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Counting the Numbers of Paths of All Lengths in Symmetric Dendrimers and Its Applications

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Abstract

The dendrimers are highly branched organic macromolecules having repeated iterations of branched units that surrounds the central core. Dendrimers are used in a variety of fields including chemistry, nanotechnology and biology. For positive integers n and k, the symmetric dendrimer $T_{n,k}$ is defined as the rooted tree of radius n whose all vertices at distance less than n from the root have degree k and all pendent vertices have equal distance n from the root. In this paper, for any positive integer ℓ, we count the number of paths of length ℓ of $T_{n,k}$. As a consequence of our main results, we obtain the average distance of $T_{n,k}$ which we can establish an alternate proof for the Wiener index of $T_{n,k}$. Further, we generalize the concept of

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medium domination, introduced by Vargör and Dündar in 2011, of $T_{n,k}$.

1 Introduction

The set of vertices in a graph $G = (V(G), E(G))$ is $V(G)$ while the set of edges is denoted by $E(G)$. All graphs in this paper are finite and simple, with no loops or multiple edges. The the set $\{u : uv \in E(G)\}$ is the *neighbor set* $N_G(v)$ of a vertex v in G. The degree $deg_G(v)$ of a vertex v in G is given by $|N_G(v)|$. If the subgraph of G induced by S has no edges, then the vertex subset S of $V(G)$ is *independent*. The maximum cardinality of an independent set is given by the *independence number* of G which denoted by $\alpha(G)$. If every vertex of G has degree k then the graph G is *k-regular*. For $u, v \in V(G)$, the length of a shortest path from u to v is the *distance* $d_G(u, v)$ between u and v in G. The maximum distance between all pairs of vertices of G is the *diameter* of G and is denoted by $diam(G)$.

A *tree* is a connected graph with no subgraphs that are cycles. A *leaf*, also known as *pendent vertex*, is a vertex with degree one. A leaf's incident edge is the *pendent edge* while a leaf's neighbouring vertex is called a *support vertex*. A *rooted tree* T is a tree whose one vertex is identified as the root r. Furthermore, if $d_T(r, v) = i$, a vertex v of T is at *level* i and T has *n-level* if the greatest level of all vertices of T is n. The symmetric dendrimer $T_{n,k}$ is defined as the rooted tree of n-level whose all vertices at distance less than n from the root have degree k and all pendent vertices have equal distance n from the root. A (general) dendrimer is a molecule with a well-defined chemical structure that is synthesised chemically. Dendrimers have three key main components: one is the core, and it's the most fundamental aspect in dendrimer development, then branches that are added at each step sequentially produce a structure like tree, the last component is end groups. Dendrimers are hyperbranched macromolecules that have a wide range of applications in domains like supramolecular, drug development, and nanotechnology. Some graph variants such as domination number and some other types of domination numbers are used to describe a range of physical characteristics, including physicochemical characteristics, thermodynamic characters, chemical and biological actions, and so on. In 1978, Buhleier, Vogtle and Wehner [5] were the first to bring these nanomolecules to researcher's attention. Bokhary, Imran and Manzoor [2] introduced the topological indices of dendrimers and some more chemical structures that can be presented by graphs, inspired by the chemical relevance of molecular networks.

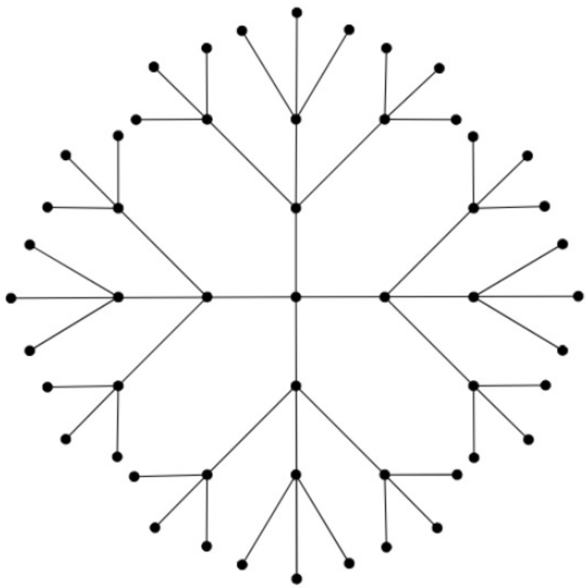

Figure 1. The symmetric dendrimer $T_{3,4}$.

The followings are examples of $T_{n,,k}$ when n or k is small. By the definition of the symmetric dendrimers, we have that $n \geq 1$ and $k \geq 2$.

When $n = 1$, $T_{1,k}$ is a *star* with $k + 1$ vertices.

When $k = 2$, $T_{n,2}$ is P_{2n+1}, a *path* of length $2n$.

When $n = 2$, it can be observed that $T_{2,k}$ can be obtained from $T_{1,k}$ by introducing $k - 1$ vertices to each leaf of $T_{1,k}$ and joining these vertices to that leaf. Hence, when $n, k \geq 2$, $T_{n,k}$ can be obtained from $T_{n-1,k}$ by introducing $k - 1$ vertices to each leaf of $T_{n-1,k}$ and joining these vertices to that leaf. Namely, when $n \geq 2$ and $k \geq 0$, $T_{n,k}$ is constructed by n iterations from the graph that has exactly one vertex. For example, the symmetric dendrimer $T_{3,4}$ is illustrated in Figure 1.

