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Introducing New Exponential Gourava Indices for Graphs

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Abstract. *We state first and second Gourava indices of a molecular Graph. We then introduce Exponential of first and second Gourava indices. In this paper we compute the stated indices for some generalized graphs along with Hypercube and Wheel Graph.*
Keywords: *Molecular graph, Gourava indices, Gourava, Exponential Gourava indices, Wheel Graph, Hypercube Graphs*

I. Introduction and Preliminaries

Let G be a simple and connected graph with vertex set V(G) = {v_1, v_2, . . ., v_n} and edge set E(G) such that |E(G)| = m. If any two vertices u, v ∈ V(G) are adjacent with an edge, they are denoted by uv ∈ E(G). Degree of any vertex v ∈ V(G) is the number of edges that are incident to v and denoted by $deg_G(v)$. In this paper, we will generally follow reference for unexplained terminology and notation.

In chemical graph theory, different chemical structures are usually modelled by a molecular graph to understand different properties of the chemical compound theoretically. A graph invariant that correlates the physio-chemical properties of a molecular graph with a number is called a molecular structure index. By use of the adjacency, degree, or distance matrices in graph theory, one can describe the structure of molecules in chemistry-Vertex Degree based topological indices and distance based topological indices [5,6,8,9,10]. Application of molecular structure indices are a standard procedure in structure-property relations. [1,7] and certain other properties in [11,12,13].

The first and second Zagreb indices, first appeared in a topological formula for the total π-energy of conjugated molecules, were introduced by Gutman et al. in [1].
These indices have been used as branching indices. The Zagrebindices have found applications in QSPR[2] and QSAR[3] studies.
The First and Second Zagreb Indices of Graphs are defined as follows:

$$M_1(G) = \sum_{uv\in G}[d_G\,(u) + d_G\,(v)] \qquad , \qquad M_2(G) = \sum_{uv\in G}[d_G\,(u).\,d_G\,(v)]$$

Motivated by the definitions of the Zagreb indices and their wide applications,
V.R Kulli introduced the first and Second Gourava index of a molecular graph in [2] as follows:

$$GO_1(G) = \sum_{uv\in G}[\{d_G\,(u) + d_G\,(v)\} + d_G\,(u).\,d_G\,(v)],$$
$$GO_2(G) = \sum_{uv\in G}[\{d_G\,(u) + d_G\,(v)\}.\,d_G\,(u).\,d_G\,(v)]$$

Rada [3] has recently introduced a function of exponential topological indices as for a vertex-degree-based index and also has studied Randic's exponential index over the set of graphs with non isolated vertices. Furthermore, by using the same approximation, Cruz and Rada [4] have investigated extremal tree graphs for exponential first and second Zagreb indices except maximal tree graph of exponential second Zagreb index. Other exponential indices are as discussed in
Inspired by the above stated work we define Exponential of first Gourava index and Exponential of second index as follows:

$$EGO_1(G) = \sum_{uv\in G} e^{[\{d_G\,(u)+d_G\,(v)\}+d_G\,(u).d_G\,(v)]} ,$$

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2. QSPR - Quantitative structure-property relationship
3. QSAR - Quantitative structure-activity relationship

$EGO_2(G) = \sum_{uv \in G} e^{[\{d_G(u)+d_G(v)\}.d_G(u).d_G(v)]}$

Gourava and Exponential of Gourava indices for various types of Graphs.

Proposition 1. Let G = C_n be a cycle of vertices n≥3, Then$GO_1(G)$ =8n and $GO_2(G)$=16n
Proof:$GO_1(G) = n\,[\,(2+2)+2.2]$=8n
$GO_2(G) = n\,[\,(2+2).\,2.2]$=16n

Result 1. For G = Cn, $EGO_1(G)$ =ne^8 , $EGO_2(G)$= ne^{16}
Proof:$EGO_1(G) = ne^{[(2+2)+2.2]}$= n$e^8$
$EGO_2(G) = ne^{[(2+2).2.2]}$ = ne^{16}

