Counting the Numbers of Paths of all Lengths in Dendrimers and its Applications

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Abstract

For positive integers\(n\) and\(k\), the 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\(k\). 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, biology. In this paper, for any positive integer \(\ell\), we count the number of paths of length \(\ell\) 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 medium domination, introduced by Vargör and Dündar in 2011, of \(T_{n,k}\).

Keywords: Dendrimer; Cayley Tree; Wiener Index; Average Distance; Medium Domination

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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 \(\text{deg}_G(v)\) of a vertex \(v\) in \(G\) is given by \(|N_G(v)|\). If the subgraph of \(G\) induced by \(S\) has no edges, then

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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 diameter $\text{diam}(G)$. The total of the distance between each pair of vertices of $G$ divided by the number of pairs of vertices is the average distance $\mu(G)$ of $G$. That is:

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

A tree is a graph with no subgraphs that are cycles. A leaf, also known as pendant vertex, is a vertex with degree one. A leaf’s incident edge is the pendant edge while a leaf’s neighbouring vertex is called a support vertex. A rooted tree $T$ is a tree whose one vertex 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 $n$. A balanced tree is a rooted tree with equal number of vertices at the same level having the same degree. A dendrimer $T_{n,k}$ is an $n$-level balanced tree with the degree $k$ for all non-leaf vertices. A 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 to 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 constants such as dominating numbers and some other types of dominating number are used to describe a range of physical characteristics, including physicochemical characteristics, thermodynamic characters, chemical and biological actions, and so on. In 1978, Fritz Vogtle’s was the first to bring these nanomolecules to researcher’s attention [5]. In [2] the topological indices of well-known dendrimers were introduced. Researchers have discovered topological indices for many chemical structures such as dendrimers, trees and other graphs, inspired by the chemical relevance of topological indices of molecular networks. In context of spectral graph theory, the sum of the absolute values of the eigenvalues of the graph $G$ is known as the energy of graph $G$ which can be given as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|$$

where $\lambda_i, i = 1, 2, \ldots, n$ are the eigenvalues of $G$. In [1], the eigenvalues of the cayley tree dendrimers are obtained with the help of the characteristic polynomials. The reduction formulas for calculating the characteristic polynomials of $d(2, k)$ and $d(3, k)$ are constructed. Also, The energy of the above mentioned dendrimers is calculated. For more studies in dendrimers see [6, 26] for example.

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

2
When $n = 1$, $T_{1,k}$ can be constructed by introducing $k$ vertices and joining each of them to the central vertex through an edge. Thus $T_{1,k}$ is a star with $n + 1$ vertices.

When $k = 2$, $T_{n,2}$ is a path consisting of $2n + 1$ vertices.

When $n = 2$, it can be observed that $T_{2,k}$ can be constructed from $T_{1,k}$ by introducing $k - 1$ vertices at each leaf of $T_{1,k}$ and then joining them to that leaf. Hence, when $n, k \geq 2$, $T_{n,k}$ is constructed from $T_{n-1,k}$ by introducing further $k - 1$ vertices at each leaf vertex of $T_{n-1,k}$ and then joining them to that leaf vertex. Namely, the procedure of construction of $T_{n,k}$ for $(n \geq 2, k \geq 0)$ consists of $n$ iterations from the graph that has exactly one vertex.

Figure 1: The dendrimers $T_{3,4}$.

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, 22, 25], 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 number, according to Wiener. Later study on quantitative structure activity linkages revealed it is connected with some other factors also 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. Wiener’s works did not make use of graph theory, and the path number was only used in acyclic systems. Hosoya, in 1971, was the first to define the Wiener index within the context of chemical graph theory. The Weiner index appears to have been studied for the first time in the mathematical literature in 1976. This index has also been referred to by the terms “graph distance” and “transmission” uses the Laplacian matrix to introduce a graph-theoretical new definition of the Wiener index for trees. Andrey A. Dobryn et. al. established the Wiener index for Cayley tree dendrimer in which states that for every \( k \geq 3 \), the Wiener index of \( T_{n,k} \) is

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

(1)

For more studies of Weiner index see for example.

