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Computation of Gutman index of some cactus chains

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Abstract

Let G be a finite connected graph of order n. The Gutman index $Gut(G)$ of G is defined as $\sum_{\{x,y\} \subseteq V(G)} deg(x)deg(y)d(x,y)$, where $deg(x)$ is the degree of vertex x in G and $d(x,y)$ is the distance between vertices x and y in G. A cactus graph is a connected graph in which no edge lies in more than one cycle. In this paper we compute the exact value of Gutman index of some cactus chains.

1. Introduction

Let $G = (V, E)$ be a finite, connected, simple graph. We denote the degree of a vertex v in G by $deg(v)$, and for two vertices u, v in G, $d(u, v)$ denotes the usual distance between u and v in G, i.e., the minimum number of edges on a path from u to v. A topological index of G is a real number related to G. It does not depend on the labeling or pictorial representation of a graph. The Wiener index $W(G)$ is the first distance based topological index defined as $W(G) = \sum_{\{u,v\} \subseteq G} d(u, v) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v)$ with the summation runs over all pairs of vertices of G [12]. The topological indices and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making

their chemical applications. The Wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds [12]. The degree distance of G, denoted by $DD(G)$, is defined as $DD(G) = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v)[d(u) + d(v)]$ with the summation runs over all pairs of vertices of G. In [4] Gutman showed that if T is a tree of order n, then $DD(T) = 4W(G) - n(n-1)$. The Gutman index $Gut(G)$ of G is defined as $Gut(G) = \sum_{\{x,y\}\subseteq V(G)} deg(x)deg(y)d(x,y)$ ([4]). The Gutman index, a Schultz-type molecular topological index and a variant of the well known and much studied Wiener Index, was introduced in 1994 by Gutman [4] as a kind of a vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. Gutman revealed that in the case of acyclic structures, the index is closely related to the Wiener Index and reects precisely the same structural features of a molecular as the Wiener Index does. A question, on whether theoretical investigations on the Gutman index focusing on the more difficult case of polycyclic molecules can be done, was posed ([8]). Mukwembi in [8] proved that $Gut(G) \leq \frac{2^4}{5^5}n^5 + O(n^4)$, where n is the order of G. V. Sheeba Agnes in [11] determined the degree distance and the Gutman index of the corona product of two graphs. Also he obtained, the exact degree distance and Gutman index of certain classes of graphs. The exact value of the Gutman indices of the Cartesian product, the wreath product of graphs, and as results the exact value of Gutman indices of the hypercube, torus, grid, Hamming graph and the fence graph are given in [9].

In this paper we consider a class of simple linear polymers called cactus chains. Cactus graphs were first known as Husimi tree, they appeared in the scientific literature some sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [5, 6, 10]. We refer the reader to papers [2, 7] for some aspects of parameters of cactus graphs. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size i, the cactus is i-uniform. A triangular cactus is a graph whose blocks are triangles, i.e., a 3-uniform cactus. A vertex shared by two or more triangles is called a cut-vertex. If each triangle of a triangular cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that G is a chain triangular cactus. By replacing triangles in this definitions with cycles of length 4 we obtain cacti whose every block is C_4. We call such cacti square cacti. Note that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square[1].

In the next section, we compute the Gutman index of triangular and square cactus chains. In Section 3, we compute Gutman index of two kind of chain hexagonal cactus.

2. Gutman index of triangular and square cactus chains

First we consider a chain triangular. An example of a chain triangular cactus is shown in Figure 1. We call the number of triangles in G, the length of the chain. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n. Here we compute the exact value of Gutman index of T_n.
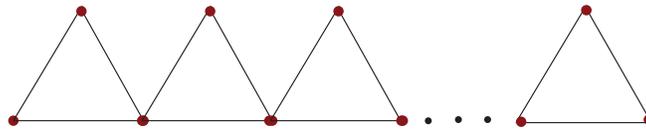
Figure 1. Chain triangular graph T_n.

