

On digraphs with maximum first outdegree Zagreb index

Hilal A. Ganie¹, Shariefuddin Pirzada^{2,*}

¹Department of Mathematics, Government Degree College Uri, Kashmir, India
hilahmad1119kt@gmail.com

²Department of Mathematics, University of Kashmir, India
*pirzadasd@kashmiruniversity.ac.in

Received: 31 May 2025; Accepted: 23 October 2025
Published Online: 5 November 2025

Abstract: Let D be a digraph with order n and a arcs. Let $d_1^+, d_2^+, \dots, d_n^+$ be the vertex outdegrees of D . The first outdegree Zagreb index of D is denoted by $Zg^+(D)$ and is defined as $Zg^+(D) = \sum_{i=1}^n (d_i^+)^2$. In this paper, we completely characterize the oriented graphs which attain the maximum value for the first outdegree Zagreb index $Zg^+(D)$ among all connected oriented graphs D of order n with $n-1 \leq a \leq 2n-3$. Further, we determine the oriented graphs which attain the second maximum value for $Zg^+(D)$ among all oriented graphs of order n with $n-1 \leq a \leq n+2$. We consider the problem of determining the orientations which attain the maximum and the minimum values for the first outdegree Zagreb index for the Path, the Cycle and the Star.

Keywords: digraph, oriented graph, topological index, first outdegree Zagreb index.

AMS Subject classification: 05C50, 05C12

1. Introduction

Throughout this paper we will consider a digraph D as $D = (V(D), E(D))$, where $V(D) = \{v_1, v_2, \dots, v_n\}$ is the vertex set and $E(D)$ is the arc set of D . A digraph D is a simple digraph if there are no loops or parallel arcs. A digraph D is said to be strongly connected if for any two vertices $v_i, v_j \in V(D)$, there is a directed path from v_i to v_j and a directed path from v_j to v_i . A digraph is considered as connected (weakly connected) if its underlying graph is connected. For any notions not defined explicitly in the paper, we will refer the reader to the standard book [11].

* Corresponding Author

In a digraph D , any two vertices u and v are said to be adjacent if there is an arc $(u, v) \in E(D)$ or $(v, u) \in E(D)$. Given an arc $e = (v_i, v_j) \in E(D)$, we call v_i the initial vertex of e , v_j the terminal vertex, and v_i a tail of v_j . The in-neighborhood and out-neighborhood of v_i is denoted, respectively, by $N_D^-(v_i) = \{v_j \in V(D) | (v_j, v_i) \in E(D)\}$ and $N_D^+(v_i) = \{v_j \in V(D) | (v_i, v_j) \in E(D)\}$. Accordingly, the indegree and outdegree are denoted by $d_i^- = |N_D^-(v_i)|$ and $d_i^+ = |N_D^+(v_i)|$, respectively. A digraph D is said to be outdegree regular if $d_1^+ = d_2^+ = \dots = d_n^+$.

A digraph D is said to be symmetric if there is an arc $(v, u) \in E(D)$ whenever there is an arc $(u, v) \in E(D)$ in D . A digraph with no symmetric pair of arcs is said to be an oriented graph or an orientation of the underlying graph.

A topological index is a number associated with a graph, which characterizes the structure of the graph and is invariant under graph isomorphism. Some major types of topological indices of graphs are degree-based topological indices (like the first, the second and the third Zagreb indices), distance-based topological indices (like Wiener and Harary indices) and counting-related topological indices. The degree-based topological indices are of great importance with a significant role in chemical graph theory, particularly in chemistry, see [8, 9].

For a graph G with n vertices having degrees $d_1 \geq d_2 \geq \dots \geq d_n$, the first Zagreb index is denoted by $M_1(G)$ and is defined as $M_1 = \sum_{i=1}^n d_i^2$. A number of papers can be found in the literature focusing on the estimates and the extremal properties for $M_1(G)$. For some recent papers in this direction, we refer to [1, 2, 12] and the references therein.

The concept of vertex-degree based topological indices was extended to digraphs by Monsalve and Rada [7]. The authors in [7] have defined a general vertex-degree based topological index for digraphs which includes as special cases the first Zagreb index, the Randić index and other vertex-based topological indices. In [7], the authors have mainly focused on the Randić index of oriented graphs and they have characterized the extremal digraphs attaining the maximum and minimum value for this index among trees and some other families of oriented graphs. In [6], Monsalve and Rada have further studied this general vertex-degree based topological index for digraphs. The authors in [6] have established several upper and lower bounds for this general vertex-degree based topological index of oriented graphs and characterized extremal digraphs. In [10], the authors have considered the first Zagreb index of a digraph D as

$$M_1(D) = \frac{1}{2} \sum_{(u,v) \in E(D)} (d_u^+ + d_v^-).$$

They have considered the orientations of a unicyclic graph with given matching number and found the oriented graphs which attain the maximum value for $M_1(D)$.

