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On a Novel Eccentricity-based Invariant of a Graph

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Abstract In this paper, for the purpose of measuring the non-self-centrality extent of non-self-centered graphs, a novel eccentricity-based invariant, named as non-self-centrality number (NSC number for short), of a graph G is defined as follows: $N(G) = \sum_{v_i,v_j \in V(G)} |e_i - e_j|$ where the summation goes over all the unordered pairs of vertices in G and e_i is the eccentricity of vertex v_i in G, whereas the invariant will be called third Zagreb eccentricity index if the summation only goes over the adjacent vertex pairs of graph G. In this paper, we determine the lower and upper bounds on $N(G)$ and characterize the corresponding graphs at which the lower and upper bounds are attained. Finally we propose some attractive research topics for this new invariant of graphs.

Keywords Eccentricity, non-self-centered graph, non-self-centrality number, third Zagreb eccentricity index, diameter

MR(2010) Subject Classification 05C12, 05C35

1 Introduction

We only consider finite, undirected and simple graphs throughout this paper. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. If $v_i, v_j \in V(G)$, then the *distance* $d_G(v_i, v_j)$ between v_i and v_j is defined as the length of a shortest path in G connecting v_i and v_j. For a vertex $v_i \in V(G)$, its *eccentricity* $e_G(v_i)$ is the largest distance between v_i and any other vertex v_j of G, i.e., $e_G(v_i) = \max_{v_j \in V(G)} d_G(v_i, v_j)$. For convenience, hereafter we

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always denote by e_i the eccentricity of $v_i \in V(G)$ if no ambiguity occurs from the context. Some applications of eccentricity in networks are given in [10]. The maximum (minimum, resp.) eccentricity over all vertices of a graph G is called the *diameter* (*radius*, resp.) of G and denoted by $d = d(G)$ ($r = r(G)$, resp.). For any graph G with vertex set $V(G)$, a *central vertex* v_i of G is just a vertex with $e_i = r(G)$ in it. Similarly, a vertex v_j with $e_j = d(G)$ is called *diametrical* vertex. Moreover, the center $C(G)$ and the periphery $P(G)$ of a graph G are defined, respectively, as follows:

$$C(G) = \{v_i \in V(G) | e_i = r(G)\},$$
$$P(G) = \{v_j \in V(G) | e_j = d(G)\}.$$

The above centrality concepts of a graph play an important role in the theory of networks, especially in facility location problems [2]. This is mainly because a property is frequently required in the networks that the maximum eccentricity of any vertex in a network or a graph is as small as possible for the most efficient facility locations at central ones. Some novel applications of eccentricity in networks are given in [5, 10, 19].

Another applicable field of eccentricity of a graph is topological index in chemical graph theory. In mathematical chemistry, Topological Index (TI), also known as molecular descriptor, is a single number that can be used to characterize some property of the graph of a molecule. Topological indices are used for modeling physicochemical, pharmacologic, toxicologic, biological, and other properties of chemical compounds and more significantly in the nonempirical quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) (see some related chapters in [21, 22]). From the viewpoint of pure graph theory, topological index can be viewed as a graph invariant under automorphisms of graphs. There is a great family of distance-based topological indices extensively studied in chemical graph theory (see for more detail in a survey [32] and a new book [31]). Some well-known ones among them include Wiener index [15, 18, 27], Harary index [8, 28, 29], degree distance [23–25] and several special distance-, just eccentricity-based topological indices, such as Zagreb eccentricity indices [6, 26], eccentric connectivity index [7], eccentricity distance sum [14, 34] and connective eccentricity index [30, 33, 35].

The first and second Zagreb eccentricity indices of a graph G are defined [26], respectively, as follows:

$$E_1(G) = \sum_{v_i \in V(G)} e_i^2,$$
$$E_2(G) = \sum_{v_i v_j \in E(G)} e_i e_j.$$

Both of them have a parallel form to two well-known topological indices, namely first and second Zagreb indices, respectively. See [9, 12, 13, 20] for some new results on these ordinary Zagreb indices of graphs.

A connected graph is called a *self-centered graph* (or SC graph for short) if all of its vertices have a same eccentricity. Otherwise, it will be called *non-self-centered*. Evidently, a connected graph G is self-centered if and only if $d(G) = r(G)$. Very recently Klavžar et al. [16, 17] introduced two class of new graphs: almost self-centered (ASC) graphs and almost-peripheral

(AP) graphs. A graph which contains only two non-central vertices is called *almost self-centered graph* [16]. And a graph G is called *almost-peripheral graph* [17] if $|P(G)| = |V(G)| - 1$, i.e., all but one vertices are diametrical in G. If an ASC graph has radius r, then it will be called r-ASC graph.

Throughout this paper our notation is standard and mainly taken from [4]. All graphs considered in this paper are connected. We denote minimum and maximum degrees of vertices of G by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. The path and the star on n vertices are denoted by P_n and S_n, respectively. We denote cycle and complete graph with n vertices by C_n and K_n, respectively. Moreover, we denote by $\overline{G}$ the complement of any graph G. For two vertex-disjoint graphs G and H are graphs, their *join* $G \oplus H$ is the graph obtained from the disjoint union of G and H by adding all edges between $V(G)$ and $V(H)$.

The third Zagreb eccentricity index of a graph G is defined as follows:

$$E_3(G) = \sum_{v_i v_j \in E(G)} |e_j - e_i|.$$

For a non-self-centered graph G, how can we measure the extent of its non-self-centrality? Now we can define a related number, denoted by $\mathrm{nsc}(G)$, to indicate the non-self-centrality of G. Certainly, $\mathrm{nsc}(G)$ must satisfy the following conditions:

(1) $\mathrm{nsc}(G) = 0$ if G is self-centered;

(2) $\mathrm{nsc}(G) = \mathrm{nsc}(H)$ if G and H are two isomorphic graphs.

Evidently, $E_3(G)$ defined above seems to be a good indicator for indicating the non-self-centrality which satisfies the above two terms. As we all know, trees can be viewed as a class of simplest graphs when studying some property of graphs. It turns out that star and path are often the extremal trees, respectively, with respect to some graphic invariants, including Wiener index [32], Harary index [28], first and second Zagreb eccentricity indices [6], and so on. Considering that star and path have a much different form in structure, we require that

(3) For any tree T of order n, we have

$$\mathrm{nsc}(S_n) \leq \mathrm{nsc}(T) \leq \mathrm{nsc}(P_n), \tag{1.1}$$

or

$$\mathrm{nsc}(P_n) \leq \mathrm{nsc}(T) \leq \mathrm{nsc}(S_n). \tag{1.2}$$

The left (right, resp.) equality in (1.1) holds if and only if $T \cong S_n$ ($T \cong P_n$, resp.), and the left (right, resp.) equality in (1.2) holds if and only if $T \cong P_n$ ($T \cong S_n$, resp.).

