GOURAVA AND HYPER-GOURAVA INDICES OF SOME CACTUS CHAINS

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Abstract. The physico-chemical characteristics of molecules are theoretically explored using the theory of graphs and mathematical chemistry. A graph’s topological index is a numerical value derived from the graph mathematically. The Gourava and hyper-Gourava indices of various cactus chains are determined in this study.

Key words and Phrases: Gourava indices, hyper-Gourava indices, cactus chains.

1. INTRODUCTION

A molecular graph, also known as a chemical graph, is a graph in which the atoms are represented by the vertices, while the bonds are represented by the edges. Topological indices are numeric quantities obtained from a molecular graph that correlate the molecular graph’s physico-chemical characteristics and have been shown to be beneficial in isomer discrimination, QSAR and QSPR analysis.

Only simple, finite, connected graphs with $V(G)$ as vertex set and $E(G)$ as edge set are considered throughout this study. The degree $d_G(a)$ of a vertex $a$ is the number of vertices adjacent to $a$.

A cactus graph is a connected graph in which no edge lies in more than one cycle. Every cactus graph cycle is chordless, and every cactus graph block is either an edge or a cycle. A cactus graph is said to be triangular if all of its blocks are triangular. A triangular cactus graph is described as a chain triangular cactus if all of its triangles have at most two cut-vertices and each cut-vertex is shared by precisely two triangles. A square cactus graph is a type of cactus graph and all of its blocks are square. A square cactus graph is said to be a chain square cactus if all of its squares have at most two cut-vertices and each cut-vertex is shared by precisely two squares. It’s worth noting that the internal squares’ connections...
to their neighbours may vary. A chain square cactus is called ortho-chain square cactus if the cut-vertices are nearby. A para-chain square cactus is one in which the cut-vertices are not contiguous in a chain square cactus. The Gourava and hyper-Gourava indices of various generic ortho and para cactus chains are studied in this paper, and particular situations such as the triangular chain cactus $T_n$, ortho-chain square cactus $O_n$, and para-chain square cactus $Q_n$ are considered. Latest investigations on several cactus chains can be found in [1, 3, 13, 14] and references cited therein. For undefined terms and notations refer to [5].

The first and second Gourava indices of a molecular graph were introduced by Kulli [6] and are defined as:

$$GO_1(G) = \sum_{ab \in E(G)} [(d_G(a) + d_G(b)) + d_G(a)d_G(b)] ,$$

$$GO_2(G) = \sum_{ab \in E(G)} [(d_G(a) + d_G(b))d_G(a)d_G(b)] .$$

Kulli proposed the first and second hyper-Gourava indices of a molecular graph $G$ in [7], and they are defined as

$$HGO_1(G) = \sum_{ab \in E(G)} [d_G(a) + d_G(b) + d_G(a)d_G(b)]^2 ,$$

$$HGO_2(G) = \sum_{ab \in E(G)} [(d_G(a) + d_G(b))d_G(a)d_G(b)]^2 .$$

Several topological indices were investigated. For further information, see [2, 4, 8, 9, 10, 11, 12].

2. MAIN RESULTS

We look at two types of cactus chains in this section: the para cacti chain and the ortho cacti chain of cycles. We start with a para cacti chain of length $n$ cycles $C_m^n$, where each block is a cycle $C_m$. Let $C_m^n$ be the symbol for it. We compute an exact expression of $GO_1, GO_2, HGO_1$ and $HGO_2$ of $C_m^n$ in the following theorem.

### Table 1. Partitioning at the edge of $C_m^n$.

| $d_{C_m^n}(a), d_{C_m^n}(b)$ : $ab \in E(C_m^n)$ | (2, 2) | (2, 4) |
|-----------------------------------------------|--------|--------|
| Edge count | $mn - 4n + 4$ | $4(n - 1)$ |

**Theorem 2.1.** For a para cacti chain of cycles $C_m^n$ ($m \geq 4$, $n \geq 2$),

1. $GO_1(C_m^n) = 8[3n + 3(n - 1)]$. 