The concept of first outdegree Zagreb index $Zg^+(D)$ and the first indegree Zagreb index $Zg^-(D)$ of a digraph D was recently introduced in [4] and are formally defined

as

$$Zg^+(D) = \sum_{i=1}^n (d_i^+)^2 \quad \text{and} \quad Zg^-(D) = \sum_{i=1}^n (d_i^-)^2,$$

where $d_1^+ \geq d_2^+ \geq \dots \geq d_n^+$ are the vertex outdegrees and $d_1^- \geq d_2^- \geq \dots \geq d_n^-$ are the vertex indegrees of D . In [4], the authors have established several upper and lower bounds for the first outdegree Zagreb index $Zg^+(D)$ of a digraph D in terms of the number of vertices n and the number of arcs a . They have characterized the extremal digraphs attaining these bounds. Further, they have determined the digraphs which attain the maximum, the second maximum and the third maximum value for $Zg^+(D)$ among all digraphs of order n and among all bipartite digraphs of order n . They have shown that among the orientations of a path P_n the minimum value for $Zg^+(D)$ is attained by the directed path. In [10] the authors have shown that $M_1(D) = \frac{1}{2} \sum_{v \in V(D)} ((d_v^+)^2 + (d_v^-)^2)$. Using the definitions of $Zg^+(D)$ and $Zg^-(D)$, it follows that

$$M_1(D) = \frac{1}{2} (Zg^+(D) + Zg^-(D)).$$

Therefore, the study of $Zg^+(D)$ and $Zg^-(D)$ is equivalent to the study of $M_1(D)$. As discussed in [4], the first outdegree Zagreb index $Zg^+(D)$ is connected with a number of digraph invariants. In fact the authors in [4] have shown that first outdegree Zagreb index $Zg^+(D)$ is connected with the number of pairs of out-arcs which have a common starting vertex in D ; the number of pairs of out-arcs with a different starting vertex in D ; the second Laplacian and the second signless Laplacian coefficient of D . In [4], the authors have motivated the study of first outdegree Zagreb index $Zg^+(D)$ under these observations. More on this topic can be seen in [5].

The rest of the paper is organized as follows. In Section 2, we characterize the oriented graphs which attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$ among all the oriented graphs D of order n with $n - 1 \leq a \leq 2n - 3$. We also characterize the oriented graphs which attains the second maximum value for the first outdegree Zagreb index $Zg^+(D)$ among all the oriented graphs D of order n with $n - 1 \leq a \leq n + 2$. We discuss the orientations of a Path graph P_n , the Cycle graph C_n and the Star graph S_n in Section 3 and characterize the orientations of these graphs which attain the maximum and the minimum values for the first outdegree Zagreb index $Zg^+(D)$.

2. Extremal digraphs for the first outdegree Zagreb index

One of the interesting problems discussed for the topological indices of graphs is the characterization of graphs which attain the maximum and the minimum values for the topological indices among all graphs of order n or among a special family of graphs

(like trees, trees with given matching number, unicyclic graphs, bicyclic graphs, graphs with given connectivity, independence number, clique number, maximum degree, etc) of order n . A number of papers can be found in this direction, for example see [3]. Therefore, the following problem will be of interest for the first outdegree Zagreb index.

Problem 1. Characterize the digraphs D of order n which attain the extremal values for $Zg^+(D)$.

In the rest of this section, we will focus on Problem 1 and characterize among some families of digraphs the digraphs, which attain the extremal values for $Zg^+(D)$.

The following result gives the effect of adding an arc between two non-adjacent vertices in D on the first Zagreb index $Zg^+(D)$.

Lemma 1. *Let D be a connected digraph of order n with a arcs having two non-adjacent vertices u and v . Let $D' = D + (u, v)$ be the digraph obtained by adding an arc from u to v in D . Then $Zg^+(D') = Zg^+(D) + 2d_u^+ + 1$.*

Proof. Let D be a digraph of order n having a arcs and let u and v be two non-adjacent vertices in D . Let $D' = D + (u, v)$ be the digraph obtained by adding an arc from u to v in D . Then, the outdegree of u increases by one and the outdegrees of rest of the vertices remains unchanged. Therefore, by the definition of the first outdegree Zagreb index, we have

$$\begin{aligned} Zg^+(D') - Zg^+(D) &= \sum_{i=1}^n (d_i^+(D'))^2 - \sum_{i=1}^n (d_i^+(D))^2 \\ &= (d_u^+ + 1)^2 - (d_u^+)^2 = 2d_u^+ + 1, \end{aligned}$$

and the result follows. □

Now, if a digraph D attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$, then the maximum outdegree of D should be $n - 1$, as is shown in the following theorem.

Theorem 1. *Let D be a connected digraph of order n with a arcs having maximum outdegree Δ^+ . If D attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$ among all digraphs with a arcs, then $\Delta^+ = n - 1$.*

Proof. Let D be a digraph of order n having a arcs and let Δ^+ be the maximum outdegree of D . Suppose that D is a digraph with a arcs which attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$ and the maximum outdegree of D is not $n - 1$. Then, $\Delta^+(D) \leq n - 2$. Let u be a vertex in D having the maximum outdegree. Then $d_i^+ \leq d_u^+$, for each vertex v_i of D . Let g be the vertex in D which

is not an out-neighbour of u . Clearly, such a vertex exists, as $d_u^+ \leq n - 2$. Let us suppose that there exists a vertex v in D having g as its out-neighbour. Let D' be the digraph obtained by deleting the arc (v, g) and by adding the arc (u, g) . By doing so the outdegree of v decreases by one, the outdegree of u increases by one while as the outdegree of rest of the vertices remains unchanged. We have

$$\begin{aligned} Zg^+(D') - Zg^+(D) &= \sum_{i=1}^n (d_i^+(D'))^2 - \sum_{i=1}^n (d_i^+(D))^2 \\ &= (d_u^+ + 1)^2 - (d_u^+)^2 + (d_v^+ - 1)^2 - (d_v^+)^2 \\ &= 2(d_u^+ - d_v^+) + 2 \\ &> 0. \end{aligned}$$

This shows that D' is a digraph on n vertices with a arcs satisfying $Zg^+(D') > Zg^+(D)$, which is a contradiction to the fact that D has the maximum first outdegree Zagreb index among all digraphs with a arcs.