But $E_3(G)$ does not satisfy the conditions (1) or (2), since $E_3(S_n) = n-1$ and $E_3(P_n) = n-1$ if $n \geq 5$ is odd. Here we construct a novel graphic invariant for better indicating the non-self-centrality of a graph as follows:

$$N(G) = \sum_{v_i \neq v_j} |e_j - e_i|,$$

where the summation goes over all the unordered pairs of vertices in a graph G. Hereafter this invariant $N(G)$ is called *non-self-centrality number*, or NSC *number* for short, of a graph G. Note that the *total irregularity* [1] of a graph is similarly defined but based on the degrees of vertices.

We prove that $N(S_n) \leq N(T) \leq N(P_n)$ for any tree T of order n with left (right, resp.) equality holding if and only if $T \cong S_n$ ($T \cong P_n$, resp.) in the subsequent sections. From this point, $N(G)$ is a better descriptor than $E_3(G)$ for indicating the non-self-centrality of a graph G.

The NSC number of a vertex v_i in a graph G is defined as $n_G(v_i) = \sum_{j=1,j\neq i}^{n} |e_j - e_i|$. Therefore we have $N(G) = \frac{1}{2}\sum_{v_i\in V(G)} n_G(v_i)$ for any connected graph G. From the definitions of $N(G)$ and $E_3(G)$, respectively, we have

$$N(G) = E_3(G) + \sum_{v_iv_j \notin E(G)} |e_j - e_i|. \tag{1.3}$$

The *eccentricity sequence* of a graph G is just a set $\mathcal{E}(G) = \{e_i : v_i \in V(G)\}$ of eccentricities of its vertices with their multiplicity listed in a non-increasing order. If the eccentricity e_i appears $l_i \geq 1$ times in $\mathcal{E}(G)$, we will write $e_i^{(l_i)}$ in it for short. Assume that $\mathcal{E}(G)$ of a graph G has exactly k distinct elements: $e_1 > e_2 > \cdots > e_k$ with $l_1, l_2, \ldots, l_k$ as their respective multiplicities. Then we have

$$N(G) = \sum_{1\leq i<j\leq k} l_il_j(e_i - e_j). \tag{1.4}$$

This paper is organized as follows. In Section 2, we prove that $E_3(T)$ is either $n-1$ or $n-2$ for any tree T of order $n \geq 3$. In Section 3, we characterize some graphs with smaller NSC numbers. And in Section 4, we determine some graphs with larger NSC numbers, in particular, we show that the path P_n has uniquely the maximum NSC number among all trees and connected graphs of order $n \geq 3$, respectively. Finally, in Section 5, we propose some attractive directions on NSC number for graphs.

2 Some Properties of Third Zagreb Eccentricity Index

In this section, we present some properties of the third Zagreb eccentricity index of a graph. It is well known [4] that any tree T has one central vertex or two adjacent central vertices. First we prove a related lemma below.

Lemma 2.1 *Let T be a tree with any edge $e = v_iv_j \in E(T)$. Then we have*

$|e_i - e_j| = 0$ if and only if v_i and v_j are two central vertices of a bicentral tree T.

Proof If v_i, v_j are two adjacent centers of a bicentral tree, then, by the definition of central vertex, we have $e_i = e_j$. Thus $|e_i - e_j| = 0$.

Conversely, assume that $|e_i - e_j| = 0$. Thus we have $e_i = e_j$. Now we have to prove that v_i, v_j are just two adjacent central vertices of a bicentral tree T. Suppose that T has the following structure (see Figure 1).

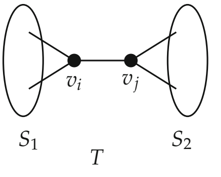

Figure 1 The tree T

Let S_1 and S_2 be two sets of vertices as shown in Figure 1 such that $S_1 \cup S_2 \cup \{v_i, v_j\} = V(T)$. Then there exist two vertices v_k and v_p such that $e_i = \max_{v_t \in V(T)} d_T(v_i, v_t) = d_T(v_i, v_k)$ and $e_j = \max_{v_t \in V(T)} d_T(v_j, v_t) = d_T(v_j, v_p)$. Thus we have $d_T(v_i, v_k) = d_T(v_j, v_p)$.

If $v_k \in S_1$, we have $d_T(v_j, v_k) = d_T(v_j, v_i) + d_T(v_i, v_k) = 1 + e_i$. It follows that

$$e_j = \max_{v_t \in V(T)} d_T(v_j, v_t) \geq d_T(v_j, v_k) = 1 + e_i = 1 + e_j,$$

which is a contradiction. Therefore, we conclude that $v_k \in S_2$. Similarly, we have $v_p \in S_1$.

Now, from the fact that $e_i = e_j$, we have $d_T(v_i, v_k) = d_T(v_j, v_p)$. Moreover, for any vertex $v_t \in S_1$, we have

$$e_t = \max_{v_s \in V(T)} d_T(v_t, v_s) \geq d_T(v_t, v_i) + d_T(v_i, v_k) \geq 1 + e_i.$$

Similarly, we get

$$e_t = \max_{v_s \in V(T)} d_T(v_t, v_s) \geq d_T(v_t, v_j) + d_T(v_j, v_p) \geq 1 + e_j \quad \text{for any vertex } v_t \in S_2.$$

Therefore, we claim that $e_i = e_j$ is smallest in the eccentricity sequence of the tree T. Thus v_i, v_j are adjacent central vertices of a bicentral tree T, finishing the proof. □

Theorem 2.2 *For any tree T of order n, we have*

$$E_3(T) = \begin{cases} n-1, & \text{if } T \text{ has one central vertex;} \\ n-2, & \text{if } T \text{ has two central vertices.} \end{cases}$$

Proof For any edge $v_s v_t \in E(T)$, one can easily see that $|e_s - e_t| \leq 1$. By Lemma 2.1, we have $|e_s - e_t| = 1$ for any edge $v_s v_t \in E(T)$, unless v_s, v_t are just two central vertices of a bicentral tree. Thus, our theorem follows immediately. □

Remark 2.3 The result in Theorem 2.2 cannot be extended to general graphs. For example, we consider the graph depicted in Figure 2. We have $E_3(G) = 4$ since three vertices in the triangle are all central vertices in G.

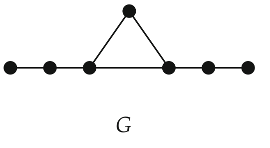

Figure 2 The graph G

The following corollary can be deduced easily from the property of eccentricity of vertex in a graph.

Corollary 2.4 *For any connected graph G with m edges, we have*

$$E_3(G) \leq m$$

with equality holding if and only if $e_i \neq e_j$ for any edge $v_i v_j \in E(G)$.

Note that a bicentral tree has an odd diameter, and vice versa. The following corollary holds clearly.

