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Research Article

Neighborhood first Zagreb index and maximal unicyclic and bicyclic graphs

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Abstract: The Neighborhood First Zagreb Index NM_1 measures the topological properties of a molecular graph. Neighborhood First Zagreb Index NM_1 is defined as $NM_1(G) = \sum_{v \in V(G)} (S(v))^2$, where $S(v)$ used to represent the sum of degrees of vertices adjacent to a vertex v in a graph G. In this study, we focus on characterizing the graphs with the maximum neighborhood first Zagreb index in the class of unicyclic/bicyclic graphs on n vertices, where n is a fixed integer greater than or equal to 5. Specifically, we are interested in identifying the graphs that have the highest value according to the recently introduced neighborhood first Zagreb index NM_1.

Keywords: extremal graph theory, neighborhood topological index, different classes of graphs.

AMS Subject classification: 05C09, 05C92

1. Introduction

In our current study, we will focus on discussing graphs that meet certain criteria. These graphs are simple, connected, undirected, and finite. Let's define some key terms related to graphs. For a graph $G = (V, E)$, the order refers to the number of vertices ($|V(G)|$) in G, while the size represents the number of edges ($|E(G)|$) in G.

To describe the set of neighbors of a vertex $v \in G$, we use the notation $N_G(v)$, which represents the set of vertices adjacent to v. The degree of a vertex $v \in G$, denoted as $d(v)$, is the count of vertices in $N_G(v)$. If a vertex w has a degree of 1, it is referred to as a pendent vertex or a leaf.

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We use the symbol P_n to represent a path graph with an order of n, while the star graph on n vertices is denoted as S_n. For a more comprehensive understanding of graph theory, we recommend referring to relevant books such as [12, 14, 27].

For a graph G, the definition of the first Zagreb index, denoted as M_1, can be found in the formula derived in Gutman's paper [19]. Similarly, in Gutman's paper [20], the second Zagreb index, represented as M_2, was introduced and can be defined as

$$M_1(G) = \sum_{\vartheta \in V(G)} d(\vartheta)^2 = \sum_{\vartheta\rho \in E(G)} (d(\vartheta) + d(\rho)) \ \ and \ \ M_2(G) = \sum_{\vartheta\rho \in E(G)} d(\vartheta)d(\rho).$$

The theory of Zagreb indices has a strong foundation in the literature, as evidenced by several papers such as [1, 2, 8, 15, 16, 18, 19, 21, 22, 24, 26]. Additionally, recent surveys like [3, 4, 6, 17, 30] provide comprehensive overviews of the topic, along with a list of related references for further exploration.

In the literature, different notations have been used by researchers to represent the sum of degrees of vertices adjacent to a vertex w in a graph G. However, for clarity and consistency, we will use the notation $S_G(w)$, $S(w)$, or S_w to denote this sum, as S represents the sum. The average degree [31] of a vertex $w \in V(G)$, also known as the dual degree [10], is defined as the ratio of the sum of degrees of vertices adjacent to a vertex w to the degree of w, and we will denote it as $a(w)$. Now, take a look on the following general graph invariants.

$$\Gamma_1(G) = \sum_{w \in V(G)} g_1(S(w)) \ \ and \ \ \Gamma_2(G) = \sum_{vw \in E(G)} g_2(S(v), S(w)).$$

In the field of mathematical chemistry, many instances of the invariants Γ_1 and Γ_2 have already been discussed. For instance, if we choose $g_1(S(u)) = S(u)$ or $\frac{1}{\sqrt{S(u)}}$, then Γ_1 corresponds to the first Zagreb index M_1 ([7]) or the first extended zeroth-order connectivity index [5, 28, 29, 32], respectively. Similarly, if we select $g_2(S(v), S(w)) = S(v) + S(w)$ or $\frac{1}{\sqrt{S(v)S(w)}}$, then Γ_2 represents M_2 (refer to Lemma 2.6 in [7]), the first extended first-order connectivity index [5]. To achieve a deeper comprehension, see [11, 13]. Following a similar approach, it is logical to consider the subsequent updated versions of the first and second Zagreb indices as proposed in [25].

$$NM_1(G) = \sum_{v \in V(G)} (S(v))^2 \ \ and \ \ NM_2(G) = \sum_{uv \in E(G)} S(u)S(v).$$

The invariants NM_1 and NM_2 in [25] were referred as the neighborhood first Zagreb index and neighborhood second Zagreb index. In the context of molecular graphs, the NM_1 has found applications in various areas of computational chemistry and drug discovery. Few of them are listed. The NM_1 can be used as a molecular descriptor to predict the biological activity or properties of chemical compounds. By incorporating NM_1 values into QSAR models, researchers can gain insights into the structure-activity relationships of molecules. It can also help in identifying molecular scaffolds or substructures that are associated with specific biological activities. By analyzing the NM_1 values of different compounds, medicinal chemists can prioritize or optimize molecules for drug design. The NM_1 can be employed as a similarity measure to compare and cluster molecules based on their structural features. By calculating NM_1 values for different compounds, researchers can identify structurally similar molecules, which can be useful in virtual screening and lead optimization processes. The NM_1 has been used to assess the reactivity and stability of molecules. Higher NM_1 values may indicate increased reactivity, while lower values may suggest greater stability. This information can aid in understanding the chemical behavior and potential reactions of compounds. It is important to note that the application of the NM_1 in molecular graphs is just one aspect of its broader usage in graph theory and network analysis. Researchers continue to explore and develop new applications for this graph invariant in various scientific domains.

