Some new results on multiplicative topological indices

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Abstract: *As a molecular descriptor, the first multiplicative Zagreb index $\Pi_1(G)$ and Narumi-Katayama index (NK) are defined as product of squares of vertex degrees and usual product of all vertex degrees of graph G respectively. In this paper, we determine upper bound of NK index of G with maximum edge connectivity k. Also we obtain $\Pi_1(G)$ values for two derived graphs namely Mycielski graph and thorn graph.*

Keywords: *First multiplicative Zagreb index, Narumi-Katayama Index, edge connectivity, derived graph.*

AMS Classification: 05C10; 05C35; 05C75

1. Introduction

Molecular descriptors play a significant role in the study of quantitative structure-property and structure-activity relationships of chemical as well as biological compounds. Among them, vertex-based topological indices occupy a particular space for it in mathematical chemistry. A topological index of G is a numerical value or parameter, related to particular structure of G which characterizes its topology i.e. carbon-atom skeleton and remains invariant under isomorphism of graphs.

Over the time, various indices have been defined depending on the demand and purpose to provide and analyse chemical compound viz. hydrocarbons etc. In chemical graph theory, mathematical modelling of certain chemical events are done using graph that is called molecular graph. Molecular graph is a simple graph (having no multiple edges and loops) such that atoms and corresponding bonds between any two atoms are represented by vertices and edges respectively. A graph $G(V,E)$ or G is a collection of vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \epsilon V(G)$, the degree of v denoted by $d_v(G)$ refers number of edges incident on v. G is r-regular if $d_v = r$ for any vertex $v \epsilon V(G)$.

Historically, though Zagreb index was the first vertex-based structure descriptor to be introduced but because of its separate utility measures, it was not regarded as a topological indices at that time and did not attract the attention of mathematicians too. In 1975, Milan Randić put forward the first genuine degree-based topological index called Randić or Connectivity index defined as

$$R = R(G) = \sum_{uv \epsilon E(G)} \left(\frac{1}{\sqrt{d_u d_v}}\right)$$

and latter it was found suitable for drug design i.e. in pharmacology and modelling physico-chemical properties of organic compounds ([8], [14]). After this, the first and second Zagreb Indices defined as

$$M_1(G) = \sum_v {d_v}^2$$

and

$$M_2(G) = \sum_{uv \epsilon E(G)} (d_u d_v)$$

respectively were found useful for quantitative measures of molecular branching of carbon-atom skeleton, chirality, ZE-isomerism in theoretical chemistry. After this, Ernesto Estrada defined another topological index associating the information of number of edges adjacent to each respective edges taken into account and termed it as 'atom-bond connectivity' (ABC) index co-related with the thermodynamic properties of alkanes, particularly its heat of formation [4]. Inspired by several positive outcomes of ABC index, Furtula et al. introduced another new version called 'Augmented Zagreb Index' (AZI). Soon AZI emerged as more prominent as it was much better than ABC index to describe many chemical features of hydrocarbons. Some other topological indices were also defined with time viz. Geometric-Arithmetic index, Harmonic index, Sum-connectivity index etc.

Over the time, the multiplicative versions of the indices were also defined. Todeschini et al. [18] who introduced the multiplicative counterparts of the additive invariants of a graph lead to the definition of first and second multiplicative Zagreb indices. Thus the first multiplicative Zagreb index is defined as

$$\Pi_1 = \Pi_1(G) = \prod_{u \epsilon V(G)} d_G(u)^2$$

And the second multiplicative Zagreb index is defined as

$$\prod_2 = \prod_2(G)=\prod_{uv\in E(G)} d_G(v)d_G(u)$$

In 1984, Narumi and Katayama [5] introduced a "simple topological index" as a multiplicative graph invariant to represent the features of carbon atom skeleton of saturated chemical compounds mainly hydrocarbon. Tomovic and Gutman [21] later recoined it as 'Narumi-Katayama index' or NK index. This Narumi-Katayama index of G denoted by $NK(G)$ is defined as

$$NK(G) = \prod_{v\in V(G)} d_G(u)$$

Clearly $\prod_1(G) = NK^2$. In this paper, we have determine upper bounds of NK index of graph G with maximum connectivity k. Also we compute first multiplicative Zagreb index of two derived graphs viz. Mycielski graph and thorn graph.

