The Extremal Values and Rankings of the Gutman Index of k-Caterpillar

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Abstract. In this paper, based on the conception of the Gutman index of graphs, we proposed the degree-distance of a graph to a vertex and the vertex-Gutman index. We studied the extremal values and rankings of the vertex-Gutman indices of the k-caterpillar, obtained the distribution of the extremal vertices; we also researched the extremal values and rankings of the Gutman index of the family of k-caterpillar, characterized the corresponding extremal graphs.

Introduction

Topological indexes of graphs are often used to study the structural properties of molecules. After H. Wiener proposed the Wiener index[1] in 1947, many variants of Wiener index were proposed according to degree and distance of vertex[2-8]. In 2016, Gutman, Furtula and Das introduced the Gutman index of graphs based on vertex degree-and-distance, which extended the research area of parameters of graphs related to vertex degree-and-distance[8].

Caterpillar trees (also known as "benzenoid trees" and "Gutman trees") are trees which will leave a path (called spine) if all the pendent vertices are deleted. In chemical graph theory, caterpillar trees are often used to describe the structure of benzenoid hydrocarbons. In 1987, El-Basil pointed out in ref.[9]: "It is amazing that nearly all graphs that played an important role in what is now called ‘chemical graph theory’ may be related to caterpillar trees."

In this paper, our aim is to study the extremal values and rankings of the vertex-Gutman index of k-caterpillar and the Gutman index of the family of the k-caterpillar.

Definitions and Notation

Let T be a connected simple graph with the vertex set V(T) and the edge set E(T), and the degree of the vertex u is denoted by d(u). The vertex with degree 1 is called the pendent vertex (the tree’s pendent vertex is called the leaf-node), and the edge associated with it is called the pendent edge. The distance between vertices u and v of T is denoted by d(u,v).

The Gutman index of T (denoted by G(T)) is defined as \[ G(T) = \sum_{(u,v) \in V(T)} (d(u) \cdot d(v))d(u,v) \] \[ \text{Namely, the sum of the products of the distance of pairs of unordered vertices and their vertex degrees.} \]

Let T be a simple connected graph, \( u \in T \). The degree-distance of the graph T to the vertex u (denoted as G(u,T)) is defined as \[ G(u,T) = \sum_{v \in V(T)} d(v)d(u,v) . \] Call \( d(u) \cdot G(u,T) \) to be the vertex-Gutman index of u (in graph T). Thus, we can get the relation between the Gutman index of the graph T and the vertex-Gutman index:

\[ G(T) = \sum_{(u,v) \in V(T)} (d(u) \cdot d(v))d(u,v) = \frac{1}{2} \sum_{u \in V(T)} d(u)G(u,T) = \frac{1}{2} \sum_{u \in V(T)} G(u). \]

Let \( P_n = v_1 v_2 \ldots v_n \) (\( k \geq 3 \)) be a path. Construct the k-caterpillar tree (short for the k-caterpillar, denoted by \( CB^n_k \), see fig. 1) by attaching k (\( k \geq 2 \)) pendent vertices to vertex \( v_i \) (\( i=1, 2, \ldots, n \)). Here, \( P_n \) is called the spine of the k-caterpillar, \( v_i \) (\( i=1, 2, \ldots, n \)) is called the spine-node of the k-caterpillar.
Main Results

Vertex-Gutman Index and Extremal Values of the $k$-Caterpillar

Lemma 1. The vertex-Gutman indices of the spine-nodes in the $k$-caterpillar $CB^k_n$ are:

$$G(v_1) = G(v_n) = (k + 1) \cdot ((k + 1)n^2 - 2n + 1);$$

$$G(v_i) = (k + 2) \cdot (2(k + 1)i^2 - 2(k + 1)(n + 1)i + (k + 1)n^2 + 2kn + 1) \ (2 \leq i \leq n - 1).$$