Corollary 2.5 *For any tree T of order n, we have*

$$E_3(T) = \begin{cases} n-1, & \text{if } T \text{ has an even diameter;} \\ n-2, & \text{if } T \text{ has an odd diameter.} \end{cases}$$

3 Some Graphs with Smaller NSC Numbers

In this section, we determine some graphs with smaller non-self-centrality numbers. First we present a lower bound of $N(G)$ in terms of $E_3(G)$ for any connected graph G.

Theorem 3.1 *For any connected graph G of order $n \geq 2$, we have*

$$N(G) \geq E_3(G) \tag{3.1}$$

with equality holding if and only if the diameter of G is $d \leq 2$.

Proof By (1.3), we get $N(G) \geq E_3(G)$ immediately for any connected graph G. Next we deal with the equality case in (3.1).

Thanks to (1.3), again, we find that the equality in (3.1) holds if and only if the following claim holds.

Claim 1 All nonadjacent (if any) vertices have the same eccentricity in the graph G.

If G has diameter $d = 1$, that is, $G \cong K_n$, the equality holds in (3.1) trivially. Now we assume that G has diameter 2. Then any vertex in G has eccentricity 1 or 2. If any vertex in G has the same eccentricity 2, then the equality in (3.1) holds clearly. Otherwise, there is at least one vertex in G with eccentricity 1. Let v_i be any vertex in G with eccentricity 2. Then there exists a corresponding vertex, say v_j, which is not adjacent to v_i in G. Thus we have $e_j = 2$. It follows that any two nonadjacent vertices have the same eccentricity 2 in G. Therefore the equality in (3.1) follows, finishing the proof of the "if" part.

For the proof of "only if" part, we assume that the equality holds in (3.1) for a connected graph G. Now we claim that the diameter of G is at most 2. If not, let $d \geq 3$ be the diameter of G. Assume that $P = v_1v_2\cdots v_dv_{d+1}$ is a diametral path in G. By Claim 1, we deduce that $e_1 = e_{d+1}$, $e_2 = e_{d+1}$. Thus we have $e_1 = e_2$, which is impossible from the definition of eccentricity of a vertex in a graph. Thus we complete the proof of the "only if" part. □

Corollary 3.2 *Let T be a tree of order n. Then we have*

$$N(T) \geq n-1$$

with equality holding if and only if $T \cong S_n$.

Proof Note that a tree with diameter $d \leq 2$ is uniquely a star. Then our result follows immediately form Theorem 3.1 and Corollary 2.5. □

For two integers n, m such that $4 \leq n \leq m \leq 2n-4$, we denote by $\mathcal{S}_n^m$ the set of graphs obtained by inserting $m-n+1$ edges to a star S_n. Also let $\mathcal{G}_n^m$ be the set of graphs of order n and with m edges. Next we present a result on the extremal graphs with minimal NSC number as a generalization of Corollary 3.2.

Theorem 3.3 *For any non-self-centered graph $G \in \mathcal{G}_n^m$ with $4 \leq n \leq m \leq 2n-4$, we have*

$$N(G) \geq n-1$$

with equality holding if and only if $G \in \mathcal{S}_n^m$.

Proof Let $G \in \mathcal{G}_n^m$ with $4 \le n \le m \le 2n-4$ be a non-self-centered graph. Then G is not a complete graph. From Theorem 3.1, we have $N(G) \ge E_3(G)$ with equality holding if and only if G has diameter 2.

Assume that G is a graph from $\mathcal{G}_n^m$ with diameter 2 where $4 \le n \le m \le 2n-4$. Now we claim that $G \in \mathcal{S}_n^m$. From the definition of $\mathcal{S}_n^m$, it suffices to prove that there is a unique vertex in G with maximum degree $n-1$. Note that G is a non-self-centered graph with diameter 2. Then there is at least one vertex, say v_i, with eccentricity 1 in G, that is, $d_G(v_i) = n-1$. If there are at least two vertices of degree $n-1$ in G, then the number of edges in G is at least $2n-3$, contradicting to the fact that $m \le 2n-4$ in G. Therefore there is only one vertex of degree $n-1$ in G. Thus we have $G \in \mathcal{S}_n^m$ from its definition.

Considering the structure of any graph $G \in \mathcal{S}_n^m$, we have $N(G) = E_3(G) = n-1$, completing the proof of this theorem. □

From its definition, an ASC graph can be viewed as a non-self-centered graph closest to SC graph. By (1.4), we have $N(G) = 2(n-2)$ for any ASC graph G of order n. Then *does there exists a non-self-centered graph G satisfying* $0 < N(G) < 2(n-2)$? To our surprise, the answer is positive to this problem. In the following more general theorem than Theorem 3.3, we determine the minimum NSC number for all non-self-centered graphs of order n.

Theorem 3.4 *For any non-self-centered graph G of order $n \ge 3$, we have*

$$N(G) \ge n-1$$

with equality holding if and only if G is an AP *graph.*

Proof Let e_i be the eccentricity of vertex v_i in G. Without loss of generality, we assume that $e_1 \ge e_2 \ge \cdots \ge e_n$. Then $e_1 > e_n$ since G is a non-self-centered graph. Therefore we get

$$\begin{aligned} N(G) &= |e_1 - e_n| + \sum_{j=2}^{n-1}(|e_1 - e_j| + |e_n - e_j|) + \sum_{2\le i<j\le n-1} |e_i - e_j| \\ &\ge 1 + n - 2 \\ &= n-1 \end{aligned}$$

with equality holding if and only if $e_1 - e_n = 1$, $|e_1 - e_j| + |e_n - e_j| = 1$ and $e_i = e_j$ for $2 \le i < j \le n-1$. Equivalently, there are exactly two distinct elements in $\mathcal{E}(G)$. From (1.4), we arrive at $N(G) = n-1 = l_1 l_n$ where l_1, l_n are the multiplicities of e_1 and e_n in $\mathcal{E}(G)$. Note that there are at least two diametrical vertices in any graph G of order $n \ge 3$, that is, $l_1 \ge 2$. Thus it follows that $l_1 = n-1$ and $l_n = 1$, that is, G is an AP graph, which completes the proof of this theorem. □

Now we introduce a new graph as a weak form of AP graph. A graph G is called weak almost-peripheral (WAP) graph if $|P(G)| = |V(G)| - 2$. In other words, G is a WAP graph if and only if all but two vertices are diametrical in G. For examples, $K_2 \oplus \overline{K_{n-2}}$ is a WAP graph with radius 1, another WAP graph with radius 2 is shown in Figure 3 where two vertices with degree 6 are its central vertices. In the theorem below, we characterize the second minimum NSC number for all non-self-centered graphs of order $n \ge 4$.

