Subtrees, BC-subtrees of generalized Bethe trees and related questions

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Abstract

Topological indices of graphs and trees in particular have been vigorously studied in the past decade due to their many applications in different fields. Among such indices, the number of subtrees (BC-subtrees), along with their variations have received much attention. In this paper we provide some new evaluation results related to these two indices on specific structures (generalized Bethe trees, Bethe trees, dendrimers), which are some of the structures of practical interests. Using "generating functions", we also examine the asymptotic behavior of subtree (resp. BC-subtree) density of dendrimers.

Keywords: Subtree, BC-subtree, Generating function, Generalized Bethe tree, Bethe tree, Dendrimer, Subtree (BC-subtree) density

1. Introduction

Various topological indices have been proposed and vigorously studied in recent years. The structure-based indices such as the number of subtrees (also called the ρ-index in [14]), leaf-containing subtrees of a tree, Merrifield-Simmons-index (number of independent vertex subsets), Hosoya-index (number of matchings) have been studied [11, 14, 21, 22, 23].

The *BC-tree*, also known as the *block-cutpoint-tree* or the *bicolorable tree*, is a tree (with at least two vertices) where the distance between any two leaves is even, introduced by Harary, Plummer, and Prins [6, 7]. One can find related work in fields including but not limited to, mathematics [1, 4, 16], information Science [3, 9, 15], and bio-chemistry [2, 17, 18]. Naturally, a BC-subtree is a subtree

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that is also a BC-tree. The number of BC-subtrees or leaf-containing BC-subtrees provide new structure based indices that are recently studied in [26].

A rooted tree is called generalized Bethe tree if degrees of vertices at the same level are the same while degrees may differ at different levels. In general, we consider the root as of level 1 and denote the generalized Bethe tree of k levels by B_k. In particular, a Bethe tree $B_{k,d}$ (also called a rooted d-ary tree in other literatures) is a rooted tree of k levels with root degree d, the vertices at level j $(2 \leq j \leq k-1)$ have degrees $(d+1)$ and the level k vertices being pendant vertices. Another special case of B_k is the regular dendrimer tree $T_{k,d}$, which satisfies that each non-leaf vertex having degree d. It is easy to see that for any $d \geq 3$, $T_{0,d}$ is a single vertex and $T_{1,d}$ is the star with $d+1$ vertices; the parameter k corresponds to what is called "number of generations".

The evaluation of various topological indices for generalized Bethe trees and special cases are of interests, one may see [5, 10, 20] for such work on distance-based indices. A linear-time algorithm to count the sum of weights of subtrees of T through "generating functions" was provided in [25]. This idea was employed in [26], where among other properties of BC-trees and BC-subtrees, enumeration of BC-subtrees and leaf-containing BC-subtrees are provided.

Motivated by the applications of these topological indices, their behavior on specific structures are of interests. The rest of the paper is organized as follows. Section 2 presents some general notations and useful previous results. We provide formulae of (leaf-containing) subtree numbers of generalized Bethe trees, Bete trees and dendrimers in Section 3. The analogous work on (leaf-containing) BC-subtrees is done in Section 4. As an example of applications, we apply our results to the enumeration of subtrees and BC-subtrees for Newkome's arborol in Section 5. Last but not least, in Section 6, with the vertex (resp. edge) generating functions of subtrees (resp. BC-subtrees), we briefly discuss the asymptotic behavior of subtree (resp. BC-subtree) density of dendrimers.

2. General notations and some previous works

In this section we introduce some technical notations and lemmas from previous work that will facilitate our discussion in the later sections. More details can be found in [25, 26].

In general, for a weighted tree $T = (V(T), E(T); f, g)$ with $V(T) = \{v_1, v_2, \ldots, v_n\}$ and $E(T) = \{e_1, e_2, \ldots, e_{n-1}\}$. When considering the subtrees of T, we could set its vertex-weight function $f := f_1$ and edge-weight function $g := g_1$ with $f_1 : V(T) \rightarrow \Re$ and $g_1 : E(T) \rightarrow \Re$ (where $\Re$ is a commutative ring with a unit element 1); when considering the BC-subtrees, *OLDV*-subtrees (to be defined more precisely later) and *ELDV*-subtrees (to be defined more precisely later) of T, we could set its vertex-weight function $f := f_2$ and edge-weight function $g := g_2$ with $f_2 : V(T) \rightarrow \Re \times \Re$ and $g_2 : E(T) \rightarrow \Re$ (where $\Re$ is a commutative ring with a unit element 1).

For convenience, we list main notations in Table 1.

Table 1. Main notations

Notation	Meaning
$L(T)$	Leaf set of T.
$S(T)$ (resp. $S_{BC}(T)$)	Set of subtrees (resp. BC-subtrees) of T.
$S(T;v)$	Set of subtrees of T containing v.
$S(T;v,odd)$	Set of subtrees of T containing v such that all leaves (not v) have odd distance from v. See Eq. (1).
$S(T;v,even)$	Set of subtrees of T containing v such that all leaves (not v) have even distance from v, the single vertex tree $\{v\}$ itself is contained in it. See Eq. (2).
$\omega\_vodd(T_1)$	ω_vodd weight of subtree $T_1 \in S(T;v,odd)$.
$\omega\_veven(T_2)$	ω_veven weight of subtree $T_2 \in S(T;v,even)$.
$\omega(T_s)$ (resp. $\omega_{bc}(T_3)$)	Weight of $T_s \in S(T)$ (resp. BC-weight of $T_3 \in S_{BC}(T)$).
$F_{BC}(\cdot)$ function	Sum of BC-weight of BC-subtrees of $S_{BC}(\cdot)$.
$\eta(\cdot)$ function	Cardinality of the above $S(\cdot)$ set of subtree.
$\eta^+(T)$	The number of leaf-containing subtrees of T
$\eta^+_{BC}(T)$	The number of leaf-containing BC-subtrees of T
$\eta_{BC}(\cdot)$ function	Cardinality of the above $S_{BC}(\cdot)$ set of BC-subtree.