The neighborhood first Zagreb index and neighborhood second Zagreb index, denoted as NM_1 and NM_2 respectively in [25], are of interest in this paper. Specifically, we focus on NM_1, which was first introduced in Refs. [9, 23] as the neighborhood first Zagreb index [23]. The expression for NM_1 can be rewritten as shown in [9]:

$$NM_1(G) = \sum_{v \in V(G)} (d(v)a(v))^2.$$

The primary goal of this study is to establish extremal findings concerning unicyclic graphs and bicyclic graphs with order n in relation to NM_1.

Section 2 introduces certain transformations that will increase the neighborhood first Zagreb index. The graphs discussed in this paper are limited to unicyclic or bicyclic graphs with n vertices, where n is a fixed integer greater than or equal to 5.

2. Maximum Neighborhood First Zagreb Index of Unicyclic and Bicyclic Graphs

In this section, we will demonstrate transformations and establish certain lemmas that contribute to enhance the neighborhood's first Zagreb index, focusing on graphs that are either unicyclic or bicyclic. A graph is considered unicyclic if it is both connected and contains precisely one cycle, whereas a graph is considered bicyclic if it is connected and contains exactly two cycles.

Transformation 2.1. *Let $uv \in E(G)$, $d(v) \geq 2$, v is on the cycle of G, $N_G(u) = \{v, u_1, u_2, \ldots, u_i\}$ and $u_1, u_2, \ldots, u_i$ are pendent vertices. Construct $G^* = G - \{uu_1, uu_2, \ldots, uu_i\} + \{vu_1, vu_2, \ldots, vu_i\}$.*

Lemma 1. *Let G^* and G represent the graphs mentioned in Transformation 2.1. Then $NM_1(G) < NM_1(G^*)$.*

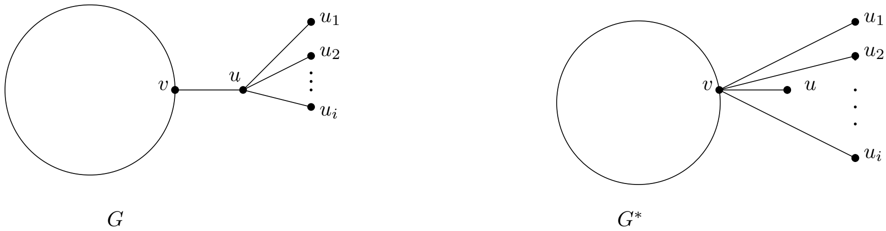


Figure 1. **Graphs G and G^* (typically refers in Transformation 2.1).**

Proof. Let $x \in N_G(v) \setminus \{u\}$, by definition of neighborhood first Zegrab index, we get

$$NM_1(G^*) - NM_1(G) = i\left[(d(v)+i)^2 - (i+1)^2\right]$$
$$(d(v)-1)\left[\left(\sum_{w\in N_G(x)} d(w)+i\right)^2 - \left(\sum_{w\in N_G(x)} d(w)\right)^2\right] > 0.$$

□

Transformation 2.2. *Let $u, v \in V(G)$, $d(v) \geq d(u)$ and suppose that u and v lie on the the same cycle. Suppose $u_1, u_2, \cdots, u_i$ are pendent vertices adjacent to u and $v_1, v_2, \cdots, v_j$ are pendent vertices adjacent to v. Construct $G^* = G - \{uu_1, uu_2, \cdots, uu_i\} + \{vu_1, vu_2, \cdots, vu_i\}$.*

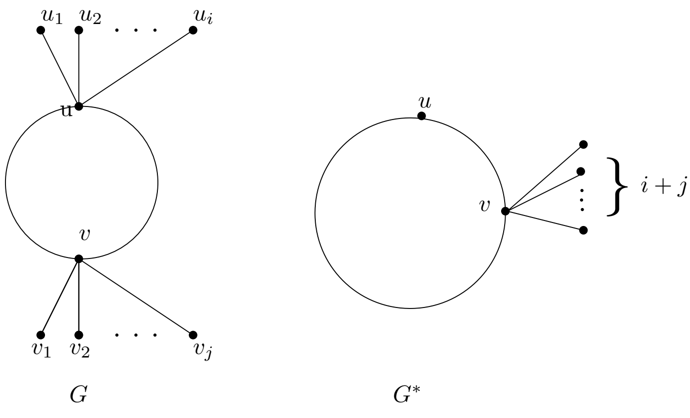


Figure 2. **Graphs G and G^* (typically refers in Transformation 2.2).**

Remark 1. If $x \geq y$ and $i \geq 1$, then

$$(x+i)^2 + (y-i)^2 - x^2 - y^2 = 2i^2 + 2i(x-y) > 0.$$

Lemma 2. *Let G^* and G be the graphs as in Transformation 2.2. Then $NM_1(G) < NM_1(G^*)$.*

Proof. Let $x \in N_G(u)$, $v \neq x$ and $\acute{x} \in N_G(v)$, $u \neq \acute{x}$, then there will exists five cases with relation to the positions of u and v.