If g is not an out-neighbour of any vertex in D , then there is at least one vertex say k in D which is out-neighbour of g . Note that this last argument is true as D is connected. Also, note that this vertex k can be the vertex u itself. Let D' be the digraph obtained by deleting the arc (g, k) and by adding the arc (u, k) . By doing so, the outdegree of g decreases by one, the outdegree of u increases by one while as the outdegree of rest of the vertices remains unchanged. We have

$$\begin{aligned} Zg^+(D') - Zg^+(D) &= \sum_{i=1}^k (d_i^+(D'))^2 - \sum_{i=1}^k (d_i^+(D))^2 \\ &= (d_u^+ + 1)^2 - (d_u^+)^2 + (d_g^+ - 1)^2 - (d_g^+)^2 \\ &= 2(d_u^+ - d_g^+) + 2 \\ &> 0. \end{aligned}$$

This shows that D' is a digraph on n vertices with a arcs satisfying $Zg^+(D') > Zg^+(D)$, which is a contradiction to the fact that D has the maximum first outdegree Zagreb index among all digraphs with a arcs.

Thus in each case we have arrived at a contradiction. Therefore, if D has the maximum first outdegree Zagreb index among all digraphs of order n with a arcs, then we must have $\Delta^+ = n - 1$. This completes the proof. \square

The following result gives the maximum values and the digraphs attaining these values, for the first outdegree Zagreb index among all oriented graphs with n vertices and $a \leq n + 2$ arcs.

Theorem 2. *Let D be a connected oriented graph of order n with $a \leq n + 2$ arcs. Let D be the oriented graph which attains the maximum value for the first outdegree Zagreb index*

$Zg^+(D)$ among all oriented graphs on n vertices with a arcs.

(i). If $a = n - 1$, then $D \cong \vec{K}_{1,n-1}$, where $\vec{K}_{1,n-1}$ is an orientation of the star $K_{1,n-1}$ with all edges oriented from vertex of degree $n - 1$.

(ii). If $a = n$, then $D \cong \vec{S}_n^*$, an orientation of $S_n^* = K_{1,n-1} + e$ shown in Figure 1.

(iii). If $a = n + 1$, then $D \cong \vec{B}_n^{(1)}$, an orientation of $K_1 \vee ((n - 4)K_1 \cup P_3)$ shown in Figure 1.

(iv). If $a = n + 2$, then $D \cong \vec{G}'_{n,n+2}$, an orientation of $K_1 \vee ((n - 5)K_1 \cup K_{1,3})$ shown in Figure 1.

Proof. Let D be a oriented graph of order n having a arcs and let Δ^+ be the maximum outdegree of D . Suppose that D is an oriented graph with $a \leq n + 2$ arcs which attains the maximum value for first outdegree Zagreb index $Zg^+(D)$. Then, by Theorem 1 the maximum outdegree Δ^+ of D is $n - 1$. If $a = n - 1$, then D is an orientation of a tree T . Clearly, among all the oriented trees the oriented star $\vec{K}_{1,n-1}$ is the only oriented tree with maximum outdegree $n - 1$. By Theorem 1, it follows that $\vec{K}_{1,n-1}$ attains the maximum value for $Zg^+(D)$ with maximum value equal to $(n - 1)^2$, in this case.

If $a = n$, then D is an orientation of a unicyclic graph. Evidently, among all the oriented unicyclic graphs the oriented graph \vec{S}_n^* is the only graph with maximum outdegree $n - 1$. So, by Theorem 1, it follows that \vec{S}_n^* attains the maximum value for $Zg^+(D)$ with maximum value equal to $(n - 1)^2 + 1$, in this case.

If $a = n + 1$, then D is an orientation of a bicyclic graph. We note that an oriented bicyclic graph with maximum outdegree $n - 1$ can be obtained from an oriented star $\vec{K}_{1,n-1}$ by adding two new arcs. Therefore, the oriented bicyclic graph which attains the maximum value for the first outdegree Zagreb index is one among the oriented graphs $\vec{B}_n^{(1)}$ or $\vec{B}_n^{(2)}$, where $\vec{B}_n^{(2)}$ is obtained from $\vec{B}_n^{(1)}$ by reversing the orientation of one of arcs incident from a vertex of outdegree 2. By direct calculation, it can be seen that $Zg^+(\vec{B}_n^{(1)}) > Zg^+(\vec{B}_n^{(2)})$, implying that the oriented graph $\vec{B}_n^{(1)}$ has the maximum while as the oriented graph $\vec{B}_n^{(2)}$ has the second maximum first outdegree Zagreb index among all oriented bicyclic graphs.

If $a = n + 2$, then D is an orientation of a tricyclic graph. Clearly, an oriented tricyclic graph with maximum outdegree $n - 1$ can be obtained from an oriented star $\vec{K}_{1,n-1}$ by adding three new arcs. By Theorem 1, it is clear that the oriented tricyclic graph which attains the maximum value for the first outdegree Zagreb index is obtained from the oriented graph $\vec{B}_n^{(1)}$ by adding an arc between two non-adjacent vertices u and v so that the outdegree of u or v is maximum possible. Since, $d_v^+, d_u^+ \leq 2$ and $Zg^+(\vec{B}_n^{(1)}) = n^2 - 2n + 5$, it follows that if D is the digraph with maximum first outdegree Zagreb index, then by Theorem 1, we have

$$Zg^+(D) = Zg^+(\vec{B}_n^{(1)}) + 2d_u^+(\vec{B}_n^{(1)}) + 1 \leq n^2 - 2n + 10.$$

Equality occurs if and only if the new arc introduced in $\vec{B}_n^{(1)}$ is from a vertex of outdegree two. As there is a single vertex of outdegree two in $\vec{B}_n^{(1)}$, it follows that

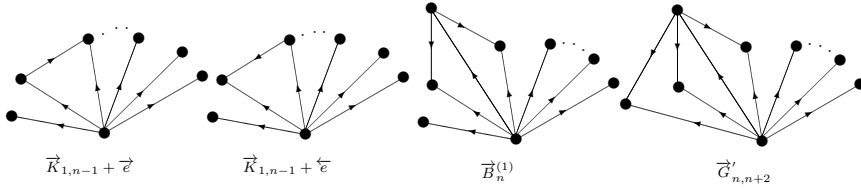


Figure 1. The oriented graphs of order n with $n - 1 \leq a \leq n + 2$ arcs which attains the maximum value for first outdegree Zagreb index.