A graph \( G \) fulfilling specific constraints can efficiently simulate 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 usually the average distance between vertices. The average distance in graph \( G \) is defined as follows:

\[
\mu(G) = \frac{\sum_{\{u,v\} \subseteq V(G)} d_G(u, v)}{\binom{|V(G)|}{2}}
\]

The study of the average distance of graphs was initiated by Plesnik in his classical result in 1976. The average distance is an important tool to analyze 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 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 improved this bound to \( \alpha(G) \geq \mu(G) \) 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 for example.

Domination in graph has been extensively researched and utilized in a variety of fields. Vargör and Dündar established the idea of “the medium domination number” which is defined as the total number of vertices that dominate every pair of vertices with the average value of it. In the same way each vertex in a graph may protect every vertex in its immediate
surroundings and in domination every vertex in neighborhood must be secured. In any connected simple graph $G$ having order $n$, the medium domination number of $G$ is defined as $\gamma_m(G) = \frac{TD_T(G)}{\binom{n}{2}}$. The medium domination number of Jahangir graph was determined by Ramachandran and Parvathi [24]. Mirajkar et. al. found the medium domination number of few poly silicates in [17]. Mahadevan et.al. proposed the concept of the Extended Medium Domination number of a graph in [20]. The total number of vertices that dominate each pair of vertices

$$ETDV(G) = \sum edom(u,v)$$

for any $u, v \in V(G)$. The extended medium domination number of a graph $G$ is defined as $EMD(G) = \frac{EDT(G)}{\binom{n}{2}}$. $ETDV(G)$ is the sum of number of path of length one, two and three.

Motivated by the above G. Mahadevan et.al. introduced the idea of Double Twin domination of a graph [20]. The total number of vertices that dominate every pair of vertices

$$SDTwin(G) = \sum DTwin(u,v)$$

for $u, v \in V(G)$. In any simple graph $G$ with $n$ number of vertices, the double Twin domination number of $G$ can be given as $DTD(G) = \frac{SDTwin(G)}{\binom{n}{2}}$ where $SDTwin(G)$ is the total of number of path having length one, two, three and four. This number was discovered by Mahadevan and Vijayalakshmi in [21], for variety of common classes of graphs like path, cycle, wheel graph, complete graph, star graph, Cartesian product of path and Corona product of path.

From the above discussion, it can be showed that 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 $\ell$, how many paths of length $\ell$ does a 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 $\ell$ 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 $\ell$-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

$$n_\ell(G): \text{ the number of paths of length } \ell \text{ of } G.$$ 

The first main result is the formula of $n_\ell(T_{n,k})$ for all possible values of $\ell$. Recall that when $k = 2$, the dendrimer $T_{n,2}$ is a path of length $2n$. Thus, we let $x_1, \ldots, x_{2n+1}$ be $T_{n,2}$. Clearly, for a positive integer $1 \leq \ell \leq 2n$, all the paths of length $\ell$ are $x_i, x_{i+1}, \ldots, x_{i+\ell}$ 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

$$n_\ell^1(T): \text{ the number of paths of length } \ell \text{ of } T \text{ with exactly one end vertex is a leaf of } T.$$ 

$$n_\ell^2(T): \text{ the number of paths of length } \ell \text{ of } T \text{ whose both end vertices are leaves of } T.$$ 

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 $\ell$ is even number, then

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

If $\ell$ is odd number, then

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

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

$$n_\ell(T_{n,k}) = \begin{cases} 
\frac{k(k-1)^{\ell-1}}{2} \left[\frac{(k-1)^n - \ell}{k-2}\right] & \text{when } \ell \text{ is even}, \\
\frac{k(k-1)^{\ell-1}}{2} \left[\frac{(k-1)^n - (k-1)^{\ell-1}}{k-2}\right] & \text{when } \ell \text{ is odd}.
\end{cases}$$
Corollary 2  For natural number $n$ and $k$ such that $k \geq 3$, we have that

$$\left(1 + \frac{k(k-1)^{n-1}}{k-2}\right) = \sum_{\ell=0}^{n-1} k(k-1)^\ell \left(\frac{(k-1)^{n} - (k-1)^\ell}{k-2}\right) + \sum_{\ell=1}^{n} \frac{k(k-1)^{2\ell-1}}{2} \left[\frac{k(k-1)^{n-\ell} - 2}{k-2}\right]$$