Case I. $uv \in E(G)$ and $N_G(u) \cap N_G(v) = \phi$.

$$\begin{aligned} NM_1(G^*) - NM_1(G) = &\left[\left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} (d(\acute{w}) + i)\right)^2 + \left(\sum_{w \in N_G(x \setminus \{v, u_i\})} (d(w) - i)\right)^2\right] \\ &- \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} d(\acute{w})\right)^2 + \left(\sum_{w \in N_G(x \setminus \{v, u_i\})} d(w)\right)^2\right] \\ &+ i\left((d(v) + i)^2 - d(u)^2\right) \\ &+ j\left((d(v) + i)^2 - d(v)^2\right) > 0. \end{aligned}$$

Case II. $uv \in E(G)$ and $\mid N_G(u) \cap N_G(v) \mid = 1$.
Let $t_1 \in N_G(u) \cap N_G(v)$,

$$\begin{aligned} NM_1(G^*) - NM_1(G) = &\left[\left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} d(\acute{w}) + i\right)^2 - \left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} d(\acute{w})\right)^2\right] \\ &+ i\left((d(v) + i)^2 - d(u)^2\right) \\ &+ j\left((d(v) + i)^2 - d(v)^2\right) > 0. \end{aligned}$$

Case III. $uv \notin E(G)$ and $N_G(u) \cap N_G(v) = \phi$.

$$\begin{aligned} NM_1(G^*) - NM_1(G) = &\left[\left(\sum_{\acute{x} \in N_G(v)} (d(\acute{x}) + i)\right)^2 + \left(\sum_{x \in N_G(u)} (d(x) - i)\right)^2\right] \\ &- \left[\left(\sum_{\acute{x} \in N_G(v)} d(\acute{x})\right)^2 + \left(\sum_{x \in N_G(u)} d(x)\right)^2\right] \\ &+ \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} (d(\acute{w}) + i)\right)^2 + \left(\sum_{w \in N_G(x \setminus \{v, u_i\})} (d(w) - i)\right)^2\right] \\ &- \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \setminus \{u, v_j\})} d(\acute{w})\right)^2 + \left(\sum_{w \in N_G(x \setminus \{v, u_i\})} d(w)\right)^2\right] \\ &+ i\left((d(v) + i)^2 - d(u)^2\right) \\ &+ j\left((d(v) + i)^2 - d(v)^2\right) > 0. \end{aligned}$$

Case IV. $uv \notin E(G)$ and $\mid N_G(u) \cap N_G(v) \mid = 1$.
Let $t_1 \in N_G(u) \cap N_G(v)$.

$$\begin{aligned}
NM_1(G^*) - NM_1(G) = & \left[\left(\sum_{\acute{x} \in N_G(v)} (d(\acute{x}) + i) \right)^2 + \left(\sum_{x \in N_G(u)} (d(x) - i) \right)^2 \right] \\
& - \left[\left(\sum_{\acute{x} \in N_G(v)} d(\acute{x}) \right)^2 + \left(\sum_{x \in N_G(u)} d(x) \right)^2 \right] \\
& + \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \backslash \{u, v_j\})} (d(\acute{w}) + i) \right)^2 + \left(\sum_{w \in N_G(x \backslash \{v, u_i\})} (d(w) - i) \right)^2 \right] \\
& - \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \backslash \{u, v_j\})} d(\acute{w}) \right)^2 + \left(\sum_{w \in N_G(x \backslash \{v, u_i\})} d(w) \right)^2 \right] \\
& + i \left((d(v) + i)^2 - d(u)^2 \right) \\
& + j \left((d(v) + i)^2 - d(v)^2 \right) > 0.
\end{aligned}$$

Case V. $uv \notin E(G)$ and $\mid N_G(u) \cap N_G(v) \mid = 2$.
Let $t_1, t_2 \in N_G(u) \cap N_G(v)$.

$$\begin{aligned}
NM_1(G^*) - NM_1(G) = & \left[\left(\sum_{\acute{x} \in N_G(v)} (d(\acute{x}) + i) \right)^2 + \left(\sum_{x \in N_G(u)} (d(x) - i) \right)^2 \right] \\
& - \left[\left(\sum_{\acute{x} \in N_G(v)} d(\acute{x}) \right)^2 + \left(\sum_{x \in N_G(u)} d(x) \right)^2 \right] \\
& + \left[\left(\sum_{\acute{w} \in N_G(\acute{x} \backslash \{u, v_j\})} (d(\acute{w}) + i) \right)^2 - \left(\sum_{\acute{w} \in N_G(\acute{x} \backslash \{u, v_j\})} d(\acute{w}) \right)^2 \right] \\
& + i \left((d(v) + i)^2 - d(u)^2 \right) \\
& + j \left((d(v) + i)^2 - d(v)^2 \right) > 0.
\end{aligned}$$

□

Lemma 1 and Lemma 2 imply the next result.

Theorem 1. *$\mathcal{U}_n^j$ represents a unicyclic graph of order n and length j with $n-j$ pendents attached to a vertex of C_j. Consider a unicyclic graph G that is distinct from $\mathcal{U}_n^j$, then $NM_1(G) < NM_1(\mathcal{U}_n^j)$.*

Since $NM_1(\mathcal{U}_n^j) = (n-j)^3 + 7(n^2 + j^2) + 14n(2-j) - 12j \leq NM_1(\mathcal{U}_n^3)$ for $3 \leq j \leq n$

and equality achieved if and only if $j = 3$.

