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Edge eccentric connectivity index of nanothorns

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The edge eccentric connectivity index of a graph G is defined as $\xi_e^c(G)=\sum_{f\in E(G)}\deg_G(f)\varepsilon c_G(f)$, where $\deg_G(f)$ is the degree of an edge f and $ec_G(f)$ is its eccentricity. In this paper, we investigate the edge eccentric connectivity index of a class of nanographs, namely, nanothorns and we present an explicit formula for the edge eccentric connectivity index of nanothorns. The results are applied to compute this eccentricity-related invariant for some important classes of chemical graphs by specializing components of this type of graphs. In addition, an algorithm is designed for calculating the edge eccentric connectivity index of graphs.

Keywords: Edge eccentric connectivity index, Eccentric connectivity index, Eccentricity, Zagreb index, Thorny graph.

INTRODUCTION

Let $G=(V,E)$ be a connected simple graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. If $|V(G)|=n$ and $|E(G)|=q$, we say that G is an (n,q)-graph. The *degree of a vertex* $v\in V(G)$, denoted by $\deg_G(v)$, is the number of edges incident to v. A vertex of degree one is called a *pendent vertex*. The edge incident to a pendent vertex is called a *pendent edge*. The *distance* $d_G(u,v)$ *between two vertices* u and v in G is the length of the shortest path between them. The *eccentricity of a vertex* $u\in V(G)$, denoted by $ec_G(u)$, is the largest distance between u and any other vertex v of G. Let $f=uv$ be an edge in $E(G)$. Then the *degree of an edge* f, denoted as $\deg_G(f)$, is defined to be $\deg_G(f)=\deg_G(u)+\deg_G(v)-2$. For two edges $f_1=u_1v_1$, $f_2=u_2v_2$ in $E(G)$, the *distance between two edges* f_1 and f_2, denoted as $d_G(f_1,f_2)$, is defined to be $d_G(f_1,f_2)=\min\{d_G(u_1,u_2),d_G(u_1,v_2),d_G(v_1,u_2),d_G(v_1,v_2)\}$. The *eccentricity of an edge* f, denoted by $ec_G(f)$, is defined as $ec_G(f)=\max\{d_G(f,e)\,|\,e\in E(G)\}$. The corona product $G\circ H$ of two graphs G and H is defined as the graph obtained by taking one copy of G and $V(G)$ copies of H and joining the ith vertex of G to every vertex in the ith copy of H [3,7]. We will omit the subscript G when the graph is clear from the context.

A topological index is a numerical descriptor of the molecular structure derived from the corresponding (hydrogen-depleted) molecular graph. Various topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [2,14,16-17,19].

The eccentric connectivity index of G, $\xi^c(G)$, proposed by Sharma, Goswami and Madan [24], has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [21-22]. It is defined as

$$\xi^c(G)=\sum_{v\in V(G)}\deg_G(v)ec_G(v),$$

where $\deg_G(v)$ denotes the degree of the vertex v in G and $ec_G(v)$ is the largest distance between v and any other vertex u of G. The quantity $ec_G(v)$ is named as the eccentricity of vertex v in G. In fact, one can rewrite the eccentric connectivity index as

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$$\xi^c(G)=\sum_{uv\in E(G)}\left(ec(u)+ec(v)\right).$$

The total eccentricity of a graph G [18], denoted by $\theta(G)$, is the sum of all the eccentricities of G, that is,

$$\theta(G)=\sum_{v\in V(G)}ec(v).$$

The eccentric connectivity and total eccentricity polynomials of G are defined as

$$\Xi(G,x)=\sum_{v\in V(G)}\deg_G(v)x^{ec_G(v)}, \text{ and}$$

$$\Theta(G,x)=\sum_{v\in V(G)}x^{ec_G(v)},$$

respectively. It is easy to see that the eccentric connectivity index and the total eccentricity of a graph can be obtained from the corresponding polynomials by evaluating their first derivatives at $x=1$.

The edge version of eccentric connectivity index of G, $\xi_e^c(G)$, proposed by Xu and Guo [25], is defined as

$$\xi_e^c(G)=\sum_{f\in E(G)}\deg_G(f)\varepsilon c_G(f),$$

where $\deg_G(f)$ is the degree of an edge f and $\varepsilon c_G(f)$ is its eccentricity.

The Zagreb indices are the most known and widely used topological indices. The first and second Zagreb index of a graph were first introduced by Gutman and Trinajstić [13], defined as

$$M_1(G)=\sum_{v\in V(G)}\deg(v)^2,$$

$$M_2(G)=\sum_{uv\in E(G)}\deg(u)\deg(v),$$

respectively.