2. Some Preliminary results

Proposition 2.1. *For* $m \geq 0$, $f(x) = \frac{(x+m)^x}{((x-1)+m)^{x-1}}$ *is an increasing function of* x.

Proposition 2.2. *Let* $u, v \in V(G)$ *and* $uv \notin E(G)$, *then*

$$NK(G) < NK(G+uv).$$

Proposition 2.3. *Let* $f(x) = \frac{x}{x+k}$, *then* $f(x)$ *is an increasing function of* x *for* $k \geq 1$.

Proposition 2.4. *(Arithmetic mean and Geometric mean) Let* $x_1, x_2, \cdots, x_n$ *be non-negative numbers, then* $\left(\frac{x_1+x_2+\cdots+x_n}{n}\right)^n \geq x_1 x_2 \cdots x_n$.

3. Upper bounds of NK index with connectivity at most k

Let G_1 and G_2 be two graphs with disjoint point sets i.e. $V(G_1) \cap V(G_2) = \varphi$, then the join of the two graphs denoted by $G_1 \oplus G_2$ is a unique graph with vertex set $V(G_1) \cup V(G_2)$ and edge set having all edges of the form

$$E(G_1) \cup E(G_2) \cup \{e_{uv} | u \in V(G_1), v \in V(G_2)\}$$
.

. For any set of vertices of G, the vertex induced subgraph or simply an induced subgraph $< S >$ is the maximal subgraph of G with vertex set S. A complete induced subgraph of a graph is called a clique. Again, for a graph G and vertex $v \in V(G)$, the neighbour set or neighbourhood $N(v)$ of v is the set of vertices (other than v) such that

$$N(v) = \{w \in V(G) | \ v \neq w, \exists\ e \in E(G): e =< v, w >\}$$

. For $k \geq 1$, a graph G is said to be $k-$ vertex connected if either G is a complete graph K_{k+1} i.e. minimum k vertices have to remove to disconnect the graph or there exist at least $(k+2)$ vertices of G with no $(k-1)$ vertex cut. Similarly, G is $k-$ edge connected ($k \geq 1$) if it has at least two vertices and contains no $(k-1)-$ edge cut. The maximum value of k for which G is $k-$ connected is said to be the connectivity of the graph and it is denoted by $\kappa(G)$ and $\kappa'(G)$ in case of vertex and edge connectivity respectively.

Lemma 3.1. *Let* $G(j, n-k-j) = A_j \oplus H_k \oplus A_{n-k-j}$ *be a graph with* n *vertices in which* A_j *and* A_{n-k-j} *are cliques, and* H_k *is a graph with* k *vertices. Then provided* $k \geq 1$ *and* $2 \leq j \leq \frac{n-k}{2}$, *we have*

$$NK(G(j, n-k-j)) < NK(G(1, n-k-1))$$

Proof. Let us consider that $G_1 = (j, n-k-j)$ and $G_2 = (j-1, n-k-j+1)$. It is obvious that for $v \in V(H_k)$ in G_2, $d_{G_2}(v) = d_{G_1}(v)$; $v \in V(A_{j-1})$ in G_2, $d_{G_2}(v) = d_{G_1}(v) - 1 = j+k-2$ and for $v \in V(A_{n-k-j+1})$ in G_2, $d_{G_2}(v) = d_{G_1}(v) + 1 = n-j$. Hence

$$\frac{NK(G_1)}{NK(G_2)} = \frac{\prod_{v\in V(A_j)} d_v \prod_{v\in V(H_k)} d_v \prod_{v\in V(A_{n-k-j})} d_v}{\prod_{v\in V(A_{j-1})} d_v \prod_{v\in V(H_k)} d_v \prod_{v\in V(A_{n-k-j+1})} d_v}$$

$$= \frac{(j+k-1)^j (n-j-1)^{n-k-j}}{(j+k-2)^{j-1}(n-j)^{n-k-j+1}}$$

$$= \frac{\frac{(j+(k-1))^j}{((j-1)+(k-1))^{j-1}}}{\frac{((n-j-k+1)+(k-1))^{n-k-j+1}}{((n-j-k)+(k-1))^{n-k-j}}}$$

Since $2 \leq j \leq \frac{n-k}{2}$ such that $j < n-k-j+1$, therefore we have $\frac{NK(G_1)}{NK(G_2)}1$ i.e. $NK(G_1) < NK(G_2)$ [from proposition 2.1] and recursively using the same procedure, we obtain

$$NK(G(j, n-k-j)) < NK(G(j-1, n-k-j+1)) < NK(G(j-2, n-k-j+2)) < \cdots < NK(G(1, n-k-1))$$
.