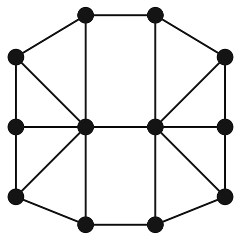

Figure 3 A WAP graph with radius 2

Theorem 3.5 *For any non-self-centered graph G of order $n \geq 4$ other than* AP *one, we have*

$$N(G) \geq 2(n-2)$$

with equality holding if and only if G is an ASC *graph or a* WAP *graph.*

Proof Let G be any non-self-centered graph G of order $n \geq 4$ other than AP one. Assume that e_i is the eccentricity of the vertex v_i in G. Denote by $\{e_{p_1}^{(l_1)}, e_{p_2}^{(l_2)}, \ldots, e_{p_k}^{(l_k)}\}$ with $\sum_{i=1}^{k} l_i = n$ the eccentricity set of graph G. Note that $k \geq 2$, since G is non-self-centered and not AP. From (1.4), we have

$$\begin{aligned} N(G) &= \sum_{1\leq i<j\leq k} l_i l_j (j-i) \\ &\geq \sum_{1\leq i<j\leq k} l_i l_j \\ &= l_1 \sum_{i=2}^{k} l_i + \sum_{2\leq i<j\leq k} l_i l_j \\ &\geq l_1(n-l_1) \\ &\geq 2(n-2). \end{aligned}$$

Note that the last inequality holds from the fact that G is non-self-centered and not AP and $f(x) = x(n-x)$ with $1 \leq x \leq \frac{n}{2}$ is an increasing function. Moreover, the above three equalities hold if and only if there are exactly two distinct numbers e_{p_1}, e_{p_2} in $\mathcal{E}(G)$ with $(l_1, l_2) = (2, n-2)$ or $(n-2, 2)$, that is, G is an ASC graph or a WAP graph. Thus we complete the proof of this theorem. □

A *double star*, denoted by DS_{n_1,n_2}, is a tree obtained by adding a new edge between the centers of stars S_{n_1+1} and S_{n_2+1}, respectively. Obviously, a tree T different from star has two distinct eccentricities if and only if T is a double star. From Theorem 3.5, the corollary below follows immediately in which the trees with second smallest NSC number are completely characterized.

Corollary 3.6 *Let T be a tree of order $n \geq 4$ other than star S_n. Then we have*

$$N(T) \geq 2(n-2)$$

with equality holding if and only if $T \cong \mathrm{DS}_{n_1,n_2}$ with $n_1 + n_2 = n$.

4 Some Graphs with Larger NSC Numbers

In this section, we determine some graphs with larger NSC numbers. After knowing Corollary 3.2, a natural problem occurs in our mind: *which tree has the largest non-self-centrality number among all trees of order* n? To solve this problem, we first introduce some notations.

A *caterpillar* [11], denoted by $P_{k+1}^n(a_2, a_3, \ldots, a_k)$ with $\sum_{i=2}^k a_i = n-k-1$, is a tree of order n with diameter k obtained from a path $P_{k+1} = v_1v_2\cdots v_{k+1}$ by attaching $a_i \geq 0$ pendant vertices to the vertex v_i for $i = 2, 3, \ldots, k$. If k is even, then P_{k+1} has a unique central vertex $v_{\frac{k}{2}+1}$. Otherwise, P_{k+1} has two adjacent central vertices. When k is even, if $a_2 + a_k + a_{\frac{k}{2}+1} = n-k-1$ with $a_2, a_k > 0$ and $a_2 + a_k$, $a_{\frac{k}{2}+1}$ are almost equal, i.e., $|a_2 + a_k - a_{\frac{k}{2}+1}| \leq 2$, then $P_{k+1}^n(a_2, a_3, \ldots, a_k)$ is called a *balanced caterpillar* and denoted by $\mathrm{BC}_{n,k}$. Moreover, the set of all balanced caterpillars of order n and with diameter k is denoted by $\mathcal{BC}_{n,k}$. Similarly, when k is odd, the balanced caterpillar from $\mathcal{BC}_{n,k}$ can be defined in parallel but two central vertices $v_{\frac{k+1}{2}}$ and $v_{\frac{k+3}{2}}$ in P_{k+1} with $|a_2 + a_k - a_{\frac{k+1}{2}} - a_{\frac{k+3}{2}}| \leq 2$ must be considered in the process. As examples, two trees from $\mathcal{BC}_{11,6}$ and $\mathcal{BC}_{12,7}$, respectively, are shown in Figure 4. In the following, we denote by $\mathcal{T}_{n,d}$ the set of trees of order n and with diameter d.

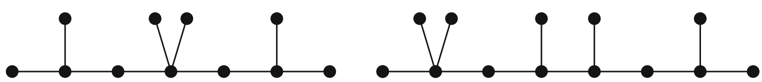

Figure 4 Two trees $T_1 \in \mathcal{BC}_{11,6}$ and $T_2 \in \mathcal{BC}_{12,7}$

If $d = 2$, the set $\mathcal{T}_{n,d}$ contains a single tree, i.e., star S_n with $N(S_n) = n-1$. Only path P_n belongs to $\mathcal{T}_{n,d}$ when $d = n-1$. A tree T of order $n \geq 4$ has diameter 3 if and only if $T \cong \mathrm{DS}_{n_1,n_2}$ where $n_1 + n_2 = n-2$ with NSC number $2(n-2)$ from Corollary 3.6. In the following two theorems we characterize the extremal trees from $\mathcal{T}_{n,d}$ $(4 \leq d \leq n-2)$ with maximal NSC numbers.

Theorem 4.1 *For any tree $T \in \mathcal{T}_{n,d}$ where $d = 2k$ with $4 \leq d \leq n-2$, we have*

$$N(T) \leq nk^2 - \frac{4}{3}k^3 + \frac{k}{3} + (k-1)\left\lfloor \frac{n-2k-2}{2} \right\rfloor \left\lceil \frac{n-2k-2}{2} \right\rceil$$

with equality holding if and only if $T \in \mathcal{BC}_{n,2k}$ with $a_2 + a_{2k} = a_{k+1}$ or $a_{k+1} + 1$.