2. \( \text{GO}_2(C^n_m) = 16[mn + 8(n - 1)]. \)
3. \( \text{HGO}_1(C^n_m) = 16[4mn + 33(n - 1)]. \)
4. \( \text{HGO}_2(C^n_m) = 256[mn + 32(n - 1)]. \)

**Proof.** 1. By utilizing the definition of \( \text{GO}_1 \) and entries in Table 1, we have

\[
\text{GO}_1(C^n_m) = \sum_{ab \in E(C^n_m)} [(d_{C^n_m}(a) + d_{C^n_m}(b)) + (d_{C^n_m}(a)d_{C^n_m}(b))] \\
= (mn - 4n + 4)(4 + 4) + 4(n - 1)(2 + 4 + 8) \\
= 8[mn + 3(n - 1)].
\]

2. By making use the definition of \( \text{GO}_2 \) and values in Table 1, we have

\[
\text{GO}_2(C^n_m) = \sum_{ab \in E(C^n_m)} [(d_{C^n_m}(a) + d_{C^n_m}(b))(d_{C^n_m}(a)d_{C^n_m}(b))] \\
= (mn - 4n + 4)(4 \times 4) + 4(n - 1)(6 \times 8) \\
= 16[mn + 8(n - 1)].
\]

3. By the usage of the definition of \( \text{HGO}_1 \) and facts in table 1, we have

\[
\text{HGO}_1(C^n_m) = \sum_{ab \in E(C^n_m)} [(d_{C^n_m}(a) + d_{C^n_m}(b)) + (d_{C^n_m}(a)d_{C^n_m}(b))]^2 \\
= (mn - 4n + 4)(4 + 4)^2 + 4(n - 1)(6 + 8)^2 \\
= 16[4mn + 33(n - 1)].
\]

4. By using the concept of \( \text{HGO}_2 \) as well as the data in Table 1, we have

\[
\text{HGO}_2(C^n_m) = \sum_{ab \in E(C^n_m)} [(d_{C^n_m}(a) + d_{C^n_m}(b))(d_{C^n_m}(a)d_{C^n_m}(b))]^2 \\
= (mn - 4n + 4)(4 \times 4)^2 + 4(n - 1)(6 \times 8)^2 \\
= 256[mn + 32(n - 1)].
\]

□

The graph \( Q_n \) is pictured in Figure 1.

**Corollary 2.2.** For a para-chain square cactus graph \( Q_n(n \geq 2) \),

1. \( \text{GO}_1(Q_n) = 8(7n - 3). \)
Figure 1. The graph $Q_n$.

2. $GO_2(Q_n) = 3n^3 + 9n^2 + 60n$.
3. $HGO_1(Q_n) = 16(49n - 33)$.
4. $HGO_2(Q_n) = 1024(9n - 8)$.

Proof. Replace $m = 4$ in Theorem 2.1 to complete the proof. □

The graph $L_n$ is indicated in Figure 2.

Figure 2. The graph $L_n$.

Corollary 2.3. For a para-chain hexagonal cactus graph $L_n (n \geq 3)$,
1. $GO_1(L_n) = 24(3n - 1)$.
2. $GO_2(L_n) = 32(7n - 4)$.
3. $HGO_1(L_n) = 16(57n - 33)$.
4. $HGO_2(L_n) = 512(19n - 16)$.

Proof. We get the required outcome if we set $m = 6$ in the Theorem 2.1. □

The ortho-chain cacti of cycles with neighbouring cut-vertices is now considered. Let $CO_m^n$ be an ortho-chain cactus graph, where $m$ is the cycle length and $n$ is the chain length. $|V(CO_m^n)| = mn - n + 1$ and $|E(CO_m^n)| = mn$ are self-evident. $GO_1$, $GO_2$, $HGO_1$ and $HGO_2$ of $CO_m^n$ are obtained by utilizing the following theorem.

