$P_y(K_{1,n}^j)$	$\eta(K_{1,n}^j)$	$D(K_{1,n}^j)$
1	50,331,670	4,194,326	0.521736621869847
2	5,683,820,588	362,797,089	0.681159363604678
3	29,685,950,982	1,787,743,521	0.721967947748206
4	52,358,400,102	3,110,400,052	0.731884047161090
5	87,226,395,622	5,103,959,426	0.743041170007376
6	56,400,430,972	3,370,318,067	0.727584934777173
7	231,968,014,120	13,141,451,319	0.767462100378713
8	36,440,865,014	2,224,820,302	0.712140856484914
9	93,645,742,414	5,511,577,694	0.738727501280144
10	240,339,417,442	13,653,922,612	0.765314128820302
11	616,080,713,876	33,825,095188	0.791900742502907
12	9,137,267,062	592,843,864	0.670113169892776
13	14,666,890,448	933,106,276	0.683406494463958
14	23,533,982,520	1,468,662,129	0.696699813456106
15	37,748,062,639	2,311,599,999	0.709993128330647
16	60,525,953,078	3,638,341,646	0.723286440182849
17	97,015,668,926	5,726,566,014	0.736579749833999
18	155,453,553,144	9,013,325,743	0.749873057893726
19	249,013,516,065	14,186,519,625	0.763166364810336
20	398,761,664,190	22,328,865,632	0.776459670910826
21	638,376,020,719	35,144,507,194	0.789752976431952
22	1,021,684,176,864	55,315,680,041	0.803046281543951

* $P_y(G)$ stands for $\left.\frac{\partial F(G;y,1)}{\partial y}\right|_{y=1}$.

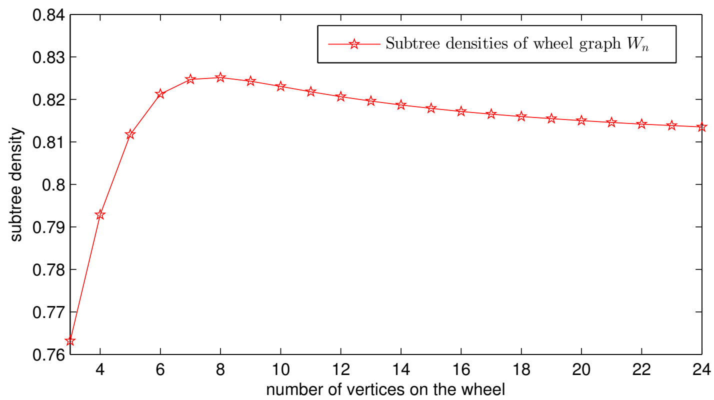


Figure 7. Subtree densities of wheel graph $W_n (3 \le n \le 24)$.

Table 3. Related data for wheel graph W_n $(n = 3, 4 \ldots, 24)$.

k	$P_y(W_k)$	$D(W_k)$	k	$P_y(W_k)$	$D(W_k)$
3	116	0.7631578947368421	14	115,215,423	0.8186895664414613
4	444	0.7928571428571428	15	386,480,089	0.8178844370865525
5	1617	0.8117469879518072	16	1,291,505,336	0.8171718247840813
6	5789	0.8212512413108243	17	4,301,328,493	0.8165375712479791
7	20,519	0.8247186495176849	18	14,282,430,812	0.8159697793983819
8	72,064	0.8251351103783091	19	47,296,291,958	0.815458656779937
9	250,841	0.8242943051493543	20	156,239,476,051	0.8149961728004785
10	865,923	0.8230636087039588	21	514,980,557,554	0.8145757185906111
11	2,967,219	0.8218031806171793	22	1,693,994,724,188	0.8141918205521789
12	10,102,071	0.8206394655271703	23	5,561,968,202,536	0.813839912225434
13	34,200,012	0.8196030381092273	24	18,230,780,418,139	0.8135161559345164

* $P_y(G)$ stands for $\left.\frac{\partial F(G;y,1)}{\partial y}\right|_{y=1}$.

