The Gutman Index of the Unicyclic Graphs with pendent edges

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Abstract. The graph-parameters mainly studies vertex degree and distance between unordered vertices. There are many graph-parameters, and this paper mainly focuses on the Gutman index. For the sake of discussion, this paper puts forward the concept of "contribution" based on the relationship between Gutman index of graph and vertex-Gutman index. On this basis, we discussed the Gutman index of unicyclic graph with pendent edges in odd and even parts, and gave the corresponding extremal graphs, which lays a foundation for the study of the Gutman index of other cycle graphs.

1. Introduction
In 1947, American chemist Harold Wiener proposed the Wiener index based on the distance between vertices for estimating the boiling point of Alkanes[1]. Since then, scholars have never stopped the research on graph-parameters. 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[2]. In this paper, we mainly discuss the Gutman index of the unicyclic graphs with pendent edges.

2. Preliminaries
For better discuss the Gutman index of the unicyclic graphs with pendent edges, we give some basic definitions.

Definition 1. Let \( T \) be a graph, the degree of the vertex \( v \) is the number of edges connected with the vertex \( v \) (Specially, each self-loop is counted as two edges).

Definition 2. A road is said to be closed if its starting vertex and ending vertex are the same and its length is greater than 0. A closed road is called cyclic ( denoted as \( C_n \)) if its starting vertex is different from its internal vertex.

Definition 3. Let \( T \) be a simple graph, the Gutman index of \( T \) is defined as:

\[ G(T) = \sum_{(u,v)\in E(T)} (d(u) \cdot d(v))d(u,v) \]  

the Gutman index \( v \) is defined as

\[ G(u) = d(u) \sum_{v\in V(T)} d(v)d(u,v) \]
so the Gutman index of graph $T$ can also be formatted as:

$$G(T) = \sum_{u \in V(T)} (d(u) \sum_{v \in V(T)} d(u,v)) / 2 = \sum_{u \in V(T)} G(u) / 2$$

(3)

**Definition 4.** The unicyclic graph with pendent edges (denoted as $C_{n_1,n}$, see below Figure) is cyclic graph (denoted as $C_n$, $1 \leq n_1 \leq n$) with $n_1$ vertices, and only one vertex of cyclic has pendent edges (Pendent vertices are denoted as $v_i (1 \leq i \leq n - n_1)$).

![Figure 1. Unicyclic graph with pendent edges $C_{n_1,n}$](image)

3. Main Results

**Theorem 1.** The Gutman index of the unicyclic graph with pendent edges $C_{n_1,n}$ is as follows:

$$G(C_{n_1,n}) = \begin{cases} 
1/2 \cdot [-n_1^3 + 2mn_1^2 + (3 - 8n)n_1 + 4n^2 - 4n], & \text{when } n_1 \text{ is odd;} \\
1/2 \cdot [-n_1^3 + 2mn_1^2 + (2 - 4n)n_1 + 4n^2 - 2n], & \text{when } n_1 \text{ is even}
\end{cases}$$

(4)

**Proof.** For discussion purposes, we label the vertices of cyclic $C_{n_1}$. Let’s start from the neighbor vertex $u_0$, and remembere as $u_1, u_2, \cdots, u_{i-1}, u_i, \cdots, u_{n-1}$. Next, we study the Gutman index of the unicyclic graph with pendent edges in odd and even parts.

Because of the complexity of structure of graph $C_{n_1,n}$, the concept of contribution is proposed in this paper. As shown below:

The contribution of any vertex $v$ to the calculation of vertex-Gutman index of vertex $u$ is called the contribution $(u,v)$ (denoted as $G(u,v)$).

In the same way, the contribution of any vertex $u$ to the calculation of the Gutman index of graph $T$ is called the contribution $(T,u)$ (denoted as $G(T,u)$).