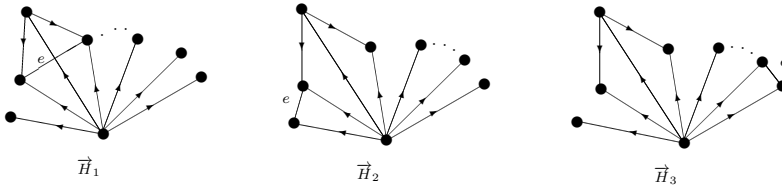


Figure 2. The oriented graphs of order n with $a = n + 2$ arcs which attains the second maximum value for first outdegree Zagreb index, where e can have any orientation.

the oriented graph $\vec{G}'_{n,n+2}$ has the maximum first outdegree Zagreb index among all oriented tricyclic graphs. Moreover, for the oriented graph which attains the second maximum value for $Zg^+(D)$, we have three choices under isomorphism. These oriented graphs are shown in Figure 2. This completes the proof. \square

The following result gives an upper bound for $Zg^+(D)$ in terms of the number of arcs a .

Theorem 3. *Let D be an oriented graph of order n with $a \geq 1$ arcs. Then*

$$Zg^+(D) \leq a^2, \tag{2.1}$$

with equality if and only if $D \cong \vec{K}_{1,a} \cup (n - a - 1)K_1$, where $\vec{K}_{1,a}$ is an orientation of $K_{1,a}$ with all edges oriented away from the central vertex..

Proof. Let D be an oriented graph of order n with a arcs. We prove this result by induction on a . If $a = 1$, then $D \cong \vec{P}_2 \cup (n - 2)K_1$ and so $d_1^+ = 1, d_i^+ = 0$, for $i \geq 2$, implying that the result holds in this case. If $a = 2$, then $D \cong \vec{H} \cup (n - 3)K_1$, where \vec{H} is an orientation of P_3 or $D \cong 2\vec{P}_2 \cup (n - 4)K_1$. In the first case $d_1^+ = 1, d_2^+ = 1, d_i^+ = 0$, for $i \geq 3$ or $d_1^+ = 2, d_i^+ = 0$, for $i \geq 2$, implying that the result holds in each case. In the second case, we have $d_1^+ = 1, d_2^+ = 1, d_i^+ = 0$, for $i \geq 3$ and so the result holds in this case as well. Assume that the result is true for all digraphs of order n with a arcs. Let D be a digraph with n vertices and a arcs and let u, v be two non-adjacent vertices in D . Let $D' = D + (u, v)$ be the digraph obtained from D by adding an arc from u to v . Let $\bar{d}_1^+ \geq \bar{d}_2^+ \geq \dots \geq \bar{d}_n^+$ be the outdegrees of D' .

Then it is clear that $\bar{d}_u^+ = d_u^+ + 1$ and $\bar{d}_i^+ = d_i^+$, for $i \neq u$. Therefore, by induction hypothesis applied to D , we get

$$Zg^+(D') = \sum_{i=1}^n (\bar{d}_i^+)^2 = \sum_{i=1}^n (d_i^+)^2 + 2d_u^+ + 1 \leq a^2 + 2a + 1 = (a + 1)^2,$$

where we have used the fact $d_u^+ \leq a$. This shows that the result is also true for the digraph D' with $a + 1$ arcs. Thus, by the induction hypothesis the result holds for all digraphs.

Suppose that equality holds in (2.1). Then

$$\left(\sum_{i=1}^n d_i^+ \right)^2 = a^2 = Zg^+(D) = \sum_{i=1}^n (d_i^+)^2. \quad (2.2)$$

Since $\left(\sum_{i=1}^n d_i^+ \right)^2 = \sum_{i=1}^n (d_i^+)^2 + 2 \sum_{i < j} d_i^+ d_j^+$, therefore for (2.2) to hold we must have $\sum_{i < j} d_i^+ d_j^+ = 0$. This last equality holds if $d_i^+ = 0$, for all i or $d_i^+ \neq 0$ for exactly one i .

In the first case D has no arc, which is not possible. So, equality holds in (2.1) if and if $d_i^+ \neq 0$ for exactly one i . Let $d_1^+ \neq 0$ and $d_i^+ = 0$, for $i \geq 2$. Then $a \leq n - 1$ and $\sum_{i=1}^n d_i^+ = a$ giving that $d_1^+ = a$, which is only possible if $D \cong \vec{K}_{1,a} \cup (n - a - 1)K_1$. This completes the proof. \square

Let $D_{n,a}^{n-1,a-n+1}$ be the digraph with no symmetric pair of arcs having the maximum outdegree $n - 1$, the second maximum outdegree $a - n + 1$ and all other outdegrees equal to zero, where $n + 3 \leq a \leq 2n - 3$. For the structure of the digraph $D_{n,a}^{n-1,a-n+1}$, see Figure 3. The next result characterizes the oriented graphs which attain the maximum value for the first outdegree Zagreb index $Zg^+(D)$, when D is an oriented graph of order n with a arcs, where $n + 3 \leq a \leq 2n - 3$.

