Computation of edge-based topological indices for zero divisor graphs of commutative rings

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Abstract. Graph constructing algorithms and their mapping with real life problems for scientific data analysis are getting popular. Standard algorithms construct the graph in a way that it can deal with all possibilities of input data to calculate the desired output. This article gives an algorithmic computational model for edge based eccentric topological indices by constructing zero divisor graph containing finite rings as $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ and $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$, where p, p_1, p_2 and q are primes numbers. At first algorithm classify vertices with common eccentricity and then computes first Zagreb, third Zagreb, geometric-arithmetic, atom-bond connectivity and harmonic index for zero divisor graphs containing commutative rings. Results of algorithms are verified using mathematical formulation so algorithm can be reuse or modify for applications of coding theory, algebraic cryptography, ICT, biology and chemistry easily.

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1. Introduction

Graphs structures as powerful tool of formal science is facilitating the deep and innovative research in pure sciences, particularly in the field of chemistry and biology. This strong relation of graph theory with pure sciences has evolved interdisciplinary fields like molecular graph theory and biological networks. Many other practical problems can be represented and solved using graphs by emphasizing their applications in real world. Chemical graph theory incorporate, investigation of particles and atoms where graph structures are used to model pair wise relationship between objects. In last two decades many graph invariants have been studied and used for correlation analysis in theoretical chemistry, pharmacology, toxicology, and environmental chemistry [10].

Topological index is a numerical parameter of a graph which characterize it's topology and considered as a graph invariant. In the study of chemical graph theory, topological indices are used in the development of quantitative structure-activity relationship (QSARs) in which the properties of molecules are correlated [7, 9]. A variety of topological indices are available and have application in chemical graph theory , computer networks, statistics, physics, robotics and biological networks [22].

Topological indices can be classified as "degree based topological indices" [1, 21] and "distance based topological indices" [28, 13] on the basis of their dealing with degree of vertices or distance between the vertices. Some well-known degree based topological indices are Zagreb indices [19], atom bond connectivity [15] , geometric arithmetic index [20] , Randi connectivity index [23], Harmonic index [24] and sum connectivity index. Similarly distance based topological indices are Wiener index, Hosaya index, the energy and Estrada index [28, 27].

Group and ring theory have been studied extensively for their close relationship with algebra, number theory and representation theory but also for their applications to other areas [6, 11]. Finite commutative rings is a part of group and ring theory. Now a days, finite commutative rings gain importance in many fields like algorithm analysis, engineering, combination theory, cryptography, coding theory, wireless communications, graph and iterative coding, data analysis and modeling, and finite geometry. Zero divisor graph is one of the important finite commutative rings [5, 6].

Topological indices as molecular descriptors have achieved an important place in the field of chemistry, pharmaceutical science. Moreover these indices have wide applications in nanotube structures [7, 9, 22]. Analysis of topological indices for a particular graph helps us to understand graph characteristics, their similarities and their differences with respect to the other graphs. Topological indices guide us that how the chemical structure can further grow and what mathematical operations on the graphs with the help of topological indices can extend multidisciplinary research.

2. Definitions and notations

For a connected graph G with vertex and edge sets $V(G)$ and $E(G)$ respectively, a numerical quantity that is invariant under graph automorphisms is called topological index or topological descriptor. For a graph G the degree of a vertex v is the number of edges incident with v and is denoted by $d(v)$. The maximum degree of a graph G, denoted by $\Delta(G)$, and the minimum degrees of a graph, denoted by $\delta(G)$. The distance between any two vertices u and v is denoted by $d(u, v)$ and is defined as the number of edges in a shortest path connecting them. Mathematical definition of eccentricity is:

$$\varepsilon_u = \max\{d(u, v) : v \in V(G)\}. \tag{1}$$

Zagreb indices and their variants are useful molecular descriptors which found considerable use in QSPR and QSAR studies as summarized by Todeschini and Consonni [25]. In an analogy with the first and the second Zagreb indices, Vukičević and Graovac [26] and Ghorbani and Hosseinzadeh [19] introduced two types of Zagreb eccentricity indices that are defined as: The first Zagreb eccentricity index of G is

$$M_1^*(G) = \sum_{uv\in E(G)} (\varepsilon_u + \varepsilon_v). \tag{2}$$

The third Zagreb eccentricity index of G is

$$M_3^*(G) \sum_{uv\in E(G)} (\varepsilon_u \times \varepsilon_v). \tag{3}$$

In 2010, Ghorbani and Khaki [20], defined the geometric-arithmetic eccentric index $GA_4(G)$ as follows:

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon_u \times \varepsilon_v}}{\varepsilon_u + \varepsilon_v}. \tag{4}$$

The atom-bond connectivity eccentric index $ABC_5(G)$ defined by Farahani [16] as follows:

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{\varepsilon_u + \varepsilon_v - 2}{\varepsilon_u \times \varepsilon_v}}. \tag{5}$$

In 2017 Farahani, Ediz and Imran [17] and Gao, Ediz, Farahani and Imran [18] in 2018 defined the the fourth type of eccentric harmonic index $H_4(G)$ as:

$$H_4(G) = \sum_{uv\in E(G)} \frac{2}{\varepsilon_u + \varepsilon_v}. \tag{6}$$

Let R be a commutative ring with identity and $Z(R)$ is the set of all zero divisors of R. $G(R)$ is said to be a zero divisor graph if $x, y \in V(G(R)) = Z(R)$ and $(x, y) \in E(G(R))$ if and only if $x.y = 0$. Beck [11] introduced the notion of zero divisor graph. Anderson and Livingston [5] proved that $G(R)$ is always connected if R is commutative. For a graph G, the concept of graph parameters have always a high interest. Numerous authors briefly studied the zero-divisor and total graphs from commutative rings [3, 4, 6].

3. Method and results

While solving a problem, choosing the correct and optimum method is basic key to attain the desired solution. In mathematics one of the captivating technique for solving any problem is algorithmic approach [8]. Algorithmic solution not only compute mathematical solution rather it leads the study to apply those algorithms in future applications addressing the same problem. *Algorithm* is a well specified set of computational procedure that transforms the input to desired output. Algorithms can perform calculation, data processing, and automated reasoning tasks related to computer and mathematical operations [12]. In this article algorithm is designed to compute edge based eccentric topological indices by constructing zero divisor graph containing finite rings for two cases that are $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ and $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$. Algorithms only takes three prime integers as input and computes first Zagreb, third Zagreb, geometric-arithmetic, atom-bond connectivity and harmonic index for zero divisor graphs. During algorithm designing a great care is taken on accuracy of the results as well as efficiency of the algorithm.

3.1 Algorithms

Input: Three prime numbers a, b and c.
Output: Edge-based eccentric topological indices.

Algorithm 1 calculateTopologicalIndices (a, b, c)

createGraphSets (a,b,c)
$firstZagreb \leftarrow 4 \times EccEdges1 + 5 \times EccEdges2$
$thirdZagreb \leftarrow 4 \times EccEdges1 + 6 \times EccEdges2$
$GA \leftarrow 2 \times EccEdges1 + 2 \times \sqrt{6/5} \times EccEdges2$
$ABC5 \leftarrow \sqrt{1/2} \times EccEdges1 + \sqrt{1/2} \times EccEdges2$
$harmonic \leftarrow 1/2 \times EccEdges1 + 2/5 \times EccEdges2$

Input: Three prime numbers a, b and c.
Output: All possible vertex sets of zero divisor graph with eccentricity of each set.