For a given subtree T_s of a weighted T, we define the weight of T_s, 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 T, denoted by $F(T;f_1,g_1)$, is the sum of weights of subtrees of T. That is,

$$F(T;f_1,g_1) = \sum\nolimits_{T_s \in S(T)} \omega(T_s).$$

Similarly, the generating function of subtrees of T containing v is denoted as

$$F(T;f_1,g_1;v) = \sum\nolimits_{T_s \in S(T;v)} \omega(T_s).$$

$$S(T;v,odd) = \{T_s | T_s \in S(T;v) \wedge d_{T_s}(v,l) \equiv 1 (mod\, 2) \;\; (\forall l \in L(T_s) \wedge l \neq v)\} \quad (1)$$

$$S(T;v,even) = \{T_s | T_s \in S(T;v) \wedge d_{T_s}(v,l) \equiv 0 (mod\, 2) \;\; (\forall l \in L(T_s) \wedge l \neq v)\} \cup \{v\} \quad (2)$$

To facilitate presentation of our work, we call subtree in $S(T;v,odd)$ (resp. $S(T;v,even)$) as *OLDV*-subtree (resp. *ELDV*-subtree). For a given vertex v_k, *OLDV*-subtree $T_1 \in S(T;v_k,odd)$, *ELDV*-subtree $T_2 \in S(T;v_k,even) \backslash v_k$, we assign each edge (resp. vertex) of T_1 and T_2 the weight z (resp. (x,y) where x

is the "odd" weight and y is the "even" weight). And we define ω_vodd (resp. ω_veven) weight of T_1 (resp. T_2), denoted by $\omega\_vodd(T_1)$ (resp. $\omega\_veven(T_2)$), as the product of the even weights of vertices in $EWSO(T_1)$ (resp. $EWSE(T_2)$) and weights of edges in T_1 (resp. T_2). Here

$$EWSO(T_1) = \{v | v \in V(T_1) \wedge d_{T_1}(v, v_k) \equiv 1 (mod\ 2)\}$$

and

$$EWSE(T_2) = \{v | v \in V(T_2) \wedge d_{T_2}(v, v_k) \equiv 0 (mod\ 2)\}.$$

Since $v_k \in S(T; v_k, even)$, for the vertex v_k itself, we define $\omega\_veven(v_k) = y$. The generating function of $S(T; v_k, odd)$ (resp. $S(T; v_k, even)$) of a weighted graph $T = (V(T), E(T); f_2, g_2)$, denoted by $F(T; f_2, g_2; v_k, odd)$ (resp. $F(T; f_2, g_2; v_k, even)$), is the sum of ω_vodd (resp. ω_veven) weight of each $OLDV$-subtree (resp. $ELDV$-subtree) of $S(T; v_k, odd)$ (resp. $S(T; v_k, even)$). That is,

$$F(T; f_2, g_2; v_k, odd) = \sum_{T_1 \in S(T; v_k, odd)} \omega\_vodd(T_1),$$

and

$$F(T; f_2, g_2; v_k, even) = \sum_{T_2 \in S(T; v_k, even)} \omega\_veven(T_2).$$

Similarly, for a given BC-subtree T_3 of a weighted graph T, we define

$$BEWS(T_3) = \{v | v \in V(T_3) \wedge d_{T_3}(v, v_l) \equiv 0 (mod\ 2)\}$$

and

$$BNEWS(T_3) = \{v | v \in V(T_3) \wedge d_{T_3}(v, v_l) \equiv 1 (mod\ 2)\}$$

where $v_l \in L(T_3)$. The BC-weight of T_3, $\omega_{bc}(T_3)$, is the product of the even weights of the vertices in $BEWS(T_3)$ and weights of edges in T_3.

The generating function of BC-subtrees of a weighted graph T, denoted by $F_{BC}(T; f_2, g_2)$, is the sum of BC-weights of BC-subtrees of T. That is,

$$F_{BC}(T; f_2, g_2) = \sum_{T_3 \in S_{BC}(T)} \omega_{bc}(T_3).$$

Following the above notations and Table 1, we have

$$\eta(T) = F(T; 1, 1), \quad \eta(T; v) = F(T; 1, 1; v),$$

$$\eta(T; v_i, odd) = F(T; (0, 1), 1; v_i, odd), \quad \eta(T; v_i, even) = F(T; (0, 1), 1; v_i, even),$$

and

$$\eta_{BC}(T) = F_{BC}(T; (0, 1), 1).$$

Let $T = (V(T), E(T); f_1, g_1)$ be a weighted tree of order $n > 1$ and u a pendant vertex of T. Suppose $e = (u, v)$ is the pendant edge of T, we define weighted tree

$T_1' = (V(T_1'), E(T_1'); f_1', g_1')$ of order $n-1$ from T as follows: $V(T_1') = V(T)\backslash u$, $E(T_1') = E(T)\backslash e$, and

$$f_1'(v_s) = \begin{cases} f_1(v)(1 + f_1(u)g_1(e)) & \text{if } v_s = v, \\ f_1(v_s) & \text{otherwise.} \end{cases}$$

for any $v_s \in V(T_1')$, and $g_1'(e) = g_1(e)$ for any $e \in E(T_1')$.

Lemma 1. *[25] With the above notations, for arbitrary vertex $u \neq v_i$, the generating functions $F(T; f_1, g_1; v_i)$ and $F(T_1'; f_1', g_1'; v_i)$ satisfy the following*

$$F(T; f_1, g_1; v_i) = F(T_1'; f_1', g_1'; v_i).$$

Let $T = (V(T), E(T); f_2, g_2)$ be a weighted tree of order $n > 1$ with root v_i and let $u \neq v_i$ be a pendant vertex of T with a unique neighbor v, we define weighted tree $T_2' = (V(T_2'), E(T_2'); f_2', g_2')$ of order $n-1$ from T as follows: $V(T_2') = V(T)\backslash u$, $E(T_2') = E(T)\backslash e$, and

$$f_2'(v_s)_o = \begin{cases} f_2(v)_o(1 + g_2(e)f_2(u)_e) + g_2(e)f_2(u)_e & \text{if } v_s = v, \\ f_2(v_s)_o & \text{otherwise.} \end{cases}$$

$$f_2'(v_s)_e = \begin{cases} f_2(v)_e(1 + g_2(e)f_2(u)_o) & \text{if } v_s = v, \\ f_2(v_s)_e & \text{otherwise.} \end{cases}$$

for any $v_s \in V(T_2')$, and $g_2'(e) = g_2(e)$ for any $e \in E(T_2')$. Here $f_2(v)_o$ and $f_2(v)_e$ are the odd and even vertex weight of $(f_2(v)_o, f_2(v)_e)$ of v.

