

On computing the general Narumi-Katayama index of some graphs

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Abstract

The Narumi-Katayama index was the first topological index defined by the product of some graph theoretical quantities. Let G be a simple graph with vertex set $V = \{v_1, \dots, v_n\}$ and $d(v)$ be the degree of vertex v in the graph G . The Narumi-Katayama index is defined as $NK(G) = \prod_{v \in V} d(v)$. In this paper, the Narumi-Katayama index is generalized using a n -vector x and it is denoted by $GNK(G, x)$ for a graph G . Then, we obtain some bounds for GNK index of a graph G by terms of clique number and independent number of G . Also we compute the GNK index of splice and link of two graphs. Finally, we use from our results to compute the GNK index of a class of dendrimers.

Keywords : Narumi-Katayama index; Molecular graph; Clique number; Independent number; Dendrimers.

1 Introduction

By a graph G we mean a finite, connected, undirected with neither loops nor multiple edges. Specifically, let $G = (V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, \dots, v_n\}$ of order n and the edge set $E(G)$. For graph theoretic terminology we follow [19]. We denote the degree of a vertex v in G by $d(v)$ or $d_G(v)$, which is the number of edges incident to v . A graph G is complete if there is an edge between every pair of the vertices of G , i.e. a graph G is called complete if any two different vertices of G are adjacent. A complete graph on n vertices is denoted by K_n . A subset X of the vertices of a graph G is called independent if there is no edge with two endpoints in X . A graph G is called bipartite if its vertex set can be partitioned into two subsets X and Y such that every edge of G has one endpoint in X and the other endpoint in Y . A clique in a graph is a set of mutually adjacent vertices. The maximum

size of a clique in a graph G is called the clique number of G and denoted by $\omega(G)$. A topological index is a number invariant under automorphisms of the graph under consideration. In [16] Narumi and Katayama considered the product of $d(v)$ over all degrees of vertices in G as "simple

topological index". Then the papers, mostly used from the name "Narumi-Katayama index" for this index. So we use from it in this paper, too. Also we denote the Narumi-Katayama index by NK . Thus, if G is a graph, then $NK(G) = \prod_{v \in V(G)} d_G(v)$. In [6, 8], the authors investigated some properties of this topological index, but the main mathematical properties of NK index was reported by Klein and Rosenfeld [14]. This paper makes a new start on research about mathematical properties and chemical meaning of NK index. We encourage the interested readers to consult [3, 7, 12, 15, 18] and references therein for computational techniques as well as mathematical properties of topological indices. Let G be a graph and $V(G) = \{v_1, \dots, v_n\}$. Consider the vector $x = [x_1, \dots, x_n]$ such that x_i 's,

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($1 \leq i \leq n$), are positive integers. To generalize the Narumi-Katayama index, we define the general Narumi-Katayama index, GNK , for the graph G as below:

$$GNK(G, x) = \prod_{i=1}^n (d_G(v_i))^{x_i}.$$

Therefore, one can see that $GNK(G, j) = NK(G)$, where $j = [1, \dots, 1]$. Also, if G is a graph, then the first multiplicative Zagreb index defined as $\Pi_1(G) = \prod_{i=1}^n (d_G(v_i))^2$, (for more details see [6]). So, $GNK(G, 2j) = \Pi_1(G)$. The second multiplicative Zagreb index [11], $\Pi_2(G)$, or the modified Narumi-Katayama index [5], $NK^*(G)$, are defined as $\prod_{i=1}^n (d_G(v_i))^{d_G(v_i)}$. So, it is easy to see that $GNK(G, d) = \Pi_2(G) = NK^*(G)$, in which $d = [d_G(v_1), \dots, d_G(v_n)]$. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [17]. One of the important classes of molecular graphs is dendrimers. Dendrimers are a new class of polymeric materials. They are highly branched, mono disperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior, dendrimers are suitable for a wide range of biomedical and industrial applications [13]. Recently, many papers are constructed to investigate the topological indices of dendrimers, for more details we refer to [1, 2, 9, 10]. In this paper, we obtain a relation between GNK index of a graph and its clique number and its independent number. Also we compute the GNK index of splice and link of two graphs, then we using them to compute the GNK index of a class of dendrimers.

2 Some Properties of GNK Index of Graphs

In this section, we compute GNK index of the sun of a graph. Then we obtain some bounds for GNK index of a graph G by terms of its clique number and its independent number. Also we generalize the formula for the

first and the second multiplicative Zagreb index of splice and link of two graphs in [11]. Let G be a graph with $V(G) = \{v_1, \dots, v_n\}$, add new vertices $\{u_1, \dots, u_n\}$ together with new edges $\{v_i u_i : 1 \leq i \leq n\}$ to G . Then the resulting graph is called sun and we denote it by $sun(G)$. Also, if we add to G the new vertices $\{u_{1,1}, \dots, u_{1,r}, \dots, u_{n,1}, \dots, u_{n,r}\}$ together with new edges $\{v_i u_{i,j} : 1 \leq i \leq n, 1 \leq j \leq r\}$, we denote the resulting graph by $sun(G, r)$. Thus, it is easy to see that $sun(G, 1) = sun(G)$.

