The Extreme Values of the Vertex-degree-distance of $k$-Caterpillar

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Abstract. In this paper, we studied the extremal values and rankings of the vertex-degree-distance of the $k$-caterpillar. We obtained the distribution of the maximum (vertices) and the minimum (vertices) of the vertex-degree-distance of the $k$-caterpillar; we also researched the rankings of the vertex-degree-distance of the spine vertices and the leaves of the $k$-caterpillar.

Introduction

Topological indexes of graphs are often used to study the structural properties of molecules. In 1947, H. Wiener proposed the Wiener index\cite{1}, and after that, many variants of Wiener index were proposed according to degree and distance of vertex\cite{2-8}. In 1994, Dobrynin and Kochetova introduced the degree-distance of graphs based on vertex degree and distance, which extended the research area of parameters of graphs related to the Wiener index \cite{2}. In chemical graph theory, caterpillar trees are often used to describe the structure of benzenoid hydrocarbons. “It is amazing that nearly all graphs that played an important role in what is now called ‘chemical graph theory’ may be related to caterpillars trees”\cite{10}.

In this paper, we study the extremal values and rankings of the vertex-degree-distance of $k$-caterpillar.

Definitions and Notation

Let $G$ be a connected simple graph with the vertex set $V(G)$ and the edge set $E(G)$, and the degree of the vertex $u$ is denoted by $d(u)$. The distance between vertices $u$ and $v$ of $T$ is denoted by $d(u,v)$. A vertex with degree 1 is called the pendent vertex, and an edge associated with a pendent vertex is called the pendent edge.

Let $G$ be a connected simple graph. $\forall v \in G$, call $d(v)\sum_{u \in V(G)}d(u,v)$ (denote as $d'_v(v)$, $d'(v)$ for short) to be the vertex-degree-distance of the vertex $v$; call $\sum_{v \in V(G)}d'(v)$ (denote as $D'(G)$) the degree-distance of the graph $G$\cite{1}.

Caterpillar trees (also known as "benzenoid trees") are trees which will leave a path if all the pendent vertices are deleted. Let $P_\ast = v_1v_2\ldots v_n$ ($n \geq 3$) be a path. Construct the $k$-caterpillar tree (short for the $k$-caterpillar, denoted by $C_n^k$, see fig. 1) by attaching $k$ ($k \geq 2$) pendent vertices to vertex $v_i$ ($i=1, 2, \ldots, n$). Here, $P_\ast$ is called the spine of the $k$-caterpillar, $v_i$ ($i=1, 2, \ldots, n$) is called the spine-vertex of the $k$-caterpillar.
Main Results

Vertex-Degree-Distance and Extremal Values of the $k$-Caterpillar

Lemma 1. The vertex-degree-distances of the spine-vertices in the $k$-caterpillar $C_n^k$ are:

$$d'(v_i) = d'(v_n) = \frac{k+1}{2}((k+1)n^2+(k-1)n),$$

$$d'(v_i) = \frac{k+2}{2}(2(k+1)i^2-2(k+1)(n+1)i+(k+1)n^2+(3k+1)n).$$

Proof. According to the structural features of $C_n^k$, we can get the vertex-degree-distance of the spine-vertices as follows:

$$d'(v_i) = d'(v_n) = (k+1)\left(\sum_{j=1}^{n-1}(k+1)j + kn\right) = \frac{k+1}{2}((k+1)n^2+(k-1)n).$$

$$d'(v_i) = d(v_i) = \sum_{v_j \in C_n^k} d(v_i, v_j) = d(v_i) \left(\sum_{j=1}^{i-1}d(v_i, v_j) + \sum_{i+1}^{n}d(v_i, v_j) + \sum_{i+1}^{n}kd(v_{i+1}, v_i) + \sum_{i+1}^{n}kd(v_{i+1}, v_i)\right)$$

$$= (k+2)\left(\sum_{j=1}^{i-1}l + \sum_{i+1}^{n}l-i + \sum_{i+1}^{n}k(i-l+1) + \sum_{i+1}^{n}k(l-i+1)\right)$$

$$= \frac{k+2}{2}(2(k+1)i^2-2(k+1)(n+1)i+(k+1)n^2+(3k+1)n).$$

Lemma 2. The vertex-degree-distances of the leaves in the $k$-caterpillar $C_n^k$ are:

$$d'(v_{ij}) = d'(v_{nj}) = \frac{1}{2}((k+1)n^2+(3k+1)n-4k)(1 \leq j \leq k),$$

$$d'(v_{ij}) = \frac{1}{2}(k+1)i^2-2(kn+n+1)i+(k+1)(n^2+3n-2))(2 \leq i \leq n; 1 \leq j \leq k).$$