2.1 Wiener Index and Average Distance

In this subsection, we have linked our main problem to distance in Cayley Tree Dendrimer. Using the results obtained in Theorem 1, Corollary 1 and 2, we have found the Wiener index and average distance of $T_{n,k}$. We obtain Corollaries 3 and 4. However, we may 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

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

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

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

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

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

7
2.2 Medium Domination

Motivated by [20, 21, 28], we generalize their results to $\varsigma$-medium domination of $T_{n,k}$. For a graph $G$ of order $n$ and for some $2 \leq \varsigma \leq \text{diam}(G)$, the $\varsigma$-medium domination number $\gamma_{\varsigma MD}(G)$ of $G$ is defined as

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

where

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

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

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

$$\gamma_{\varsigma MD}(T_{n,k}) = \frac{\varsigma(T_{n,k})}{\left|V(T_{n,k})\right|}$$

where

$$\varsigma(T_{n,k}) = \sum_{\ell=0}^{s} k(k-1)^{\ell}\left[\frac{(k-1)^n-(k-1)^{\ell}}{k-2}\right] + \sum_{\ell=1}^{\left\lceil \frac{\varsigma}{2} \right\rceil} k(k-1)^{2\ell-1}\left[\frac{k(k-1)^{n-\ell}-2}{k-2}\right]$$

and

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

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

$$S_n = \frac{n-1}{a(1-r^n)}$$

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 \( k \) are \( \frac{k(k-1)^n-2}{k-2} \),

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 \( \ell \) of \( T_{n,k} \) having exactly one end vertex as a leaf of \( T_{n,k} \). Then

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

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

\( P_x \) : 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 \( \ell \).

Case 1: \( 1 \leq \ell \leq n \).

For a path \( P \in P_x \), 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 $\mathcal{P}_{x,0}, \mathcal{P}_{x,1}, \ldots, \mathcal{P}_{x,\lfloor \frac{\ell - 1}{2} \rfloor}$ partition $\mathcal{P}_x$.

When $i = 0$, we have that $|\mathcal{P}_{x,0}| = 1$ as there is exactly one path of length $\ell$ starting from $x$, goes through vertices in $L_{n-1}, L_{n-2}, \ldots, L_{n-\ell+1}$ 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 through vertices in $L_{n-1}, \ldots, L_{n-\ell+i+1}, L_{n-\ell+i}$ 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 $L_{n-\ell+i+1}, \ldots, L_{n-\ell+2i}$. As $y$ is already in every of such path, there are $k - 2$ possibilities for all the paths in $\mathcal{P}_{x,i}$. Further, there are $k - 1$ possibilities for all the paths to pass each of $L_{n-\ell+i+2}, \ldots, L_{n-\ell+2i}$. Hence,
\[ |\mathcal{P}_{x,i}| = (k - 2)(k - 1)^{i-1} \]
which implies that
\[ |\mathcal{P}_x| = |\mathcal{P}_{x,0}| + |\mathcal{P}_{x,1}| + \cdots + |\mathcal{P}_{x,\lfloor \frac{\ell - 1}{2} \rfloor}| \]
\[ = 1 + (k - 2) + (k - 2)(k - 1) + \cdots + (k - 2)(k - 1)^{\lfloor \frac{\ell - 3}{2} \rfloor}. \]

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 possibilities. Then, from $r$, all the paths pass through $L_1, \ldots, L_{\ell-n-1}$ and terminate in $L_{\ell-n}$, each of which with the possibilities $k - 1$. 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, $S_{x, \ell-n+1}, \ldots, S_{x, \left\lfloor \frac{\ell-1}{2}\right\rfloor}$ partitions $S_x$.