Theorem 2. *For $n \geq 4$, among the collection of U_n, $\mathcal{U}_n^3$ has the maximum neighborhood first Zegrab index, its value is $(n-3)^3 + 7n^2 - 14n + 27$.*

Now we consider the class of non-isomorphic connected graphs which have property $m = n + 1$-graph, where m,n represent counts of edges and vertices respectively , denoted by $G(n, m = n + 1)$ and we will find the extremal(maximal) $(n, m = n + 1)$-graph relative to neighborhood first Zegrab index.
For any element $G \in G(n, m = n + 1)$ there will be two cycles C_ϑ and C_ς. We split up the class of non-isomorphic simply connected $(n, m = n + 1)$-graph into further three sub-classes.
(i) The sub-class from $G(n, m = n+1)$ is denoted by $B_n^1(\vartheta, \varsigma)$ in which cycles C_ϑ and C_ς have one commonplace vertex.
(ii) The sub-class from $G(n, m = n + 1)$ is denoted by $B_n^0(\vartheta, \varsigma)$ in which cycles C_ϑ and C_ς have no commonplace vertex.
(iii) The sub-class from $G(n, m = n+1)$ is denoted by $B_n^l(\vartheta, \varsigma)$ in which cycles C_ϑ and C_ς have a common path of length l. First of all, we will find out the maximal graph from the Sub-class $B_n^1(\vartheta, \varsigma)$. Let $S_n^1(\vartheta, \varsigma)$ be the graph in $B_n^1(\vartheta, \varsigma)$ with $n+1-(\vartheta+\varsigma)$ pendents (vertices or edges) are attached to the join (common vertex) of C_ϑ and C_ς.

Theorem 3. *The graph with maximum neighborhood first Zegrab index in the class of $B_n^1(\vartheta, \varsigma)$ is $S_n^1(\vartheta, \varsigma)$.*

Proof. By utilizing Transformation 2.1 and 2.2 on graph G and applying Lemmas 1 and 2, a graph G^* can be obtained such that $NM_1(G) \leq NM_1(G^*)$ equality achieved if and only if all edges not located on cycles are pendent edges connected to the same vertex in G. If $G^* = S_n^1(\vartheta, \varsigma)$, the proof is complete. If not, then $u \neq w$, where w represents the shared vertex of C_ϑ and C_ς. In general, assuming that u lies on cycle C_ς, there are five cases to consider regarding the positions of u and w.
Case I. $uw \in E(G)$ and $N_G(u) \cap N_G(w) = \phi$.
Suppose that t be the count of pendent vertices affixed to u.

$$\begin{aligned} NM_1(S_n^1(\vartheta, \varsigma)) - NM_1(G^*) = t &\left[(n+5-\vartheta-\varsigma)^2 - (n+3-\vartheta-\varsigma)^2\right] \\ &+ \left[(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 - 20\right] \\ &+ 2\,(n+7-\vartheta-\varsigma)^2 - 2(6^2) \geq 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 \geq 20$, $n+1-\vartheta-\varsigma \geq 0$, also equality achieved if and only if $n = \vartheta + \varsigma - 1$ and $G^* = S_n^1(\vartheta, \varsigma)$.

Case II. $uw \in E(G)$ and $\mid N_G(u) \cap N_G(w) \mid = 1$.
Let $t_1 \in N_G(u) \cap N_G(w)$, then

$$\begin{aligned} NM_1(S_n^1(\vartheta,\varsigma)) - NM_1(G^*) &= t\left[(n+5-\vartheta-\varsigma)^2 - (n+3-\vartheta-\varsigma)^2\right] \\ &\quad + 2\left[(n+7-\vartheta-\varsigma)^2 - 6^2\right] \geq 0, \end{aligned}$$

with equality holds if and only if $n = \vartheta + \varsigma - 1$ and $G^* = S_n^1(\vartheta,\varsigma)$.
Case III. $uw \notin E(G)$ and $N_G(u) \cap N_G(w) = \phi$.

$$\begin{aligned} NM_1(S_n^1(\vartheta,\varsigma)) - NM_1(G^*) &= (n+9-\vartheta-\varsigma)^2 - 64 \\ &\quad + t\left[(n+5-\vartheta-\varsigma)^2 - (n+3-\vartheta-\varsigma)^2\right] \\ &\quad + 3\left[(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 - 20\right] \\ &\quad + (n+7-\vartheta-\varsigma)^2 - (6^2) \geq 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 \geq 20$, also equality achieved if and only if $n = \vartheta + \varsigma - 1$ and $G^* = S_n^1(\vartheta,\varsigma)$.
Case IV. $uw \notin E(G)$ and $\mid N_G(u) \cap N_G(w) \mid = 1$.
Let $t_1 \in N_G(u) \cap N_G(w)$.

$$\begin{aligned} NM_1(S_n^1(\vartheta,\varsigma)) - NM_1(G^*) &= (n+9-\vartheta-\varsigma)^2 - 64 \\ &\quad + t\left[(n+5-\vartheta-\varsigma)^2 - (n+3-\vartheta-\varsigma)^2\right] \\ &\quad + 2\left[(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 - 20\right] \\ &\quad + (n+7-\vartheta-\varsigma)^2 - (6^2) \geq 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 \geq 20$, also equality achieved if and only if $n = \vartheta + \varsigma - 1$ and $G^* = S_n^1(\vartheta,\varsigma)$.
Case V. $uw \notin E(G)$ and $\mid N_G(u) \cap N_G(w) \mid = 2$.
Let $t_1, t_2 \in N_G(u) \cap N_G(w)$.

$$\begin{aligned} NM_1(S_n^1(\vartheta,\varsigma)) - NM_1(G^*) &= (n+9-\vartheta-\varsigma)^2 - 64 \\ &\quad + t\left[(n+5-\vartheta-\varsigma)^2 - (n+3-\vartheta-\varsigma)^2\right] \\ &\quad + [(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 - 20] \\ &\quad + (n+7-\vartheta-\varsigma)^2 - (6^2) \geq 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2 \geq 20$, also equality achieved if and only if $n = \vartheta + \varsigma - 1$ and $G^* = S_n^1(\vartheta,\varsigma)$. □

Lemma 3. *(i) If $\vartheta > 3$, then $NM_1(S_n^1(\vartheta,\varsigma)) < NM_1(S_n^1(\vartheta-1,\varsigma))$.*
(ii) If $\varsigma > 3$, then $NM_1(S_n^1(\vartheta,\varsigma)) < NM_1(S_n^1(\vartheta,\varsigma-1))$.