The first Zagreb index can be also expressed as a sum over edges of G,

$$M_1(G)=\sum_{uv\in E(G)}\left(\deg_G(u)+\deg_G(v)\right)$$

It is important and of interest to understand how certain invariants of composite graphs are related to the corresponding invariants of the original graphs. The concept of thorny graphs was proposed by Gutman [12]. Let G be a connected graph on n vertices. The thorn graph G^* of G is obtained by attaching p_i new vertices of degree one to the vertex u_i of the graph G, where $p_i>0$ and $i=1,\ldots,n$. The p_i pendent vertices attached to vertex u_i are called the thorns of u_i. Recall the definition of the corona product. In particular, if $p_1=p_2=\ldots=p_n=p$, then the thorny graph $G^*=G\circ\overline{K_p}$, where $\overline{K_p}$ denotes the complement of a complete graph K_p.

The concept of thorn graphs was found in a variety of chemical applications as given in Refs. [4-6,11-12,15,20]. Interesting classes of graphs can also be obtained by specializing the parent graph in thorny graphs. Plerograms and kenograms are the two types of molecular graphs. Molecular graphs will be depicted in a usual way – atoms will be replaced by vertices and bonds by edges. In modern chemical graph theory, the plerograms are molecular graphs in which all atoms are represented by vertices whilst the kenograms are referred to as a hydrogen-suppressed or hydrogen-depleted molecular graphs [1]. The name thorn graphs for plerographs was introduced by Gutman [12]. What Cayley [1] calls a plerogram and Pólya [10] a C-H graph is just a thorn graph [12] and the parent graph would then be referred to as kenogram or a C-graph. In addition, caterpillars are the thorn graphs whose parent graph is a path [9]. For a given graph G, its t-fold bristled graph $Brs_t(G)$ is obtained by attaching t vertices of degree 1 to each vertex of G. This graph can be represented as the corona of G and the complement graph on t vertices $\overline{K_t}$. The t-fold bristled graph of a given graph is also known as its t-thorny graph.

The paper proceeds as follows. In Section 2, the edge eccentric connectivity index of thorn graphs is investigated. Then, the results are applied to compute this eccentricity-related invariant for some important classes of graphs in terms of the underlying parent graph by specializing components and consider some special cases. A polynomial time algorithm is proposed in order to calculate the edge eccentric connectivity index for any simple finite connected graph without loops and multiple edges in Section 3.

MAIN RESULTS

Let G be an (n,m)-graph and G^* be the thorn graph of G with parameters p_i, $p_i>0$, $i=1,\ldots,n$, We let t_{ij} be the jth thorn attached to the vertex u_i of G, where $j=1,\ldots,p_i$. By the definition of thorn graphs, for every edge f in G^*, it holds that

$$\deg_{G^*}(f)=\begin{cases}\deg_G(u_i)+p_i+\deg_G(u_j)+p_j-2,\\ \text{if } f=u_iu_j\in E(G);\\ \deg_G(u_i)+p_i-1,\\ \text{if } f=u_it_{ij} \text{ is a pendent edge in } G^*.\end{cases}$$

and

$$ec_{G^*}(f)=\begin{cases}ec_G(f)+1,\\ \text{if } f\in E(G);\\ ec_G(u_i),\\ \text{if } f=u_it_{ij} \text{ is a pendent edge in } G^*.\end{cases}$$

Now, we start to compute the edge version of eccentric connectivity index of thorn graphs.

Theorem 2.1. Let G be an (n,m)-graph. If G^* is the thorn graph of G with parameters p_i, $p_i>0$, $i=1,\ldots,n$, then

$$\xi_e^c(G^*)=\xi_e^c(G)+M_1(G)-2m+\sum_{f=u_iu_j\in E(G)}(p_i+p_j)\left(ec_G(u_iu_j)+1\right)+\sum_{i=1}^{n}p_i\left(\deg_G(u_i)+p_i-1\right)ec_G(u_i)$$

Proof. By the definition of edge eccentric connectivity index, we have:

$$\xi_e^c(G^*)=\sum_{f\in E(G^*)}\deg_{G^*}(f)ec_{G^*}(f)$$

$$=\sum_{f=u_iu_j\in E(G)}\deg_{G^*}(u_iu_j)ec_{G^*}(u_iu_j)+\sum_{i=1}^{n}\sum_{j=1}^{p_i}\deg_{G^*}(u_it_{ij})ec_{G^*}(u_it_{ij})$$