Table 2. Partitioning at the edge of $CO_m^n$.

| $d_{CO_m^n}(a), d_{CO_m^n}(b) : ab \in E(CO_m^n)$ | (2, 2) | (2, 4) | (4, 4) |
|----------------|--------|--------|--------|
| Edge count     | $mn - 3m + 2$ | $2n$   | $n - 1$ |

Theorem 2.4. For a ortho cacti chain of cycles $CO_m^n (m \geq 3, n \geq 2)$,
1. $GO_1(CO_m^n) = 8mn - 24m + 52n - 8$. 
2. \( GO_2(CO^n_m) = 16mn - 48m + 224n - 96. \)
3. \( HGO_1(CO^n_m) = 64mn - 192m + 968n - 448. \)
4. \( HGO_2(CO^n_m) = 256mn - 768m + 20992n - 15872. \)

**Proof.**

1. By using the concept of \( GO_1 \) as well as the data in Table 2, we have

\[
GO_1(CO^n_m) = \sum_{ab \in E(CO^n_m)} \left[ (d_{CO^n_m}(a) + d_{CO^n_m}(b)) + (d_{CO^n_m}(a)d_{CO^n_m}(b)) \right]
\]

\[
= (mn - 3m + 2)(4 + 4) + 2n(6 + 8) + (n - 1)(8 + 16)
\]

\[
= 8mn - 24m + 52n - 8.
\]

2. By making use the definition of \( GO_2 \) and values in Table 2, we have

\[
GO_2(CO^n_m) = \sum_{ab \in E(CO^n_m)} \left[ (d_{CO^n_m}(a) + d_{CO^n_m}(b)) + (d_{CO^n_m}(a)d_{CO^n_m}(b)) \right]
\]

\[
= (mn - 3m + 2)(4 \times 4) + 2n(6 \times 8) + (n - 1)(8 \times 16)
\]

\[
= 16mn - 48m + 224n - 96.
\]

3. By utilizing the description of \( HGO_1 \) and entries in Table 2, we have

\[
HGO_1(CO^n_m) = \sum_{ab \in E(CO^n_m)} \left[ (d_{CO^n_m}(a) + d_{CO^n_m}(b)) + (d_{CO^n_m}(a)d_{CO^n_m}(b)) \right]^2
\]

\[
= (mn - 3m + 2)(4 + 4)^2 + 2n(6 + 8)^2 + (n - 1)(8 + 16)^2
\]

\[
= 64mn - 192m + 968n - 448.
\]

4. By the usage of the definition of \( HGO_2 \) and facts in table 2, we have

\[
HGO_2(CO^n_m) = \sum_{ab \in E(CO^n_m)} \left[ (d_{CO^n_m}(a) + d_{CO^n_m}(b)) + (d_{CO^n_m}(a)d_{CO^n_m}(b)) \right]^2
\]

\[
= (mn - 3m + 2)(4 \times 4)^2 + 2n(6 \times 8)^2 + (n - 1)(8 \times 16)^2
\]

\[
= 256mn - 768m + 20992n - 15872.
\]

\( \square \)

Then, as illustrated in Figure 3, we consider a chain triangular cactus, designated by \( T_n \), where \( n \) is the length of the \( T_n \). For \( m = 3 \), \( T_n \) is a special case of \( CO^n_m \).
Corollary 2.5. For a chain triangular cactus $T_n$ ($n \geq 2$),
1. $GO_1(T_n) = 76n - 80$.
2. $GO_2(T_n) = 272n - 240$.
3. $HGO_1(T_n) = 1160n - 1024$.
4. $HGO_2(T_n) = 21760n - 18176$.