For a graph G, the sum of the distance between any pair of vertices of G is known as the *Weiner index* $W(G)$ of G. That is:

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

In the quantitative structure-property relationships (QSPR) [3,18,21], the Wiener index was the first and most well researched topological index. Since then dozens of new indices have been developed to link topological indices with various physical features. The boiling temperatures of alkane molecules are closely associated with the Wiener index. Later, a study on quantitative structure activity linkages revealed it is also connected with some other factors such as the critical point parameters, density, surface tension, viscosity of the liquid phase and the molecule's van der Waals surface area. It was originally called the path number since it was defined as the total of the lengths between any two carbon atoms in an alkane in terms of carbon-carbon bonds [24]. Wiener's works did not make use of graph theory, and the path number was only used in acyclic systems. In 1971, Hosoya [11] was the first to define the Wiener index within the context of chemical graph theory. In 1976, the Weiner index was studied for the first time by Entringer, Jackson and Snyder [9]. This index has also been referred by the terms "graph distance" [9] and "transmission" [12, 19]. Further, Plesnik [19] applied the Laplacian matrix to introduce a new graph-theoretical definition of the Wiener index for trees. Dobryin, Entringer and Gutman [8] established the Wiener index for symmetic dendrimers which states that for every $k \geq 3$, the Wiener index of $T_{n,k}$ is

$$W(T_{n,k}) = \frac{1}{(k-2)^3}[(k-1)^{2n}[nk^3 - 2(n+1)k^2 + k] + 2k^2(k-1)^n - k]. \tag{1}$$

A graph G fulfilling specific constraints can efficiently simulates numerous scenarios in communication, facility locating, cryptology and other fields. Due to cost constraint, it is frequently sought to have a spanning tree of G that is optimal with respect to one or more attributes. One of these attributes is the *average distance* of a graph which is defined to be the sum of all distances between any pair of vertices divided by the number of pairs of vertices of the graphs. That is,

$$\mu(G) = \frac{\displaystyle\sum_{u,v \in V(G)} d_G(u,v)}{\dbinom{|V(G)|}{2}}.$$

The study of the average distance of graphs was initiated by Plesnik in his classical result in [19]. The average distance is an important tool to analyse entire structure of the graph. The parameter globally presents expected number of edges that an object needs to travel between nodes (vertices) of networks. This reflects data transmission efficiency of communication networks as well as capability to deliver objects of transportation networks. Hence, the average distance has been continuously studied in both theoretical, algorithm and application areas. For example of the studies of average distance of graphs, Fajtlowicz and Waller [10] established the inequality between the average distance and the independence number in their classical paper since 1986 that $\alpha(G) \geq \mu(G) - 1$ for every connected graph G. Chung [6] improved this bound to be $\alpha(G) \geq \mu(G)$ and further characterized that the equality holds if and only if G is a complete graph. For more studies of the average distance of graphs see [7, 22] for example.

Domination in graph has been extensively researched and utilised in a variety of fields. Vargör and Dündar [23], established the idea of "the medium domination" which is defined as follows. For a graph G of order n and for any vertices $u, v \in V(G)$, $dom(u,v)$ is the number of vertices that dominate both u and v (but u and v will contribute eaxctly 1 to $dom(u,v)$ if $uv \in E(G)$). Then $TDV(G) = \sum_{u,v \in V(G)} dom(u,v)$ and the *medium domination number* of G is defined as

$$\gamma_m(G) = \frac{TDV(G)}{\binom{n}{2}}.$$

The medium domination number of graphs has been studied by [13, 20] for examples. It can be observed that $dom(u, v)$ is the number of paths of lengths one and two between u and v. Hence, for a given positive integer $\varsigma \geq 2$, the concept of $dom(u, v)$ can be generalized to $P\varsigma(u, v)$, the number of paths of lengths at most ς between u and v. Because $dom(u, v)$ is the main part of the medium domination number, the value $P\varsigma(G)$ generalizes the concept of medium domination number as well. For examples of the studies when $1 \leq \varsigma \leq 4$ see [16, 17].

From the above discussion, it can be showed that the Weiner index, the average distance and the medium domination number of dendrimers can be found if we know the number of paths of all lengths. Thus, the problems that arises is:

Problem 1. *For non-negative integers n, k and ℓ, how many paths of length ℓ does a symmetric dendrimer $T_{n,k}$ have?*

Surprisingly, to the best of our knowledge, Problem 1 has not been answered.

In this paper, we solve Problem 1 by establishing the exact and recursive formulas to count the number of paths of length ℓ of $T_{n,k}$ for all $1 \leq \ell \leq 2n$. As a consequence, we easily obtain average distance of $T_{n,k}$. Further, we generalize the concept of medium domination to ς-medium domination in graphs.

2 Main results and applications

In this section, we state our main results of this paper as well as their applications in Subsections 2.1 and 2.2 while most of the proofs are given in Section 4. First, for a graph G, we let

$n_\ell(G)$ be the number of paths of length ℓ of G.

Further, we may call a symmetric dendrimer shortly a dendrimer throughout. The first main result is the formula of $n_\ell(T_{n,k})$ for all possible values of ℓ. Recall that when $k = 2$, the dendrimer $T_{n,2}$ is a path of length $2n$. Thus, we let $x_1, ..., x_{2n+1}$ be $T_{n,2}$. Clearly, for a positive integer $1 \leq \ell \leq 2n$, all the paths of length ℓ are $x_i, x_{i+1}, ..., x_{i+\ell}$ for all $1 \leq i \leq 2n + 1 - \ell$. Hence, we obtain the following observation.

Observation 1. *Let $T_{n,k}$ be the dendrimer. If $k = 2$, then*

$$n_\ell(T_{n,2}) = 2n + 1 - \ell.$$

Thus, throughout of this paper, we may assume that $k \geq 3$. Further, for a tree T, we let

$n^1_\ell(T)$: the number of paths of length ℓ of T with exactly one end vertex is a leaf of T.