Theorem 2.1. *The Gutman index of the chain triangular cactus T_n ($n \geq 2$) is*

$$Gut(T_n) = 6n^2(n+1).$$

Proof. Let u and v be two arbitrary vertices of T_n. Suppose that $d(u,v) = k$. We have the following cases:

(1) If $d(u,v) = 1$ then there are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$, and $2n$ pairs of vertices $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$, and there are $n-2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.

(2) If $d(u,v) = k$ and $2 \leq k \leq n-1$ then there are $n-k+3$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$, there are $2(n-k+1)$ pairs of vertices $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$, and $n-k-1$ pairs of vertices $u, v \in V(G)$ with $d(u) = d(v) = 4$.

(3) If $d(u,v) = n$ then there are four pairs of vertices $u, v \in V(G)$ with $d(u) = d(v) = 2$.

So by definition of Gutman index, we have:

$$
\begin{aligned}
Gut(T_n) \quad &= \sum_{\{u,v\} \subseteq V(G)} d(u,v)d(u)d(v) \\
&= \sum_{\{u,v\} \subseteq V(G), d(u,v)=k, k \in \{2,\ldots,n-1\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\} \subseteq V(G), d(u,v)=1} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\} \subseteq V(G), d(u,v)=n} d(u,v)d(u)d(v) \\
&= \sum_{k=2}^{n-1} 4k(n-k+3) + \sum_{k=2}^{n-1} 16k(n-k+1) + \sum_{k=2}^{n-1} 16k(n-k-1) \\
&+ 2(4) + 2n(8) + (n-2)(16) + 4(2)(2)n \\
&= 48n - 24 + \left(36 \sum_{k=2}^{n-1} k(n-k-1)\right) + 48 \sum_{k=2}^{n-1} k
\end{aligned}
$$
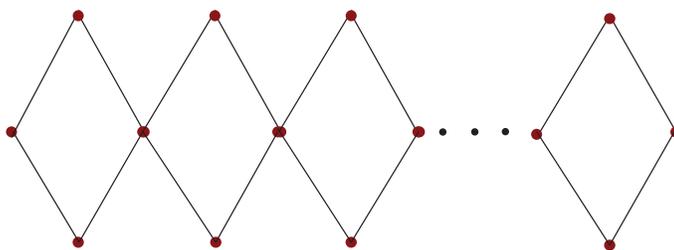
Figure 2. Para-chain square cactus graph Q_n.

$$= 48(\frac{n(n-1)}{2} - 1) + 48n - 24 + 36 \sum_{k=2}^{n-1} k(n-k-1)$$

$$= 24n^2 + 24n - 72 + 36 \sum_{k=2}^{n-1} k(n-k-1)$$

$$= 24n^2 + 24n - 72 + 6n^3 - 18n^2 - 24n + 72$$

$$= 6n^2(n+1). \quad \square$$

By replacing triangles in the definitions of triangular cactus T_n, with cycles of length 4 we obtain cacti whose every block is C_4. We call such cacti, square cacti. An example of a square cactus chain is shown in Figure 2. We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square. We consider a para-chain of length n, which is denoted by Q_n as shown in Figure 2. The following theorem gives the exact value of Gutman index of Q_n.

Theorem 2.2. *The Gutman index of the Para-chain square cactus graph Q_n ($n \geq 2$) is*

$$Gut(Q_n) = \frac{32}{3}n(2n^2 + 1).$$

Proof. Suppose that u and v are two arbitrary vertices of Q_n and let $d(u,v) = k$. We have the following cases:

(1) If $d(u,v) = k$ and $k = 2s+1$ ($0 \leq s \leq n-2$) then we have the following pairs of vertices:
   (i) There are four pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $4(n-s-1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(2) If $d(u,v) = 2$ then we have the following pairs of vertices:
   (i) There are $5(n-1)+1$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
   (iii) There are $n-2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.
(3) If $d(u,v) = k$ and $k = 2s$ ($2 \leq s \leq n-1$) then we have the following pairs of vertices:

   (i) There are $4(n-s)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.

   (ii) There are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.

  (iii) There are $n - s - 1$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.

(4) If $d(u, v) = 2n - 1$, then there are four pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.