Proof. Replace $m = 3$ in Theorem 2.4 to complete the proof. □

By identifying every node of $K_m$ with a node of one $K_y$, the graph $Q(m, y)$ is formed from $K_m$ and $m$ copies of $K_y$. $GO_1$, $GO_2$, $HGO_1$ and $HGO_2$ of $Q(m, y)$ are computed in the following theorem. Figure 5 depicts the graph $Q(m, y)$.

Table 3. Partitioning at the edge of $Q(m, y)$.

| $d_{Q(m,y)}(a), d_{Q(m,y)}(b) : ab \in E(Q(m,y))$ | Edge count |
|-------------------------------------------------|------------|
| $(y - 1, y - 1)$                                 | $\frac{m(y-1)(y-2)}{2}$ |
| $(y - 1, m + y - 2)$                             | $m(y - 1)$ |
| $(m + y - 2, m + y - 2)$                         | $\frac{m(y-1)}{2}$ |

Theorem 2.7. For an ortho-chain $Q(m, y)$ ($m, y \geq 2$),
1. $GO_1(Q(m, y)) = \frac{m(y-1)(y-2)(y^2-1)}{2} + m(y-1)(y^2 + ym - y - 1)$

2. $GO_2(Q(m, n)) = m(y - 1)^4(y - 2) + m(y - 1)[(2y^2 - 9y + 13) + m(5 - m) + m(y - 1)(m + y - 2)^3]$.

3. $HGO_1(Q(m, y)) = \frac{m(y-1)(y-2)(y^2-1)}{2} + m(y-1)(y^2 + ym - y - 1)^2$

4. $HGO_2(Q(m, y)) = 2m(y - 1)[(y - 1)^6(y - 2) + (m + y - 2)^6] + m(n - 1)[(m + 2y - 3)(y - 1)(m + y - 2)]^2$.

Proof. 1. By using the concept of $GO_1$ as well as the data in Table 3, we have

$$GO_1(Q(m, y)) = \sum_{ab \in E(Q(m, y))} [(d_{Q(m,y)}(a) + d_{Q(m,y)}(b)) + (d_{Q(m,y)}(a)d_{Q(m,y)}(b))]$$

$$= \frac{m(y-1)(y-2)(y^2-1)}{2} + m(y-1)(y^2 + ym - y - 1)$$

$$+ \frac{m(y-1)(m+y-2)(m+y)}{2}.$$

2. By utilizing the description of $GO_2$ and entries in Table 3, we have

$$GO_2(Q(m, n)) = \sum_{ab \in E(Q(m,n))} [(d_{Q(m,y)}(a) + d_{Q(m,y)}(b)) (d_{Q(m,y)}(a)d_{Q(m,y)}(b))]$$

$$= m(y - 1)^4(y - 2) + m(n - 1)[(2y^2 - 9y + 13) + m(5 - m) + m(y - 1)(m + y - 2)^3].$$

3. By the usage of the definition of $HGO_1$ and facts in Table 3, we have
$$HGO_1(Q(m, y)) = \sum_{a \in E(Q(m, y))} \left[(dQ(m, y)(a) + dQ(m, y)(b)) + (dQ(m, y)(a)dQ(m, y)(b))\right]^2$$

$$= \frac{m(y - 1)(y - 2)(y^2 - 1)}{2} + m(y - 1)(y^2 + ym - n - 1)^2 + m(y - 1)(m + y - 2)(m + y)^2.$$