Lemma 2. *[26] With the above notations, we have $F(T; f_2, g_2; v_i, odd) = F(T_2'; f_2', g_2'; v_i, odd)$; $F(T; f_2, g_2; v_i, even) = F(T_2'; f_2', g_2'; v_i, even)$.*

Lemma 3. *[21] The path P_n (resp. star $K_{1,n-1}$) has $\binom{n+1}{2}$ (resp. $2^{n-1} + n - 1$) subtrees, fewer (resp. more) than any other trees of n vertices.*

Lemma 4. *[26] The star $K_{1,n-1}$ has $2^{n-1} - n$ BC-subtrees, more than any other trees on n vertices.*

Lemma 5. *[26] The number of BC-subtrees of the path P_n is $\lfloor \frac{n-1}{2} \rfloor \cdot \lfloor \frac{n}{2} \rfloor$, less than that of any other n-vertex tree.*

3. $\eta(.)$ of generalized Bethe trees, Bethe trees, and dendrimers

Let $T_1, T_2, \ldots, T_m (m \geq 1)$ be trees with disjoint vertex sets and w_i be the root of T_i $(i = 1, 2, \ldots, m)$. A tree T on more than two vertices could be considered as being obtained by joining a new vertex w to each of the vertices $w_1, w_2, \ldots, w_m$. With Lemma 1, the following theorem is immediate.

Theorem 3.1. *Let T be a tree on $n \geq 3$ vertices, whose structure is specified above. Then*

$$\eta(T) = \sum_{i=1}^{m} \eta(T_i) + \prod_{i=1}^{m} (1 + \eta(T_i; w_i)). \tag{3}$$

Next, we present a closed formula for the number of subtrees of generalized Bethe trees.

Theorem 3.2. *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. If d_1 denotes the degree of rooted vertex and $d_i + 1$ denotes the degree of vertices on ith level $(1 < i \leq k)$, then*

$$\eta(B_{k+1}) = \sum_{i=1}^{k-1} n_{i+1} m_{i+1} + m_1 + \prod_{i=1}^{k} d_i, \tag{4}$$

where $n_{i+1} = d_1 d_2 \dots d_i$, $m_k = 2^{d_k}$ and $m_{k-i} = (1 + m_{k+1-i})^{d_{k-i}}$ for $i = 1, 2, \dots, k-1$.

Proof. For convenience, denote by n_i the number of vertices on the ith level of B_{k+1}. Then we have $n_1 = 1$ and $n_i = d_1 d_2 d_3 \dots d_{i-1}$ for $i = 2, 3, \dots, k+1$. Let v_{k+1} be the root of B_{k+1} and l be an arbitrary leaf vertex, the path connecting v_{k+1} and l is denoted by $v_{k+1} v_k v_{k-1} \dots, v_1(l)$. Define A_{k+1} to be the tree B_{k+1} itself and A_{k-j} the component that contains v_{k-j} after the deletion of edge (v_{k-j}, v_{k-j+1}) from A_{k+1-j} for $j = 0, 1, \dots, k-2$.

By Theorem 3.1 and for $j = 0, 1, \dots, k-1$, the subtrees in the set $S(A_{k+1-j})$ could be characterized into two categories:

(i) containing vertex v_{k+1-j};

(ii) not containing vertex v_{k+1-j}.

Obviously, the number of subtrees of case (ii) equals

$$d_{j+1} \eta(A_{k-j}). \tag{5}$$

From Lemma 1, the number of subtrees of case (i) equals

$$(1 + \eta(A_{k-j}; v_{k-j}))^{d_{j+1}}. \tag{6}$$

And for $j = 0, 1, \dots, k-2$ we have

$$\eta(A_{k+1-j}; v_{k+1-j}) = (1 + \eta(A_{k-j}; v_{k-j}))^{d_{j+1}} \tag{7}$$

and

$$\eta(A_2; v_2) = 2^{d_k}. \tag{8}$$

For simplicity, define $m_j = \eta(A_{k+2-j}; v_{k+2-j})$ $(j = 1, 2, \dots, k)$.

Then with the above notations and combining Eqs. (5) to (8), we have the formula of subtrees number of a generalized Bethe tree B_{k+1} as in Eq. (4). □

By definition we know that $T_{k,d}$ is a generalized Bethe tree of $k+1$ levels, with Theorem 3.2, the following corollary follows after simple algebra.

Corollary 3.3. *The subtree number of dendrimer $T_{k,d}$ is*

$$\eta(T_{k,d}) = d\sum_{i=2}^{k-1}(d-1)^{i-2}m_i + m_1 + d(d-1)^{k-2}(2^{d-1}+d-1),$$

where $m_1 = (1+m_2)^d$, $m_k = 2^{d-1}$ and $m_{k-i} = (1+m_{k+1-i})^{d-1}$ for $i = 1,2,\ldots,k-2$.

Let v_k be the root vertex of Bethe tree $B_{k,d}$ and A_k the tree $B_{k,d}$ itself. Similar to the the proof of Theorem 3.2, suppose the path connecting v_k and l (an arbitrary leaf vertex) is $v_k v_{k-1}\ldots v_1(l)$ and denote by A_{k-j} the component of $A_{k+1-j}\backslash(v_{k-j}, v_{k-j+1})$ that contains v_{k-j} and define $m_j = \eta(A_{k+1-j}; v_{k+1-j})$ for $j = 1,2\ldots,k-1$. Theorem 3.2 and simple algebra indicate the following.