$n^2_\ell(T)$: the number of paths of length ℓ of T whose both end vertices are leaves of T.

Our main results in this subsection are Theorem 1, Corollaries 1 and 2. As informed earlier, the proofs are given in Section 4.

Theorem 1. *Let $T_{n,k}$ be the dendrimer and $k \geq 3$. If ℓ is even number, then*

$$n_\ell(T_{n,k}) = (k-1)n^1_{\ell-1}(T_{n-1,k}) + (k-1)^2 n^2_{\ell-2}(T_{n-1,k}) + n_\ell(T_{n-1,k}).$$

If ℓ is odd number, then

$$n_\ell(T_{n,k}) = (k-1)n^1_{\ell-1}(T_{n-1,k}) + 2(k-1)n^2_{\ell-1}(T_{n-1,k}) + n_\ell(T_{n-1,k}).$$

By Theorem 1, we obtain the following corollaries. It is worth noting that Corollary 2 is a combinatorial identity which is obtained by the counting two way principle.

Corollary 1. *Let $T_{n,k}$ be the dendrimer and $k \geq 3$. Then*

$$n_\ell(T_{n,k}) = \begin{cases} \frac{k(k-1)^{\ell-1}}{2}[\frac{k(k-1)^{n-\frac{\ell}{2}}-2}{k-2}] & \textit{when } \ell \text{ is even,} \\ \\ k(k-1)^{\frac{\ell-1}{2}}[\frac{(k-1)^n-(k-1)^{\frac{\ell-1}{2}}}{k-2}] & \textit{when } \ell \text{ is odd.} \end{cases}$$

Corollary 2. *For natural numbers n and k such that $k \geq 3$, we have that*

$$\binom{1+\frac{k[(k-1)^n-1]}{k-2}}{2} = \sum_{l=0}^{n-1} k(k-1)^l[\frac{(k-1)^n-(k-1)^l}{k-2}] + \sum_{l=1}^{n} \frac{k(k-1)^{2l-1}}{2}[\frac{k(k-1)^{n-l}-2}{k-2}].$$

2.1 Wiener index and average distance

In this subsection,We have linked our main problem to distance in dendrimers. Using the results obtained in Theorem 1, Corollaries 1 and 2, we have found the Wiener index and average distance of $T_{n,k}$. We obtain Corollaries 3 and 4. However, we still need Theorem 2 and the proof of this theorem is given in Section 4.

Theorem 2. *Let T be a tree having the diameter $diam(T)$. Then*

$$\sum_{\{u,v\}\subseteq V(T)} d_T(u,v) = \sum_{\ell=1}^{diam(T)} \ell n_\ell(T).$$

By Corollary 1, we have that

$$\sum_{\ell=1}^{2n} \ell n_\ell(T_{n,k}) = \sum_{l=0}^{n-1}(2l+1)k(k-1)^l[\frac{(k-1)^n-(k-1)^l}{k-2}] + \sum_{l=1}^{n}(2l)\frac{k(k-1)^{2l-1}}{2}[\frac{k(k-1)^{n-l}-2}{k-2}]. \tag{2}$$

As $diam(T_{n,k}) = 2n$, by (2) and Theorem 2, we immediately obtain the following corollaries.

Corollary 3. *Let $T_{n,k}$ be the dendrimer with the Weiner index $W(T_{n,k})$. Then*

$$W(T_{n,k}) = \sum_{l=0}^{n-1}(2l+1)k(k-1)^l[\frac{(k-1)^n-(k-1)^l}{k-2}] + \sum_{l=1}^{n}(2l)\frac{k(k-1)^{2l-1}}{2}[\frac{k(k-1)^{n-l}-2}{k-2}].$$

It is worth noting that the right hand side of the equation in Corollary 3 can be simplified to Equation (1).

Corollary 4. *Let $T_{n,k}$ be the dendrimer with the average distance $\mu(T_{n,k})$. Then*

$$\mu(T_{n,k}) = \Big(\sum_{l=0}^{n-1}(2l+1)k(k-1)^l[\frac{(k-1)^n-(k-1)^l}{k-2}] + \sum_{l=1}^{n}(2l)\frac{k(k-1)^{2l-1}}{2}[\frac{k(k-1)^{n-l}-2}{k-2}]\Big)/\Bigg(\frac{1+\frac{k[(k-1)^n-1]}{k-2}}{2}\Bigg).$$

2.2 Medium domination

Motivated by [16, 17, 23], we generalize their results to ς-medium domination of $T_{n,k}$. For a graph G of order n and for some $2 \leq \varsigma \leq diam(G)$, the *$\varsigma$-medium domination number* $\gamma_{\varsigma MD}(G)$ of G is defined as

$$\gamma_{\varsigma MD}(G) = \frac{P\varsigma(G)}{\binom{n}{2}},$$

where

$$P\varsigma(G) = \sum_{\ell=1}^{\varsigma} n_\ell(G),$$

the number of all paths whose lengths less than or equal to ς. Hence, when G is a dendrimer $T_{n,k}$, we obtain the ς-medium domination number of $T_{n,k}$ as follow:

Corollary 5. *Let $T_{n,k}$ be the dendrimer with the ς-medium domination number $\gamma_{\varsigma MD}(G)$. Then*

$$\gamma_{\varsigma MD}(T_{n,k}) = \frac{P\varsigma(T_{n,k})}{\binom{|V(T_{n,k})|}{2}},$$

where

$$P\varsigma(T_{n,k}) = \sum_{\ell=0}^{s} k(k-1)^{\ell}[\frac{(k-1)^n-(k-1)^{\ell}}{k-2}] + \sum_{\ell=1}^{\lfloor\frac{\varsigma}{2}\rfloor} \frac{k(k-1)^{2\ell-1}}{2}[\frac{k(k-1)^{n-\ell}-2}{k-2}]$$

and

$$s = \begin{cases} \lfloor\frac{\varsigma}{2}\rfloor & \text{when } \varsigma \text{ is odd,} \\ \lfloor\frac{\varsigma}{2}\rfloor - 1 & \text{when } \varsigma \text{ is even.} \end{cases}$$

3 Preliminaries

In this section, we provide some results that are used in establishing our main theorems. We begin with a simple but yet useful formula for geometric series. For a geometric series $S_n = a + ar + ar^2 + \cdots + ar^{n-1}$, we have that

$$S_n = \sum_{i=0}^{n-1} ar^i = \frac{a(1-r^n)}{1-r}$$

where n is the number of terms, a is the coefficient and $r \neq 1$ is the common ratio.

Further, for $T_{n,k}$, we may have the following formulas by simple counting arguments and geometric series,

- the total number of vertices of degree k is equal to $\frac{k(k-1)^{n-1}-2}{k-2}$,
- the total number of vertices of degree 1 (i.e. pendent vertices) is equal to $k(k-1)^{n-1}$,

- the total number of vertices is equal to $1 + \frac{k[(k-1)^n - 1]}{k-2}$ and
- the total number of edges is equal to $\frac{k[(k-1)^n - 1]}{k-2}$.

4 Proofs

In this section, we give the proofs of Theorem 1, Corollary 1, Corollary 2 and Theorem 2.

4.1 Proof of Theorem 1

To prove this theorem, we need to establish Lemmas 1 and 2 which are the exact formulas of $n^1_\ell(T_{n,k})$ and $n^2_\ell(T_{n,k})$.

Lemma 1. *for $n, k \geq 1$ and $1 \leq \ell \leq 2n$, we let $n^1_\ell(T_{n,k})$ be the number of paths of length ℓ of $T_{n,k}$ having exactly one end vertex as a leaf of $T_{n,k}$. Then*

$$n^1_\ell(T_{n,k}) = k(k-1)^{n+\lceil \frac{\ell}{2} \rceil - 2}.$$

Proof. First, we let r be the root and let x be an arbitrary leaf of the graph $T_{n,k}$. Further, for $0 \leq j \leq n$, we let

L_j : the set of all vertices of $T_{n,k}$ at distance i from r,

and

$\mathcal{P}_x$: the family of all paths of $T_{n,k}$ starting from x and the other end vertex is not
a leaf of $T_{n,k}$.

We distinguish two cases according to the value of ℓ.

Case 1: $1 \leq \ell \leq n$.
For a path $P \in \mathcal{P}_x$, we let

$$min(P) = \min\{j : V(P) \cap L_j \neq \emptyset\}.$$

Further, for $0 \leq i \leq \lfloor \frac{\ell-1}{2} \rfloor$, we let

$$\mathcal{P}_{x,i} = \{P \in \mathcal{P}_x : min(P) = n - \ell + i\}.$$

It can be observed that $\mathcal{P}_{x,0}, \mathcal{P}_{x,1}, ..., \mathcal{P}_{x,\lfloor \frac{\ell-1}{2} \rfloor}$ partition $\mathcal{P}_x$.

When $i = 0$, we have that $|\mathcal{P}_{x,0}| = 1$ as there is exactly one path of length ℓ starting from x, goes through vertices in $L_{n-1}, L_{n-2}, ..., L_{n-\ell+1}$ and terminates in $L_{n-\ell}$.

For each $1 \leq i \leq \lfloor \frac{\ell-1}{2} \rfloor$, all the paths in $\mathcal{P}_{x,i}$ start from x and go trough vertices in $L_{n-1}, ..., L_{n-\ell+i+1}, L_{n-\ell+i}$ with exactly one possibility. We may let $y \in L_{n-\ell+i+1}$ and $z \in L_{n-\ell+i}$ be the vertices that are in all the paths. Then, from the vertex z, all the paths move back to $L_{n-\ell+i+1}, ..., L_{n-\ell+2i}$. As y is already in every of such path, there are $k-2$ possibilities for all the paths in $P_{x,i}$. Further, there are $k-1$ possibilities for all the paths to pass each of $L_{n-\ell+i+2}, ..., L_{n-\ell+2i}$. Hence,

$$|\mathcal{P}_{x,i}| = (k-2)(k-1)^{i-1}$$

which implies that

$$\begin{aligned} |\mathcal{P}_x| &= |\mathcal{P}_{x,0}| + |\mathcal{P}_{x,1}| + \cdots + |\mathcal{P}_{x,\lfloor \frac{\ell-1}{2} \rfloor}| \\ &= 1 + (k-2) + (k-2)(k-1) + \cdots + (k-2)(k-1)^{\lfloor \frac{\ell-3}{2} \rfloor}. \end{aligned}$$

After simplifying this geometric series, we get

$$|\mathcal{P}_x| = (k-1)^{\lfloor \frac{\ell-1}{2} \rfloor}$$

and this proves Case 1.

Case 2: $\ell = n+1 \leq l \leq 2n$.
In this case, we let

$$\mathcal{R}_x = \{P \in \mathcal{P}_x : r \in V(P)\}$$

and

$$\mathcal{S}_x = \{P \in \mathcal{P}_x : r \notin V(P)\}.$$

We first count the number of paths in $\mathcal{R}_x$. All the paths in $\mathcal{R}_x$ start from x and pass to the root r with one possibility each. Then, from r, all the paths pass trough $L_1, ..., L_{\ell-n-1}$ and terminate in $L_{\ell-n}$ with $k-1$ possibilities. Thus, $|\mathcal{R}_x| = (k-1)^{\ell-n}$.