Proof. According to the structural features of $CB^k_n$, we can get the degree-distance of $CB^k_n$ to the spine-nodes as follows:

$$G(v_1, CB^k_n) = G(v_n, CB^k_n) = (k + 1)(n - 1) + (k + 2) \sum_{i=1}^{n-2} i + k \sum_{i=1}^{n} i = (k + 1)n^2 - 2n + 1;$$

$$G(v_i, CB^k_n) = (k + 1)(i - 1 + n - i) + (k + 2) \sum_{i=1}^{i-2} i + (k + 2) \sum_{t=1}^{n-i} t + k(\sum_{t=1}^{i} t + \sum_{t=2}^{n-i+1} t)$$

$$= 2(k + 1)i^2 - 2(k + 1)(n + 1)i + (k + 1)n^2 + 2kn + 1.$$  

Thus, the vertex-Gutman indices of the spine-nodes are:

$$G(v_1) = G(v_n) = d(v_1) \cdot G(v_1, CB^k_n) = (k + 1)((k + 1)n^2 - 2n + 1);$$

$$G(v_i) = d(v_i) \cdot G(v_i, CB^k_n) = (k + 2)((k + 1)(2i^2 - 2(n + 1)i + n^2) + 2kn + 1)(2 \leq i \leq n - 1).$$

Lemma 2. The vertex-Gutman indices of the leaf-nodes in the $k$-caterpillar $CB^k_n$ are:

$$G(v_j) = (3k + 2)i^2 - (3k + 2)(n + 1)i + \frac{3k+2}{2}n^2 + \frac{7k+4}{2}n + k - 3 \ (1 \leq i \leq n; 1 \leq j \leq k).$$

Proof. According to the structural features of $CB^k_n$, we can get that

$$G(v_j, CB^k_n) = (k + 1)(i + n - i + 1) + 2(k - 1) + (k + 2)(\sum_{t=1}^{i-1} t + \sum_{t=2}^{n-i} t) + k(\sum_{r=1}^{i-1} (2r + 1) + \sum_{r=2}^{n-i} (2r + 1))$$

$$= (3k + 2)i^2 - (3k + 2)(n + 1)i + \frac{3k+2}{2}n^2 + \frac{7k+4}{2}n + k - 3.$$  

$$G(v_j) = d(v_j) \cdot G(v_j, CB^k_n) = G(v_j, CB^k_n) = (3k + 2)i^2 - (3k + 2)(n + 1)i + \frac{3k+2}{2}n^2 + \frac{7k+4}{2}n + k - 3.$$  

Theorem 1. The maximum values of the vertex-Gutman index of $k$-caterpillar are as follows:
max\{G(u)\} = \begin{cases} 
G(v_i) = G(v_n), & 3 \leq n \leq \left\lfloor x^* \right\rfloor; \\
G(v_2) = G(v_{n-1}), & n \geq \left\lceil x^* \right\rceil.
\end{cases}

where, \(x^* = \left(k^2 + 3k + 3 + \sqrt{k(k^2 + 2k^2 - k - 3)}\right)/(k+1)\).

**Proof.** (1) Firstly, we consider the vertex-Gutman index of the spine-node. From Lemma 1, \(G(v_i)\) \((2 \leq i \leq n-1)\) is a quadratic function on \(i\), and takes maximum values at \(i=2\) or \(i=n-1\).

\[
G(v_2) = G(v_{n-1}) = (k + 2) \cdot ((k + 1)n^2 - 2(k + 2)n + 4(k + 1) + 1);
\]

\[
G(v_2) - G(v_1) = (k + 1)n^2 - 2(k^2 + 3k + 3)n + 4(k^2 + 3k + 2) + 1.
\]

Let \(f(x) = (k + 1)x^2 - 2(k^2 + 3k + 3)x + 4(k^2 + 3k + 2) + 1\), where \(x \in \mathbb{Z}, x \geq 3\). It is easy to see that the symmetric axis of function \(f(x)\) is \(\hat{x} = k + 2 + \frac{1}{x-1}\). Obviously, \(\hat{x} > 3\) and \(f(3) = -k(2k - 3) < 0\). Because the larger zero point of the function is \(x^* = (k^2 + 3k + 3 + \sqrt{k(k^2 + 2k^2 - k - 3)})/(k+1)\), so

a) When \(3 \leq n \leq \left\lfloor x^* \right\rfloor\), there is \(G(v_2) - G(v_1) = f(n) < 0\), the maximum value of the vertex-Gutman index of the spine-node is \(G(v_i) = G(v_{n-1})\);

b) When \(n \geq \left\lceil x^* \right\rceil\), there is \(G(v_2) - G(v_1) = f(n) > 0\), the maximum value of the vertex-Gutman index of the spine-node is \(G(v_2) = G(v_n)\).