(5) If $d(u, v) = 2n$, then there is one pair of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.

So by definition of Gutman index we have:

$$
\begin{aligned}
Gut(Q_n) \quad &= \sum_{\{u,v\}\subseteq V(G)} d(u,v)d(u)d(v) \\
&= \sum_{\{u,v\}\subseteq V(G), d(u,v)=2s+1, s\in\{0,\dots,n-2\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=2} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=2s, s\in\{2,\dots,n-1\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=2n-1} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=2n} d(u,v)d(u)d(v) \\
&= \sum_{s=0}^{n-2} 4(2s+1)(2)(2) + \sum_{s=0}^{n-2} 4(n-s-1)(2s+1)(2)(4) \\
&+ (5(n-1)+1)(2)(2)(2) + 2(2)(2)(4) + (n-2)(2)(4)(4) \\
&+ \sum_{s=2}^{n-1} 4(n-s)(2s)(2)(2) + \sum_{s=2}^{n-1} 2(2s)(2)(4) + \sum_{s=2}^{n-1} (n-s-1)(2s)(4)(4) \\
&+ 4(2n-1)(2)(2) + 2n(2)(2) \\
&= \frac{32}{3}n(2n^2+1). \quad \square
\end{aligned}
$$

Now we consider another kind of square cactus chain and compute its Gutman index (Figure 3).

Theorem 2.3. *The Gutman index of the Ortho-chain square cactus graph O_n ($n \geq 5$) is*

$$
Gut(O_n) = \frac{32}{3}n^3 + 24n^2 - \frac{8}{3}n + 48.
$$

Proof. Suppose that u and v are two vertices of O_n and let $d(u, v) = k$. We have the following cases:
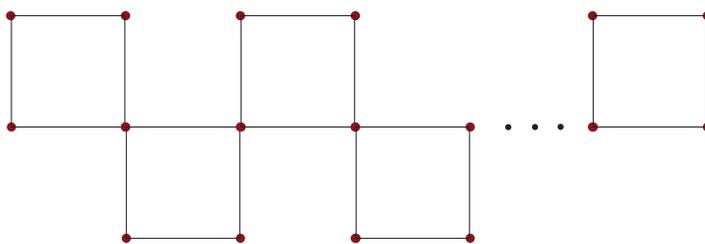
Figure 3. Ortho-chain square cactus graph O_n.

(1) If $d(u,v) = 1$, then we have the following pairs of vertices:
    (i) There are $n+2$ of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
    (ii) There are $2n$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
    (iii) There are $n-2$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 4$.
(2) If $d(u,v) = 2$, then we have the following pairs of vertices:
    (i) There are $n+3$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
    (ii) There are $4(n-1)$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
    (iii) There are $n-3$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 4$.
(3) If $d(u,v) = 3$ then we have the following pairs of vertices:
    (i) There are $3n$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
    (ii) There are $4(n-3) + 2$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
    (iii) There are $n-4$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 4$.
(4) If $d(u,v) = k$ $(4 \leq k \leq n-1)$ then we have the following pairs of vertices:
    (i) There are $4(n-k+3)$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
    (ii) There are $4(n-k) + 2$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
    (iii) There are $n-k-1$ pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 4$.
(5) If $d(u,v) = n$ then we have the following pairs of vertices:
    (i) There are thirteen pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
    (ii) There are two pairs of vertices such as $u,v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(6) If $d(u,v) = n+1$ then there are six pairs of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.
(7) If $d(u,v) = n+2$ then there is one pair of vertices such as $u,v \in V(G)$ with $d(u) = d(v) = 2$.