Theorem 4. *Let D be an oriented graph of order n with a arcs, where $n + 3 \leq a \leq 2n - 3$. Then,*

$$Zg^+(D) \leq (n - 1)^2 + (a - n + 1)^2, \quad (2.3)$$

with equality if and only if $D \cong D_{n,a}^{n-1,a-n+1}$.

Proof. Let D be an oriented graph of order n having a arcs. Assume that D attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$. Then, by Theorem 1, the maximum outdegree of D is $n - 1$. This implies that the orientation $\vec{K}_{1,n-1}$ of the star is a spanning subdigraph of D . In other words, this implies that D is obtained from the digraph $\vec{K}_{1,n-1}$ by adding $a - n + 1$ arcs. Let D' be the digraph obtained from D by deleting the vertex of maximum outdegree and the arcs incident

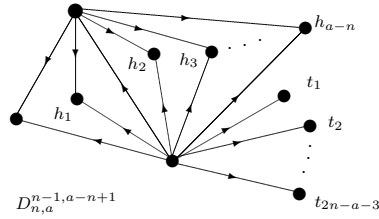


Figure 3. The digraph $D_{n,a}^{n-1, a-n+1}$.

from it. Let $\bar{d}_1^+ \geq \bar{d}_2^+ \geq \dots \geq \bar{d}_{n-1}^+$ be the outdegrees of D' . Then it is clear that $d_1^+ = n - 1$ and $d_{i+1}^+ = \bar{d}_i^+$, for $i = 1, 2, \dots, n - 1$. Therefore using Theorem 3, we have

$$\begin{aligned} Zg^+(D) &= \sum_{i=1}^n (d_i^+)^2 = (n - 1)^2 + \sum_{i=2}^n (d_i^+)^2 \\ &= (n - 1)^2 + \sum_{i=1}^{n-1} (\bar{d}_i^+)^2 \leq (n - 1)^2 + (a - n + 1)^2. \end{aligned}$$

Note that we have used the fact that $Zg^+(D') = \sum_{i=1}^{n-1} (\bar{d}_i^+)^2 \leq (a - n + 1)^2$, as D' has $a - n + 1$ arcs.

Assume that equality occurs in (2.3). Then equality occurs in $Zg^+(D') \leq (a - n + 1)^2$. Since by Theorem 3 equality occurs in $Zg^+(D') \leq (a - n + 1)^2$ if and only if $D' \cong \bar{K}_{1, a-n+1} \cup (2n - a - 3)K_1$. Now, adding the vertex of outdegree $n - 1$ to D' it follows that equality occurs in (2.3) if and only if $D \cong D_{n,a}^{n-1, a-n+1}$. This completes the proof. \square

From Theorem 4, it follows that among all orientations D of the graph G with n vertices and $n + 3 \leq m \leq 2n - 3$ edges, the oriented graph $D_{n,a}^{n-1, a-n+1}$ attains the maximum value for the first outdegree Zagreb index $Zg^+(D)$.

3. Extremal values of first outdegree Zagreb index among the orientations of some graphs

In this section, we discuss the problem of determining the extremal digraphs for the first outdegree Zagreb index among orientations of Paths, the orientations of Cycles and the orientations of Stars.

The following theorem gives a lower bound for the first outdegree Zagreb index $Zg^+(D)$ in terms of the number of vertices n and the number of arcs a of a digraph D and can be seen in [4].

Theorem 5. [4] *Let D be a digraph of order n with a arcs having first outdegree Zagreb index $Zg^+(D)$. Let k be the largest positive integer such that $d_k^+ > 0$, where $1 \leq k \leq n$. Then*

$$Zg^+(D) \geq a(2p + 1) - pk(p + 1), \quad (3.1)$$

where $p = \lfloor \frac{a}{k} \rfloor$ is the integer value of $\frac{a}{k}$. Equality occurs in (3.1) if and only if $d_i^+ - d_j^+ \leq 1$, for any pair of vertices v_i and v_j having non-zero outdegrees in D .

Orientations of a Path. Let P_n be a path on n vertices with $m = n - 1$ edges. We will show that among all the orientations D of P_n , the orientation with $n - 1$ vertices of outdegree 1 attains the minimum value for $Zg^+(D)$ and the orientation with $\lfloor \frac{n}{2} \rfloor$ vertices of outdegree 2 attains the maximum value for $Zg^+(D)$. Since the maximum degree is 2 in P_n , it follows that the outdegree of any vertex in D is either 2 or 1 or 0. Therefore, the condition $d_i^+ - d_j^+ \leq 1$, for any pair of vertices v_i and v_j having non-zero outdegrees is always satisfied for D . So, by Theorem 5, we have