(2) It is easy to see that \(G(v_{n-1}) = G(v_2) = G(v_3) = \cdots = G(v_{k-1})\) for \(1 \leq i \leq n\). And from Lemma 2, \(G(v_j)\) \((1 \leq i \leq n, 1 \leq j \leq k)\) takes maximum values at \(i=1\) or \(i=n\). There is:

\[
G(v_{i,j}) = G(v_{n,j}) = (3k + 2) - (3k + 2)(n + 1) + \frac{3k+2}{2}n^2 + \frac{7k+4}{2}n + k - 3
\]

\[
= \frac{1}{2}((3k + 2)n^2 + kn + 2k - 6).
\]

(3) Following we compare the size of \(G(v_i), G(v_2)\) and \(G(v_{i,j})\). Because,

\[
G(v_i) - G(v_{i,j}) = \frac{1}{2}((2k^2 + k)n^2 - (5k + 4)n + 8) > 0.
\]

\[
G(v_2) - G(v_{i,j}) = \frac{1}{2}((2k^2 + 3k + 2)n^2 - (4k^2 + 17k + 16)n + (4k^2 + 12k + 13)) > 0.
\]

Therefore, \(G(v_i) > G(v_{i,j}), G(v_2) > G(v_{i,j})\).

**Theorem 2** The minimum values of the vertex-Gutman index of \(k\)-caterpillar are as follows:

\[
\min\{G(u)\} = \begin{cases} 
G(v_{\frac{n+1}{2}}) = G(v_{\frac{n+1}{2}-1}) = \cdots = G(v_{\frac{n+1}{2}-1}), & \text{when } n \text{ is odd;}
\\
G(v_{\frac{n}{2}}) = G(v_{\frac{n}{2}-1}) = \cdots = G(v_{\frac{n}{2}+1}), & \text{when } n \text{ is even.}
\end{cases}
\]

**Proof.** According to the structure distribution of the \(k\)-caterpillar and the characteristics of its own parity of Gutman index, it is necessary to discuss the parity of the number \(n\) of spine-node of the \(k\)-caterpillar.

(1) If \(n\) is odd. From Lemma 1, \(G(v_i)(2 \leq i \leq n-1)\) takes minimum values at \(i = (n+1)/2\). Since

\[
G(v_{\frac{n+1}{2}}) = \frac{k+2}{2}((k + 1)n^2 + 2(k - 2)n - (k - 1)),
\]

\[
G(v_{\frac{n+1}{2}}) - G(v_{\frac{n}{2}}) = \frac{k}{2}((k + 1)n^2 - 2(k + 3)n + k + 3) > 0.
\]

Therefore, \(G(v_i) > G(v_{\frac{n+1}{2}})\). From Lemma 2, \(G(v_j)(1 \leq i \leq n, 1 \leq j \leq k)\) takes minimum values at \(i = (n+1)/2\). Since
\[ G(v_{\alpha}) = \frac{1}{4}((3k^2 + 2k + 4)n^3 + \frac{1}{4}(3k^2 + 6k - 4)n^2 - \frac{1}{3}(k^2 + 37k - 7)n - 1). \]

\[ G(v_{\alpha}) - G(v_{\beta}) = \frac{1}{4}((2k^2 + 3k + 2)n^3 + 4(k^2 - k - 3)n - 2(k^2 + 2k - 16)) > 0. \]

So, \( G(v_{\alpha}) > G(v_{\beta}) \).

In conclusion, if \( n \) is odd, we have \( \min_{u \in CB_n^k} \{G(u)\} = G(v_{\alpha}) \).