So we have:

$$
\begin{aligned}
Gut(O_n) \quad &= \sum_{\{u,v\}\subseteq V(G), d(u,v)=1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G), d(u,v)=2} d(u,v)d(u)d(v) \\
&= \sum_{\{u,v\}\subseteq V(G), d(u,v)=3} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=k, k\in\{4,\dots,n-1\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=n} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G), d(u,v)=n+1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G), d(u,v)=n+2} d(u,v)d(u)d(v) \\
&= (n+2)(2)(2) + 2n(2)(4) + (n-2)(4)(4) \\
&\quad + (n+3)(2)(2)(2) + 4(n-1)(2)(2)(4) + (n-3)(2)(4)(4) \\
&\quad + 3n(3)(2)(2) + (4(n-3)+2)(3)(2)(4) + (n-4)(3)(4)(4) \\
&\quad + \sum_{k=4}^{n-1} 4(n-k+3)(k)(2)(2) + \sum_{k=4}^{n-1}(4(n-k)+2)(k)(2)(4) \\
&\quad + \sum_{k=4}^{n-1}(n-k-1)(k)(4)(4) \\
&\quad + 13n(2)(2) + 2n(2)(4) + 6(n+1)(2)(2) + (n+2)(2)(2) \\
&= 8n^3 + 32n^2 + 88n - 272 + \frac{8}{3}(n-4)(n-5)(n+6). \\
&= \frac{32}{3}n^3 + 24n^2 - \frac{8}{3}n + 48. \quad \square
\end{aligned}
$$

3. Gutman index of chain hexagonal cactus

In this section we shall compute the exact value of Gutman index of some hexagonal cactus chains. Replacing triangles in the definitions of triangular cactus, by cycles of length 6 we obtain cacti whose every block is C_6. We call such cacti, hexagonal cacti. An example of a hexagonal cactus chain is shown in Figure 4. We see that the internal hexagonal may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-hexagonal; if the cut-vertices are not adjacent, we call the square a para-hexagonal. We consider a para-chain of length n, which is denoted by L_n as shown in Figure 4. The following theorem gives the exact value of Gutman index of L_n. In this section we shall compute the Gutman index of two kinds of para-chain hexagonal cactus. The following theorem gives the Gutman index of L_n.

Theorem 3.1. *The Gutman index of the Para-chain hexagonal cactus graph L_n ($n \geq 3$) is*

$$
Gut(L_n) = 36n(2n^2 + 1).
$$
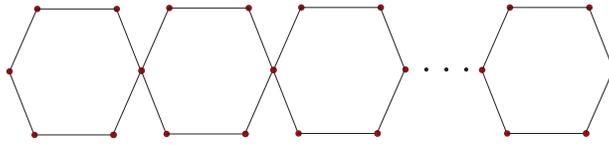
Figure 4. Para-chain hexagonal cactus graph L_n.

Proof. Suppose that u and v are two vertices of L_n and let $d(u,v) = k$. We have the following cases:

(1) If $d(u,v) = 1$, then we have the following pairs of vertices:
  (i) There are $2n + 4$ of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are $4(n-1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(2) If $d(u,v) = 2$, then we have the following pairs of vertices:
  (i) There are $6n$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are $4(n-1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(3) If $d(u,v) = 3$ then we have the following pairs of vertices:
  (i) There are $10(n-1) + 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
  (iii) There are $n - 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.
(4) If $d(u,v) = k$ and $k = 3s + 1$ $(1 \le s \le n - 2)$ then we have the following pairs of vertices:
  (i) There are $4(n - s + 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are $4(n - s - 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(5) If $d(u,v) = k$ and $k = 3s + 2$ $(1 \le s \le n - 2)$ then we have the following pairs of vertices:
  (i) There are $4(n - s)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are $4(n - s - 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(6) If $d(u,v) = k$ and $k = 3s$ $(2 \le s \le n - 1)$ then we have the following pairs of vertices:
  (i) There are $8(n - s)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
  (ii) There are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
  (iii) There are $n - s - 1$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.

(7) If $d(u,v) = 3n - 2$ then there are eight pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
(8) If $d(u,v) = 3n - 1$ then there are four pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
(9) If $d(u,v) = 3n$ then there is one pair of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
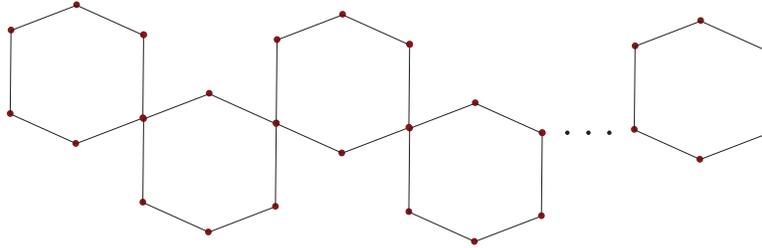
Figure 5. Meta-chain graph M_n.