For each $\ell-n+1 \leq i \leq \left\lfloor \frac{\ell-1}{2}\right\rfloor$, all paths in $S_{x,i}$ start from $x$ pass through $L_{n-1}, \ldots, L_{n-\ell+i+1}$ 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 $L_{n-\ell+2i}$, each of which with $k-1$ possibilities. Thus

$$|S_{x,i}| = (k-2)(k-1)^{i-1}$$

which implies that

$$|S_x| = |S_{x,\ell-n+1}| + \cdots + |S_{x,\left\lfloor \frac{\ell-1}{2}\right\rfloor}|$$

$$= (k-2)(k-1)^{\ell-n} + (k-2)(k-1)^{\ell-n+1} + \cdots + (k-2)(k-1)^{\left\lfloor \frac{\ell-1}{2}\right\rfloor}$$

$$= (k-2)\left(\frac{(k-1)^{\left\lfloor \frac{\ell-1}{2}\right\rfloor} - 1}{k-2} - \frac{(k-1)^{\ell-n} - 1}{k-2}\right)$$

$$= (k-1)^{\left\lfloor \frac{\ell-1}{2}\right\rfloor} - (k-1)^{\ell-n}.$$

Hence,

$$|P_x| = |R_x| + |S_x| = (k-1)^{\left\lfloor \frac{\ell-1}{2}\right\rfloor}$$

and this proves Case 2.

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

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

and this proves Lemma 1. □

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

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

**Proof.** First, we let

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

Clearly, $\ell$ must be even. For a path $P \in Q_{\ell}$, 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 $\ell/2$. We distinguish 2 cases according to the value of $\ell$.

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

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

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

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

$$n^2_{\ell}(T_{n,k}) = |Q_{\ell}| = k(k-1)^{n-\ell/2-3}\binom{k-1}{2}.$$

**Case 2:** $\ell = 2n$

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

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

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:** $\ell$ is an even number.

Every path of length $\ell$ 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 $\ell$ while the Case (ii) gives $(k-1)n_{\ell-1}(T_{n-1,k})$ paths of length $\ell$ as the end vertex at a leaf of $T_{n-1,k}$ can be extended with $k-1$ ways. Finally, the Case (iii) gives $(k-1)^2n^2_{\ell-2}(T_{n-1,k})$ paths as every path of length $\ell-2$ whose both end vertices...
vertices are at the leaves of $T_{n-1,k}$ can be extended to the path of length $\ell$ by $(k - 1)^2$ ways, $k - 1$ for each end vertex. Thus, we have the following recursive formula

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

This proves Case 1.

**Case 2:** $\ell$ is an odd number

Similarly, every path of length $\ell$ 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 $(k - 1)n_{\ell}(T_{n-1,k})$ 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 $\ell$ by extending only one end vertex, $k - 1$ ways for each end vertex. Thus there are $2(k - 1)n_{\ell-1}(T_{n-1,k})$ paths in this case. Thus, we have a recursive formula

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

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

### 4.2 Proof of Corollary

We distinguish two cases according to the parity of $\ell$.

**Case 1:** $\ell$ is an even number.

By Theorem, we have that

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

For $\ell = 0$, we have $n_0(T_{n,k}) = 1$. For $\ell = 1$, we have $n_1(T_{n,k}) = 1$. For $\ell = 2$, we have $n_2(T_{n,k}) = (k - 1)n_1(T_{n-1,k}) + (k - 1)^2n_0(T_{n-1,k}) + n_2(T_{n-1,k})$. We can continue this process for all even $\ell$.

As $\frac{\ell - 2}{2} < \frac{\ell}{2}$, we have $n_\ell(T_{\frac{\ell-2}{2},k}) = 0$. Further, $n_{\ell-1}(T_{\frac{\ell-2}{2},k}) = 0$ because $\frac{\ell - 2}{2} < \frac{\ell - 1}{2}$. Thus, summing the above equations we have
\begin{equation}
n_{\ell}(T_{n,k}) = (k - 1) \sum_{i=\ell/2}^{n-1} n_{\ell-1}^1(T_{i,k}) + (k - 1)^2 \sum_{j=\ell/2}^{n-1} n_{\ell-2}^2(T_{j,k}). \tag{3}
\end{equation}