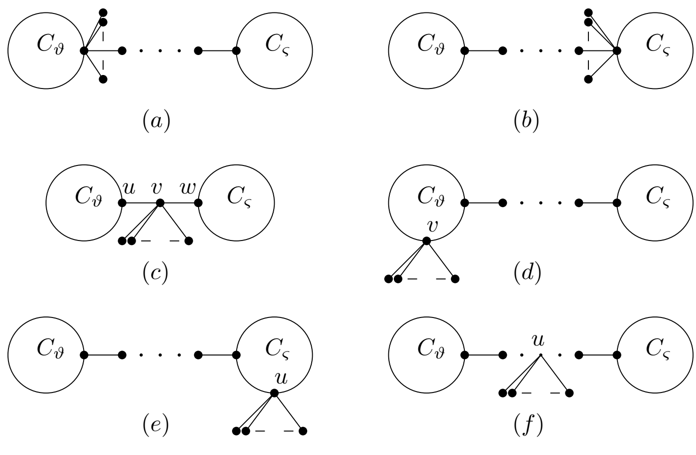
Proof. (i)

$$\begin{aligned} NM_1(S_n^1(\vartheta-1,\varsigma)) - NM_1(S_n^1(\vartheta,\varsigma)) &= (n+10-\vartheta-\varsigma)^2 - (n+9-\vartheta-\varsigma)^2 \\ &\quad + 4\left[(n+8-\vartheta-\varsigma)^2 - (n+7-\vartheta-\varsigma)^2\right] \\ &\quad + t\left[(n+6-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2\right] \\ &\quad + (n+6-\vartheta-\varsigma)^2 - 4^2 > 0. \end{aligned}$$

Since $n+1-\vartheta-\varsigma > 0$.
(ii) The proof is same as in part (i) due to symmetry of ϑ and ς. $\square$

Theorem 4. *The optimal graph with maximum neighborhood first Zegrab index in the class of $B_n^1(\vartheta,\varsigma)$ is $S_n^1(3,3)$ for all $\vartheta \geq 3$ and $\varsigma \geq 3$.*

Now, we are considering the class $B_n^0(\vartheta,\varsigma)$ in order to find the maximum bicyclic graph. To do this, we define $A_n^k(\vartheta,\varsigma)$ as the resulting $(n, m = n+1)$-graph by connecting C_ϑ and C_ς with a path of length k, and attaching the remaining $n+1-\vartheta-\varsigma-k$ edges to C_ϑ. The graph where C_ϑ and C_ς are joined by a path uvw of length 2, and the other $n-\vartheta-\varsigma-1$ edges are connected to the vertex w, which is the common vertex of the path and C_ϑ, is denoted as $A_n(\vartheta,\varsigma)$.



$(a)A_n^k(\vartheta,\varsigma)$; $(b)A_n^k(\vartheta,\varsigma)$; $(c)A_n(\vartheta,\varsigma)$.

Figure 3. **The members of the class $B_n^0(\vartheta,\varsigma)$.**

Theorem 5. *If $G \in B_n^0(\vartheta,\varsigma)$, the length of the shortest path linking C_ϑ and C_ς in G is k, then*
(i) $NM_1(G) \leq NM_1(A_n^k(\vartheta,\varsigma))$ equality sign holds true if and only if $G \cong A_n^1(\vartheta,\varsigma)$. or
(ii) $NM_1(G) \leq NM_1(A_n^k(\varsigma,\vartheta))$ equality sign holds true if and only if $G \cong A_n^1(\varsigma,\vartheta)$. or
(iii) $NM_1(G) \leq NM_1(A_n(\vartheta,\varsigma))$ equality sign holds true if and only if $G \cong A_n(\vartheta,\varsigma)$.

Proof. (i) Suppose that the shortest path establishing link between the cycles C_ϑ and C_ς is denoted by $U = u_1, u_2, \ldots, u_k, u_{k+1}$ and commonplace vertex of U and C_ϑ is marked as u_1 and commonplace vertex of U and C_ς is marked as u_{k+1}. If u is on the cycle C_ϑ, as shown in figure $3(d)$.
By applying Transformations 2.1 and 2.2 to a graph G and utilizing Lemmas 1 and 2, we can obtain a graph G^* for which $NM_1(G) \leq NM_1(G^*)$. The equality sign holds only if all edges that are not part of cycles in G are pendent edges attached to the same vertex u in G. The location of u on the cycle C_ϑ can result in several possible outcomes.