Next, we count the number of paths in $\mathcal{S}_x$ by similar arguments as in Case 1. For $\ell-n+1 \leq i \leq \lfloor\frac{\ell-1}{2}\rfloor$, we let

$$\mathcal{S}_{x,i} = \{P \in \mathcal{S}_x : min(P) = n-\ell+i\}.$$

Clearly, $\{\mathcal{S}_{x,\ell-n+1}, ..., \mathcal{S}_{x,\lfloor\frac{\ell-1}{2}\rfloor}\}$ partitions $\mathcal{S}_x$.

For each $\ell-n+1 \leq i \leq \lfloor\frac{\ell-1}{2}\rfloor$, all paths in $\mathcal{S}_{x,i}$ start from x pass trough $L_{n-1}, ..., L_{n-\ell+i+1}$ to $L_{n-\ell+i}$ with one possibility. Then, the paths pass back to $L_{n-\ell+i+1}$ with $k-2$ possibilities and continue in $L_{n-\ell+i+2}$ until terminating in $L_{n-\ell+2i}$ with $k-1$ possibilities. Thus

$$|\mathcal{S}_{x,i}| = (k-2)(k-1)^{i-1}$$

which implies that

$$\begin{aligned}
|S_x| &= |\mathcal{S}_{x,\ell-n+1}| + \cdots + |\mathcal{S}_{x,\lfloor\frac{\ell-1}{2}\rfloor}| \\
&= (k-2)(k-1)^{\ell-n} + (k-2)(k-1)^{\ell-n+1} + \cdots + (k-2)(k-1)^{\lfloor\frac{\ell-3}{2}\rfloor} \\
&= (k-2)\Big(\frac{(k-1)^{\lfloor\frac{\ell-1}{2}\rfloor}-1}{k-2} - \frac{(k-1)^{\ell-n}-1}{k-2}\Big) \\
&= (k-1)^{\lfloor\frac{\ell-1}{2}\rfloor} - (k-1)^{\ell-n}.
\end{aligned}$$

Hence,

$$|\mathcal{P}_x| = |\mathcal{R}_x| + |\mathcal{S}_x| = (k-1)^{\lfloor\frac{\ell-1}{2}\rfloor}$$

and this proves Case 2.

In both cases, we have that $|\mathcal{P}_x| = (k-1)^{\lfloor\frac{\ell-1}{2}\rfloor}$. As x is an arbitrary leaf of $T_{n,k}$ and $T_{n,k}$ has $k(k-1)^{n-1}$ leaves, it follows that

$$n_\ell^1(T_{n,k}) = \begin{cases} k(k-1)^{n+\frac{\ell}{2}-2} & \text{when } \ell \text{ is even,} \\ \\ k(k-1)^{n+\frac{\ell-1}{2}-1} & \text{when } \ell \text{ is odd.} \end{cases}$$

This implies that

$$n_\ell^1(T_{n,k}) = k(k-1)^{n+\lceil\frac{\ell}{2}\rceil-2}$$

which proves Lemma 1. ■

Lemma 2. *Let $n_\ell^2(T_{n,k})$ be the number of paths of length ℓ that start and end on a leaf vertex of the graph $T_{n,k}$. Then, for $n, k \geq 1$,*

$$n_\ell^2(T_{n,k}) = \begin{cases} k(k-1)^{n+\frac{\ell}{2}-3}\binom{k-1}{2} & \text{when } 2 \leq \ell \leq 2n-2 \\ \\ (k-1)^{\ell-2}\binom{k}{2} & \text{when } \ell = 2n. \end{cases}$$

Proof. First, we let

$\mathcal{Q}_\ell$: the family of paths of length ℓ of $T_{n,k}$ whose both end vertices are leaves of $T_{n,k}$.

Clearly, ℓ must be even. For a path $P \in \mathcal{Q}_\ell$, we let x_P be the center of P which the distance from x_p to the end vertices of P are both equal to $\frac{\ell}{2}$. We distinguish 2 cases according to the value of ℓ.

Case 1: $2 \leq \ell \leq 2n-2$.

It can be observed that every path in $\mathcal{Q}_\ell$ has the center in $L_{n-\frac{\ell}{2}}$. Let x be a vertex in $L_{n-\frac{\ell}{2}}$. There are $k-1$ neighbors of x in $L_{n-\frac{\ell}{2}+1}$. Each pair of these $k-1$ neighbors can be passed by a path in $\mathcal{Q}_\ell$. Hence, there are $\binom{k-1}{2}$ possibilities for the paths in $\mathcal{Q}_\ell$. We may let x_1 and x_2 be a pair among these $\binom{k-1}{2}$ possibilities. There are $(k-1)^{\frac{\ell}{2}-1}$ paths from each of x_1 and x_2 to the leaves of $T_{n,k}$. Hence, there are

$$\binom{k-1}{2}(k-1)^{\frac{\ell}{2}-1}(k-1)^{\frac{\ell}{2}-1} = (k-1)^{\ell-2}\binom{k-1}{2}$$

paths whose center is x and both end vertices are leaves. Since x is arbitraty and there are $k(k-1)^{n-\frac{\ell}{2}-1}$ vertices in $L_{n-\frac{\ell}{2}}$, it follows that

$$n_\ell^2(T_{n,k}) = |\mathcal{Q}_\ell| = k(k-1)^{n-\frac{\ell}{2}-3}\binom{k-1}{2}.$$

Case 2: $\ell = 2n$

In this case, the root r is the center of all paths in $\mathcal{Q}_{2n}$. There are $\binom{k}{2}$ possibilities for the paths in $\mathcal{Q}_{2n}$ to pass these vertices. Similarly, we let x_1 and x_2 be a pair among these $\binom{k}{2}$ possibilities. There are $(k-1)^{\frac{\ell}{2}-1}$

paths from each of x_1 and x_2 to the leaves of $T_{n,k}$. Hence,

$$n_\ell^2(T_{n,k}) = |\mathcal{Q}_{2n}| = (k-1)^{\ell-2}\binom{k}{2}$$

and this proves Lemma 2. ■

Now we are ready to prove Theorem 1.