So by definition Gutman index we have:

$$
\begin{aligned}
Gut(L_n) \quad &= \sum_{\{u,v\}\subseteq V(G)} d(u,v)d(u)d(v) = \sum_{\{u,v\}\subseteq V(G),d(u,v)=1} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=2} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=3} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=3s+1,s\in\{1,...,n-2\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=3s+2,s\in\{1,...,n-2\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=3s,s\in\{2,...,n-1\}} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=3n-2} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=3n-1} d(u,v)d(u)d(v) \\
&+ \sum_{\{u,v\}\subseteq V(G),d(u,v)=3n} d(u,v)d(u)d(v) \\
&= (2n+4)(2)(2) + 4(n-1)(2)(4) + 6n(2)(2)(2) + 4(n-1)(2)(2)(4) \\
&+ (10(n-1)+2)(3)(2)(2) + 2(3)(2)(4) + (n-2)(3)(4)(4) \\
&+ \sum_{s=1}^{n-2} 4(n-s+1)(3s+1)(2)(2) + \sum_{s=1}^{n-2} 4(n-s-1)(3s+1)(2)(4) \\
&+ \sum_{s=1}^{n-2} 4(n-s)(3s+2)(2)(2) + \sum_{s=1}^{n-2} 4(n-s-1)(3s+2)(2)(4) \\
&+ \sum_{s=2}^{n-1} 8(n-s)(3s)(2)(2) + \sum_{s=2}^{n-1} 2(3s)(2)(4) + \sum_{s=2}^{n-1} (n-s-1)(3s)(4)(4) \\
&+ 8(3n-2)(2)(2) + 4(3n-1)(2)(2) + 3n(2)(2) \\
&= 36n(2n^2+1). \quad \square
\end{aligned}
$$

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Theorem 3.2. *The Gutman index of the Para-chain hexagonal cactus graph M_n ($n \geq 4$) is $Gut(M_n) = 48n^3 + 72n^2 - 28n + 16$.*

Proof. Let $d(u, v) = k$. We have the following cases:

(1) If $d(u, v) = 1$ then we have the following pairs of vertices:
   (i) There are $2n + 4$ of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $4(n - 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(2) If $d(u, v) = 2$ then we have the following pairs of vertices:
   (i) There are $5n$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $2n$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
   (iii) There are $n - 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.
(3) If $d(u, v) = 3$ then we have the following pairs of vertices:
   (i) There are $5n + 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $6n - 10$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(4) If $d(u, v) = 4$ then we have the following pairs of vertices:
   (i) There are $9(n - 1) - 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $2(n - 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
   (iii) There are $n - 3$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.
(5) If $d(u, v) = k$ and $k = 2s + 1$ ($2 \leq s \leq n - 2$) then we have the following pairs of vertices:
   (i) There are $6(n - s + 1) + 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $6(n - s - 1) + 2$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(6) If $d(u, v) = k$ and $k = 2s$ ($3 \leq s \leq n - 1$) then we have the following pairs of vertices:
   (i) There are $10(n - s + 1) - 1$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are $2(n - s + 1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
   (iii) $n - s - 1$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 4$.
(7) If $d(u, v) = 2n - 1$ then we have the following pairs of vertices:
   (i) There are fourteen pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
   (ii) There are two pairs of vertices such as $u, v \in V(G)$ with $d(u) = 2$ and $d(v) = 4$.
(8) If $d(u, v) = 2n$ then there are ten pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
(9) If $d(u, v) = 2n + 1$ then there are four pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.
(10) If $d(u, v) = 2n + 2$ then there is one pair of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = 2$.