Proposition 2. Let G = Kn be a complete graph of n≥2, Then
$GO_1(G) = \frac{1}{2}n(n+1)(n-1)^2$, $GO_2(G) = n(n-1)^4$
Proof: Let Kn be a complete graph with n vertices, then it has $\frac{n(n-1)}{2}$ edges

$$GO_1(G) = \frac{n(n-1)}{2}[\,(n-1)+(n-1)) + (n-1).(n-1)]$$

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

Result 2. For Kn, $EGO_1(G) = \frac{n(n-1)}{2}e^{n^2-1}$ and $EGO_2(G) = \frac{n(n-1)}{2}e^{(n-1)^3}$
Proof:$EGO_1(G) = \frac{n(n-1)}{2}e^{(n-1)+(n-1)+(n-1)(n-1)}$
=$\frac{n(n-1)}{2}e^{2(n-1)+(n-1)^2}$
=$\frac{n(n-1)}{2}e^{(n-1)(2+n-1)}$
= $\frac{n(n-1)}{2}e^{(n-1)(n+1)}$
=$\frac{n(n-1)}{2}e^{n^2-1}$

$$EGO_2(G) = \frac{n(n-1)}{2}e^{[((n-1)+(n-1)).(n-1)(n-1)]}$$
$$= \frac{n(n-1)}{2}e^{[2(n-1).(n-1)(n-1)]}$$

= $\frac{n(n-1)}{2}e^{(n-1)^3}$

Proposition 3. Let G = $K_{m,n}$be a complete bipartite graph with 1≤m≤n, Then
$GO_1(G) = mn(m+n+mn)$, $GO_2(G) = m^2n^2(m+n)$
Proof: Let Km, nbe a complete bipartite graph with 1≤m≤n.
Km, nhas (m+n) vertices and mn edges. The vertices can be divided into 2 sets such that │V1│=m, │V2│=n, V1UV2=V, clearly every vertex of V1 is adjacent with n vertices and every vertex of V2 is adjacent with m vertices.
Then $GO_1(G) = mn(m+n+mn)$
and $GO_2(G) = mn[(m+n).mn]$
=$m^2n^2(m+n)$

Result 3. For complete bipartite graph Km, n
$EGO_1(G) = mne^{(m+n+mn)}$, $EGO_2(G) = mne^{((m+n).mn)}$
Proof: Let Km, nbe a complete bipartite graph with 1≤m≤n
Km, n has(m+n) vertices and mn edges. The vertices can be divided into 2 sets such that │V_1│=m, │V_2│=n, V_1UV_2, clearly every vertex of V1 is adjacent with n vertices and every vertex of V2 is adjacent with m vertices.

$$EGO_1(G) = mne^{(m+n+mn)}$$
$$EGO_2(G) = mne^{((m+n).mn)}$$

Proposition 4. Let G be a r-regular Graph with n vertices. Then
$GO_1(G) = \frac{nr^2}{2}(2+r)$, $GO_2(G) = nr^4$

Proof: If G is a regular graph with n vertices, it has nr/2 edges. The degree of each vertex is 'r', then

$$GO_1(G) = \frac{nr}{2}[(r+r)+r.r]$$
$$= \frac{nr}{2}[2r+r^2]$$
$$= \frac{nr^2}{2}(2+r)$$
$$GO_2(G) = \frac{nr}{2}[(r+r).r.r]$$
$$= \frac{nr}{2}[2r.r^2]$$
$$= nr^4$$

Result 4: For a Hypercube Graph G = Qn, $EGO_1(G) = \frac{n.2^n}{2}e^{2n+n^2}$,$EGO_2(G) = \frac{n.2^n}{2}e^{2n^3}$

Proof: Q_n is a n-regular graph with 2^n vertices So using the formula in proof of proposition 4 for no. of edges of a regular graph, we get no. of edges in a hypercube = $\frac{n.2^n}{2}$.

So $GO_1(G) = \frac{n.2^n}{2}[(n+n)+n.n]$

$$= \frac{n.2^n}{2}[2n+ n^2]$$
$$= \frac{n^2.2^n}{2}(n+2)$$

And $GO_2(G) = \frac{n.2^n}{2}[(n+n).n.n]$

$$= \frac{n.2^n}{2}[2n.n^2]$$

Based on the similar lines the Exponential Gourava Indices are computed to be

$$EGO_1(G) = \frac{n.2^n}{2}e^{[(n+n)+n.n]}$$
$$= \frac{n.2^n}{2}e^{[2n+n^2]}$$

And

$$EGO_2(G) = \frac{n.2^n}{2}e^{[(n+n).n.n]}$$
$$= \frac{n.2^n}{2}e^{[2n.n^2]}$$
$$= \frac{n.2^n}{2}e^{2n^3}$$

Result 5: For a Path graph G = P_n, The Indices are as follows:

$GO_1(G)$ = 8n-14, $GO_2(G)$=16n-36

$EGO_1(G) = 2e^3 + (n-3)e^8$, $EGO_2(G) = 2e^6 + (n-3)e^{16}$

Proof: Let P_n be a Path Graph with n≥3 vertices, then no. of edges of a path graph are (n-1).