Lemma 3.2. *Let* G *be a connected graph such that* $u, v \in V(G)$. *Suppose that* $u_1, u_2, \cdots, u_k \in N(u) \backslash N((v)$ *and* $1 \leq k \leq d(u)$. *Let* $G' = G - \{uu_1, uu_2, \cdots, uu_k\} + \{vu_1, vu_2, \cdots vu_k\}$. *Then if* $d(v) \geq d(u)$ *and* v *and* u *are not adjacent to each other,*

$$NK(G) > NK(G')$$

Proof. We have,

$$\frac{NK(G)}{NK(G')} = \frac{d_u d_v}{(d_u-k)(d_v+k)} = \frac{\left(\frac{d_v}{d_v+k}\right)}{\left(\frac{d_u-k}{d_u}\right)}$$

$$= \frac{\left(\frac{d_v}{d_v+k}\right)}{\left(\frac{d_u-k}{(d_u-k)+k}\right)}$$

As $d_v \geq d_u > d_u - k$, it implies that

$\frac{d_v}{d_v+k} > \frac{d_u-k}{(d_u-k)+k}$ [from proposition 2.3] Hence $NK(G) > NK(G')$ is established.

Let $\mathbb{V}_n^k$ and $\mathbb{E}_n^k$ be the set of graphs having n vertices with connectivity almost k such that $\kappa(G) \leq k \leq n-1$ and $\kappa'(G) \leq k \leq n-1$ respectively.

Theorem 3.3. *For any graph G in $\mathbb{V}_n^k$, we have*

$$NK(G) \leq k(n-1)^k(n-2)^{n-k-1}$$

with equality holds for $G \cong K_n^k$.

Proof. The sequence of degrees in K_n^k is $k, \underbrace{n-2, n-2, \cdots, n-2}_{n-k-1}, \underbrace{n-1, n-1, \cdots, n-1}_{k}$.

Therefore we obtain

$$NK(K_n^k) = k(n-1)^k(n-2)^{n-k-1}.$$

So it is sufficient to proof that $NK(G) \leq NK(K_n^k)$ and equality establish if and only if $G \cong K_n^k$.

Now, for $k = n-1$, we get $G \cong K_n^{n-1} = K_n$ and hence the theorem the true.

For $1 \leq k \leq n-2$, then we consider a graph $\bar{G}$ in $\mathbb{V}_n^k$ such that $NK(\bar{G})$ is maximum.

Obviously, $\bar{G} \ncong K_n$ (for $1 \leq k \leq n-2$)

Therefore , $\bar{G}$ has a vertex cut set of size k. Let $V' = \{v'_1, v'_2, \cdots, v'_k\}$ be the set of cut vertex of $\bar{G}$. Let us denote $\omega(\bar{G} - V')$ be the number of components of ($\bar{G} - V'$). Hence we claim the followings:

Claim 1. *$\omega(\bar{G} - V')$=2*

Proof. We proof it by method of contradiction.

If possible, let $\omega(\bar{G} - V') \geq 3$ and let $G_1, G_2, \cdots, G_{\omega(\bar{G}-V')}$ be the components of $(\bar{G} - V')$. As $\omega(\bar{G} - V') \geq 3$, we can choose vertices $v \in V(G_1)$ and $u \in V(G_2)$ such that V' is still a k-vertex cut of $\bar{G} + uv$. Therefore $NK(\bar{G} + uv) > NK(\bar{G})$ [from proposition 2.2] which is a contradiction to our choice of $\bar{G}$. Hence the claim is established.

Without loss of generality (WLOG), assume that $(\bar{G} - V')$ has two connected components namely G_{11} and G_{12}.

Claim 2. *The induced subgraph of $V(G_{11}) \cup V'$ and $V(G_{12}) \cup V'$ in $\bar{G}$ are complete subgraphs.*

Proof. Again we will proof it by method of contradiction. Let us assume that $\bar{G}[V(G_{11}) \cup V']$ is not a complete subgraph of $\bar{G}$. Then there exists $uv \notin \bar{G}[V(G_{11}) \cup V']$. As $\bar{G}[V(G_{11}) \cup V'] + uv \in \mathbb{V}_n^k$, therefore we get $NK(\bar{G}[V(G_{11}) \cup V'] + uv) > NK(\bar{G}[V(G_{11}) \cup V'])$ [from proposition 2.2], which is a contradiction. Hence the claim.