Algorithm 2 createGraphSets (a,b,c)

```
for i ← 0 to a × b
  for j ← 0 to c
    if (i ≠ 0 OR j ≠ 0)
     if (a ≠ b)
         if (i mod a ≠ 0 AND i mod b ≠ 0 AND i ≠ 0 AND j = 0)
           D[di] ← AddPoint(i, j)
         else if (i = 0 AND j ≠ 0)
           A[ai] ← AddPoint(i, j)
         else if (i mod a = 0)
             if (j = 0)
               B[bi] ← AddPoint(i, j)
             else
               E[ei] ← AddPoint(i, j)
         else if (i mod b = 0)
             if (j ≠ 0)
               F[fi] ← AddPoint(i, j)
             else
               C[ci] ← AddPoint(i, j)
     else
         if (i mod a ≠ 0 AND i ≠ 0 AND j = 0)
           D[di] ← AddPoint(i, j)
         else if (i = 0 AND j ≠ 0)
           A[ai] ← AddPoint(i, j)
         else if (i mod a = 0)
             if (j = 0)
               B[bi] ← AddPoint(i, j)
             else
               C[ci] ← AddPoint(i, j)
if (a ≠ b)
      EccEdges1 ← ai × bi + ai × ci + bi × ci
      EccEdges2 ← ai × di + bi × fi + ci × ei
else
      EccEdges1 ← ai × bi
      EccEdges2 ← ai × di + bi × ci
return EccEdges1, EccEdges2
```

4. Verification of algorithmic results

For any two positive integers a and b, where $G(R)$ be a zero divisor graph containing commutative ring $R = \mathbb{Z}_a \times \mathbb{Z}_b$ with vertex set $V(G(R))$ and edge set $E(G(R))$ then $V(G(R)) = \{(x, y) \in R : x|a \text{ or } y|b \text{ or } x = 0 \text{ or } y = 0\} \setminus \{(0, 0)\}$

and $E(G(R)) = \big\{\big((x_1,y_1),(x_2,y_2)\big) \in V(G(R)) \times V(G(R)) : (x_1x_2, y_1y_2) = (0,0) \text{ in } R\big\}$.

4.1 Case 1: $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$

For $a = p^2$ and $b = q$, where p, q are prime numbers. Let G_1 be a zero divisor graph containing commutative ring $R = \mathbb{Z}_{p^2} \times \mathbb{Z}_q$. From [2], we obtain $\vee_t(G_1)$ with $t = p-1, q-1, p^2-1, pq-2$ and $|\vee_{p-1}| = (p-1)(q-1)$, $|\vee_{q-1}| = p(p-1)$, $|\vee_{p^2-1}| = q-1$, $|\vee_{pq-2}| = p-1$. By hand shaking lemma $|E(G_1)| = \frac{(p-1)(4pq-3p-2)}{2}$.

Let $\Xi_{r,s} = \{uv \in E(G_1) : \varepsilon_u = r, \varepsilon_v = s\}$ be the set contain the edges with endpoints has the eccentricity r and s. From the above discussion, we have $|\Xi_{2,2}| = \frac{(p-1)(p+2q-4)}{2}$, $|\Xi_{2,3}| = (p-1)(q-1)(2p-1)$. Mathematical formulation of above edge-based eccentric topological indices can be represent for graph G_1 in the following theorem.

Theorem 4.1. *For p, q be prime numbers. Let G_1 be the zero divisor graph containing commutative ring $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$, then First Zagreb eccentric index of G_1,*

$$M_1^*(G_1) = (p-1)(10pq - 8p - q - 3)$$

the third Zagreb eccentric index

$$M_3^*(G_1) = 2(p-1)(6pq - 5p - q - 1)$$

the geometric-arithmetic eccentric index

$$GA_4(G_1) = (p-1)\left(\frac{p+2q-4}{2} + \frac{2\sqrt{6}}{5}(2p-1)(q-1)\right)$$

the atom-bond connectivity eccentric index

$$ABC_5(G_1) = \frac{1}{\sqrt{2}}|E(G_1)|$$

the fourth type of eccentric harmonic index

$$H_4(G_1) = \frac{p-1}{20}\left(16pq - 11p + 2q - 12\right).$$

Proof. By putting $|\Xi_{2,2}| = \frac{(p-1)(p+2q-4)}{2}$, $|\Xi_{2,3}| = (p-1)(q-1)(2p-1)$ in equations (2), (3), (4), (5) and (6), we obtain the required results. □

For verification purpose algorithmic results are compared by substituting some instances of the values of $a = p^2$ and $c = q$ in Theorem 4.1. It is observed that both results are same that proves the accuracy of algorithm. Some of the results are are given in Table 1 for sake of computing fidelity and their use in future applications.