By substituting the values of parameters due to the definition of thorn graphs, we compute

$$\xi_e^c(G^*)=\sum_{f=u_iu_j\in E(G)}\left(\deg_G(u_i)+p_i+\deg_G(u_j)+p_j-2\right)\left(ec_G(u_iu_j)+1\right)+\sum_{i=1}^{n}\sum_{j=1}^{p_i}\left(\deg_G(u_i)+p_i-1\right)ec_G(u_i)$$

$$=\sum_{f=u_iu_j\in E(G)}\left(\deg_G(u_i)+\deg_G(u_j)-2\right)ec_G(u_iu_j)+\sum_{f=u_iu_j\in E(G)}\left(\deg_G(u_i)+\deg_G(u_j)-2\right)+$$

$$\sum_{f=u_iu_j\in E(G)}(p_i+p_j)ec_G(u_iu_j)+\sum_{f=u_iu_j\in E(G)}(p_i+p_j)+\sum_{i=1}^{n}p_i\left(\deg_G(u_i)+p_i-1\right)ec_G(u_i)$$

Since

$$\sum_{e\in E(G)}\deg_G(e)=\sum_{v\in V(G)}\left(\deg_G(v)\right)^2-2\left|E(G)\right| \quad [8],$$

we get

$$\xi_e^c(G^*)=\xi_e^c(G)+M_1(G)-2m+\sum_{f=u_iu_j\in E(G)}(p_i+p_j)\left(ec_G(u_iu_j)+1\right)+\sum_{i=1}^{n}p_i\left(\deg_G(u_i)+p_i-1\right)ec_G(u_i)$$

Hence, the desired result of $\xi_e^c(G^*)$ holds.

The following corollaries for thorny graphs follow easily by direct calculations.

Corollary 2.1. If G^* is the thorn graph of an (n,m)-graph G with parameters $p_1=p_2=\ldots=p_n=p$, then

$$\xi_e^c(G^*)=\xi_e^c(G)+M_1(G)+2m(p-1)+p\left(\xi^c(G)+(p-1)\theta(G)\right)+2p\sum_{f=u_iu_j\in E(G)}ec_G(u_iu_j).$$

Corollary 2.2. If G^* is the thorn graph of an (n,m)-graph G with parameters $p_1=p_2=\ldots=p_n=1$, then

$$\xi_e^c(G^*)=\xi_e^c(G)+M_1(G)+\xi^c(G)+2\sum_{f=u_iu_j\in E(G)}ec_G(u_iu_j).$$

Observation 2.1.

By Corollary 2.1, the edge eccentric connectivity index of t-fold bristled graph of a given graph G can easily be computed.

Example 2.1. Let G be an (n,m)-graph. Then

$$\xi_e^c(Brs_t(G))=\xi_e^c(G)+M_1(G)+2m(t-1)+t\left(\xi^c(G)+(t-1)\theta(G)\right)+2t\sum_{f=u_iu_j\in E(G)}ec_G(u_iu_j).$$

For the simple bristled graph ($t=1$)

$$\xi_e^c\left(Brs_t\left(G\right)\right)=\xi_e^c\left(G\right)+M_1\left(G\right)+\xi^c\left(G\right)+2\sum_{f=u_iu_j\in E(G)} ec_G\left(u_iu_j\right).$$

From the above formula and Observation 2.1, the edge eccentric connectivity index of the t-fold bristled graph of P_n and C_n can easily be computed.

$$\xi_e^c\left(Brs_t\left(P_n\right)\right)=\begin{cases}\dfrac{3n\left(n\left(t^2+3t+2\right)-8\right)-t\left(2n\left(t+13\right)+t-17\right)+26}{4}, & \text{if } n \text{ is odd;}\\ \dfrac{n\left(3n\left(t^2+3t+2\right)-2\left(t^2+13t+12\right)\right)}{4+4t+6}, & \text{if } n \text{ is even.}\end{cases}$$

and

$$\xi_e^c\left(Brs_t\left(C_n\right)\right)=\begin{cases} n\left(n\left(1+t\left(t+5\right)/2\right)-2t\right), & \text{if } n \text{ is even;}\\ n\left(n-1+t\left(nt-t+3n-3\right)/2\right), & \text{if } n \text{ is odd.}\end{cases}$$

Note that the 2-fold bristled graph of P_4 is the molecular graph related to polyethene.