Therefore G_{11} and G_{12} are two complete subgraph of $\bar{G}$. Let $G_{11} = K_n{}'$ and $G_{12} = K_n{}''$. Thus

$$\bar{G} = K_n{}' \oplus \bar{G}[V'] \oplus K_n{}''$$

Claim 3. $n' = 1$ *or* $n'' = 1$

Proof. If possible, let $n', n'' \geq 2$. Therefore WLOG $n' \leq n''$. Then by lemma 3.1, we get a new graph $\bar{G}' = K_1 \oplus \bar{G}[V'] \oplus K_{n-k-1}$ such that $NK(\bar{G}') > NK(\bar{G})$ and $\bar{G}' \in \mathbb{V}_n^k$ which is a contradiction to our choice of $\bar{G}$ such that $NK(\bar{G})$ is maximal. Hence either $n' = 1$ or $n'' = 1$ and the claim is established.

Therefore,

$NK(K_1 \oplus K_{|H_k|} \oplus K_{n-k-1}) > NK(K_1 \oplus \bar{G}[V(H_k)] \oplus K_{n-k-1})$

[from proposition 2.2] where $V' = H_k$. Since

$$K_n^k = NK(K_1 \oplus K_{|V'|} \oplus K_{n-k-1})$$

hence $NK(K_n^k)$ is maximal and hence the theorem is proofed.

4. First Multiplicative Zagreb index of some derived graphs

Now we calculate the First multiplicative Zagreb Index of the Mycielski graph $\mu(G)$ of a given graph G and thorn graph respectively.

4.1. The Mycielski Graph

The Mycielski graph $\mu(G)$ of G contains G itself as an isomorphic subgraph and additional $(n+1)$ vertices; a vertex u_i corresponding to each vertex v_i and additional vertex w. Each vertex u_i is connected by an edge to the vertex w, so that these vertices form a subgraph in the form of a star $K_{1,n}$. In addition, for each edge v_iv_j of G, the Mycielski graph includes two edges u_iv_j and v_iu_j. So, the vertex set of $\mu(G)$ is $V(\mu(G)) = V(G) \cup X \cup \{w\}$ where $V(G) = \{v_1, v_2, \cdots, v_n\}$ and $X = \{u_1, u_2, \cdots, u_n\}$. Edge set $E(\mu(G)) = E(G) \cup \{v_iu_j | v_iv_j \in E(G)\} \cup \{u_jw | 1 \leq j \leq n\}$. Hence if the initial graph G has n vertices and m edges, then the The Mycielski graph $\mu(G)$ of G contains $(2n+1)$ vertices and $(3m+n)$ edges.

Theorem 4.1.1. *The first multiplicative Zagreb index of Mycielski graph $\mu(G)$ of G satisfies the inequality*

$$\prod_1(\mu(G)) \leq n^2 4^n r^{2n} \left(\frac{2m+n}{n}\right)^{2n}$$

with equality holds if and only if G is a $r-$ regular graph.

Proof. Let for any non-trivial graph G, $|V(G)| = n$ and $|E(G)| = m$ and let $\mu(G)$ be its Mycielski graph. For each $i, i \in \{1,2,\cdots n\}$, $d_{\mu(G)}(v_i) = 2d_G(v_i)$, $d_{\mu(G)}(u_i) = d_G(v_i) + 1$ and $d_{\mu(G)}(w) = n$. Then first multiplicative Zagreb index of $\mu(G)$ is calculated as

$$\prod_1(\mu(G)) = \left(d_{\mu(G)}(w)\right)^2 \prod_{i=1}^{n}\left(d_{\mu(G)}(v_i)\right)^2 \prod_{i=1}^{n}\left(d_{\mu(G)}(u_i)\right)^2$$

$$= \left(d_{\mu(G)}(w)\right)^2 \prod_{i=1}^{n} 2(d_G(v_i))^2 \prod_{i=1}^{n}(d_G(v_i)+1)^2$$