Corollary 3.4. *The subtree number of Bethe tree $B_{k,d}$ is*

$$\eta(B_{k,d}) = \sum_{i=1}^{k-3} d^i(1+m_{i+2})^d + m_1 + d^{k-2}(2^d+d),$$

where $m_{k-1} = 2^d$ and $m_i = (1+m_{i+1})^d$ for $i = 1,2,\ldots,k-2$.

Noting that the number of leaf-containing subtrees of a Bethe tree or dendrimer is simply the number of subtrees of the tree minus that of the "skeleton" (obtained from removing all leaves), it is easy to obtain the formulas for $\eta^+(.)$.

Corollary 3.5. *The leaf-containing subtree number of dendrimer $T_{k,d}$ equals*

$$\eta^+(T_{k,d}) = d(d-2)\sum_{i=3}^{k}(d-1)^{i-3}m_i + m_1 + (d-1-m_3)(1+m_3)^{d-1} + d(d-1)^{k-2}(d-2), \quad (9)$$

where $m_1 = (1+m_2)^d$, $m_k = 2^{d-1}$ and $m_{k-i} = (1+m_{k+1-i})^{d-1}$ for $i = 1,2,\ldots,$ $k-2$.

Proof. By Corollary 3.3, we have

$$\eta(T_{k,d}) = d\sum_{i=3}^{k-1}(d-1)^{i-2}m_i + d(1+m_3)^{d-1} + m_1 + d(d-1)^{k-2}(2^{d-1}+d-1), \quad (10)$$

and

$$\begin{aligned}\eta(T_{k-1,d}) &= d\sum_{i=2}^{k-2}(d-1)^{i-2}m_{i+1} + (1+m_3)^d + d(d-1)^{k-3}(2^{d-1}+d-1)\\ &= d\sum_{i=3}^{k-1}(d-1)^{i-3}m_i + (1+m_3)^d + d(d-1)^{k-3}(2^{d-1}+d-1).\end{aligned} \quad (11)$$

Subtracting Eq. (11) from Eq. (10) yields Eq. (9). □

4. $\eta_{BC}(.)$ of the generalized Bethe trees, Bethe trees, and dendrimers

Similar to the previous section, Lemma 2 implies the following theorem. For simplicity of notations, we employ the convention that $\prod_{t=i}^{j} a_t = 1$ and $\sum_{t=i}^{j} a_t = 0$ if $j < i$.

Theorem 4.1. *Let T be a tree on $n \geq 3$ vertices rooted at w with children w_i's ($i = 1, 2, \ldots, m$) and let T_i be the connected component of $T \backslash w$ that contains w_i, then*

$$\begin{aligned}\eta_{BC}(T) = \sum_{i=1}^{m} \eta_{BC}(T_i) + \sum_{i=1}^{m} \Big(\eta(T_i; w_i, odd) \prod_{j=i+1}^{m} (1 + \eta(T_j; w_j, odd)) \\ + \eta(T_i; w_i, even) \sum_{s=1}^{m-i} \Big[\sum_{i+1 \leq j_1 < j_2 < \cdots < j_s \leq m} \prod_{k=1}^{s} \eta(T_{j_k}; w_{j_k}, even) \Big] \Big).\end{aligned} \tag{12}$$

Proof. For the sake of convenience, first we define T_w^m the tree T itself and denote T_w^{m-i} the component of $T_w^{m+1-i} \backslash (w, w_i)$ that contains w for $i = 1, 2, \ldots, m$. Obviously, T_w^0 is the isolated vertex w. For $i = 1, 2, \ldots, m$, the BC-subtrees of T_w^{m+1-i} could be characterized into two categories:

(i) containing the edge $e_i = (w_i, w)$;

(ii) not containing the edge $e_i = (w_i, w)$.

It is easy to see that the generating function corresponding to case (ii) is $F_{BC}(T_i; f_2, g_2) + F_{BC}(T_w^{m-i}; f_2, g_2)$ and the number equals

$$\eta_{BC}(T_i) + \eta_{BC}(T_w^{m-i}). \tag{13}$$

On the other hand, the generating function corresponding to case (i) is

$$g_2(e_i) F(T_i; f_2, g_2; w_i, odd) F(T_w^{m-i}; f_2, g_2; w, even) + g_2(e_i) F(T_i; f_2, g_2; w_i, even) F(T_w^{m-i}; f_2, g_2; w, odd),$$

which equals

$$\eta(T_i; w_i, odd) \eta(T_w^{m-i}; w, even) + \eta(T_i; w_i, even) \eta(T_w^{m-i}; w, odd). \tag{14}$$

By Lemma 2, we have

$$\eta(T_w^{m-i}; w, even) = \prod_{j=i+1}^{m} (1 + \eta(T_j; w_j, odd)) \tag{15}$$

and

$$\eta(T_w^{m-i}; w, odd) = \sum_{s=1}^{m-i} \Big[\sum_{i+1 \leq j_1 < j_2 < \cdots < j_s \leq m} \prod_{k=1}^{s} \eta(T_{j_k}; w_{j_k}, even) \Big]. \tag{16}$$

Combining the Eqs. (13) to (16), we have Eq. (12). □

With Theorem 4.1, the formulae for the BC-subtree number of generalized Bethe trees B_{k+1}, Bethe trees $B_{k,d}$ and $T_{k,d}$ could be obtained.

Theorem 4.2. *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels, then*

$$\eta_{BC}(B_{k+1}) = \sum_{j=0}^{k-2} n_{j+1}\left[\sum_{r=1}^{d_{j+1}-1}\left[\sum_{s=1}^{r}\binom{r}{s}m_{j+2,even}^{s+1} + m_{j+2,odd}\left(1+m_{j+2,odd}\right)^{r}\right] + m_{j+2,odd}\right] + \prod_{j=1}^{k-1} d_j(2^{d_k} - d_k - 1)$$

where $n_1 = 1$, $n_{j+1} = d_1 d_2 \ldots d_j$ $(j \geq 1)$, $m_{k,odd} = 2^{d_k} - 1$, $m_{k,even} = 1$ and $m_{j,odd} = \sum_{s=1}^{d_j}\binom{d_j}{s} m_{j+1,even}^{s}$, $m_{j,even} = (1 + m_{j+1,odd})^{d_j}$ for $j = 2, 3, \ldots, k-1$.