$$Zg^+(D) = (2p + 1)(n - 1) - pk(p + 1) \quad (3.2)$$

where k is the number of vertices with positive outdegree. We first show that the value of k varies from $\lfloor \frac{n}{2} \rfloor$ to $n - 1$ for any orientation D of P_n . The upper bound is trivially true as at the most $n - 1$ vertices in D can have outdegree positive. Note that in this case D is a directed path. Let v_1, v_2, \dots, v_n be the vertices of P_n with edges $v_i v_{i+1}$, for $i = 1, 2, \dots, n - 1$. To show that the lower bound holds, we consider the cases when n is even or odd. It is clear that an orientation D of P_n can have minimum number of vertices with positive outdegree if and only if it has the maximum number of vertices with outdegree 2. Let us first suppose that n is even. Consider the vertices $v_2, v_4, \dots, v_{n-2}, v_n$ with even subscripts. Orient the edges incident at these vertices directed outwards, we obtain an orientation P_1 of P_n with maximum number of vertices of outdegree 2. In fact, the number of vertices with outdegree 2 is $\frac{n}{2} - 1$ and there is one vertex with outdegree 1, in this case. This implies that the minimum value for k is $\frac{n}{2}$ and this value is achieved in the orientation P_1 . Let us now suppose that n is odd. Consider the vertices v_2, v_4, \dots, v_{n-1} with even subscripts and orient the edges incident at these vertices directed outwards. We obtain an orientation P_2 of P_n with maximum number of vertices of outdegree 2. In fact, the number of vertices with outdegree 2 is $\frac{n-1}{2}$ in this case. So the minimum value for k is $\frac{n-1}{2}$ and this value is achieved in the orientation P_2 . Thus, we have shown that $\lfloor \frac{n}{2} \rfloor \leq k \leq n - 1$, with equality on the left if and only if $D \cong P_1$ or P_2 , according to as n is even or odd and equality on right holds if and only if D is a directed path \vec{P}_n . If n is even, then $k \geq \frac{n}{2}$ implies that $k = \frac{n}{2} + c$, where $c = 0, 1, \dots, \frac{n}{2} - 1$. So, $p = \lfloor \frac{n-1}{\frac{n}{2} + c} \rfloor = \lfloor \frac{2(n-1)}{n+2c} \rfloor = \lfloor \frac{2(n+2c)-2-4c}{n+2c} \rfloor = \lfloor 2 - \frac{(4c+2)}{n+2c} \rfloor = 1$. On the other hand, if n is odd, then $k \geq \frac{n-1}{2}$ gives $k = \frac{n-1}{2} + c$, where $c = 0, 1, \dots, \frac{n-1}{2}$. Therefore, $p = \lfloor \frac{n-1}{\frac{n-1}{2} + c} \rfloor = \lfloor \frac{2(n-1)}{n+2c-1} \rfloor = \lfloor \frac{2(n+2c-1)-4c}{n+2c-1} \rfloor = \lfloor 2 - \frac{(4c)}{n+2c-1} \rfloor = 1$, for $c \neq 0$ and equal to

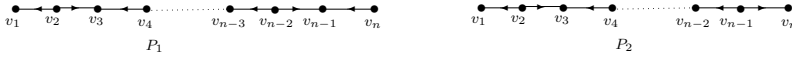


Figure 4. The orientations P_1 and P_2 of the path P_n which attain the maximum value for the first outdegree Zagreb index for n even and n odd, respectively.

2, for $c = 0$. Thus, it follows that $p = 1$ for $\frac{n}{2} \leq k \leq n-1$, n even; $\frac{n-1}{2} + 1 \leq k \leq n-1$, n odd and $p = 2$, for $k = \frac{n-1}{2}$, n odd. Inserting the values of p in (3.2), we arrive at

$$Zg^+(D) = 3(n-1) - 2k, \quad (3.3)$$

for $\frac{n}{2} \leq k \leq n-1$, n even; or $\frac{n+1}{2} \leq k \leq n-1$, n odd and

$$Zg^+(D) = 5(n-1) - 6k, \quad (3.4)$$

for $k = \frac{n-1}{2}$, n odd. If $\frac{n}{2} \leq k \leq n-1$, for n even, then (3.3) gives $n-1 \leq Zg^+(D) \leq 2n-3$, with equality on left if and only if $k = n-1$ and equality on right if and only if $k = \frac{n}{2}$. If $\frac{n-1}{2} - 1 \leq k \leq n-1$, for n odd, then (3.3) gives $n-1 \leq Zg^+(D) \leq 2n-4$, with equality on the left if and only if $k = n-1$ and equality on the right if and only if $k = \frac{n+1}{2}$; and $Zg^+(D) = 2n-2$, if $k = \frac{n-1}{2}$, for n odd. Thus, summarizing all these observations we arrive at the following result.

Theorem 6. *Among all the orientations of the Path P_n , the directed path \vec{P}_n attains the minimum value for $Zg^+(D)$ with the minimum value equal to $n-1$. Among all the orientations of the Path P_n with n even, the orientation P_1 attain the maximum value for $Zg^+(D)$ with the maximum value equal to $2n-3$. Among all the orientations of the Path P_n with n odd, the orientation P_2 attain the maximum value for $Zg^+(D)$ with the maximum value equal to $2n-2$.*

Orientations of a Cycle. Let C_n be a cycle on n vertices with $m = n$ edges. Among all the orientations D of C_n , we show that the directed cycle attains the minimum value for $Zg^+(D)$ and the orientation with $\frac{n-2}{2}$ vertices of outdegree 2 attains the maximum value for $Zg^+(D)$, when n is even and the orientation with $\frac{n+1}{2}$ vertices of outdegree 2 attains the maximum value for $Zg^+(D)$, when n is odd. Since the maximum degree in C_n is 2, it follows that the outdegree of any vertex in D is either 2 or 1 or 0. Therefore, the condition $d_i^+ - d_j^+ \leq 1$, for any pair of vertices v_i and v_j having non-zero outdegrees is always satisfied for D . So, by Theorem 5, we have

$$Zg^+(D) = (2p+1)(n-1) - pk(p+1), \quad (3.5)$$

where k is the number of vertices with positive outdegree. First we show that the value of k varies from $\frac{n}{2}$ to n for any orientation D of C_n , when n is even and it varies from $\frac{n+1}{2}$ to n , when n is odd. The upper bound is trivially true as at most n