Proof of Theorem 1 Recall that the graph $T_{n,k}$ can be constructed from $T_{n-1,k}$ by introducing $k-1$ vertices to each leaf, and joining these $k-1$ vertices to the leaf. We have considered two cases.

Case 1: ℓ is an even number.

Every path of length ℓ in this case is either (i) lies completely in $T_{n-1,k}$, (ii) can be formed from a path of length $\ell-1$ whose exactly one end vertex is a leaf of $T_{n-1,k}$ or (iii) can be formed from a path of length $\ell-2$ whose both end vertices are at the leaves of $T_{n-1,k}$. The Case (i) gives $n_\ell(T_{n-1,k})$ paths of length ℓ while the Case (ii) gives $(k-1)n_\ell^1(T_{n-1,k})$ paths of length ℓ as the end vertex at a leaf of $T_{n-1,k}$ can be extended with $k-1$ ways. Finally, the Case (iii) gives $(k-1)^2 n_{\ell-2}^2(T_{n-1,k})$ paths as every path of length $\ell-2$ whose both end vertices are at the leaves of $T_{n-1,k}$ can be extended to the path of length ℓ by $(k-1)^2$ ways, $k-1$ for each end vertex. Thus, we have the following recursive formula

$$n_\ell(T_{n,k}) = (k-1)n_{\ell-1}^1(T_{n-1,k}) + (k-1)^2 n_{\ell-2}^2(T_{n-1,k}) + n_\ell(T_{n-1,k}).$$

This proves Case 1.

Case 2: ℓ is an odd number

Similarly, every path of length ℓ in this case is either (i) lies completely in $T_{n-1,k}$, (ii) can be formed from a path of length $\ell-1$ whose exactly one end vertex is a leaf of $T_{n-1,k}$ or (iii) can be formed from a path of length $\ell-1$ whose both end vertices are at the leaves of $T_{n-1,k}$. The Case (i) gives $n_\ell(T_{n-1,k})$ paths while the Case (ii) gives $(k-1)n_\ell^1(T_{n-1,k})$ paths. For the Case (iii), we can only extend these paths of length $\ell-1$ in $T_{n-1,k}$ to be a path of length ℓ by extending only one end vertex, $k-1$ ways for each end vertex. Thus there are $2(k-1)n^2_{\ell-1}(T_{n-1,k})$ paths in this case. Thus, we have a recursive formula:

$$n_\ell(T_{n,k}) = (k-1)n^1_{\ell-1}(T_{n-1,k}) + 2(k-1)n^2_{\ell-1}(T_{n-1,k}) + n_\ell(T_{n-1,k}).$$

This proves Case 2 and completes the proof of our theorem. ■

4.2 Proof of Corollary 1

We distinguish two cases according to the parity of ℓ.

Case 1: ℓ is an even number.

By Theorem 1, we have that

$$\begin{aligned}
n_\ell(T_{n,k}) &= (k-1)n^1_{\ell-1}(T_{n-1,k}) + (k-1)^2 n^2_{\ell-2}(T_{n-1,k}) + n_\ell(T_{n-1,k}) \\
n_\ell(T_{n-1,k}) &= (k-1)n^1_{\ell-1}(T_{n-2,k}) + (k-1)^2 n^2_{\ell-2}(T_{n-2,k}) + n_\ell(T_{n-2,k}) \\
n_\ell(T_{n-2,k}) &= (k-1)n^1_{\ell-1}(T_{n-3,k}) + (k-1)^2 n^2_{\ell-2}(T_{n-3,k}) + n_\ell(T_{n-3,k}) \\
&\vdots \\
n_\ell(T_{\frac{\ell}{2}+1,k}) &= (k-1)n^1_{\ell-1}(T_{\frac{\ell}{2},k}) + (k-1)^2 n^2_{\ell-2}(T_{\frac{\ell}{2},k}) + n_\ell(T_{\frac{\ell}{2},k}) \\
n_\ell(T_{\frac{\ell}{2},k}) &= (k-1)n^1_{\ell-1}(T_{\frac{\ell-2}{2},k}) + (k-1)^2 n^2_{\ell-2}(T_{\frac{\ell-2}{2},k}) + n_\ell(T_{\frac{\ell-2}{2},k}).
\end{aligned}$$

As $\frac{\ell-2}{2} < \frac{\ell}{2}$, we have $n_\ell(T_{\frac{\ell-2}{2},k}) = 0$. Further, $n^1_{\ell-1}(T_{\frac{\ell-2}{2},k}) = 0$ because $\frac{\ell-2}{2} < \frac{\ell-1}{2}$. Thus, summing the above equations we have

$$n_\ell(T_{n,k}) = (k-1)\sum_{i=\frac{\ell}{2}}^{n-1} n^1_{\ell-1}(T_{i,k}) + (k-1)^2 \sum_{j=\frac{\ell-2}{2}}^{n-1} n^2_{\ell-2}(T_{j,k}). \qquad (3)$$