Proof. With the same notations as specified in Theorem 3.2, By Theorem 4.1 and Lemma 2, for $j = 0, 1, \ldots, k-1$, BC-subtrees in the set $S_{BC}(A_{k+1-j})$ could be characterized into two categories:

(i) containing the vertex v_{k+1-j};

(ii) not containing the vertex v_{k+1-j}.

It is easy to know that the number of BC-subtrees of case (ii) equals

$$d_{j+1}\eta_{BC}(A_{k-j}). \tag{17}$$

By Theorem 4.1, the number of BC-subtrees of case (i) equals

$$\begin{aligned}&\sum_{r=1}^{d_{j+1}-1}\left[\sum_{s=1}^{r}\binom{r}{s}F(A_{k-j};(0,1),1;v_{k-j},even)^{s+1} + F(A_{k-j};(0,1),1;v_{k-j},odd)\right.\\ &\left.\times\left(1+F(A_{k-j};(0,1),1;v_{k-j},odd)\right)^{r}\right] + F(A_{k-j};(0,1),1;v_{k-j},odd).\end{aligned} \tag{18}$$

By Lemma 4, we have

$$\eta_{BC}(A_2) = F_{BC}(A_2;(0,1),1) = 2^{d_k} - d_k - 1. \tag{19}$$

With Lemma 2, for $j = 0, 1, \ldots, k-2$, we have the following recurrent formulas

$$F(A_{k+1-j};(0,1),1;v_{k+1-j},odd) = \sum_{s=1}^{d_{j+1}}\binom{d_{j+1}}{s}F(A_{k-j};(0,1),1;v_{k-j},even)^{s}, \tag{20}$$

$$F(A_{k+1-j};(0,1),1;v_{k+1-j},even) = (1 + F(A_{k-j};(0,1),1;v_{k-j},odd))^{d_{j+1}}, \tag{21}$$

and

$$F(A_2;(0,1),1;v_2,odd) = 2^{d_k} - 1, F(A_2;(0,1),1;v_2,even) = 1. \tag{22}$$

For simplicity, denote

$$m_{j,odd} = F(A_{k+2-j};(0,1),1;v_{k+2-j},odd)\ (j = 1,2,\ldots,k); \tag{23}$$

$$m_{j,even} = F(A_{k+2-j};(0,1),1;v_{k+2-j},even)\ (j = 1,2,\ldots,k). \tag{24}$$

The conclusion then follows from Eqs. (17) to (24). □

Again, the number of BC-subtrees of more specific structures follow as immediate consequences. We skip the details here.

Corollary 4.3. *The BC-subtree number of dendrimer $T_{k,d}$ is*

$$\begin{aligned}\eta_{BC}(T_{k,d}) =& d\sum_{j=1}^{k-2}(d-1)^{j-1}\Bigg[\sum_{r=1}^{d-2}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{j+2,even}^{s+1} + m_{j+2,odd}\left(1+m_{j+2,odd}\right)^{r}\Bigg]\\ &+ m_{j+2,odd}\Bigg] + \sum_{r=1}^{d-1}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{2,even}^{s+1} + m_{2,odd}\left(1+m_{2,odd}\right)^{r}\Bigg] + m_{2,odd}\\ &+ d(d-1)^{k-2}(2^{d-1}-d).\end{aligned}$$

where $m_{k,odd} = 2^{d-1}-1$, $m_{k,even} = 1$ *and* $m_{j,odd} = \sum_{s=1}^{d-1}\binom{d-1}{s}m_{j+1,even}^{s}$, $m_{j,even} = (1+m_{j+1,odd})^{d-1}$ *for* $j = 2,3,\ldots,k-1$.

Corollary 4.4. *The BC-subtree number of Bethe tree $B_{k,d}$ is*

$$\eta_{BC}(B_{k,d}) = \sum_{j=0}^{k-3}d^{j}\Bigg[\sum_{r=1}^{d-1}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{j+2,even}^{s+1} + m_{j+2,odd}\left(1+m_{j+2,odd}\right)^{r}\Bigg] + m_{j+2,odd}\Bigg]$$

$$+ d^{k-2}(2^{d}-d-1),$$

where $m_{k-1,odd} = 2^{d}-1$, $m_{k-1,even} = 1$ *and* $m_{j,odd} = \sum_{s=1}^{d}\binom{d}{s}m_{j+1,even}^{s}$, $m_{j,even} = (1+m_{j+1,odd})^{d}$ *for* $j = 1,2,\ldots,k-2$.

From Corollary 4.3 we also have the following.

Corollary 4.5. *The leaf-containing BC-subtree number of dendrimer $T_{k,d}$ is*

$$\begin{aligned}\eta_{BC}^{+}(T_{k,d}) =& d(d-2)\sum_{j=2}^{k-2}(d-1)^{j-2}\Bigg[\sum_{r=1}^{d-2}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{j+2,even}^{s+1} + \left(1+m_{j+2,odd}\right)^{r}\\ &\times m_{j+2,odd}\Bigg] + m_{j+2,odd}\Bigg] + (d-1)\Bigg[\sum_{r=1}^{d-2}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{3,even}^{s+1} + \left(1+m_{3,odd}\right)^{r}\\ &\times m_{3,odd}\Bigg] + m_{3,odd}\Bigg] + \sum_{r=1}^{d-1}\Bigg[\sum_{s=1}^{r}\binom{r}{s}m_{2,even}^{s+1} + m_{2,odd}\left(1+m_{2,odd}\right)^{r}\Bigg]\\ &+ m_{2,odd} - m_{3,even}m_{2,odd} - m_{3,odd}m_{2,even} + d(d-2)(d-1)^{k-3}(2^{d-1}-d).\end{aligned}$$

where $m_{k,odd} = 2^{d-1}-1$, $m_{k,even} = 1$ *and* $m_{j,odd} = \sum_{s=1}^{d-1}\binom{d-1}{s}m_{j+1,even}^{s}$, $m_{j,even} = (1+m_{j+1,odd})^{d-1}$ *for* $j = 2,3,\ldots,k-1$.