vertices in D can have outdegree positive. Note that in this case D is a directed cycle \vec{C}_n . Let v_1, v_2, \dots, v_n be the vertices of C_n with edges $v_i v_{i+1}$, for $i = 1, 2, \dots, n-1$ and the edge $v_n v_1$. To show that the lower bound is true, we consider the cases n even or odd one by one. It is clear that an orientation D of C_n can have minimum number of vertices with positive outdegree if and only if it has the maximum number of vertices with outdegree 2. Let us first suppose that n is even. Consider the vertices $v_2, v_4, \dots, v_{n-2}, v_n$ with even subscripts. Orient the edges incident at these vertices directed outwards, we obtain an orientation C_1 of C_n with maximum number of vertices of outdegree 2. In fact, the number of vertices with outdegree 2 is $\frac{n}{2}$ in this case. This gives that the minimum value for k is $\frac{n}{2}$ and this value is achieved in the orientation C_1 . Now, suppose that n is odd. Consider the vertices v_2, v_4, \dots, v_{n-1} with even subscripts. Orient the edges incident at these vertices directed outwards and orient the edge $v_n v_1$ from v_1 to v_n or from v_n to v_1 , we obtain an orientation C_2 or C'_2 of C_n with maximum number of vertices of outdegree 2. In fact, the number of vertices with outdegree 2 is $\frac{n+1}{2}$ in this case. This implies that the minimum value for k is $\frac{n+1}{2}$ and this value is achieved in the orientation C_2 or C'_2 . Thus, we have shown that $\frac{n}{2} \leq k \leq n$, for n even, with equality on the left if and only if $D \cong C_1$ and equality on the right if and only if D is a directed cycle \vec{C}_n and $\frac{n+1}{2} \leq k \leq n$, for n odd, with equality on the left if and only if $D \cong C_2$ or C'_2 and equality on right if and only if D is a directed cycle \vec{C}_n . If n is even, then $k \geq \frac{n}{2}$ gives that $k = \frac{n}{2} + c$, where $c = 0, 1, \dots, \frac{n}{2}$ and so $p = \lfloor \frac{n}{\frac{n}{2} + c} \rfloor = \lfloor \frac{2n}{n+2c} \rfloor = \lfloor \frac{2(n+2c)-4c}{n+2c} \rfloor = \lfloor 2 - \frac{(4c)}{n+2c} \rfloor = 1$, if $c \neq 0$ and equal to 2, if $c = 0$. On the other hand, if n is odd, then $k \geq \frac{n+1}{2}$ which gives $k = \frac{n+1}{2} + c$, where $c = 0, 1, \dots, \frac{n+1}{2}$. Therefore, $p = \lfloor \frac{n}{\frac{n+1}{2} + c} \rfloor = \lfloor \frac{2n}{n+2c+1} \rfloor = \lfloor \frac{2(n+2c+1)-4c-2}{n+2c+1} \rfloor = \lfloor 2 - \frac{(4c+2)}{n+2c+1} \rfloor = 1$. Thus, it follows that $p = 1$ for $\frac{n}{2} \leq k \leq n$, n even; $\frac{n+1}{2} \leq k \leq n$, n odd and $p = 2$, for $k = \frac{n}{2}$, n even. Inserting the values of p in (3.5), we arrive at

$$Zg^+(D) = 3n - 2k, \quad (3.6)$$

for $\frac{n}{2} + 1 \leq k \leq n$, n even or $\frac{n+1}{2} \leq k \leq n$, n odd and

$$Zg^+(D) = 5n - 6k, \quad (3.7)$$

for $k = \frac{n}{2}$, n even. If $\frac{n+2}{2} \leq k \leq n$, for n even, then (3.6) gives $n \leq Zg^+(D) \leq 2n - 2$, with equality on the left if and only if $k = n$ and equality on the right if and only if $k = \frac{n-2}{2}$; and $Zg^+(D) = 2n$, if $k = \frac{n}{2}$, for n even. If $\frac{n+1}{2} \leq k \leq n$ for n odd, then (3.6) gives $n \leq Zg^+(D) \leq 2n - 1$, with equality on left if and only if $k = n$ and equality on right if and only if $k = \frac{n+1}{2}$. Thus, summarizing all these observations we arrive at the following result.

Theorem 7. *Among all the orientations of the Cycle C_n , the directed cycle \vec{C}_n attains the minimum value for $Zg^+(D)$ with the minimum value equal to n . Among all the orientations*

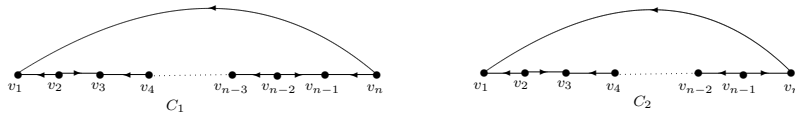


Figure 5. The orientations C_1 and C_2 of cycle C_n which attain the maximum value for the first outdegree Zagreb index for n even and n odd, respectively. Note that C_2' can be obtained from C_2 by reversing the direction of last edge $v_n v_1$.

of the cycle C_n with n even, the orientation C_1 attains the maximum value for $Zg^+(D)$ with the maximum value equal to $2n$. Among all the orientations of the cycle C_n with n odd, the orientation C_2 or C_2' attains the maximum value for $Zg^+(D)$ with the maximum value equal to $2n - 1$.