A.1. If $n_1$ is odd. Due to the special location, the calculation of the vertex-Gutman index of $u_0$ is a little difficult to obtain. By calculating the contribution $\sum_{v \in f} (u,v)$, we can get the vertex-Gutman index of $u_0$:

$$G(u_0) = d(u_0) \cdot [2 \cdot \sum_{j=1}^{n_1-1} G(u_0,u_j) + \sum_{k=1}^{n-n_1} G(u_0,v_k)]$$

$$= [-n_1^3 + (n + 4)n_1^2 - (4n + 3)n_1 + 2n^2 + 3n - 2] / 2$$

(5)

Considering the symmetry of the vertices of $C_{n_1,n}$, we all have to do is calculate the vertex-Gutman index of top half vertices of the unicyclic graph with pendent edges. The vertex-Gutman index of $u_i$ $(1 \leq i \leq n_1 - 1/2)$ is as follows:
In the same method, we can get the vertex-Gutman index of pendent vertex $v_j$:

$$G(v_j) = d(v_j) \cdot \left[ \sum_{k \in j, k \neq j} G(v_j, v_k) + G(v_j, u_{0i}) + 2 \cdot \sum_{i=1}^{n_i-1/2} G(v_j, u_i) \right]$$

$$= (n_i^2 - 2n_i + 6n - 5)/2$$

(7)

In summary, the calculation of the Gutman index of the unicyclic graphs with pendent edges can be broken down into the calculations-contributions of all vertices. So we finally can get:

$$G(C_{n_i,n}) = [G(C_{n_i,n}, u_0) + \sum_{j=1}^{n_i} G(C_{n_i,n}, v_j) + 2 \cdot \sum_{i=1}^{n_i-1/2} G(C_{n_i,n}, u_i)]/2$$

$$= [-n_i^3 + 2nn_i^2 + (3 - 8n)n_i + 4n^2 - 4n]/2$$

(8)

A.2. If $n_i$ is even. Similar to the proof of A.1, we can also get the vertex-Gutman index of $u_i$ $(1 \leq i \leq n_i/2)$:

$$G(u_i) = d(u_i) \cdot \left[ 2 \sum_{j \neq i} G(u_i, u_j) + G(u_i, u_{0i}) - 2d(u_i, u_0) + G(u_i, u_0) + \sum_{k=1}^{n_i} G(u_i, v_k) \right]$$

$$= n_i^2 - 2n_i + 2n + 4(n - n_i)i$$

(9)

Specially, we have $G(u_{n_i/2}) = -n_i^2 + (2n - 2)n_i + 2n$. We can also come to the following conclusions using same analyses way.

Vertex-Gutman index of $u_0$ and $v_j$ are as follows:

$$G(u_0) = d(u_0) \cdot \left[ 2 \sum_{j \neq 0} G(u_0, u_j) + G(u_0, u_{0i}) + \sum_{k=1}^{n_i} G(u_0, v_k) \right]$$

$$= [-n_i^3 + (n + 4)n_i^2 - (4n + 4)n_i + 2n^2 + 4n]/2$$

(10)

$$G(v_j) = d(v_j) \cdot \left[ \sum_{k \in j} G(v_j, v_k) + G(v_j, u_0) + 2 \sum_{i=1}^{n_i-2/2} G(v_j, u_i) + G(v_j, u_{0i}/2) \right]$$

$$= (n_i^2 - 2n_i + 6n - 4)/2$$

(11)

So the Gutman index of the unicyclic graph with pendent edges $C_{n_i,n}$ is:

$$G(C_{n_i,n}) = [G(C_{n_i,n}, u_0) + \sum_{j=1}^{n_i} G(C_{n_i,n}, v_j) + 2 \cdot \sum_{i=1}^{n_i-2/2} G(C_{n_i,n}, u_i) + G(C_{n_i,n}, u_{0i}/2)]/2$$

$$= [-n_i^3 + 2nn_i^2 + (2 - 4n)n_i + 4n^2 - 2n]/2$$

(12)

Theorem 2. The extreme values of the unicyclic graph with pendent edges $C_{n_i,n}$ are as follows:

$$\max \{G(C_{n_i,n})\} = \begin{cases} (n_i^3 - 4n_i^2 - n)/2, & \text{when } n_i \text{ is odd;} \\ n_i^2/2, & \text{when } n_i \text{ is even} \end{cases}$$

(13)

$$\min \{G(C_{n_i,n})\} = \begin{cases} 2n_i^2 - 6n - 1, & \text{when } n_i \text{ is odd;} \\ 2n_i^2 - 2n + 1/2, & \text{when } n_i \text{ is even} \end{cases}$$

(14)

Proof B.1. If $n_i$ is odd:
From theorem 2, we have \( G(C_{n_1,n}) = [-n_1^3 + 2nn_1^2 + (3-8n)n_1 + 4n^2 - 4n]/2 \).