Now out of these (n-1) edges, vertices ofthe 2 terminal edges have vertex degree 1 and 2 respectively each and the vertices of remaining (n-3) edges have vertex degree 2 each.

Then $GO_1(G)$ = 2[(1+2) +1.2] +(n-3) [(2+2) +2.2]

=2[3+2] +(n-3) (8)

=10+8n-24

=8n-14

$GO_2(G)$ = 2[(1+2).1.2] +(n-3) [(2+2).2.2]

=2 (6) +(n-3) (16)

=12+16n-48

=16n-36

$EGO_1(G) = 2e^{[(1+2)+1.2]} + (n-3)e^{[(2+2)+2.2]}$

$$= 2e^3 + (n-3)e^8$$

$EGO_2(G) = 2e^{[(1+2).1.2)]} + (n-3)e^{[(2+2).2.2]}$

$$= 2e^6 + (n-3)e^{16}$$

Result 6: For a Wheel graph G = W_n, The Indices are as follows:

$GO_1(G)$=$(n-1)(4n+14)$, $GO_2(G)$ =3(n-1)(n^2+n-16)

$EGO_1(G)$=(n-1)$e^{15}+(n-1)e^{4n-1}$, $EGO_2(G)$=(n-1)$e^{54}+(n-1)e^{3n^2+3n-6}$

Proof: A wheel graph is a graph formed by connecting a single universal vertex to all vertices of a cycle (a universal vertex is a vertex of an undirected graph that is adjacent to all other vertices of the graph.)

As Shown in Fig 1 is W_9 which is made from C_8 and a universal vertex.

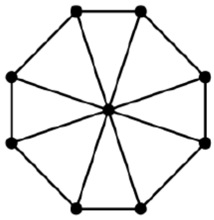

Fig 1

so, a Wheel Graph of n vertices consists of a cyclic graph of (n-1) vertices along with 1 universal vertex. It has 2(n-1) edges which can be divided into 2 sets.(n-1) edges of the cyclic part and rest (n-1) edges which are connected to the universal vertex.

Now vertices of (n-1) edges of the cyclic part have vertex degree 3 each and the vertices of remaining(n-1) edges has vertex degree of 3 and (n-1) respectively.

$GO_1(G)$ =(n-1) [$(3+3)+3.3$]+(n-1) [3+(n-1)+3. (n-1)]
=(n-1)15+(n-1) [n+2+3n-3]
=(n-1)15+(n-1) (4n-1)
= (n-1) [15+4n-1]
=(n-1) (4n+14)

$GO_2(G)$ =(n-1) [$(3+3).3.3$]+(n-1) [{(3+(n-1)}.3. (n-1)]

=(n-1) 54+(n-1) [(2+n). (3n-3)]

=(n-1)54+3$(n-1)^2(n+2)$

=(n-1) [54+3(n-1) (n+2)]

=3(n-1) (n^2+n-16)

$EGO_1(G)$=(n-1)$e^{[(3+3)+3.3]}+(n-1)e^{[(3+(n-1))+3.(n-1)]}$
=(n-1)$e^{15}+(n-1)e^{[n+2+3n-3]}$
=(n-1)$e^{15}+(n-1)e^{4n-1}$

$EGO_2(G)$=(n-1)$e^{[(3+3).3.3]}+(n-1)e^{[(3+(n-1)).3.(n-1)]}$
=(n-1)$e^{54}+(n-1)e^{(2+n).(3n-3)}$
=(n-1)$e^{54}+(n-1)e^{3n^2+3n-6}$

II. Conclusion:

New exponential indices i.e., Gourava exponential indices of various graphs have been computed for several well-known graphs. This study holds the scope of the real-life applications of the index. Few other functions of the indices (just like the exponential function) can also be computed. The same index can be calculated for various other graphs.

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