Table 2.1. Invariants of path and cycle

G	P_n	C_n
$\xi_e^c\left(G\right)$	$\begin{cases}\left(3n^2-16n+21\right)/2, & \text{if } n \text{ is odd;}\\ \left(3n^2-16n+20\right)/2, & \text{if } n \text{ is even.}\end{cases}$	$2n\lfloor (n-2)/2 \rfloor$
$\xi^c\left(G\right)$	$\begin{cases}\left(3n^2-6n+4\right)/2, & \text{if } n \text{ is even;}\\ 3\left(n-1\right)^2/2, & \text{if } n \text{ is odd.}\end{cases}$	$\begin{cases}n^2, & \text{if } n \text{ is even;}\\ n\left(n-1\right), & \text{if } n \text{ is odd.}\end{cases}$
$\theta\left(G\right)$	$\begin{cases}3/4\,n^2-1/2\,n, & \text{if } n \text{ is even;}\\ 3/4\,n^2-1/2\,n-1/4, & \text{if } n \text{ is odd.}\end{cases}$	$\begin{cases}1/2\,n^2, & \text{if } n \text{ is even;}\\ 1/2\,n\left(n-1\right), & \text{if } n \text{ is odd.}\end{cases}$
$M_1\left(G\right)$	$4n-6$	$4n$
$\sum_{f=u_iu_j\in E(G)} ec_G\left(u_iu_j\right)$	$\begin{cases}\left(3n^2-12n+9\right)/4, & \text{if } n \text{ is odd;}\\ \left(3n^2-12n+8\right)/4, & \text{if } n \text{ is even.}\end{cases}$	$n\lfloor (n-2)/2 \rfloor$

COMPUTING THE EDGE ECCENTRIC CONNECTIVITY INDEX OF A GRAPH

In this section, a polynomial time algorithm is proposed in order to calculate the edge eccentric connectivity index for any simple finite undirected connected graph without loops and multiple edges by using the exploration algorithm BFS [23]. The adjacency matrix A is used to store the neighbors of each vertex.

Algorithm. The Edge Eccentric Connectivity Index

```
for all v ∈ V do
        BFS(G,v);
        δ[v] ← 0;
        for all u ∈ V do
                D[v,u] ← dist[u];
                δ[v] ← δ[v] + A[v,u];
        end
end
ξ_e^c(G) ← 0;
for all f1(u1,v1) ∈ E do
        deg_G(f1) ← δ[u1] + δ[v1] − 2
        for all f2(u2,v2) ∈ E do
d_G[f2] ← min{D[u1,u2], D[u1,v2], D[v1,u2], D[v1,v2]}
        end
        ec_G(f1) ← max{d_G[f] | ∀f ∈ E}
        ξ_e^c(G) ← ξ_e^c(G) + deg_G(f1) * ec_G(f1)
end
```

The below function BFS returns the distances from a source vertex v to all other vertices in the graph.

function $BFS(G,v)$;

Input: Graph $G=(V,E)$, start vertex v

Output: for all vertices u reachable from v, dist[u] is set to the distance from v to u

```
for all u ∈ V do
        dist[u] ← ∞;
end
dist[v] ← 0;
Q ← [v];
while Q is not empty do
        u ← eject(Q);
        for all edges (u,w) ∈ E do
                if dist[v] = ∞ then
                        INJECT(Q,v);
                        dist[w] ← dist[u] + 1;
                end
        end
end
```

The Edge Eccentric Connectivity Index calculation algorithm runs in polynomial time. The running time of function BFS(G , v) is $\mathrm{O}(|V|+|E|)$ and the function BFS(G , v) runs for all $v \in V(G)$. Since the binary combinations of the edge set, that are $C(|E|,2)=|E|(|E|-1)/2$, are handled one by one in the algorithm and since $|E| \le |V|(|V|-1)/2$, the complexity for the algorithm described is $\mathrm{O}(|E|^2)=\mathrm{O}(|V|^4)$

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Индекс на ексцентрична реброва свързаност на наноторни

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Индексът на ексцентрична реброва свързаност на един граф G се дефинира като $\xi_e^c(G)=\sum_{f\in E(G)}\deg_G(f)\varepsilon c_G(f)$, където $\deg_G(f)$ е степента на едно ребро f и $ec_G(f)$ е неговата ексцентричност. В тази статия изследваме индекса на ексцентрична реброва свързаност на един клас нанографи, а именно наноторни и представяме една експлицитна формула за индекса на ексцентрична реброва свързаност на наноторни. Резултатите се прилагат за изчисляване на този инвариант, свързан с ексцентричността за някои важни класове химически графи от специализирани компоненти на този тип графи. В допълнение, е конструиран алгоритъм, предназначен за изчисляване на индекса на ексцентричната реброва свързаност на графи.