Basing on the above results, the values of $\eta(.)$, $\eta^{+}(.)$, $\eta_{BC}(.)$ and $\eta_{BC}^{+}(.)$ can be efficiently calculated for any (generalized) Bethe trees or dendrimers. It is easy to see that number of subtrees or BC-subtrees grow exponentially as the number of levels (of the tree) increases, so does the leaf-containing subtrees (resp. BC-subtrees) number.

5. Newkome's arborol

As an application, we apply our results to Newkome's arborol [19], synthesized by Newkome and others (see Fig. 1). Note that T has 36 vertices of degree one and 253 vertices in total. The vertex whose degree is greater than two is called branching vertex. It is obvious that there are three types of branching vertices: α, β and γ (see Fig. 1). The neighbours of α, β and γ are denoted as α_i, β_i and γ_i for $i = 1, 2, 3, 4$ respectively. Denote T_i the connected component of $T \setminus \bigcup_{i=1}^{4} (\alpha, \alpha_i)$ that contains α_i $(i = 1, 2, 3, 4)$, obviously T_i $(i = 1, 2, 3, 4)$ are identical with each other. Similarly, denote $T_{1,i}$ (resp. $T_{1,1,i}$) the connected component of $T_1 \setminus \bigcup_{i=1}^{4} (\beta, \beta_i)$ (resp. $T_{1,1} \setminus \bigcup_{i=1}^{4} (\gamma, \gamma_i)$) that contains β_i (resp. γ_i) $(i = 1, 2, 3, 4)$.

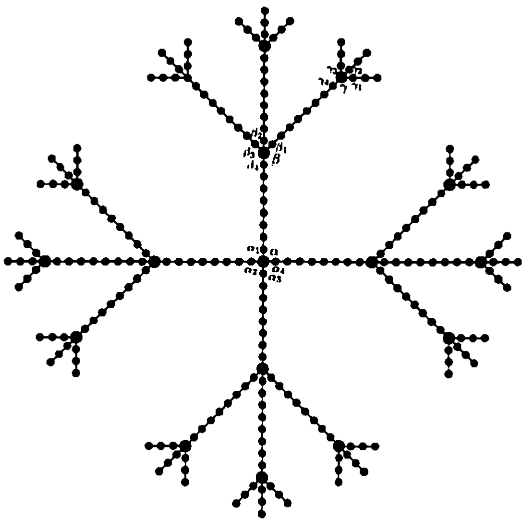


Figure 1. The molecular graph T of Newkome's arborol.

By Theorem 3.1, we have

$$\eta(T) = 4\eta(T_1) + (1 + \eta(T_1; \alpha_1))^4; \tag{25}$$

$$\eta(T_1) = 3\eta(T_{1,1}) + \eta(T_{1,4}) + 9(1 + \eta(T_{1,1}; \beta_1))^3, \tag{26}$$

and

$$\eta(T_{1,1}) = 3\eta(T_{1,1,1}) + \eta(T_{1,1,4}) + 9(1 + \eta(T_{1,1,1}; \gamma_1))^3. \tag{27}$$

By Lemma 3, we have $\eta(T_{1,1,4}) = \eta(T_{1,4}) = 36$, $\eta(T_{1,1,1}) = 6$; by Lemma 1, we have $\eta(T_{1,1,1}; \gamma_1) = 3$, $\eta(T_{1,1}; \beta_1) = 72$ and $\eta(T_1; \alpha_1) = 373256$. Hence, combining Eqs (25) to (27), we have $\eta(T) = 14012316 + 373257^4$.

Similarly, by Theorem 4.1, we have

$$\begin{aligned}\eta_{BC}(T) =&4\eta_{BC}(T_1) + \eta(T_1;\alpha_1,odd)^4 + \eta(T_1;\alpha_1,even)^4 + 4\eta(T_1;\alpha_1,odd)\\&+ 4(\eta(T_1;\alpha_1,odd)^3 + \eta(T_1;\alpha_1,even)^3) + 6(\eta(T_1;\alpha_1,odd)^2\\&+ \eta(T_1;\alpha_1,even)^2),\end{aligned} \tag{28}$$

$$\begin{aligned}\eta_{BC}(T_1) =&3\eta_{BC}(T_{1,1}) + \eta_{BC}(T_{1,4}) + 5(\eta(T_{1,1};\beta_1,odd)^3 + \eta(T_{1,1};\beta_1,even)^3)\\&+ 4 + 15(\eta(T_{1,1};\beta_1,odd)^2 + \eta(T_{1,1};\beta_1,even)^2) + 15\eta(T_{1,1};\beta_1,odd)\\&+ 12\eta(T_{1,1};\beta_1,even),\end{aligned} \tag{29}$$

$$\begin{aligned}\eta_{BC}(T_{1,1}) =&3\eta_{BC}(T_{1,1,1}) + \eta_{BC}(T_{1,1,4}) + 5(\eta(T_{1,1,1};\gamma_1,odd)^3 + \eta(T_{1,1,1};\\&\gamma_1,even)^3) + 4 + 15(\eta(T_{1,1,1};\gamma_1,odd)^2 + \eta(T_{1,1,1};\gamma_1,even)^2)\\&+ 15\eta(T_{1,1,1};\gamma_1,odd) + 12\eta(T_{1,1,1};\gamma_1,even).\end{aligned} \tag{30}$$

By Lemma 5, we have $\eta_{BC}(T_{1,1,4}) = \eta_{BC}(T_{1,4}) = 12$, $\eta_{BC}(T_{1,1,1}) = 1$; by Lemma 2, we have $\eta(T_{1,1,1};\gamma_1,odd) = 1$, $\eta(T_{1,1,1};\gamma_1,even) = 2$, $\eta(T_{1,1};\beta_1,odd) = 30$, $\eta(T_{1,1};\beta_1,even) = 12$, $\eta(T_1;\alpha_1,odd) = 2200$ and $\eta(T_1;\alpha_1,even) = 29795$. Therefore, $\eta_{BC}(T_1) = 160444$. Combining Eqs. (28) to (30), we have $\eta_{BC}(T) = 29795^4 + 2200^4 + 4(2200^3 + 29795^3) + 5356142726$.