So we have:

$$
\begin{aligned}
Gut(M_n) \quad &= \sum_{\{u,v\}\subseteq V(G),d(u,v)=1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2} d(u,v)d(u)d(v) \\
&= \sum_{\{u,v\}\subseteq V(G),d(u,v)=3} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=4} d(u,v)d(u)d(v) \\
&\quad + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2s,s\in\{2,\dots,n-2\}} d(u,v)d(u)d(v) \\
&\quad + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2s+1,s\in\{3,\dots,n-1\}} d(u,v)d(u)d(v) \\
&\quad + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2n-1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2n} d(u,v)d(u)d(v) \\
&\quad + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2n+1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G),d(u,v)=2n+2} d(u,v)d(u)d(v) \\
&= (2n+4)(2)(2) + 4(n-1)(2)(4) \\
&\quad + 5n(2)(2)(2) + 2n(2)(2)(4) + (n-2)(2)(4)(4) \\
&\quad + (5n+2)(3)(2)(2) + (6n-10)(3)(2)(4) \\
&\quad + (9(n-1)-2)(4)(2)(2) + 2(n-1)(4)(2)(4) + (n-3)(4)(4)(4) \\
&\quad + \sum_{s=2}^{n-2}(6(n-s+1)+2)(2s+1)(2)(2) + \sum_{s=2}^{n-2}(6(n-s-1)+2)(2s+1)(2)(4) \\
&\quad + \sum_{s=3}^{n-1}(10(n-s+1)-1)(2s)(2)(2) + \sum_{s=3}^{n-1}2(n-s+1)(2s)(2)(4) \\
&\quad + \sum_{s=3}^{n-1}(n-s-1)(2s)(4)(4) + 14(2n-1)(2)(2) + 2(2n-1)(2)(4) \\
&\quad + 10(2n)(2)(2) + 4(2n+1)(2)(2) + (2n+2)(2)(2) \\
&= 48n^3 + 72n^2 - 28n + 16. \quad \square
\end{aligned}
$$

Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1,\dots,G_k$ as follows. Select a vertex of G_1, a vertex of G_2, and identify these two vertices. Then continue in this manner inductively. Note that the graph G constructed in this way has a tree-like structure, the G_i's being its building stones. Usually say that G is obtained by point-attaching from $G_1,\dots,G_k$ and that G_i's are the primary subgraphs of G. A particular case of this construction is the decomposition of a connected graph into blocks (see [3]). Cactus chains which we considered in this paper are particular cases of point attaching of cycles of length three, four and six. As another example consider the graph $Q(m,n)$ constructed in the following manner: consider the graph K_m and m copies of K_n. The graph $Q(m,n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n (see Figure 6). We end this paper by computing the Gutman index of the graph $Q(m,n)$.
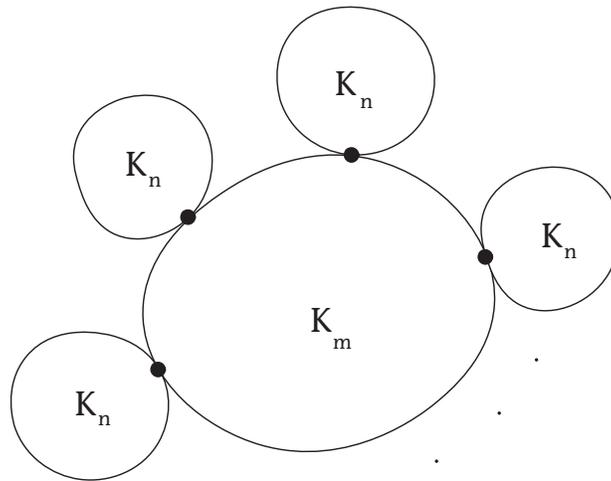
Figure 6. The graph $Q(m,n)$.