$$= n^2 4^n \prod_{i=1}^{n}(d_G(v_i))^2 \prod_{i=1}^{n}(d_G(v_i)+1)^2$$

$$= n^2 4^n \prod_1(G) \prod_{i=1}^{n}(d_G(v_i)+1)^2$$

Now,

$$\prod_{i=1}^{n}(d_G(v_i)+1)^2 = \left(\prod_{i=1}^{n}(d_G(v_i)+1)\right)^2$$

$$\leq \left\{\left(\frac{1}{n}\sum(d_G(v_i)+1)\right)^n\right\}^2$$

$$= \left(\frac{\sum(d_G(v_i)+1)}{n}\right)^{2n}$$

$$= \left(\frac{2m+n}{n}\right)^{2n}$$

Therefore, $\prod_1(\mu(G)) \leq n^2 4^n \prod_1(G)\left(\frac{2m+n}{n}\right)^{2n}$ and equality holds if and only if G is $r-$ regular graph where

$$\prod_1(\mu(G)) = n^2 4^n r^{2n}\left(\frac{2m+n}{n}\right)^{2n} = n^2 4^n r^{2n}(r+1)^{2n}$$

(as for r -regular graph , we have $r = \frac{2m}{n}$).

4.2. Thorn Graphs

Thorn graphs denoted by G^T was first introduced by Gutman [9] and it is derived from initial graph G by adding a number of thorns or edges to each vertex of G. Here vertex set of G^T, $V(G^T) = V(G) \cup V_1 \cup \cdots \cup V_n$ where V_i, $i = 1,2,\cdots,n$ be the set of vertices of degree one joined to the vertex v_i in G^T. Thus if v_{ij} represents the vertices of the set V_i for $i = 1,2,\cdots,n$ and $j = 1,2,\cdots,k_i$, then $d_{G^T}(v_i) = d_G(v_i) + k_i$ and $|V(G^T)| = n + p$ where $p = \sum_{i=1}^{n} k_i$.

Theorem 4.2.1. *The first multiplicative Zagreb index of G^T satisfies the following inequality*

$$\prod_1(G^T) = \left(\frac{2m+p}{n}\right)^{2n}$$

with equality holds if and only if $d_G(v_1) + k_1 = d_G(v_2) + k_2 = \cdots d_G(v_n) + k_n$.

Proof. As

$$\prod_1(G^T) = \prod_{i=1}^{n} d_{G^T}(v_i)^2$$

$$= \prod_{i=1}^{n}(d_G(v_i) + k_i)^2$$

$$\leq \left\{\left[\frac{1}{n}\sum(d_G(v_i) + k_i)\right]^n\right\}^2$$

$$= \left(\frac{2m+p}{n}\right)^{2n} \quad \text{[from proposition 2.4]}$$

And clearly the above equality holds if and only if $d_G(v_1) + k_1 = d_G(v_2) + k_2 = \cdots d_G(v_n) + k_n$ (since G^T is regular itself.

Corollary 4.2.2. *Let G^T be thorn graph where $k_i = t$, for all i. Then*

$$\prod_1(G^T) \leq \left(\frac{2m}{n} + t\right)^{2n}$$

with equality holds if G is a regular graph.

Proof. As

$$\prod_1(G^T) = \prod_{i=1}^{n}(d_G(v_i) + t)^2$$

$$\leq \left(\frac{\sum(d_G(v_i)+t)}{n}\right)^{2n} \quad \text{[from proposition 2.4]}$$

$$= \left(\frac{2m+tn}{n}\right)^{2n} = \left(\frac{2m}{n} + t\right)^{2n}$$

and for $r-$ regular graph $\prod_1(G^T) = (r+t)^{2n}$.

Corollary 4.2.3. *Let Let G^T be thorn graph where k_i (≥ 1) is equal to the degree of the corresponding vertex v_i for all i, then*

$$\prod_1(G^T) \leq \left(\frac{4m}{n}\right)^{2n}$$

with equality exists if G is a regular graph.

Conclusion

In recent times, vertex-based multiplicative topological indices have drawn the attention along with other topological indices. In this paper, we have computed some upper bound of NK index with connectivity at most k. Similarly, lower bounds and some sharp bounds can also be computed for the same index. For further study first multiplicative Zagreb index of some other derived graph viz. subdivision graphs, double graphs and extended double graph etc. and for different composite graphs can also be computed.

Acknowledgement

We convey our sincere thanks to Dr. Ankur Bharali, Assistant Professor, Department of Mathematics, Dibrugarh University for his guidance and supervision throughout our research.

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