Proof Let $P_{2k+1} = v_1v_2\cdots v_{2k}v_{2k+1}$ be a diametral path in $T \in \mathcal{T}_{n,d}$ with $4 \leq d = 2k \leq n-2$. In this case, T has only one central vertex v_{k+1}. Then we have $e_i = 2k+1-i = e_{2k+2-i}$ for $i = 1, 2, \ldots, k$ and $e_{k+1} = k$. Therefore, we denote the eccentricity sequence of T by

$$\{(2k)^{(l_1+2)}, (2k-1)^{(l_2+2)}, \ldots, (k+1)^{(l_k+2)}, k^{(1)}\}$$

with $l_i \geq 0$ being integer for $i = 1, 2, \ldots, k$ and $\sum_{i=1}^k l_i = n-2k-1$. By (1.4), we have

$$N(T) = (l_1+2)k + (l_2+2)(k-1) + \cdots + (l_k+2) \times 1 + \sum_{1 \leq i < j \leq k} (l_i+2)(l_j+2)(j-i)$$

$$= k(k+1) + \sum_{i=1}^k l_i(k+1-i) + \sum_{1 \leq i < j \leq k} [l_il_j(j-i) + 2(l_i+l_j)(j-i) + 4(j-i)]$$

$$= k(k+1) + 2\sum_{i=1}^{k-1} i(i+1) + [k + k(k-1)]l_1 + [k-1+(k-1)(k-2)+2\times 1]l_2 + \cdots$$
$$+ l_i[k+1-i+(k+1-i)(k-i)+i(i-1)] + \cdots + l_k[1+k(k-1)] + \sum_{1\le i<j\le k} l_i l_j (j-i)$$
$$= \frac{k(k+1)(2k+1)}{3} + \sum_{i=1}^{k}[(k+1-i)^2 + i(i-1)]l_i + \sum_{1\le i<j\le k} l_i l_j (j-i).$$

Now we define a function

$$f(l_1, l_2, \ldots, l_k) = \sum_{i=1}^{k}[(k+1-i)^2 + i(i-1)]l_i + \sum_{1\le i<j\le k} l_i l_j (j-i)$$

with $l_i \ge 0$ for $i = 1, 2, \ldots, k$ and $\sum_{i=1}^{k} l_i = n - 2k - 1$. Let $A = (a_{ij})_{k\times k}$ be a symmetric matrix of order k whose entry a_{ij} is $\frac{1}{2}|j-i|$ for $1 \le i \le j \le k$. Then we have

$$f(l_1, l_2, \ldots, l_k) = \sum_{i=1}^{k}[(k+1-i)^2 + i(i-1)]l_i + L^T A L \tag{4.1}$$

where $L = (l_1, l_2, \ldots, l_k)^T$ is a column vector with k variables $l_i \ge 0$ for $i = 1, 2, \ldots, k$ and $\sum_{i=1}^{k} l_i = n - 2k - 1$. To determine the maximum of $N(T)$, it suffices to get the maximum of the above function $f(l_1, l_2, \ldots, l_k)$.

Assume that the above function $f(l_1, l_2, \ldots, l_k)$ reaches its maximum at the k-tuple $(l_1^*, l_2^*, \ldots, l_k^*)$. Now we determine the exact value of $(l_1^*, l_2^*, \ldots, l_k^*)$. First we prove the following claim.

Claim 1 $l_i^* = 0$ for $i = 2, \ldots, k-1$.

Proof of Claim 1 For any k-tuple $(l_1, l_2, \ldots, l_k)$ with $l_i \ge 0$ for $i = 1, 2, \ldots, k$ and $\sum_{i=1}^{k} l_i = n - 2k - 1$, if there is at least one number $q \in \{2, 3, \ldots, k-1\}$ such that $l_q \ge 1$, we can get a larger value of $f(l_1, l_2, \ldots, l_q, \ldots, l_k)$ from some transformations on the k-tuple $(l_1, l_2, \ldots, l_k)$ based on the values of l_1 and l_k. If $l_1 \le l_k$, then we replace (l_1, l_q) by (l_1+1, l_q-1) in the k-tuple $(l_1, l_2, \ldots, l_k)$. Set $\nabla_1 = f(l_1+1, l_2, \ldots, l_q-1, \ldots, l_k) - f(l_1, l_2, \ldots, l_q, \ldots, l_k)$. Then, by (4.1), we obtain

$$\nabla_1 = (l_1+1)\sum_{i=1, i\ne q-1}^{k-1} i l_{i+1} + (l_q-1)\sum_{i=1}^{k-q} i l_{q+i} + (l_1+1)(l_q-1)(q-1)$$
$$- \left[l_1 \sum_{i=1, i\ne q-1}^{k-1} i l_{i+1} + l_q \sum_{i=1}^{k-q} i l_{q+i} + l_1 l_q (q-1)\right] + k^2 - (k+1-q)^2 - q(q-1)$$
$$= \sum_{i=1, i\ne q-1}^{k-1} i l_{i+1} - \sum_{i=1}^{k-q} i l_{q+i} + (l_q - l_1 - 1)(q-1) + (2k+1-2q)(q-1)$$
$$= (q-1)(l_{q+1} + \cdots + l_k - l_1 + l_q - 1) + \sum_{i=1}^{q-2} i l_{i+1} + (2k+1-2q)(q-1)$$
$$\ge (q-1)(l_q + l_{q+1} + \cdots + l_{k-1}) + 2(k-q)(q-1) + \sum_{i=1}^{q-2} i l_{i+1} > 0.$$

If $l_1 > l_k$, i.e., $l_1 \geq l_k+1$, then we replace (l_q, l_k) by (l_q-1, l_k+1) in the k-tuple $(l_1, l_2, \ldots, l_k)$. Set $\nabla_2 = f(l_1, l_2, \ldots, l_q - 1, \ldots, l_k + 1) - f(l_1, l_2, \ldots, l_q, \ldots, l_k)$. Thus, from (4.1), we have

$$\begin{aligned}
\nabla_2 &= (l_k+1)\sum_{i=1, i\neq q}^{k-1}(k-i)l_i + (l_q-1)\sum_{i=1}^{q-1}(q-i)l_{q+i} + (l_k+1)(l_q-1)(k-q) \\
&\quad - \left[l_k \sum_{i=1, i\neq q}^{k-1}(k-i)l_i + l_q\sum_{i=1}^{q-1}(q-i)l_i + l_k l_q(k-q)\right] + k(k-1) + 1 - (k+1-q)^2 - q(q-1) \\
&= \sum_{i=1, i\neq q}^{k-1}(k-i)l_i - \sum_{i=1}^{q-1}(q-i)l_{q+i} - (l_k - l_q + 1)(k-q) + (2q-3)(k-q) \\
&= (k-q)(l_1 + \cdots + l_{q-1} - l_k + l_q - 1) + \sum_{i=q+1}^{k-1}(k-i)l_i + (2q-3)(k-q) \\
&\geq \sum_{i=q+1}^{k-1}(k-i)l_i + (2q-3)(k-q) > 0.
\end{aligned}$$

Repeating the above process, we find that any k-tuple $(l_1, l_2, \ldots, l_k)$ can be changed into $(l_1^*, 0, \ldots, 0, l_k^*)$ with $l_1^* + l_k^* = n - 2k - 1$ and $l_1^*, l_k^* \geq 0$ such that $f(l_1^*, 0, \ldots, 0, l_k^*) > f(l_1, l_2, \ldots, l_k)$. Thus we finish the proof of Claim 1.