6. The asymptotic behavior of subtree and BC-subtree densities of dendrimers $T_{k,d}$

For a tree T of order n and k subtrees (not including the empty tree) of orders $n_1, n_2, \dots, n_k$, let $\mu(T) = \frac{1}{k}\sum_{i=1}^{k} n_i$ denote the average order of subtrees of T and call $D(T) = \frac{\mu(T)}{n}$ the subtree density of T. It is not hard to see that the subtree density of a tree is also the probability that a vertex chosen at random from T will belong to a randomly chosen subtree of T.

These two invariants were introduced by Jamison [12], who showed that $D(T) > \frac{1}{3}$ for any tree T, among trees of a fixed order, and there also exist trees with $D(T)$ arbitrarily close to 1. For trees whose internal vertices have degree at least three (i.e. series-reduced trees), Jamison [12] conjectured that $D(T) > \frac{1}{2}$. Vince and Wang [24] proved this conjecture and gave a sharp upper bound $D(T) < \frac{3}{4}$ for such trees. Meir and Moon [13] determined the average density over all trees of order n to be $1 - e^{-1} \approx 0.6321$ as $n \to \infty$. Haslegrave [8] presented simple necessary and sufficient conditions for a sequence of series-reduced trees to have average subtree density tending to $\frac{1}{2}$ or $\frac{3}{4}$.

We define the BC-subtree density similarly. Suppose tree T has k BC-subtrees of orders $m_1, m_2, \dots, m_k$, then let $\mu_{BC}(T) = \frac{1}{k}\sum_{i=1}^{k} m_i$ denote the average order of BC-subtree of T. If T has order n, call $D_{BC}(T) = \frac{\mu_{BC}(T)}{n}$ the BC-subtree density of

T. In the following, we first discuss the subtree and BC-subtree densities of path P_n and star $K_{1,n-1}$ as simple examples. Then we consider the asymptotic behavior of subtree and BC-subtree densities of dendrimers $T_{k,d}$.

Lemma 6. *[25] The vertex generating functions of subtrees of P_n and $K_{1,n-1}$ are $F(P_n; x, 1) = \sum_{i=1}^{n}(n-i+1)x^i$ and $F(K_{1,n-1}; x, 1) = nx + \sum_{i=1}^{n-1}\binom{n-1}{i}x^{i+1}$ respectively.*

Lemma 7. *[26] The edge generating functions of BC-subtrees of P_n and $K_{1,n-1}$ are $F_{BC}(P_n; (0,1), y) = \sum_{i=1}^{\lceil\frac{n}{2}\rceil-1}(n-2i)y^{2i}$ and $F_{BC}(K_{1,n-1}; (0,1), y) = \sum_{i=2}^{n-1}\binom{n-1}{i}y^i$ respectively.*

From Lemmas 3 and 6, we have the subtree density of P_n and $K_{1,n-1}$ as:

$$D(P_n) = \frac{\sum_{i=1}^{n}(n-i+1)i}{n\binom{n+1}{2}} = \frac{1}{3} + \frac{1}{3n} \tag{31}$$

and

$$D(K_{1,n-1}) = \frac{n + \sum_{i=1}^{n-1}\binom{n-1}{i}(i+1)}{n(2^{n-1}+n-1)} = \frac{2^{n-1}+n-1+(n-1)2^{n-2}}{n(2^{n-1}+n-1)}. \tag{32}$$

From Lemmas 4, 5 and 7, we have the BC-subtree density of P_n and $K_{1,n-1}$ as:

$$D_{BC}(P_n) = \frac{\sum_{i=1}^{\lceil\frac{n}{2}\rceil-1}(n-2i)(2i+1)}{n\lfloor\frac{n}{2}\rfloor(\lceil\frac{n}{2}\rceil-1)} = \frac{\lceil\frac{n}{2}\rceil(n-\frac{1+4\lceil\frac{n}{2}\rceil}{3})+n}{n\lfloor\frac{n}{2}\rfloor} \tag{33}$$

and

$$D_{BC}(K_{1,n-1}) = \frac{\sum_{i=2}^{n-1}\binom{n-1}{i}(i+1)}{n(2^{n-1}-n)} = \frac{2^{n-1}-n+(2^{n-2}-1)(n-1)}{n(2^{n-1}-n)}. \tag{34}$$

By Eqs. (31) and (33), we have $\lim_{n\to\infty} D_{BC}(P_n) = \frac{1}{3}$, $\lim_{n\to\infty} D(P_n) = \frac{1}{3}$ and

$$D_{BC}(P_n) - D(P_n) = \begin{cases} \frac{4}{3n} & n \equiv 0(mod\ 2), \\ \frac{4n-2}{3n(n-1)} & n \equiv 1(mod\ 2). \end{cases} \tag{35}$$

By Eqs. (32) and (34), we have $\lim_{n\to\infty} D_{BC}(K_{1,n-1}) = \frac{1}{2}$, $\lim_{n\to\infty} D(K_{1,n-1}) = \frac{1}{2}$ and

$$D_{BC}(K_{1,n-1}) - D(K_{1,n-1}) = \frac{(n-1)(2^{n-2}(2n-3)-n+1)}{n(2^{n-1}-n)(2^{n-1}+n-1)} \tag{36}$$

From Eqs. (35) and (36), we know that the BC-subtree densities of P_n and $K_{1,n-1}$ are bigger than their corresponding subtree densities.

Weighting each vertex and edge by y and 1 respectively, with Theorem 3.2 and Corollary 3.3, we get the vertex generating function of subtrees of $T_{k,d}$ (see [25] for details) as

$$F(T_{k,d}; y, 1) = d\sum_{i=2}^{k}(d-1)^{i-2}m_i + m_1 + d(d-1)^{k-1}y, \tag{37}$$

where $m_1 = y(1+m_2)^d$, $m_{k+1} = y$ and $m_{k-i} = y(1+m_{k+1-i})^{d-1}$ for $i = 0, 1, \dots, k-2$.