By Lemma 1 when $\ell-1$ is odd, we have that

$$\sum_{i=\frac{\ell}{2}}^{n-1} n^1_{\ell-1}(T_{i,k}) = \sum_{i=\frac{\ell}{2}}^{n-1} k(k-1)^{i+\frac{\ell-2}{2}-1}$$
$$= k(k-1)^{\frac{\ell}{2}-2}[\sum_{i=0}^{n-1}(k-1)^i - \sum_{i=0}^{\frac{\ell}{2}-1}(k-1)^i].$$

By Geometric Series, we have that

$$\sum_{i=\frac{\ell}{2}}^{n-1} n^1_{\ell-1}(T_{i,k}) = k(k-1)^{\frac{\ell}{2}-2}[\frac{(k-1)^n-(k-1)^{\frac{\ell}{2}}}{k-2}]. \tag{4}$$

For the sum $\sum_{j=\frac{\ell-2}{2}}^{n-1} n^2_{\ell-2}(T_{j,k})$, we may split the first term as

$$\sum_{j=\frac{\ell-2}{2}}^{n-1} n^2_{\ell-2}(T_{j,k}) = n^2_{\ell-2}(T_{\frac{\ell-2}{2},k}) + \sum_{j=\frac{\ell}{2}}^{n-1} n^2_{\ell-2}(T_{j,k}).$$

By Lemma 2, we have that

$$\sum_{j=\frac{\ell-2}{2}}^{n-1} n^2_{\ell-2}(T_{j,k}) = (k-1)^{\ell}\binom{k}{2} + \sum_{j=\frac{\ell}{2}}^{n-1} k(k-1)^{\frac{\ell}{2}-4+j}\binom{k-1}{2}$$
$$= (k-1)^{\ell}\binom{k}{2} + k(k-1)^{\frac{\ell}{2}-4}\binom{k-1}{2}\sum_{j=\frac{\ell}{2}}^{n-1}(k-1)^j.$$

By Geometric Series, we have that

$$\sum_{j=\frac{\ell-2}{2}}^{n-1} n^2_{\ell-2}(T_{j,k}) =(k-1)^{\ell-4}\binom{k}{2}$$
$$+ k(k-1)^{\frac{\ell}{2}-4}\binom{k-1}{2}[\frac{(k-1)^n-(k-1)^{\frac{\ell}{2}}}{k-2}]. \tag{5}$$

Putting values from Equation (4) and (5) into Equation (3) and simplifying, we get

$$n_\ell(T_{n,k}) = \frac{k(k-1)^{\ell-1}}{2}[\frac{k(k-1)^{n-\frac{\ell}{2}}-2}{k-2}]. \tag{6}$$

This proves Case 1.

Case 2: ℓ is an odd number
By Theorem 1, we have that

$$\begin{aligned}
n_\ell(T_{n,k}) &= (k-1)n^1_{\ell-1}(T_{n-1,k}) + 2(k-1)n^2_{\ell-1}(T_{n-1,k}) + n_\ell(T_{n-1,k})\\
n_\ell(T_{n-1,k}) &= (k-1)n^1_{\ell-1}(T_{n-2,k}) + 2(k-1)n^2_{\ell-1}(T_{n-2,k}) + n_\ell(T_{n-2,k})\\
n_\ell(T_{n-2,k}) &= (k-1)n^1_{\ell-1}(T_{n-3,k}) + 2(k-1)n^2_{\ell-1}(T_{n-3,k}) + n_\ell(T_{n-3,k})\\
&\vdots\\
n_\ell(T_{\frac{\ell+1}{2},k}) &= (k-1)n^1_{\ell-1}(T_{\frac{\ell-1}{2},k}) + 2(k-1)n^2_{\ell-1}(T_{\frac{\ell-1}{2},k}) + n_\ell(T_{\frac{\ell-1}{2},k}).
\end{aligned}$$

Since $\frac{\ell-1}{2} < \frac{\ell}{2}$, it follows that $n_\ell(T_{\frac{\ell-1}{2},k}) = 0$. Further, $n^1_{\ell-1}(T_{\frac{\ell-1}{2},k}) = 0$ because every path of length $\ell-1$ always has both end vertices at leaves of $T_{\frac{\ell-1}{2},k}$. Thus, summing the above equations, we have

$$\begin{aligned}
n_\ell(T_{n,k}) =& (k-1)\sum_{i=\frac{\ell+1}{2}}^{n-1} n^1_{\ell-1}(T_{i,k}) + 2(k-1)\sum_{j=\frac{\ell+1}{2}}^{n-1} n^2_{\ell-1}(T_{j,k})\\
&+ 2(k-1)n^2_{\ell-1}(T_{\frac{\ell-1}{2},k}).
\end{aligned} \tag{7}$$

By Lemma 1 when $\ell-1$ is even, we have that

$$\begin{aligned}
\sum_{i=\frac{\ell+1}{2}}^{n-1} n^1_{\ell-1}(T_{i,k}) &= \sum_{i=\frac{\ell+1}{2}}^{n-1} k(k-1)^{i+\frac{\ell-1}{2}-2}\\
&= k(k-1)^{\frac{\ell-1}{2}-2}\sum_{i=\frac{\ell+1}{2}}^{n-1}(k-1)^i\\
&= k(k-1)^{\frac{\ell-1}{2}-2}[\sum_{i=0}^{n-1}(k-1)^i - \sum_{i=0}^{\frac{\ell-1}{2}}(k-1)^i].
\end{aligned}$$