Case I. $u_1u \in E(G)$ and $N_G(u_1) \cap N_G(u) = \phi$.
Suppose that t be the count of pendent vertices affixed to u.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) - NM_1(G^*) = t&\left[(n+4-\vartheta-\varsigma-k)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ &+ [(n+6-\vartheta-\varsigma-k)^2 - (n+5-\vartheta-\varsigma-k)^2 - 9] \\ &+ (n+4-\vartheta-\varsigma-k+d(u_3))^2 - (d(u_3)+3)^2 > 0. \end{aligned}$$

Since $(n+6-\vartheta-\varsigma-k)^2 - (n+5-\vartheta-\varsigma-k)^2 \geq 9$.
Case II. $u_1u \in E(G)$ and $\mid N_G(u_1) \cap N_G(u) \mid= 1$.
Suppose that t be the count of pendent vertices affixed to u and Let $t_1 \in N_G(u) \cap N_G(u_1)$.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) - NM_1(G^*) = t&\left[(n+4-\vartheta-\varsigma-k)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ &+ (n+4-\vartheta-\varsigma-k+d(u_3))^2 - (d(u_3)+3)^2 > 0. \end{aligned}$$

Case III. $u_1u \notin E(G)$ and $N_G(u_1) \cap N_G(u) = \phi$.
Suppose that t be the count of pendent vertices affixed to u.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) - NM_1(G^*) = t&\left[(n+4-\vartheta-\varsigma-k)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ &+ 2\left[(n+6-\vartheta-\varsigma-k)^2 - (n+5-\vartheta-\varsigma-k)^2 - 9\right] \\ &+ (n+5-\vartheta-\varsigma-k+d(u_2))^2 - (d(u_2)+4)^2 \\ &+ (n+4-\vartheta-\varsigma-k+d(u_3))^2 - (d(u_3)+3)^2 \\ &+ \left[(n+7-\vartheta-\varsigma-k)^2 - (n+5-\vartheta-\varsigma-k)^2 - 20\right] \\ &> 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma-k)^2-(n+5-\vartheta-\varsigma-k)^2 \geq 20$.

Case IV. $u_1u \notin E(G)$ and $\mid N_G(u)\cap N_G(u_1) \mid = 1$.
Let $t_1 \in N_G(u)\cap N_G(u_1)$.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) - NM_1(G^*) &= t\left[(n+4-\vartheta-\varsigma-k)^2-(n+3-\vartheta-\varsigma-k)^2\right] \\ &\quad + [(n+6-\vartheta-\varsigma-k)^2-(n+5-\vartheta-\varsigma-k)^2-9] \\ &\quad + (n+5-\vartheta-\varsigma-k+d(u_2))^2-(d(u_2)+4)^2 \\ &\quad + (n+4-\vartheta-\varsigma-k+d(u_3))^2-(d(u_3)+3)^2 \\ &\quad + \left[(n+7-\vartheta-\varsigma-k)^2-(n+5-\vartheta-\varsigma-k)^2-20\right] \\ &> 0. \end{aligned}$$

Since $(n+7-\vartheta-\varsigma-k)^2-(n+5-\vartheta-\varsigma-k)^2 \geq 20$.

Case V. $u_1u \notin E(G)$ and $\mid N_G(u)\cap N_G(u_1) \mid = 2$.
Let $t_1, t_2 \in N_G(u)\cap N_G(u_1)$.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) - NM_1(G^*) &= t\left[(n+4-\vartheta-\varsigma-k)^2-(n+3-\vartheta-\varsigma-k)^2\right] \\ &\quad + \left[(n+7-\vartheta-\varsigma-k)^2-(n+5-\vartheta-\varsigma-k)^2-20\right] \\ &\quad + (n+5-\vartheta-\varsigma-k+d(u_2))^2-(d(u_2)+4)^2 \\ &\quad + (n+4-\vartheta-\varsigma-k+d(u_3))^2-(d(u_3)+3)^2 > 0. \end{aligned}$$

(ii) Let u is on the cycle C_ς, as shown in figure 7(e). The proof is similar as in Case I.
(iii) If $u = u_j$, $1 < j \leq k$, as shown in figure 7(f).

Case I. $j = 2$ or $j = k$ and $k = 3$.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) - NM_1(G^*) &= t\left[(n-\vartheta-\varsigma+1)^2-(n+3-\vartheta-\varsigma-k)^2\right] \\ &\quad + \left[2\,(n-\vartheta-\varsigma+5)^2-(n-\vartheta-\varsigma-k+7)^2-36\right] \\ &\quad + (n-\vartheta-\varsigma+5)^2-(n-\vartheta-\varsigma-k+6)^2 \\ &\quad + (k-2)\,(n-\vartheta-\varsigma+1)^2-(n+6-\vartheta-\varsigma-k)^2 > 0. \end{aligned}$$

Case II. $j = 2$ or $j = k$ and $k \geq 4$.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) - NM_1(G^*) &= t\left[(n-\vartheta-\varsigma+1)^2-(n+3-\vartheta-\varsigma-k)^2\right] \\ &\quad + (n-\vartheta-\varsigma+5)^2-(n-\vartheta-\varsigma-k+6)^2 \\ &\quad + [2\,(n-\vartheta-\varsigma+5)^2-(n-\vartheta-\varsigma-k+7)^2-36] \\ &\quad + [2\,(n-\vartheta-\varsigma+1)^2-(n-\vartheta-\varsigma-k+5)^2-5^2] \\ &\quad + (k-4)[(n-\vartheta-\varsigma+1)^2-4^2] > 0. \end{aligned}$$

Case III. $j = 3$ or $j = k-1$ and $k = 4$.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) - NM_1(G^*) = {} & t\left[(n-\vartheta-\varsigma+1)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ & + 2\left[(n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+6)^2\right] \\ & + (n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+5)^2 \\ & + (k-2)\,(n-\vartheta-\varsigma+1)^2 - 2(6^2) > 0. \end{aligned}$$

Case IV. $j = 3$ or $j = k-1$ and $k \geq 5$.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) - NM_1(G^*) = {} & t\left[(n-\vartheta-\varsigma+1)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ & + [2\,(n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+5)^2 \\ & - (n-\vartheta-\varsigma-k+6)^2] \\ & + (n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+5)^2 \\ & + [3\,(n-\vartheta-\varsigma+1)^2 - (5^2) - 2(6^2)] \\ & + (k-5)[(n-\vartheta-\varsigma+1)^2 - 4^2] > 0. \end{aligned}$$