Similarly, weighting each vertex and edge by $(0, 1)$ and y respectively, from Theorem 4.2 and Corollary 4.3 we obtain the edge generating function of BC-subtrees of $T_{k,d}$ (see [26] for details)

$$\begin{aligned} F_{BC}(T_{k,d}; (0,1), y) = {} & d\sum_{j=1}^{k-2}(d-1)^{j-1}\left[\sum_{r=1}^{d-2}\left[\sum_{s=1}^{r}\binom{r}{s}m_{j+2,even}^{s+1}y^{s+1} + y\cdot m_{j+2,odd}\right.\right. \\ & \left.\left.\left(1 + y\cdot m_{j+2,odd}\right)^r\right] + y\cdot m_{j+2,odd}\right] + \sum_{r=1}^{d-1}\left[\sum_{s=1}^{r}\binom{r}{s}m_{2,even}^{s+1}y^{s+1} + y\left(1 + y\cdot m_{2,odd}\right)^r\right. \\ & \left. m_{2,odd}\right] + y\cdot m_{2,odd} + d(d-1)^{k-2}\sum_{s=2}^{d-1}\binom{d-1}{s}y^s. \end{aligned} \tag{38}$$

where $m_{k,odd} = \sum_{s=1}^{d-1}\binom{d-1}{s}y^s$, $m_{k,even} = 1$ and $m_{j,odd} = \sum_{s=1}^{d-1}\binom{d-1}{s}y^s m_{j+1,even}^s$, $m_{j,even} = (1 + y\cdot m_{j+1,odd})^{d-1}$ for $j = 2, 3, \dots, k-1$.

It is easy to see that the total number of vertices of $T_{k,d}$ is

$$n(T_{k,d}) = \frac{d((d-1)^k - 1)}{d-2}. \tag{39}$$

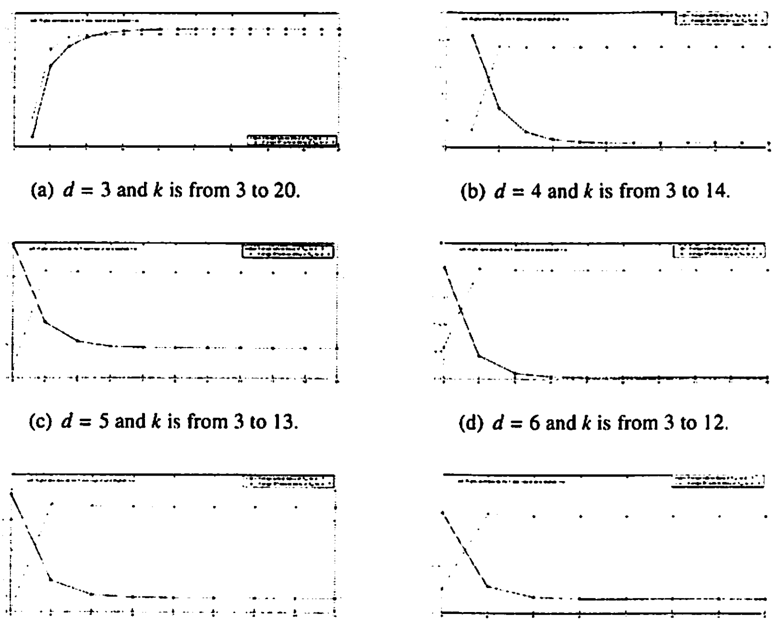
By the definitions of subtree and BC-subtree densities and Eqs. (37) to (39), we have the subtree density and BC-subtree density of $T_{k,d}$ respectively as

$$D(T_{k,d}) = \frac{\left.\frac{\partial F(T_{k,d}; y, 1)}{\partial y}\right|_{y=1}}{F(T_{k,d}; 1, 1)\times n(T_{k,d})} \tag{40}$$

and

$$D_{BC}(T_{k,d}) = \frac{\left.\frac{\partial (F_{BC}(T_{k,d}; (0,1), y)\times y)}{\partial y}\right|_{y=1}}{F_{BC}(T_{k,d}; (0,1), 1)\times n(T_{k,d})}. \tag{41}$$

Since both the vertex generating function of subtrees and the edge generating function of BC-subtrees of dendrimer $T_{k,d}$ are implicit, recursive and the values increase faster than exponential growth, computations of the $D(T_{k,d})$ and $D_{BC}(T_{k,d})$ are memory-consuming and time-consuming. We present the cases of $d = 3, 4, 5, 6, 7, 8$ and maximum level k to 20, 14, 13, 12, 11, and 10 respectively (see Fig. 2). More complex asymptotic analysis can be done but we stop here to keep the manuscript within a reasonable length.



(a) $d = 3$ and k is from 3 to 20.

(b) $d = 4$ and k is from 3 to 14.

(c) $d = 5$ and k is from 3 to 13.

(d) $d = 6$ and k is from 3 to 12.

(e) $d = 7$ and k is from 3 to 11.

(f) $d = 8$ and k is from 3 to 10.

Figure 2. Asymptotic subtree (BC-subtree) densities of $T_{k,d}$ with $d = 3$ to 8.

7. Concluding remarks

We provide some new evaluation results on number of (leaf-containing) subtrees (resp. BC-subtrees) of generalized Bethe trees, Bethe trees and regular dendrimer tree $T_{k,d}$. At the same time, through vertex (resp. edge) generation function of subtrees (resp. BC-subtrees) of dendrimers $T_{k,d}$, we consider the subtree (resp. BC-subtree) density of $T_{k,d}$ with low order of d and k.

As future work, we plan to further examine the subtree and BC-subtree densities, hoping to provide bounds on these values of special structures. We would also like to extend our current work to other categories of trees of similar nature.

Acknowledgment

This work is partially supported by the Simons Foundation (Grant No. 245307), the National Natural Science Foundation of China (Grant No. 61173035, 61472058) and the Program for New Century Excellent Talents in University (Grant No. NCET-11-0861).

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