Table 1: Algorithmic results of edge-based topological indices for zero divisor graph with $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$

		Algorithmic Results				
$a = p^2$	$c = q$	1^{st}-Zagreb	3^{rd}-Zagreb	GA	ABC_5	Harmonic
2	3	38	44	7.879	5.657	3
3	5	232	272	47.192	33.941	20
5	7	1176	1392	235.636	169.706	98
7	11	4140	4920	824.241	593.970	342
11	13	13080	15600	2589.086	1866.762	1068
11	7	6540	7800	1294.543	933.381	534
13	5	6192	7392	1223.755	882.469	504
17	5	10816	12928	2133.329	1538.664	876
19	3	6804	8136	1341.088	967.322	550
23	3	10076	12056	1983.996	1431.184	814

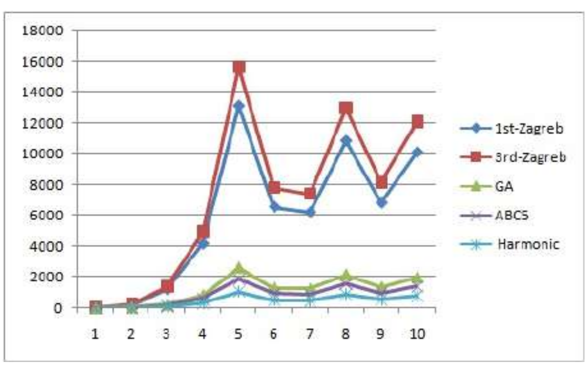

Figure 1: Pictorial representation of Table 1 results.

4.2 Case 2: $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$

For $a = p_1p_2$ and $b = q$, where p_1, p_2, q are prime numbers. Let G_2 be a zero divisor graph containing commutative ring $R = \mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$. From [14], we obtain $\vee_t(G_2)$ with $t = p_1p_2 - 1, p_1q - 1, p_2q - 1, q - 1, p_1 - 1, p_2 - 1$ and $|\vee_{p_1p_2-1}| = q-1$, $|\vee_{p_1q-1}| = p_2-1$, $|\vee_{p_2q-1}| = p_1-1$, $|\vee_{q-1}| = (p_1-1)(p_2-1)$, $|\vee_{p_1-1}| = (p_2-1)(q-1)$, $|\vee_{p_2-1}| = (p_1-1)(q-1)$. By hand shaking lemma $|E(G_2)| = 3p_1p_2q - 2p_1p_2 - 2p_1q - 2p_2q + p_1 + p_2 + q$. Let $\Xi_{r,s} = \{uv \in E(G_2) : \varepsilon_u = r, \varepsilon_v = s\}$ be the set contain the edges with endpoints has the eccentricity r and s. From the above discussion, we have $|\Xi_{2,2}| = p_1p_2 + p_1q + p_2q - 2p_1 - 2p_2 - 2q + 3$, $|\Xi_{2,3}| = 3p_1p_2q - 3p_1p_2 - 3p_1q - 3p_2q + 3p_1 + 3p_2 + 3q - 3$. Mathematical formulation of above edge-based eccentric topological indices can be represent for graph G_2 in the following theorem.

Theorem 4.2. *For $p_1 < p_2$ and q be prime numbers. Let G_2 be the zero divisor graph containing commutative ring $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$, then First Zagreb eccentric index of G_2,*

$$M_1^*(G_2) = 15p_1p_2q - 11\,(p_1p_2 + p_1q + p_2q) + 7\,(p_1 + p_2 + q) - 3$$

the third Zagreb eccentric index

$$M_3^*(G_2) = 18p_1p_2q - 14\,(p_1p_2 + p_1q + p_2q) + 10\,(p_1 + p_2 + q) - 6$$