To obtain the maximum of $f(l_1, l_2, \ldots, l_k)$, by Claim 1, we only need to determine the value of $f(l_1, 0, \ldots, 0, l_k)$ with $l_1, l_k \geq 0$ and $l_1 + l_k = n - 2k - 1$. Without loss of generality, we can assume that $l_1 \geq l_k$. In view of (4.1), we have

$$\begin{aligned}
f(l_1, 0, \ldots, 0, l_k) &= k^2 l_1 + (k^2 - k + 1)l_k + (k-1)l_1 l_k \\
&= k^2(l_1 + l_k) + (k-1)l_k(l_1 - 1) \\
&\leq k^2(n - 2k - 1) + (k-1)\left\lfloor \frac{n-2k-2}{2} \right\rfloor \left\lceil \frac{n-2k-2}{2} \right\rceil
\end{aligned}$$

with equality holding if and only if $l_1 = l_k$ or $l_1 = l_k + 1$. Thus we conclude that $f(l_1, l_2, \ldots, l_k)$ reaches its maximum when $l_i = 0$ for $i = 2, 3, \ldots, k-1$ and $(l_1, l_k) = (\frac{n-2k-1}{2}, \frac{n-2k-1}{2})$ or $(\frac{n-2k}{2}, \frac{n-2k-2}{2})$. Therefore the extremal tree is obtained from P_{2k+1} by attaching l_k pendant vertices to the central vertex v_{k+1} and attaching a_2 and a_{2k} pendant vertices to the vertices v_2 and v_{2k}, respectively, with $a_2 + a_{2k} = l_1$. Considering the definition of the set $\mathcal{BC}_{n,2k}$, we complete the proof of this theorem. □

Now we turn to consider the trees with odd diameter. For any tree T of order n with diameter $2k+1 \geq 5$, we assume that the eccentricity sequence of T is $\{(2k+1)^{(l_1+2)}, (2k)^{(l_2+2)}, \ldots, (k+2)^{(l_k+2)}, (k+1)^{(2)}\}$ with $l_i \geq 0$ for $i = 1, 2, \ldots, k$ and $\sum_{i=1}^{k} l_i = n - 2k - 2$. Then

$$\begin{aligned}
N(T) &= 2(l_1+2)k + 2(l_2+2)(k-1) + \cdots + 2(l_k+2)\times 1 + \sum_{1\leq i<j\leq k}(l_i+2)(l_j+2)(j-i) \\
&= 2k(k+1) + 2\sum_{i=1}^{k-1} i(i+1) + 2\sum_{i=1}^{k} l_i(k+1-i) + \sum_{1\leq i<j\leq k}[l_i l_j(j-i) + 2(l_i+l_j)(j-i)] \\
&= \frac{2k(k+1)(k+2)}{3} + \sum_{i=1}^{k}[(k+1-i)(k+2-i) + i(i-1)]l_i + \sum_{1\leq i<j\leq k} l_i l_j (j-i).
\end{aligned}$$

By a similar reasoning as that in the proof of Theorem 4.1, we obtain that

$$\begin{aligned} N(T) &\le \frac{2k(k+1)(k+2)}{3} + (k^2-k+2)(n-2k-2) + (k-1)(l_k+2)l_1 \\ &\le n(k^2-k+2) - \frac{2}{3}(k+1)(2k^2-5k+6) + (k-1)\left\lfloor \frac{n-2k}{2} \right\rfloor \left\lceil \frac{n-2k}{2} \right\rceil \end{aligned}$$

with both equalities holding if and only if $(l_1, l_2, \dots, l_k) = (\frac{n-2k}{2}, 0, \dots, 0, \frac{n-2k}{2} - 2)$ or $(\frac{n-2k-1}{2}, 0, \dots, 0, \frac{n-2k-3}{2})$. Therefore we arrive at the following theorem and omit its detailed proof here.

Theorem 4.2 *For any tree $T \in \mathcal{T}_{n,d}$ where $d = 2k+1$ with $5 \le d \le n-2$, we have*

$$N(T) \le n(k^2-k+2) - \frac{2}{3}(k+1)(2k^2-5k+6) + (k-1)\left\lfloor \frac{n-2k}{2} \right\rfloor \left\lceil \frac{n-2k}{2} \right\rceil$$

with equality holding if and only if $T \in \mathcal{BC}_{n,2k+1}$ with $a_2 + a_{2k+1} = a_{k+1} + a_{k+2} + 1$ or $a_{k+1} + a_{k+2} + 2$.

Let

$$\begin{aligned} h_1(n,k) &= nk^2 - \frac{4}{3}k^3 + \frac{k}{3} + (k-1)\left\lfloor \frac{n-2k-2}{2} \right\rfloor \left\lceil \frac{n-2k-2}{2} \right\rceil, \\ h_2(n,k) &= n(k^2-k+2) - \frac{2}{3}(k+1)(2k^2-5k+6) + (k-1)\left\lfloor \frac{n-2k}{2} \right\rfloor \left\lceil \frac{n-2k}{2} \right\rceil. \end{aligned}$$

By some simple calculations, we have

$$h_i(n,k) - h_i(n,k-1) > 0 \quad \text{for } i = 1,2. \tag{4.2}$$

Now we determine the NSC number of path P_n. From (1.4), for $n = 2k \ge 6$, we have

$$\begin{aligned} N(P_n) &= 4(1+2+\cdots+k-1) + 4(1+2+\cdots+k-2) + \cdots + 4(1+2) + 4\times 1 \\ &= 2\sum_{q=1}^{\frac{n}{2}-1} q(q+1) \\ &= \frac{(n-2)n(n+2)}{12}. \end{aligned}$$

Similarly, if $n = 2k+1 \ge 5$, we have

$$\begin{aligned} N(P_n) &= 4(1+2+\cdots+k-1) + 2k + 4(1+2+\cdots+k-2) + 2(k-1) \\ &\quad + \cdots + 4(1+2) + 2\times 3 + 4\times 1 + 2\times 2 + 2\times 1 \\ &= 2\sum_{q=1}^{\lfloor \frac{n}{2} \rfloor -1} q(q+1) + \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lfloor \frac{n}{2} \right\rfloor + 1 \right) \\ &= \frac{(n-1)n(n+1)}{12}. \end{aligned}$$

Hereafter we denote

$$f(n) = \begin{cases} \dfrac{(n-2)n(n+2)}{12}, & \text{if } n \ge 6 \text{ is even;} \\ \dfrac{(n-1)n(n+1)}{12}, & \text{if } n \ge 5 \text{ is odd.} \end{cases} \tag{4.3}$$

Therefore it follows that $N(P_n) = f(n)$.

Now we are ready to prove a main result in the following theorem.