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

\begin{equation}
\sum_{i=\ell/2}^{n-1} n_{\ell-1}^1(T_{i,k}) = \sum_{i=\ell/2}^{n-1} k(k - 1)^{i + \ell/2 - 1} = k(k - 1)^{\ell/2 - 2}\left[\sum_{i=0}^{n-1} (k - 1)^{i} - \sum_{i=0}^{\ell-1} (k - 1)^{i}\right]. \tag{4}
\end{equation}

By Geometric Series, we have that

\begin{equation}
\sum_{i=\ell/2}^{n-1} n_{\ell-1}^1(T_{i,k}) = k(k - 1)^{\ell/2 - 2}\left[\frac{(k - 1)^n - (k - 1)^{\ell/2}}{k - 2}\right]. \tag{4}
\end{equation}

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

\begin{equation}
\sum_{j=\ell/2}^{n-1} n_{\ell-2}^2(T_{j,k}) = n_{\ell-2}^2(T_{\ell/2,k}) + \sum_{j=\ell/2}^{n-1} n_{\ell-2}^2(T_{j,k}).
\end{equation}

By Lemma 2, we have that

\begin{equation}
\sum_{j=\ell/2}^{n-1} n_{\ell-2}^2(T_{j,k}) = (k - 1)^{\ell/2 - 4}\left[\frac{1}{2}\right] + \sum_{j=\ell/2}^{n-1} k(k - 1)^{\ell/2 - 4 + j}\left(\frac{k - 1}{2}\right) = (k - 1)^{\ell/2 - 4}\left[\frac{1}{2}\right] + k(k - 1)^{\ell/2 - 4}\left(\frac{1}{2}\right)\sum_{j=\ell/2}^{n-1} (k - 1)^{j}.
\end{equation}

By Geometric Series, we have that

\begin{equation}
\sum_{j=\ell/2}^{n-1} n_{\ell-2}^2(T_{j,k}) = (k - 1)^{\ell/2 - 4}\left[\frac{1}{2}\right] + k(k - 1)^{\ell/2 - 4}\left(\frac{1}{2}\right)\left[\frac{(k - 1)^n - (k - 1)^{\ell/2}}{k - 2}\right]. \tag{5}
\end{equation}
Putting values from Equation (4) and (5) into Equation (3) and simplifying, we get

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

(6)

This proves Case 1.

**Case 2:** \( \ell \) is an odd number

By Theorem 1, we have that

\[
n_\ell(T_{n,k}) = (k-1)n^{\ell-1}_1(T_{n-1,k}) + 2(k-1)n^{\ell-2}_1(T_{n-1,k}) + n_\ell(T_{n-1,k})
\]

\[
n_\ell(T_{n-2,k}) = (k-1)n^{\ell-1}_1(T_{n-3,k}) + 2(k-1)n^{\ell-2}_1(T_{n-3,k}) + n_\ell(T_{n-3,k})
\]

\[
\vdots
\]

\[
n_\ell(T_{\ell+1,k}) = (k-1)n^{\ell-1}_1(T_{\ell+1,k}) + 2(k-1)n^{\ell-2}_1(T_{\ell+1,k}) + n_\ell(T_{\ell+1,k}).
\]

Since \( \frac{\ell-1}{2} < \frac{\ell}{2} \), it follows that \( n_\ell(T_{\ell+1,k}) = 0 \). Further, \( n^{\ell-1}_1(T_{\ell+1,k}) = 0 \) because every path of length \( \ell - 1 \) always has both end vertices at leaves of \( T_{\ell+1,k} \). Thus, summing the above equations we have

\[
n_\ell(T_{n,k}) = (k-1) \sum_{i=\frac{\ell+1}{2}}^{n-1} n^{\ell-1}_1(T_{i,k}) + 2(k-1) \sum_{j=\frac{\ell+1}{2}}^{n-1} n^{\ell-2}_1(T_{j,k}) + 2(k-1)n^{\ell-1}_1(T_{n-1,k}).
\]

(7)