the geometric-arithmetic eccentric index

$$GA_4(G_1) = \frac{6\sqrt{6}}{5}\,(p_1p_2q - 1) + \left(1 - \frac{6\sqrt{6}}{5}\right)(p_1p_2 + p_1q + p_2q) + \left(\frac{6\sqrt{6}}{5} - 2\right)(p_1 + p_2 + q) + 3.$$

the atom-bond connectivity eccentric index

$$ABC_5(G_2) = \frac{1}{\sqrt{2}}|E(G_2)|$$

the fourth type of eccentric harmonic index

$$H_4(G_2) = \frac{6}{5}\,(p_1p_2q) - \frac{7}{10}\,(p_1p_2 + p_1q + p_2q) + \frac{1}{5}\,(p_1 + p_2 + q) + \frac{3}{10}.$$

Proof. By putting $|\Xi_{2,2}| = p_1p_2 + p_1q + p_2q - 2p_1 - 2p_2 - 2q + 3$, $|\Xi_{2,3}| = 3p_1p_2q - 3p_1p_2 - 3p_1q - 3p_2q + 3p_1 + 3p_2 + 3q - 3$ in equations (2), (3), (4), (5) and (6), we obtain the required results. □

For verification purpose algorithmic results are compared by substituting some instances of the values of $a = p_1, b = p_2$ and $c = q$ in Theorem 4.1. It is observed that both results are same that proves the accuracy of algorithm. Some of the results are are given in Table 2 for sake of computing fidelity and their use in future applications.

Table 2: Algorithmic results of edge-based topological indices for zero divisor graph with $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$

			Algorithmic Results				
a	b	c	1^{st}-Zagreb	3^{rd}-Zagreb	GA	ABC_5	Harmonic
2	3	5	176	200	37.515	26.870	16
3	5	5	608	704	126.060	50.912	54
5	7	5	1696	1984	346.181	248.902	147
5	11	7	4096	4816	829.453	596.798	350
7	11	7	6024	7104	1214.180	873.984	510
11	13	7	11808	13968	2368.359	1705.542	990
13	17	5	12736	15040	2561.450	1844.135	1073.6
17	19	5	18976	22432	3810.175	2743.574	1594
19	23	3	13784	16160	2803.995	2016.669	1188
23	29	2	11904	13752	2476.663	1777.666	1072

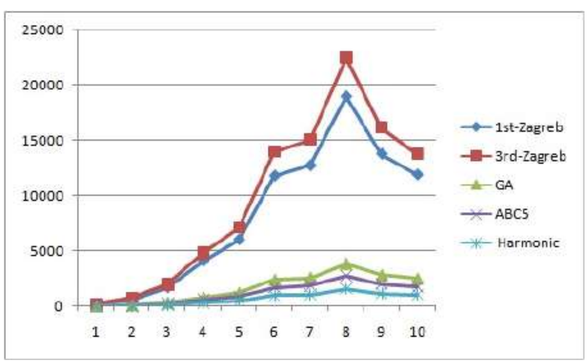

Figure 2: Pictorial representation of Table 2 results.

5. Conclusion

In this paper, we computed first Zagreb, third Zagreb, geometric-arithmetic, atom-bond connectivity and harmonic index for zero divisor graphs containing commutative rings $\mathbb{Z}_{p_1p_2} \times \mathbb{Z}_q$ and $\mathbb{Z}_{p^2} \times \mathbb{Z}_q$ algorithmically. Later on results of algorithms are verified by comparing them with mathematical calculations. Figure 1 and Figure 2 shows the trend in form of line chart about edge eccentric topological indices. In all cases, 3^{rd} Zagreb index and Harmonic index have the maximum and minimum values, respectively. ABC_5 index is greater than Harmonic Index, GA index is greater than ABC_5 index and 1^{st} Zagreb index is greater than GA index but lesser than 3^{rd} Zagreb index for all zero divisor graphs. This study is further useful in understanding the attributes of various physical structures like carbohydrates, silicone structures, polymers, hexagonal chains, cylindrical fullerenes. They can likewise be useful in creating productive physical structure in mechanics as well as for different computer network problems.

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