Case V. $4 \leq j \leq k-2$ and $k \geq 6$.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) - NM_1(G^*) = {} & t\left[(n-\vartheta-\varsigma+1)^2 - (n+3-\vartheta-\varsigma-k)^2\right] \\ & + 2\left[(n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+5)^2\right] \\ & + (n-\vartheta-\varsigma+5)^2 - (n-\vartheta-\varsigma-k+5)^2 \\ & + [4\,(n-\vartheta-\varsigma+1)^2 - 2(5^2) - 2(6^2)] \\ & + (k-6)[(n-\vartheta-\varsigma+1)^2 - 4^2] > 0. \end{aligned}$$

□

Lemma 4. *$NM_1(A_n(\vartheta,\varsigma)) \leq NM_1(A_n(3,3))$ with equality holds if and only if $\vartheta = \varsigma = 3$.*

Proof.

$$\begin{aligned} NM_1(A_n(\vartheta,\varsigma)) &= (n-1-\vartheta-\varsigma)\,(n+1-\vartheta-\varsigma)^2 + 3\,(n+5-\vartheta-\varsigma)^2 \\ &\quad + (\vartheta+\varsigma-6)4^2 + 4(5^2). \\ NM_1(A_n(3,3)) &= (n-7)\,(n-5)^2 + 3\,(n-1)^2 + 4(5^2). \end{aligned}$$

$$\begin{aligned} NM_1(A_n(3,3)) - NM_1(A_n(\vartheta,\varsigma)) &= (\vartheta+\varsigma-6)\,(2n-\vartheta-\varsigma-4)\,(n-\vartheta-\varsigma-1) \\ &\quad + (\vartheta+\varsigma-6)((n-5)^2-4^2) \\ &\quad + 3(\vartheta+\varsigma-6)\,(2n-\vartheta-\varsigma+4) > 0. \end{aligned}$$

□

Lemma 5. *$NM_1(A_n^k(\vartheta,\varsigma)) < NM_1(A_n^{k-1}(\vartheta,\varsigma))$ for $k \geq 2$.*

Proof. There will be two possible cases relating the length of path.
Case I. $k = 2$.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) &= (n-1-\vartheta-\varsigma)\,(n+2-\vartheta-\varsigma)^2 + 2\,(n+5-\vartheta-\varsigma)^2 \\ &\quad + 2\,(n+4-\vartheta-\varsigma)^2 + 6^2. \end{aligned}$$

$$\begin{aligned} NM_1(A_n^{k-1}(\vartheta,\varsigma)) &= (n-1-\vartheta-\varsigma)\,(n+3-\vartheta-\varsigma)^2 + (n+3-\vartheta-\varsigma)^2 \\ &\quad + 2\,(n+7-\vartheta-\varsigma)^2 + 2\,(n+5-\vartheta-\varsigma)^2. \end{aligned}$$

$$\begin{aligned} NM_1(A_n^{k-1}(\vartheta,\varsigma)) - NM_1(A_n^k(\vartheta,\varsigma)) &= (n-1-\vartheta-\varsigma)\left[(n+3-\vartheta-\varsigma)^2 - (n+2-\vartheta-\varsigma)^2\right] \\ &\quad + 2\left[(n+7-\vartheta-\varsigma)^2 - (n+5-\vartheta-\varsigma)^2\right] \\ &\quad + 2[(n+5-\vartheta-\varsigma)^2 - (n+4-\vartheta-\varsigma)^2] \\ &\quad + (n+3-\vartheta-\varsigma)^2 - 6^2 > 0. \end{aligned}$$

Case II. $k > 2$.

$$\begin{aligned} NM_1(A_n^k(\vartheta,\varsigma)) &= (n+1-\vartheta-\varsigma-k)\,(n+4-\vartheta-\varsigma-k)^2 + 3\,(n+6-\vartheta-\varsigma-k)^2 \\ &\quad + (n+7-\vartheta-\varsigma-k)^2 + (k-3)4^2. \end{aligned}$$

$$\begin{aligned} NM_1(A_n^{k-1}(\vartheta,\varsigma)) &= (n+1-\vartheta-\varsigma-k)\,(n+5-\vartheta-\varsigma-k)^2 + 3\,(n+7-\vartheta-\varsigma-k)^2 \\ &\quad + (n+8-\vartheta-\varsigma-k)^2 + (n+5-\vartheta-\varsigma-k)^2 + (k-4)4^2. \end{aligned}$$

$$\begin{aligned} NM_1(A_n^{k-1}(\vartheta,\varsigma)) - NM_1(A_n^k(\vartheta,\varsigma)) &= (n+1-\vartheta-\varsigma-k)\,[(n+5-\vartheta-\varsigma-k)^2 \\ &\quad - (n+4-\vartheta-\varsigma-k)^2] \\ &\quad + 2\left[(n+7-\vartheta-\varsigma-k)^2 - (n+6-\vartheta-\varsigma-k)^2\right] \\ &\quad + (n+8-\vartheta-\varsigma-k)^2 - (n+6-\vartheta-\varsigma-k)^2 \\ &\quad + (n+5-\vartheta-\varsigma-k)^2 + (k-4)4^2 - (k-3)4^2 > 0. \end{aligned}$$

□

Lemma 6. *$NM_1(A_n^1(\vartheta,\varsigma)) \leq NM_1(A_n^1(3,3))$ with equality holds true if and only if $\vartheta = \varsigma = 3$.*