4. Concluding Remarks

In this paper we established the subtree generating functions of the wheel graph W_n and "partitions" $K_{1,n}^j$ $(1 \leq j \leq n)$, along with other related structures such as the fan graphs. With the subtree generating functions, we are able to study the subtree number and subtree densities of these graphs. From our computational analysis, several theoretical conclusions are drawn, especially on the extremal problems with respect to the subtree number. These results provide a fundamental basis for studying subtree problems of multi-cyclic graphs, chemical compounds, and complex graphs.

As one can see, the computational results in Section 3.2 show interesting observations on the characteristics of these structures. Attempting to verify some of them, especially on those related to the subtree densities, and exploring the BC-subtree number index, Wiener index, Harary index, atom-bond connectivity trends of wheel graph W_n, "partitions" $K_{1,n}^j$ $(1 \leq j \leq n)$, and their generalizations would make very interesting projects for future work. Exploring the novel structural properties from the evolutionary perspective of graphs with more complicated cycle structures, particularly some important nanomaterials such as the pentagonal carbon nanocone, is also a very attractive future topic.

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Appendix A. Matlab Code, Python Code, And Data

In what follows, we provide the source codes related to Figure 4. Python code **Pythoncode1** (derived from Corollary 2) can output the data files "n=33.txt", "n=58.txt", "n=75.txt", and "n=80.txt" by inputting the integer 33, 58, 75, 80, respectively. MATLAB codes **MCF1a**, **MCF1b** can draw the Figure 4a,b, respectively.

Pythoncode1. The Python code for computing the subtree number of $K_{1,n}^j$ $(1 \leq j \leq n)$.

```
n=int(input())
b=[-1 for i in range(n+1)]
b[0]=1
b[1]=2
for j in range(1,n+1):
sum1=0
for r in range(1,j+1):
sum1=sum1+r*b[j-r]
b[j]=b[j-1]+sum1
file_name="n="+str(n)+".txt"
file = open(file_name,'w')
for j in range(1,n+1):
i = n%j
s=(j+1)*(n-i)/2+i+2**(i)*b[j]**((n-i)/j)
file.write(str(s))
file.write('\n')
print(s)
```

MCF1a. MATLAB source code for Figure 1a.

```
clear;
clc;
s1 = load('n=33.txt');
s2 = load('n=58.txt');
s3 = load('n=75.txt');
s4 = load('n=80.txt');
format long;
A =cell(1,10);
A{1,1}='-bo';
A{1,2}='-go';
A{1,3}='-mo';
A{1,4}='-ro';
subplot(2,2,1);
plot(s1,A{1,1});
axis normal;
set(legend('n=33'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,2);
plot(s2,A{1,2});
set(legend('n=58'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,3);
plot(s3,A{1,3});
axis normal;
set(legend('n=75'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,4);
plot(s4,A{1,4});
set(legend('n=80'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
```

MCF1b: The MATLAB source code for Figure 1b.

```
clear;
clc;
s1 = load('n=33.txt');
s2 = load('n=58.txt');
s3 = load('n=75.txt');
s4 = load('n=80.txt');
format long;
A =cell(1,10);
A{1,1}='-bo';
A{1,2}='-go';
A{1,3}='-mo';
A{1,4}='-ro';
```

```
subplot(2,2,1);
semilogy(s1,A{1,1});
axis normal;
set(legend('n=33','location','southeast'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,2);
semilogy(s2,A{1,2});
set(legend('n=58','location','southeast'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,3);
semilogy(s3,A{1,3});
axis normal;
set(legend('n=75','location','southeast'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
subplot(2,2,4);
semilogy(s4,A{1,4});
set(legend('n=80','location','southeast'),'fontsize',8);
xlabel('number of non-central vertices');
ylabel('subtree number');
```

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