(2) In the same way, if \( n \) is even, we have \( \min_{u \in CB_n^k} \{G(u)\} = G(v_{\beta}) = G(v_{\alpha}) \).

**Corollary 1.** The rankings of the vertex-Gutman index of the spine-node in \( k \)-caterpillar are that:

1. \( G(v_1) > G(v_2) > \cdots > G(v_{n-1}) \) for odd \( n \);
2. \( G(v_1) > G(v_2) > \cdots > G(v_{n-1}) < G(v_{n+1}) < \cdots < G(v_{n}) \) for even \( n \).

**Corollary 2.** The rankings of the vertex-Gutman index of the leaf-node in \( k \)-caterpillar are that:

1. \( G(v_1) > G(v_2) > \cdots > G(v_{n-1}) < G(v_{n+1}) < \cdots < G(v_{n}) \) for odd \( n \);
2. \( G(v_1) > G(v_2) > \cdots > G(v_{n+1}) < G(v_{n+2}) < \cdots < G(v_{n}) \) for even \( n \).

**Gutman Index and Rankings of the Family of \( k \)-Caterpillar**

**Theorem 3** The Gutman index of the \( k \)-Caterpillar \( CB_n^k \) is as follows:

\[ G(CB_n^k) = \frac{1}{6}(5k^2 + 14k + 4)n^3 + \frac{1}{4}(3k^2 + 6k - 4)n^2 - \frac{1}{3}(k^2 + 37k - 7)n - 1. \]

**Proof.**

\[
G(CB_n^k) = \frac{1}{2} \sum_{u \in CB_n^k} d(u) \cdot G(u, CB_n^k)
= \frac{1}{2} \left( d(v_1)G(v_1, CB_n^k) + \sum_{i=2}^{n-1} d(v_i)G(v_i, CB_n^k) + d(v_n)G(v_n, CB_n^k) + \sum_{j=1}^{k} \sum_{i=1}^{n} G(v_j, CB_n^k) \right)
= \frac{1}{6}(5k^2 + 14k + 4)n^3 + \frac{1}{4}(3k^2 + 6k - 4)n^2 - \frac{1}{3}(k^2 + 37k - 7)n - 1.
\]

**Corollary 3.** For the family of \( k \)-Caterpillar \( \left\{ CB_n^k \right\}_{k \geq 2} \):

1. For fixed number \( k \), \( G(CB_n^k) \geq 35k^2 + 53k + 7 \), and equality holds iff \( CB_n^k \equiv CB_3^k \).
2. For fixed number \( n \), \( G(CB_n^k) \geq (26n^3 + 30n^2 - 71n - 3)/3 \), and quality holds iff \( CB_n^k \equiv CB_n^2 \).

**Corollary 4.** The rankings of the Gutman index of the family of \( k \)-Caterpillar \( \left\{ CB_n^k \right\}_{k \geq 2} \) is as follows: \( G(CB_3^k) < G(CB_4^k) < G(CB_5^k) < \cdots G(CB_n^k) < \cdots \). i.e., the Gutman index of the family of \( k \)-Caterpillar \( \left\{ CB_n^k \right\}_{k \geq 2} \) increases with the increase of \( n \) and \( k \).

**Conclusions**

The degree-distance of a graph to a vertex proposed in this paper is a local parameter index of graphs, which may reveal some related local physicochemical properties of molecules represented by graphs. By studying the vertex-Gutman index of the \( k \)-caterpillar, we demonstrated that the distributions of the vertex-Gutman index of the spine-nodes and leaf-nodes are concave. We also obtained the extremal values (vertex) and rankings of the vertex-Gutman index of the \( k \)-caterpillar, and the
extremal graphs and rankings of the Gutman index of the family of the $k$-caterpillar. These results partly revealed the relations between the vertex-Gutman index of trees and the Gutman index of tree families, and the size and parity of the numbers of vertex of tree, which provided a useful idea for the study of the extremal values (vertex) and extremal graphs of the Gutman index of other similar trees.

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References