Theorem 4.3 *Let T be a tree of order $n \geq 4$. Then we have $N(T) \leq f(n)$ with equality holding if and only if $T \cong P_n$.*

Proof By a computer search we can find that P_n has uniquely the maximal NSC number among all trees of order n where $4 \leq n \leq 7$. Therefore in the following we consider the case when $n \geq 8$. Let $\mathcal{T}_n$ be the set of all trees of order $n \geq 8$. From the definition of the set $\mathcal{T}_{n,d}$, we have $\mathcal{T}_n = \bigcup_{d=4}^{n-2} \mathcal{T}_{n,d} \cup \{S_n, \mathrm{DS}_{n_1,n_2}, P_n\}$ with $n_1 + n_2 = n - 2 \geq 6$. Clearly we find that $N(P_n) > N(\mathrm{DS}_{n_1,n_2}) > N(S_n)$. Hence in the next step we assume that T is a tree of order $n \geq 8$ with diameter d $(4 \leq d \leq n-1)$.

If $d = n-1$, then our result follows trivially. Otherwise, $d \leq n-2$. Then, from Theorems 4.1 and 4.2 and the inequalities in (4.2), we have

$$N(T) < h_i\left(n, \left\lfloor \frac{d}{2} \right\rfloor + 1\right) < h_i\left(n, \left\lfloor \frac{d}{2} \right\rfloor + 2\right) < \cdots < \begin{cases} h_1\left(n, \left\lfloor \dfrac{n-2}{2} \right\rfloor\right); \\ h_2\left(n, \left\lfloor \dfrac{n-3}{2} \right\rfloor\right). \end{cases}$$

Note that $i = 1$ if d is even and $i = 2$ if d is odd in the above inequalities. Moreover, we have $h_1(n, \lfloor \frac{n-2}{2} \rfloor) < N(P_n)$ and $h_2(n, \lfloor \frac{n-3}{2} \rfloor) < N(P_n)$ from the formula in (4.3) and the definitions of $h_i(n,k)$ for $i = 1, 2$. This completes the proof of this theorem. □

A *starlike tree* of order n, denoted by $T_n(n_1, n_2, \ldots, n_k)$ with $\sum_{i=1}^{k} n_i = n - 1$, is a tree obtained by attaching at a single vertex k pendant paths of lengths $n_1, n_2, \ldots, n_k$, respectively. When n_i appears $a_i > 1$ times in $T_n(n_1, n_2, \ldots, n_k)$, we will write as $n_i^{(a_i)}$ for short in it. Let

$$h(n) = \begin{cases} \dfrac{(n-2)[(n-2)(n+4)+2]}{12}, & \text{if } n \geq 6 \text{ is even;} \\ \dfrac{(n-1)(n-3)(n+4)}{12}, & \text{if } n \geq 5 \text{ is odd.} \end{cases} \tag{4.4}$$

In the following theorem we determine the extremal trees with second maximum NSC numbers.

Theorem 4.4 *Let T be tree of order $n > 4$ different from P_n. Then we have $N(T) \leq h(n)$ with equality holding if and only if $T \cong T_n(1^{(2)}, n-3)$.*

Proof Assume that T is a tree of order n different from P_n with diameter d and $N(T)$ as large as possible. Combining Theorems 4.1, 4.2 and the inequalities in (4.2), we claim that the value of $N(T)$ is $h_1(n, \frac{n-2}{2})$ if n is even or $h_2(n, \frac{n-3}{2})$ if n is odd. Moreover, we have $T \cong T_n(1^{(2)}, n-3)$ from the choice of l_1 and l_k in the proof of Theorem 4.1 and in the argument before Theorem 4.2, respectively. By some simple calculations we find that $h(n)$ equals to $h_1(n, \frac{n-2}{2})$ if n is even or $h_2(n, \frac{n-3}{2})$ if n is odd. Thus our result follows immediately. □

Let

$$g(n) = \begin{cases} \dfrac{(n-2)(n^2+2n-12)}{12} + 1, & \text{if } n \geq 6 \text{ is even;} \\ \dfrac{(n-3)(n^2+3n-16)}{12} + 2, & \text{if } n \geq 7 \text{ is odd.} \end{cases} \tag{4.5}$$

Below we determine the extremal trees with third maximum NSC numbers.

Theorem 4.5 *Let T be tree of order $n > 5$ different from P_n and $T_n(1^{(2)}, n-3)$. Then we have $N(T) \leq g(n)$ with equality holding if and only if $T \cong T_n(1, \lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)$.*

Proof Assume that T is a tree of order n other than P_n and $T_n(1^{(2)}, n-3)$ with $N(T)$ as large as possible. In view of Theorems 4.1, 4.2 and the inequalities in (4.2), we claim that T belongs to $\mathcal{BC}_{n,n-3}$ with $N(T) = h_1(n, \frac{n-3}{2})$ if n is odd or $N(T) = h_2(n, \frac{n-4}{2})$ if n is even, or belongs to $\mathcal{T}_{n,n-2} \setminus \{T_n(1^{(2)}, n-3)\}$ with maximum NSC number.

By a similar reasoning as that in the proof of Theorem 4.1, the tree from $\mathcal{T}_{n,n-2}\setminus\{T_n(1^{(2)}, n-3)\}$ with maximum NSC number is $T_n(1, \lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil)$. From the formula (1.4), we have

$$N\left(T_n\left(1, \left\lfloor\frac{n-2}{2}\right\rfloor, \left\lceil\frac{n-2}{2}\right\rceil\right)\right) = \begin{cases} \dfrac{(n-2)(n^2+2n-12)}{12} + 1, & \text{if } n \geq 6 \text{ is even;} \\ \dfrac{(n-3)(n^2+3n-16)}{12} + 2, & \text{if } n \geq 7 \text{ is odd.} \end{cases}$$

Both of them are greater than $h_1(n, \frac{n-3}{2}) = \frac{(n-3)(n^2+3n-16)}{12}$ when n is odd or $h_2(n, \frac{n-4}{2}) = \frac{(n-2)(n-4)(n+6)}{12}$ if n is even from some simple calculations. Thus we complete the proof of this theorem. □

Denote by $\mathcal{G}_{n,d}$ the set of graphs obtained by possibly inserting some new edges between the pendant vertices of balanced caterpillar $\mathrm{BC}_{n,d}$ attached at a same vertex in P_{d+1}. By a very analogous reasoning as that in the proof of Theorems 4.1, 4.2, we conclude that any graph from $\mathcal{G}_{n,d}$ attains uniquely the maximum NSC number among all graphs of order n and with diameter d. Similarly as that in Theorem 4.3, we arrive at the following theorem with omitting its proof.

Theorem 4.6 *Let G be a connected graph of order $n \geq 3$. Then we have $N(G) \leq f(n)$ with equality holding if and only if $G \cong P_n$.*

Recall that a unicyclic graph is a connected graph of order n and with n edges. Denote by $C_k(n-k)$ a graph obtained by attaching at a vertex of C_k a pendant path of length $n-k$. Let $C_k(l_1, l_2)$ be a graph obtained by attaching two pendant paths of lengths l_1 and l_2 to two adajacent vertices of C_k. Clearly, we have $N(T_n(1^{(2)}, n-3)) = N(C_3(n-3))$ since they have the same eccentricity sequence. Moreover, by some elementary calculations, we find that $N(C_3(n-3)) = N(C_3(\frac{n-3}{2}, \frac{n-3}{2}))$ for odd $n \geq 5$. Similarly as above, we obtain the following theorem without proof in which the extremal graphs with second maximum NSC numbers have been determined among all connected graphs.