Proof.

$$\begin{aligned} NM_1(A_n^1(\vartheta,\varsigma)) = &(n-\vartheta-\varsigma)(n+3-\vartheta-\varsigma)^2 + 2(n+7-\vartheta-\varsigma)^2 \\ &+ 2(n+5-\vartheta-\varsigma)^2 + (\vartheta+\varsigma-6)4^2. \end{aligned}$$

$$NM_1(A_n^1(3,3)) = (n-6)(n-3)^2 + 2(n+1)^2 + 2(n-1)^2.$$

$$\begin{aligned} NM_1(A_n^1(3,3)) - NM_1(A_n^1(\vartheta,\varsigma)) = &(\vartheta+\varsigma-6)(2n-\vartheta-\varsigma)(n-\vartheta-\varsigma) \\ &+ 4(\vartheta+\varsigma-6)(2n-\vartheta-\varsigma+6) > 0 \\ &+ (\vartheta+\varsigma-6)((n-3)^2-4^2) > 0. \end{aligned}$$

□

Lemma 7. *$NM_1(A_n^1(3,3)) > NM_1(A_n(3,3))$.*

Proof. The proof is identical to that of Lemma 6. □

Theorem 5 and Lemma 4-7 reflect the following result.

Theorem 6. *The optimal(maximal) graph with neighborhood first Zegrab index from the class of $B_n^0(\vartheta,\varsigma)$ for all $\vartheta \geq 3$ and $\varsigma \geq 3$ is $NM_1(A_n^1(3,3))$.*

Now the class under consideration is $B_n^l(\vartheta,\varsigma)$ to find bicyclic graph with the maximum NM_1 in which cycles C_ϑ and C_ς have a common path of length l.

Theorem 7. *Let $H \in B_n^l(\vartheta,\varsigma)$. Then $NM_1(H) \leq NM_1(H^*)$ equality sign holds true if and only if $H = H^*$, where H^* is the graph in Figure 4.*

Proof. By applying the Transformation 2.1 and 2.2 on a graph H and using Lemmas 1 and 2, we will get a graph H^* such that $NM_1(H) \leq NM_1(H^*)$ equality is achieved if and only if all edges, except those in the cycles, are attached to the same vertex u in graph H as pendent edges. Let $e = xy$ be an edge in H_1 where both x and y have a degree of two,, We may then get a H_1^* graph by merging the edge e and

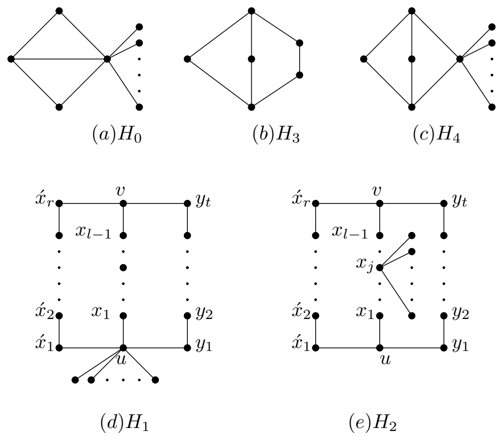


Figure 4. **The graphs H_i, $i = 0, 1, 2, 3, 4$.**

joining a pendant edge $\acute{e} = u\acute{u}$ to u, and we have $NM_1(H_1^*) > NM_1(H_1)$, since $d_{H_1}(x)d_{H_1}(y) = 4$ and $d_{H_1^*}(u)d_{H_1^*}(\acute{u}) \geq 4$ and $d_{H_1}(u) < d_{H_1^*}(u)$.

$$\begin{aligned} NM_1(H^*) - NM_1(H_1) = t((d(u)+1)^2 - d(u)^2) + (d(u)+1)^2 - 16 \\ + \left(\sum_{w \in N_z \setminus \{t\}} d(w) + 1\right)^2 - \left(\sum_{w \in N_z \setminus \{t\}} d(w)\right)^2 \\ + \left(\sum_{z \in N_u} dz + 1\right)^2 - \left(\sum_{z \in N_u} dz\right)^2 > 0. \end{aligned}$$

So, $NM_1(H_1) \leq NM_1(H_0)$ equality sign holds if and only if $H_1 \cong H_0$.
If there are m_1 edges within H_2 so that their end-vertices degrees are equal two, then the resulting graph H_2^* is obtained by contracting the m_1 edges and joining m_1 pendant edges to u. And we get $NM_1(H_2^*) > NM_1(H_2)$. So, $NM_1(H_0) > NM_1(H_2)$, $NM_1(H_1) > NM_1(H_3)$ and $NM_1(H_2) > NM_1(H_3)$. Also, it can be calculated easily that $NM_1(H_0) > NM_1(H_3)$ and $NM_1(H_0) > NM_1(H_4)$. Which completes the proof. □

Theorem 8. *Among all the classes of bicyclic graph with n vertices, H_0 has maximal neighborhood first Zegrab index .*

Proof. From Theorem 5, Theorem 7 and Theorem 8, we just need to prove the following inequality by comparing values of $NM_1(A_n^1(3,3))$, $NM_1(S_n^1(3,3))$ and $NM_1(H_0)$.

$$NM_1(A_n^1(3,3)) < NM_1(S_n^1(3,3)) < NM_1(H_0).$$

$$NM_1(H_0) = n^2(n-2) + 29n + 22.$$

$$NM_1(S_n^1(3,3)) = n^2(n-2) + 25n + 8.$$

$$NM_1(A_n^1(3,3)) = n^2(n-14) + 89n - 72.$$

which completes the proof. □

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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