Hence, we have by Geometric Series that

$$\sum_{i=\frac{\ell+1}{2}}^{n-1} n_{\ell-1}^{1}(T_{i,k}) = k(k-1)^{\frac{\ell-1}{2}-2}[\frac{(k-1)^n-(k-1)^{\frac{\ell+1}{2}}}{k-2}]. \tag{8}$$

Further, we have by Lemma 2 that

$$\begin{aligned}\sum_{j=\frac{\ell+1}{2}}^{n-1} n_{\ell-1}^{2}(T_{j,k}) &= \sum_{j=\frac{\ell+1}{2}}^{n-1} k(k-1)^{\frac{\ell+1}{2}-2+j}\binom{k-1}{2} \\ &= k(k-1)^{\frac{\ell+1}{2}-2}\binom{k-1}{2}\sum_{j=\frac{\ell+1}{2}}^{n-1}(k-1)^j.\end{aligned}$$

We have by Geometric Series that

$$\sum_{j=\frac{\ell+1}{2}}^{n-1} n_{\ell-1}^{2}(T_{j,k}) = k(k-1)^{\frac{\ell+1}{2}-2}\binom{k-1}{2}[\frac{(k-1)^n-(k-1)^{\frac{\ell+1}{2}}}{k-2}]. \tag{9}$$

Putting values from Equations (8) and (9) into Equation (7) and simplifying, we get

$$n_\ell(T_{n,k}) = k(k-1)^{\frac{\ell-1}{2}}[\frac{(k-1)^n-(k-1)^{\frac{\ell-1}{2}}}{k-2}]. \tag{10}$$

This proves Case 2 and completes the proof of Corollary 1. ■

4.3 Proof of Corollary 2

We let $\binom{V(T_{n,k})}{2}$ be the set of all sets of two vertices of $T_{n,k}$. Namely,

$$\binom{V(T_{n,k})}{2} = \{\{u,v\} : u, v \in V(T_{n,k})\}$$

and

$$\left|\binom{V(T_{n,k})}{2}\right| = \binom{|V(T_{n,k})|}{2} = \binom{1+\frac{k[(k-1)^n-1]}{k-2}}{2}.$$

Construct the $(0,1)$-matrix whose rows are the pairs $\{u,v\}$ of $\binom{V(T_{n,k})}{2}$, columns are the path length ℓ for all $1 \leq \ell \leq 2n$ and the entries $a_{\{u,v\},\ell}$ are defined as follows:

$$a_{\{u,v\},\ell} = \begin{cases} 1 & \text{if } d_T(u,v) = \ell, \\ \\ 0 & \text{otherwise.} \end{cases}$$

We first consider Row $\{u,v\}$. There is exactly one column, called ℓ, such that

$$a_{\{u,v\},\ell} = 1$$

but

$$a_{\{u,v\},j} = 0$$

for all $j \in \{1, ..., 2n\} \setminus \{\ell\}$. Thus, the summation of all entries in this matrix is

$$\sum_{\{u,v\} \subseteq V(T)} 1 = \left| \binom{V(T_{n,k})}{2} \right| = \binom{1 + \frac{k[(k-1)^n - 1]}{k-2}}{2}.$$

We then consider Column ℓ. By the definition of $n_\ell(T_{n,k})$, there are $n_\ell(T_{n,k})$ rows whose entries are equal to 1 while the entries of the other rows are all 0. Hence, the summation of all entries of Column ℓ is equal to $n_\ell(T)$ implying that the summation of all etries in this matrix is $\sum_{\ell=1}^{2n} n_\ell(T)$.

By the counting two way principle, we have that

$$\binom{1 + \frac{k[(k-1)^n - 1]}{k-2}}{2} = \sum_{\ell=1}^{2n} n_\ell(T_{n,k}).$$

This proves Corollary 2.

4.4 Proof of Theorem 2

We prove this theorem by similar argument as in the proof of Corollary 2. First, we let T be a tree with the diameter $diam(T) = t$. We let $\binom{V(T)}{2}$ be the set of all sets of two vertices of T. Construct the matrix whose rows are the pairs $\{u, v\}$ of $\binom{V(T)}{2}$, columns are the path length ℓ for all $1 \leq \ell \leq t$ and the entries $a_{\{u,v\},\ell}$ are defined as follows:

$$a_{\{u,v\},\ell} = \begin{cases} \ell & \text{if } d_T(u, v) = \ell, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Thus, in the column j, all the entries are either j or 0.

We first consider Row $\{u, v\}$. There is exactly one column, called ℓ, such that

$$a_{\{u,v\},\ell} = \ell = d_T(u, v)$$

but

$$a_{\{u,v\},j} = 0$$

for all $j \in \{1, ..., t\} \setminus \{\ell\}$. Thus, the summation of all entries of Row $\{u, v\}$ is equal to $\ell = d_T(u, v)$ implying that the summation of all entries in this matrix is $\sum_{\{u,v\} \subseteq V(T)} d_T(u, v)$.

We then consider Column ℓ. By the definition of $n_\ell(T)$, there are $n_\ell(T)$ rows whose entries are equal to ℓ while the entries of the other rows are all 0. Hence, the summation of all entries of Column ℓ is equal to $\ell n_\ell(T)$ implying that the summation of all etries in this matrix is $\sum_{\ell=1}^{diam(T)} \ell n_\ell(T)$.

By the counting two way principle, we have that

$$\sum_{\{u,v\} \subseteq V(T)} d_T(u, v) = \sum_{\ell=1}^{diam(T)} \ell n_\ell(T).$$

This proves Theorem 2.

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