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

\[
\sum_{i=\frac{\ell+1}{2}}^{n-1} n^{\ell-1}_1(T_{i,k}) = \sum_{i=\frac{\ell+1}{2}}^{n-1} k(k-1)^{i+\frac{\ell-1}{2}-2}
\]

\[
= k(k-1)^{\frac{\ell-1}{2}-2} \sum_{i=\frac{\ell+1}{2}}^{n-1} (k-1)^i
\]

\[
= k(k-1)^{\frac{\ell-1}{2}-2} \left[ \sum_{i=0}^{n-1} (k-1)^i - \sum_{i=0}^{\frac{\ell-1}{2}} (k-1)^i \right].
\]

Hence, we have by Geometric Series that

\[
\sum_{i=\frac{\ell+1}{2}}^{n-1} n^{\ell-1}_1(T_{i,k}) = k(k-1)^{\frac{\ell-1}{2}-2} \left[ \frac{(k-1)^n - (k-1)^{\frac{\ell+1}{2}}}{k-2} \right],
\]

(8)
Further, we have by Lemma 2 that
\[
\sum_{j=\ell+1}^{n-1} n^{2}_{T_{j,k}} = \sum_{j=\ell+1}^{n-1} k(k-1) \frac{\ell+1}{2} - 2j \left( \frac{k-1}{2} \right) \\
= k(k-1) \frac{\ell+1}{2} - 2 \left( \frac{k-1}{2} \right) \sum_{j=\ell+1}^{n-1} (k-1)^j.
\]

We have by Geometric Series that
\[
\sum_{j=\ell+1}^{n-1} n^{2}_{T_{j,k}} = k(k-1) \frac{\ell+1}{2} - 2 \left( \frac{k-1}{2} \right) \left[ \left( k-1 \right)^n - (k-1)^{\frac{\ell+1}{2}} \right]. \quad (9)
\]

Putting values from Equations (8) and (9) into Equation (7) and simplifying, we get
\[
n_{\ell}(T_{n,k}) = k(k-1) \frac{\ell+1}{2} \left[ \left( k-1 \right)^n - (k-1)^{\frac{\ell+1}{2}} \right]. \quad (10)
\]

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

\[\Box\]

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

Construct the \((0, 1)\)-matrix whose rows are the pairs \( \{u, v\} \) of \( \binom{V(T_{n,k})}{2} \), columns are the path length \( \ell \) 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, \( \ell \) say, such that
\[
a_{\{u,v\}, \ell} = 1
\]
but
\[ a_{\{u,v\},j} = 0 \]
for all \( j \in \{1, \ldots, 2n\} \setminus \{\ell\} \). Thus, the summation of all entries in this matrix is
\[
\sum_{\{u,v\} \subseteq V(T)} 1 = |\binom{V(T,n,k)}{2}| = \left(1 + \frac{k([k-1]n-1)}{k-2}\right). 
\]

We then consider Column \( \ell \). 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 \( \ell \) is equal to \( n_{\ell}(T) \) implying that the summation of all entries in this matrix is \( \sum_{\ell=1}^{2n} n_{\ell}(T) \).

By the counting two way principle, we have that
\[
\left(1 + \frac{k([k-1]n-1)}{k-2}\right) = \sum_{\ell=1}^{2n} n_{\ell}(T_{n,k}).
\]
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 \( \text{diam}(T) = t \). 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 \( \ell \) 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, \( \ell \) say, such that
\[
a_{\{u,v\},\ell} = \ell = d_{T}(u,v)
\]
but
\[
a_{\{u,v\},j} = 0
\]
for all \( j \in \{1, \ldots, t\} \setminus \{\ell\} \). 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 \( \ell \). By the definition of \( n_{\ell}(T) \), there are \( n_{\ell}(T) \) rows whose entries are equal to \( \ell \) while the entries of the other rows are all 0. Hence, the summation of all entries
of Column $\ell$ is equal to $\ell n_\ell(T)$ implying that the summation of all entries in this matrix is
$$\sum_{\ell=1}^{\text{diam}(T)} \ell n_\ell(T).$$

By the counting two way principle, we have that
$$\sum_{(u,v) \in V(T)} d_T(u,v) = \sum_{\ell=1}^{\text{diam}(T)} \ell n_\ell(T).$$

This proves Theorem 2.

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