Proof. According to the structural features of $C_n^k$, it is easy to see that, for $1 \leq i \leq n$, $d'(v_{i1}) = d'(v_{i2}) = \cdots = d'(v_{ik})$, so we can get that
\[ d'(v_{ij}) = d'(v_{ij}) = d(v_{ij}) \sum_{v \in C'_{C_n^{k}}} d(v, v_{ij}) = \sum_{l=1}^{n} d(v_{ij}, v_{ij}) + \sum_{l=1, l \neq j}^{n} d(v_{ij}, v_{ij}) + \sum_{l=2}^{n} k d(v_{ij}, v_{ij}) \]

\[ = \sum_{l=1}^{n} l + \sum_{l=1, l \neq j}^{n} 2 + \sum_{l=2}^{n} k(l+1) \]

\[ = \frac{1}{2}((k+1)n^2 + (3k+1)n - 4k)(1 \leq j \leq k). \]

For \( 2 \leq i \leq n-1 \) and \( 1 \leq j \leq k \), we get

\[ d'(v_{ij}) = d(v_{ij}) = \sum_{v \in C'_{C_n^{k}}} d(v, v_{ij}) \]

\[ = \sum_{l=1}^{n} d(v_{ij}, v_{ij}) + \sum_{l=1}^{n} d(v_{ij}, v_{ij}) + \sum_{l=1, l \neq j}^{n} d(v_{ij}, v_{ij}) + \sum_{l=2}^{n} k d(v_{ij}, v_{ij}) \]

\[ = \sum_{l=1}^{n} (i-l+1) + \sum_{l=1}^{n} (l-i+1) + \sum_{l=1, l \neq j}^{n} k(l-i+2) + \sum_{l=2}^{n} 2 + \sum_{l=1, l \neq j}^{n} k(l-i+1) \]

\[ = \frac{1}{2}((k+1)i^2 - 2(kn+n+1)i + (k+1)(n^2+3n-2)). \]

**Theorem 1.** The maximum value of the vertex-degree-distances of \( k \)-caterpillar is as follows:

\[ d'(v_2) = \max_{v \in C'_{C_n^{k}}} \{d'(v)\}. \]

**Proof.** (1) Firstly, we consider the vertex-degree-distances of the spine-vertices. From Lemma 1, \( d'(v_i) \) (\( 2 \leq i \leq n-1 \)) is a quadratic function on \( i \), and takes maximum values at \( i=2 \) or \( i=n-1 \):

\[ d'(v_i) = d'(v_{n-1}) = \max_{2 \leq i \leq n-1} \{d'(v_i)\} = \frac{k+2}{2}((k+1)n^2 - (k+3)n + 4(k+1)). \]

(2) From Lemma 2, for \( j \in \{1, 2, \ldots, k\} \), \( d'(v_{ij}) \) (\( 2 \leq i \leq n-1 \)) takes maximum values at \( i=1 \) or \( i=n \). That is,

\[ d'(v_{ij}) = d'(v_{n-1,j}) = \max_{2 \leq i \leq n-1} \{d'(v_{ij})\} = \frac{1}{2}((k+1)n^2 - (k+1)n + 6k - 5)). \]

(3) Comparing the size of \( d'(v_{ij}) \), \( d'(v_{ij}) \), \( d'(v_{ij}) \) and \( d'(v_{ij}) \). Since

\[ d'(v_{ij}) - d'(v_{ij}) = \frac{1}{2}(2(2n-3)k + 2n+1) > 0, \]

\[ d'(v_i) - d'(v_{ij}) = \frac{1}{2}(k(k+1)n^2 + (k^2 - 3k - 2)n + 4k) > 0 \mbox{ \( (k \geq 2) \).} \]

\[ d'(v_2) - d'(v_i) = \frac{k+1}{2}(n(n-5) + 4(k+2)) > 0(n \geq 3, k \geq 2). \]

So,

\[ d'(v_2) = d'(v_{n-1}) = \max_{u \in C'_{C_n^{k}}} \{d'(u)\}. \]