Theorem 3.3. *The Gutman index of the graph $Q(m,n)$ $(m,n \geq 2)$ is*

$$\frac{1}{2}m(4m^2n^2 + 4mn^3 + n^4 + m^3 - 6m^2n - 14mn^2 - 7n^3 - m^2 + 12mn + 13n^2 + m - 7n - 1).$$

Proof. Suppose that u and v are two vertices of $Q(m,n)$ and let $d(u,v) = k$. We have the following cases:

(1) If $d(u,v) = 1$, then there are $\frac{m(n-1)(n-2)}{2}$ of vertices $u, v \in V(G)$ with $d(u) = d(v) = n-1$, $m(n-1)$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = n-1$, $d(v) = m+n-2$, and there are $\frac{m(m-1)}{2}$ pairs of vertices such as $u, v \in V(G)$ with $d(u) = d(v) = m+n-2$.

(2) If $d(u,v) = 2$, then there are $m(m-1)(n-1)$ pairs of vertices $u, v \in V(G)$ with $d(u) = n-1$ and $d(v) = m+n-2$.

(3) If $d(u,v) = 3$, then there are $\frac{m(n-1)^2(m-1)}{2}$ pairs of vertices $u, v \in V(G)$ with $d(u) = d(v) = n-1$.

So we have:

$$
\begin{aligned}
Gut(O(m,n)) \quad &= \sum_{\{u,v\}\subseteq V(G), d(u,v)=1} d(u,v)d(u)d(v) + \sum_{\{u,v\}\subseteq V(G), d(u,v)=2} d(u,v)d(u)d(v) \\
&= \sum_{\{u,v\}\subseteq V(G), d(u,v)=3} d(u,v)d(u)d(v) \\
&= \frac{m(n-1)(n-2)}{2}(n-1)(n-1) + m(n-1)(n-1)(m+n-2) \\
&+ \frac{m(m-1)}{2}(m+n-2)^2 \\
&+ 2m(m-1)(n-1)(n-1)(m+n-2)
\end{aligned}
$$

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$$+3\frac{m(m-1)}{2}(n-1)^2$$
$$=\frac{1}{2}m(4m^2n^2 + 4mn^3 + n^4 + m^3 - 6m^2n$$
$$-14mn^2 - 7n^3 - m^2 + 12mn + 13n^2 + m - 7n - 1). \quad \square$$

Acknowledgements

References

[1] S. Alikhani, S. Jahari, M. Mehryar and R. Hasni, Counting the number of dominating sets of cactus chains, *Opt. Adv. Mat. Rapid Comm.* **8** (9-10) (2014), 955–960.

[2] M. Chellali, Bounds on the 2-domination number in cactus graphs, *Opuscula Math.* **2** (2006), 5–12.

[3] E. Deutsch and S. Klavžar, Computing the Hosoya polynomial of graphs from primary subgraphs, *MATCH Commun. Math. Comput. Chem.* **70** (2013), 627–644.

[4] I. Gutman, Selected Properties of the Schultz Molecular Topological Index, *J. Chem. Inf. Comput. Sci.* **34** (1994), 1087–1089.

[5] F. Harary and B. Uhlenbeck, On the number of Husimi trees, I, *Proc. Nat. Acad. Sci.* **39** (1953), 315–322.

[6] K. Husimi, Note on Mayer's theory of cluster integrals, *J. Chem. Phys.* **18** (1950), 682–684.

[7] S. Majstorović, T. Došlić and A. Klobučar, k-domination on hexagonal cactus chains, *Kragujevac J. Math.* **36** (2) (2012), 335–347.

[8] S. Mukwembi, On the upper bound of Gutman index of graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012), 343–348.

[9] P. Paulraja and V. Sheeba Agnes, Gutman index of product graphs, *Discrete Math. Alg. Appl.* **6** (4) (2014), 1450058.

[10] R.J. Riddell, Contributions to the theory of condensation, *Ph.D. Thesis*, Univ. of Michigan, Ann Arbor, 1951.

[11] V. Sheeba Agnes, Degree distance and Gutman index of corona product of graphs, *Trans. Combin.* **4** (3) (2015), 11–23.

[12] H. Wiener, Structural determination of the Paraffin Boiling Points, *J. Amer. Chem. Soc.* **69** (1947), 17–20.