Theorem 4.7 *Let G be a connected graph of order $n \geq 5$ other than P_n. Then $N(G) \leq h(n)$ with equality holding if and only if G is isomorphic to $T_n(1^{(2)}, n-3)$ or $C_3(n-3)$ and one more graph $C_3(\frac{n-3}{2}, \frac{n-3}{2})$ for odd n.*

Note that $h(n)$ is defined in (4.4) and $N(C_3(n-3)) = h(n)$ and $N(C_3(\frac{n-3}{2}, \frac{n-3}{2})) = h(n)$ for odd $n \geq 5$. The following corollary holds immediately.

Corollary 4.8 *For any unicyclic graph G of order $n \geq 5$, we have $N(G) \leq h(n)$ with equality holding if and only if $G \cong C_3(n-3)$ and one more graph $C_3(\frac{n-3}{2}, \frac{n-3}{2})$ for odd n.*

As introduced in [14], the *double graph* G^* of a given graph G is formed from two copies G' and G'' of G including the vertex set and edge set of each of them by adding edges $v_i'v_j''$ and $v_j'v_i''$ where $v_i', v_j' \in V(G')$ and $v_i'', v_j'' \in V(G'')$ for every edge $v_iv_j \in E(G)$. In the theorem below we give an exact formula of $N(G^*)$ for any connected graph G.

Theorem 4.9 *Let G be a connected graph of order $n \geq 3$ with G^* being its double graph. Then we have $N(G^*) = 0$ if G has maximum degree $n-1$, and $N(G^*) = 4N(G)$ otherwise.*

Proof Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $V(G') = \{v_1', v_2', \ldots, v_n'\}$, $V(G'') = \{v_1'', v_2'', \ldots, v_n''\}$

in G^*. If G has a vertex, say v_1, with degree $n-1$, then $e_G(v_1) = 1$ and $e_G(v_i) \leq 2$ for $i = 2, 3, \ldots, n$. And in G^*, we have $e_{G^*}(v'_1) = 2 = e_{G^*}(v''_1)$ because they are not adjacent and just at the distance 2 in G^*. Moreover, $e_{G^*}(v'_i) = e_{G^*}(v''_i) = 2 \geq e_G(v_i)$ for $i = 2, 3, \ldots, n$. Then G is a self-centered graph with $N(G^*) = 0$.

Otherwise, we have $e_G(v_i) \geq 2$ for $i = 1, 2, \ldots, n$. Then $e_{G^*}(v'_i) = e_{G^*}(v''_i) = e_G(v_i)$ for each $i \in \{1, 2, \ldots, n\}$ from the structure of G^*. From the formula (1.4), we get $N(G^*) = 4N(G)$, finishing the proof of this theorem. □

Recall that $f(n)$ is defined in (4.3). The following corollary is obvious.

Corollary 4.10 *For any non-self-centred graph Gof order $n \geq 3$ with G^* being its double graph, we have $N(G^*) \leq 4f(n)$ with equality holding if and only if $G^* \cong P_n^*$.*

5 Concluding Remarks

In this paper, we have introduced a novel eccentricity-based graph invariant, namely NSC number $N(G)$, together with the third Zagreb eccentricity index $E_3(G)$ of a graph G for indicating the non-self-centrality of graphs.

We focus more on the NSC number of graphs and establish some extremal properties of this graph invariant. In particular, we prove that, for any tree T, $N(T)$ uniquely attains the maximum at $T \cong P_n$ and the minimum value at $T \cong S_n$. From this fact, $N(G)$ is better reasonable than the third Zagreb eccentricity index $E(G)$ which has been shown with only two values: $n-1$ for odd n and $n-2$ for even n for any trees of order $n \geq 3$. Furthermore, we characterize some graphs with first and second minimum NSC numbers, respectively, which are specially eccentricity-based graphs, like ASC graphs, AP and WAP graphs. Moreover, we determine the extremal trees with second and third maximum NSC numbers and some general graphs with larger NSC numbers.

Since $N(G)$ is a newly-introduced graph invariant based on the eccentricity of vertex, only a few (extremal) mathematical results have been obtained on this invariant. As for a new measure for indicating the non-self-centrality of a graph, we would end this paper by proposing several attractive directions for it in the future as follows:

(i) Finding some relations between NSC number and other eccentricity-based graph invariants, like connective eccentricity index [33, 35], or generally distance-based graph invariants such as Wiener index [15, 19], degree distance [23–25], and so on. A challenging problem is to give a relationship between $N(G)$ and $E_3(G)$ for connected graph G, more exactly, to find a sharp upper bound of $N(G)$ in terms of $E_3(G)$ and other graph parameters, like the diameter.

(ii) Exploring some (potential) applications of NSC number to other scientific fields, including (classic or complex) networks, computer science, etc. Possibly, in addition to the present terms (1), (2) and (3), some more ones will be established for NSC number according to the real needs of scientific fields. For this new invariant for measuring the non-self-centrality of a graph (or network), we much expect to see its significant application to related scientific branches.

(iii) Studying the consistent behavior of NSC number of a graph when the addition or deletion of an edge are made on it. Actually, only from the definition of NSC number, it is a bit difficult to find a consistent behavior of it from the deletion or addition of an edge. For example, if $G = C_3(n-3)$ $(n \geq 5)$ including a triangle $C_3 = v_1v_2v_3v_1$ with $d_G(v_1) = d_G(v_2) = 2$,

$d_G(v_3) = 3$ and $d_G(v_n) = 1$, we have $N(G - v_1v_2) = N(G)$, $N(G - v_1v_3) > N(G)$ and $N(G - v_{n-1}v_n) < N(G)$ where v_{n-1} is the unique neighbor of v_n in G. Therefore it will be more interesting to characterize a set of graphs for which we have a consistent effect on NSC number from the deletion or addition of an edge.

(iv) Characterizing some extremal graphs w.r.t. NSC number in a given class of graphs in which some graph parameter is fixed. As a popular topic in extremal graph theory, it is much fundamental to determine the extremal graphs with respect to some graph invariant in a given set of graphs. For this new invariant, there are some interesting topics of this kind to study in the near future. For example, we can determine the extremal trees with maximum NSC numbers among all trees of order n with maximum degree Δ ($2 < \Delta < n - 1$). Probably the corresponding extremal tree will be the broom $T_n(1^{(\Delta-1)}, n - \Delta)$. From Theorem 4.4, the result is trivially true with $\Delta = 3$. But, for the general case of Δ, it seems more difficult for us to characterize the corresponding extremal trees.

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