Orientations of a star. Let $S_n = K_{1,n-1}$ be a star on n vertices with $m = n - 1$ edges. Among all the orientations D of S_n , we show that the orientation with all edges directed towards the central vertex or the orientation with all edges directed towards the central vertex except one edge which is directed outwards attains the minimum value for $Zg^+(D)$ and the orientation with all edges directed outwards from the central vertex attains the maximum value for $Zg^+(D)$. The maximum value is attained by the orientation with all edges directed outwards from the central vertex follows from the part (i) of (2). Therefore, we will find the orientation which attains the minimum value for $Zg^+(D)$. Clearly, the star S_n has a vertex of degree $n - 1$ and all other vertices of degree 1. So, by Theorem 5, the minimum value for $Zg^+(D)$ is attained by the orientation which satisfies $d_i^+ - d_j^+ \leq 1$, for any pair of vertices v_i and v_j having non-zero outdegrees. Clearly, this condition will be satisfied by an orientation D of S_n if the maximum degree vertex has the outdegree either 2 or 1 or 0. Therefore, there are three orientations namely the orientation S_1 with all edges directed towards the vertex of degree $n - 1$ except two edges which are directed outwards; the orientation S_2 with all edges directed towards the vertex of degree $n - 1$ except one edge which is directed outwards and the orientation S_3 with all edges directed towards the vertex of degree $n - 1$. For the digraphs S_1 , S_2 and S_3 , we have $k = n - 2$, $n - 1$ and $n - 1$, respectively. This implies that $p = \lfloor \frac{a}{k} \rfloor = \lfloor \frac{n-1}{k} \rfloor = 1$ in each case. Now applying Theorem 5 to digraphs, we get $Zg^+(S_1) = n + 1$, $Zg^+(S_2) = n - 1 = Zg^+(S_3)$. This shows that among the orientation of star S_n the minimum value is attained by the orientations S_2 and S_3 with minimum value $n - 1$.

Theorem 8. Among all the orientations of the star S_n , the orientation with all edges directed from the vertex of degree $n-1$ attains the maximum value for $Zg^+(D)$ with maximum value $(n - 1)^2$. Among all the orientation of the star S_n , the minimum value for the first outdegree Zagreb index is attained by the orientations S_2 and S_3 with minimum value $n - 1$.

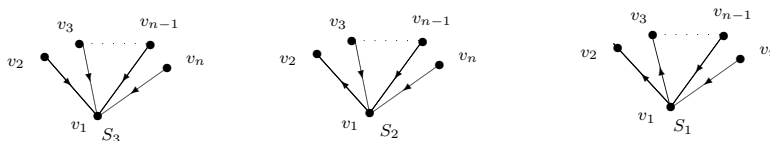


Figure 6. The orientations S_1, S_2 and S_3 of star S_n which are the candidates to attain the minimum value for the first outdegree Zagreb index.

Acknowledgements. We are highly thankful to anonymous referees for their valuable comments and suggestions which led to the improvement in the presentation of the paper. The research of S. Pirzada is supported by the NBHM-DAE research project number NBHM/02011/20/2022.

Statements and Declarations

The authors declare that no funds, grants, or other support were received during the preparation of this manuscript. The authors have no relevant financial or non-financial interests to disclose. All authors contributed to the study conception and design and commented on previous versions of the manuscript. All authors read and approved the final manuscript. This research did not generate or analyze any datasets.

References

- [1] M.H. Aftab, M. Rafaqat, M. Hussain, and T. Zia, *On the computation of some topological descriptors to find closed formulas for certain chemical graphs*, J. Chem. **2021** (2021), no. 1, 5533619.
<https://doi.org/10.1155/2021/5533619>.
- [2] A. Ali, B. Furtula, I. Gutman, and D. Vukićević, *Augmented Zagreb index: extremal results and bounds*, MATCH Commun. Math. Comput. Chem. **85** (2021), no. 2, 211–244.
- [3] B. Borovićanin, B. Furtula, and I. Gutman, *Bounds for Zagreb indices*, MATCH Commun. Math. Comput. Chem. **78** (2017), no. 1, 17–100.
- [4] H.A. Ganie and S. Pirzada, *On the first outdegree Zagreb index of a digraph*, Discrete Math. **347** (2024), no. 1, 113726.
<https://doi.org/10.1016/j.disc.2023.113726>.
- [5] H.A. Ganie, B.A. Rather, and Y. Shang, *Bounds on the first outdegree Zagreb index of digraphs*, Aequationes Math. (2025), In press.
<https://doi.org/10.1007/s00010-025-01233-x>.
- [6] J. Monsalve and J. Rada, *Sharp upper and lower bounds of VDB topological indices of digraphs*, Symmetry **13** (2021), no. 10, 1903.
<https://doi.org/10.3390/sym13101903>.

-
- [7] ———, *Vertex-degree based topological indices of digraphs*, *Discrete Appl. Math.* **295** (2021), 13–24.
<https://doi.org/10.1016/j.dam.2021.02.024>.
- [8] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, John Wiley & Sons, 2008.
- [9] ———, *Molecular Descriptors for Chemoinformatics: volume I: alphabetical listing/volume ii: appendices, references*, John Wiley & Sons, 2009.
- [10] J. Yang and H. Deng, *Maximum first Zagreb index of orientations of unicyclic graphs with given matching number*, *Appl. Math. Comput.* **427** (2022), 127131.
<https://doi.org/10.1016/j.amc.2022.127131>.
- [11] P. Zhang and G. Chartrand, *Introduction to Graph Theory*, Tata McGraw-Hill New York, 2006.
- [12] Y. Zhang, J. Wang, and M. Brunetti, *Topological indices of the wreath product of graphs*, *Discrete Math. Algorithms Appl.* **15** (2023), no. 1, 2250056.
<https://doi.org/10.1142/S1793830922500562>.