4. By making use the definition of $HGO_2$ and values in Table 3, we have

$$HGO_2(Q(m, y)) = \sum_{a \in E(Q(m, y))} \left[(dQ(m, y)(a) + dQ(m, y)(b))(dQ(m, y)(a)dQ(m, y)(b))\right]^2$$

$$= 2m(y - 1)^2(y - 2) + m(y - 1)[(m + 2y - 3)(y - 1)(m + y - 2)]^2 + 2m(y - 1)(m + y - 2)^6.$$
Proof. 1. By making use the definition of $GO$ and values in Table 4, we have

$$
GO_1(W^m_n) = \sum_{ab \in E(W^m_n)} [(d_{W^m_n}(a) + d_{W^m_n}(b)) + (d_{W^m_n}(a)d_{W^m_n}(b))]
$$

$$
= (mn - 4n + 4)[6 + 9] + 4(n - 1)[9 + 18] + (mn - 2n + 2)[3 + m + 3m] + 2(n - 1)[6 + m + 6m]
$$

$$
= 4m^2n + 24mn + 54n - 6m - 54.
$$

2. By the usage of the definition of $GO_2$ and facts in Table 4, we have

$$
GO_2(W^m_n) = \sum_{ab \in E(W^m_n)} [(d_{W^m_n}(a) + d_{W^m_n}(b))(d_{W^m_n}(a)d_{W^m_n}(b))]
$$

$$
= (mn - 4n + 4)[6 + 9] + 4(n - 1)[9 	imes 18] + (mn - 2n + 2)[3 + m + 3m] + 2(n - 1)[6 + m + 6m]
$$

$$
= 3m^3n + 15m^2n - 6m^2 + 108mn + 432n - 54m - 432.
$$

3. By using the expression for $HGO_1$ and data in Table 4, we have

$$
HGO_1(W^m_n) = \sum_{ab \in E(W^m_n)} [(d_{W^m_n}(a) + d_{W^m_n}(b)) + (d_{W^m_n}(a)d_{W^m_n}(b))]^2
$$

$$
= (mn - 4n + 4)[6 + 9]^2 + 4(n - 1)[9 + 18]^2 + (mn - 2n + 2)[3 + m + 3m]^2 + 2(n - 1)[6 + m + 6m]^2
$$

$$
= 16m^3n + 54mn + 2070n + 90m^2n - 66m^2 - 120m - 2070.
$$

4. By utilizing the description of $HGO_2$ and entries in Table 4, we have

$$
HGO_2(W^m_n) = \sum_{ab \in E(W^m_n)} [(d_{W^m_n}(a) + d_{W^m_n}(b))(d_{W^m_n}(a)d_{W^m_n}(b))]
$$

$$
= (mn - 4n + 4)[6 + 9]^2 + 4(n - 1)[9 	imes 18]^2 + (mn - 2n + 2)[3 + m + 3m]^2 + 2(n - 1)[6 + m + 6m]^2
$$

$$
= 9mn^5 + 108mn^4 + 837nm^3 + 2430nm^2 - 72m^4 - 864m^3 - 2592m^2
$$

$$
+ 2916mn + 93312n - 93312.
$$

□

3. COMPARATIVE ANALYSIS

The plotting of $GO_1$, $GO_2$, $HGO_1$ and $HGO_2$ for the cactus graphs are shown in Figures 7 and 8. We have built the figures using Origin software taking $m=4$. $GO_1(C^n_m)$, $GO_1(C^{mn}_m)$, $GO_1(CO^n_m)$, $GO_1(W^n_m)$, $GO_2(C^{mn}_m)$, $GO_2(CO^n_m)$, $GO_2(W^n_m)$, $HGO_1(C^n_m)$, $HGO_1(C^{mn}_m)$, $HGO_1(CO^n_m)$, $HGO_1(W^n_m)$, $HGO_2(C^{mn}_m)$, $HGO_2(CO^n_m)$, $HGO_2(W^n_m)$.
and $HGO_2(W_n^m)$ are linearly increasing and $GO_1(Q(m,y))$, $GO_2(Q(m,y))$, $HGO_1(Q(m,y))$ and $HGO_2(Q(m,y))$ are exponentially increasing.

4. CONCLUDING REMARKS

In this paper, para cactus chain, ortho cactus chain and wheel cactus chain are discussed and explicit expressions of $GO_1$, $GO_2$, $HGO_1$ and $HGO_2$ are derived for them.

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