**Theorem 2.** The minimum value of the vertex-degree-distances of \( k \)-caterpillar is as follows:
\[ \min_{v \in C_n^k} \{d'(v)\} = \begin{cases} 
 d'(v_{\frac{n+1}{2}}), & \text{when } n \text{ is odd, } j = 1, 2, \ldots, k; \\
 d'(v_{\frac{n+j}{2}}), & \text{when } n \text{ is even, } j = 1, 2, \ldots, k. 
 \end{cases} \]

**Proof.** We can see that, from the proof of Theorem 1,

\[ d'(v_2) > d'(v_1) > d'(v_{ij}) > d'(v_{2j}) = \max_{2 \leq i \leq n-1} \{d'(v_{ij})\}. \]

And \(d'(v_i)(2 \leq i \leq n-1)\) is a quadratic function on \(i\), it takes minimum value at \(i = (n-1)/2\) and \(i = (n+1)/2\) for odd \(n\), and \(i = n/2\) for even \(n\). So,

\[ \min_{v \in C_n^k} \{d'(v)\} = \begin{cases} 
 d'(v_{\frac{n+1}{2}}), & \text{when } n \text{ is odd, } j = 1, 2, \ldots, k; \\
 d'(v_{\frac{n+j}{2}}), & \text{when } n \text{ is even, } j = 1, 2, \ldots, k. 
 \end{cases} \]

**Corollary 1.** The rankings of the vertex-degree-distances of the spine-vertices in \(k\)-caterpillar \(C_n^k\) are that:

1. \(d'(v_2) > d'(v_1) > \cdots > d'(v_{ij}) > d'(v_{n+j}) < \cdots < d'(v_{n-1})\) for odd \(n\);

2. \(d'(v_2) > d'(v_1) > \cdots > d'(v_{ij}) > d'(v_{n+j}) = d'(v_{n+j+1}) < \cdots < d'(v_{n-1})\) for even \(n\).

**Corollary 2.** The rankings of the vertex-degree-distances of the leaves in \(k\)-caterpillar \(C_n^k\) are that:

1. \(d'(v_{ij}) > d'(v_{ij+1}) > \cdots > d'(v_{ij+j}) > d'(v_{ij+j+1}) < \cdots < d'(v_{ij+n})\) for odd \(j = 1, 2, \ldots, k\).

2. \(d'(v_{ij}) > d'(v_{ij+1}) > \cdots > d'(v_{ij+j}) > d'(v_{ij+j+1}) = d'(v_{ij+j+2}) < \cdots < d'(v_{ij+n})\) for even \(j = 1, 2, \ldots, k\).

**Vertex-Degree-Distance and Rankings of the Family of \(k\)-Caterpillar**

**Theorem 3.** The vertex-degree-distance of the \(k\)-Caterpillar \(C_n^k\) is as follows:

\[ d'(C_n^k) = \frac{1}{12} \left( 2(k^2 + 4k + 4)n^3 + 3(k^2 - 5k - 6)n^2 + (21k^2 - 101k - 104)n - (9k^2 - 3k - 4) \right). \]

**Proof.**

\[
\begin{align*}
   & d'(C_n^k) \\
   &= \sum_{v \in C_n^k} d'(v) - \sum_{i=1}^{n} (d'(v_i) + kd'(v_{i+1})) \\
   &= 2 \cdot \frac{k+1}{2} \left( (k+1)n^2 + (k-1)n \right) + \sum_{i=2}^{n-1} \frac{k+2}{2} \left( 2(k+1)i^2 - 2(k+1)(n+1)i + (k+1)n^2 + (3k+1)n \right) \\
   &\quad + 2k \cdot \frac{1}{2} \left( (k+1)n^2 + (3k+1)n - 4k \right) + k \sum_{i=2}^{n-1} \frac{1}{2} \left( (k+1)i^2 - 2(kn+n+1)i + (k+1)(n^2 + 3n - 2) \right) \\
   &= \frac{1}{12} \left( 2(k^2 + 4k + 4)n^3 + 3(k^2 - 5k - 6)n^2 + (21k^2 - 101k - 104)n - (9k^2 - 3k - 4) \right).
\end{align*}
\]
Conclusions

By studying the vertex-degree-distance of the $k$-caterpillar, we demonstrated that the distributions of the vertex-degree-distance of the spine-vertices and leaf-vertices are concave. We also obtained the extremal values (vertex) and rankings of the vertex-degree-distance of the $k$-caterpillar. These results partly revealed the relations between the vertex-degree-distance of trees, which provided a useful idea for the study of the extremal values (vertex) and extremal graphs of the vertex-degree-distance of other similar trees.

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References