Let \( f(x) = [-x^3 + 2nx^2 + (3-8n)x + 4n^2 - 4n]/2 \), \((x \in Z, 1 \leq x \leq n)\) . The first derivative for the function \( f(x) \) gives \( f'(x) = (-3x^2 + 4nx + 3-8n)/2 \) (Let's talk about the function in the case of \( n > 9 \)).

It is clear that:
- \( f'(x) < 0 \), (when \( 1 \leq x \leq 2 \)).
- \( f'(x) > 0 \), (when \( 3 \leq x \leq n \)).

So \( f(x) \) takes minimum values at \( x = 2 \) or \( x = 3 \), and we have \( f(2) = 2n^2 - 6n - 1 \) and \( f(3) = 2n^2 - 5n - 9 \).

Obviously \( f(2) < f(3) \) (when \( n > 9 \)), we can get
\[
\min \{C_{n_1,n}\} = \min_{x \in Z, 1 \leq x \leq n} \{f(x)\} = f(2) = 2n^2 - 6n - 1
\]
(15)

By analyzing the structure of function image, we can get \( f(x) \) takes maximum values at \( x = 1 \) or \( x = n \). And there are: \( f(1) = 2n^2 - 5n + 1 \); \( f(n) = (n^3 - 4n - n)/2 \).

Because \( f(n) > f(1) \) (when \( n > 9 \)), we also can get
\[
\max \{C_{n_1,n}\} = \max_{x \in Z, 1 \leq x \leq n} \{f(x)\} = f(n) = n^3 - 4n - n/2
\]
(16)

B.2. If \( n_1 \) is even:

From theorem 2, we have \( G(C_{n_1,n}) = [-n_1^3 + 2nn_1^2 + (2-4n)n_1 + 4n^2 - 2n]/2 \).

Let \( g(x) = (-x^3 + 2nx^2 + (2-4n)x + 4n^2 - 2n)/2 \), \((x \in Z, 1 \leq x \leq n)\) , similar to the proof of A.1, we can also get the extreme values:
\[
\min \{C_{n_1,n}\} = \min_{x \in Z, 1 \leq x \leq n} \{g(x)\} = g(1) = 2n^2 - 4n + 1/2
\]
(17)
\[
\max \{C_{n_1,n}\} = \max_{x \in Z, 1 \leq x \leq n} \{g(x)\} = g(n) = n^3 /2
\]
(18)

**Corollary 1.** For the unicyclic graph with pendent edges \( C_{n_1,n} \), there are:
\[
2n^2 - 6n - 1 \leq G(C_{n_1,n}) \leq n^3 /2
\]
(19)
- For fixed number \( n \), left equality holds if and only if \( C_{n_1,n} \cong C_{2,n-2} \);
- For fixed number \( n \), right equality holds if and only if \( C_{n_1,n} \cong C_{n} \).

4. **Conclusions**

Based on the Gutman index of graph and vertex-Gutman Index, this paper puts forward the concept of "contribution", which provides a new idea for the discussion of graph-parameters. On this basis, we studied the "contribution" of all vertices of the unicyclic graph with pendent edges, and obtained the Gutman index and the extreme values of graph \( C_{n_1,n} \). Minimal and maximal graph of \( C_{n_1,n} \) are \( C_{2,n} \) and \( C_{n} \)—For \( C_{n_1,n} \), the Gutman index of graph is Minimal, when the number of vertices of \( C_{n_1} \) is \( n_1 = 2 \); the Gutman index of graph is Maximal, when the number of vertices of \( C_{n} \) is \( n_1 = n \).
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