Theorem 2.1 *If G is a graph such that $V(G) = \{v_1, \dots, v_n\}$, then*

$$GNK(sun(G, r), x) = \prod_{i=1}^n (d_G(v_i) + r)^{x_i}.$$

Since the degree of each vertex $u_{i,j} \in V(sun(G))$, $1 \leq i \leq n, 1 \leq j \leq r$, is equal to 1, we have:

$$\begin{aligned} &GNK(sun(G, r), x) \\ &= \prod_{i=1}^n (d_{sun(G,r)}(v_i))^{x_i} \prod_{j=1}^r (d_{sun(G,r)}(u_{i,j}))^{x_{i,j}} \\ &= \prod_{i=1}^n (d_G(v_i) + r)^{x_i} \prod_{j=1}^r (1)^{x_{i,j}} \\ &= \prod_{i=1}^n (d_G(v_i) + r)^{x_i}. \end{aligned}$$

Example 2.1 *A caterpillar tree or caterpillar is a tree in which all the vertices are within distance 1 of a central path. If each vertex of the central path P_n has r pendant edges, we denote this caterpillar by $cat(r)$. Therefore, it is easy to see that $cat(r) = sun(P_n, r)$. Now, by Theorem 2.1, we have $GNK(cat(r), x) = GNK(sun(P_n, r), x)$ and so*

$$\begin{aligned} GNK(cat(r), x) &= \prod_{i=1}^n (d_{P_n}(v_i) + r)^{x_i} \\ &= (1 + r)^{x_1 + x_n} \prod_{i=2}^{n-1} (2 + r)^{x_i}. \end{aligned}$$

Theorem 2.2 *Let G be a connected graph and $\omega(G) = t$. Then $GNK(G, x) \geq (t - 1)^{\sum_{i=1}^t x_i}$ and the equality holds if and only if $G = K_t$.*

In graph G , let $C = \{v_1, \dots, v_t\}$ be a subset of vertices of G in which C is a clique. Since C is a clique, we have $d_G(v_i) \geq t - 1$, $(1 \leq i \leq t)$, and so

$$\begin{aligned} GNK(G, x) &= \prod_{i=1}^n (d_G(v_i))^{x_i} \\ &\geq \prod_{i=1}^t (d_G(v_i))^{x_i} \geq \prod_{i=1}^t (t-1)^{x_i} \\ &= (t-1)^{\sum_{i=1}^t x_i}. \end{aligned}$$

If the equality in the previous inequality holds, since $\omega(G) = t$, it implies that G has exactly t vertices in which they are mutually joined by an edge. Thus, G is a complete graph with t vertices. The proof of other side is straightforward.

Theorem 2.3 *If G is a connected graph with n vertices and $\alpha(G) = t$, such that $\{v_1, \dots, v_t\}$ is an independent set of G , then $GNK(G, x) \leq (n-t)^{\sum_{i=1}^t x_i} (n-1)^{\sum_{i=t+1}^n x_i}$ and the equality holds if and only if $G = K_n - E(K_t)$.*

Since $I = \{v_1, \dots, v_t\}$ is an independent set of G , so $d_G(v_i) \leq n - t$, $(1 \leq i \leq t)$, and $d_G(v_j) \leq n - 1$, $(t + 1 \leq j \leq n)$. Therefore,

$$\begin{aligned} GNK(G, x) &= \prod_{i=1}^n (d_G(v_i))^{x_i} \\ &= \left(\prod_{i=1}^t (d_G(v_i))^{x_i} \right) \left(\prod_{j=t+1}^n (d_G(v_j))^{x_j} \right) \\ &\leq \prod_{i=1}^t (n-t)^{x_i} \prod_{j=t+1}^n (n-1)^{x_j} \\ &= (n-t)^{\sum_{i=1}^t x_i} (n-1)^{\sum_{j=t+1}^n x_j}. \end{aligned}$$

In the above inequality, if the equality is hold, then for each vertex $v \in I$, $d_G(v) = n - t$ and for each $v \in V(G) - I$, $d_G(v) = n - 1$. So each vertex in $V(G) - I$ is joined to all of vertices in G and since I is an independent set, each vertex in I is joined only to each vertex in $V(G) - I$. These mean that G is isomorphic to a complete graph K_n in which the edges of K_t are removed from it. The proof of other side is straightforward.

Suppose that G and H are two graphs of order n and m , respectively. Also, $x = [x_1, \dots, x_n]$ and

$y = [y_1, \dots, y_m]$ are two vectors such that they are associated to G and H , respectively. For given vertices $v_n \in V(G)$ and $u_1 \in V(H)$ a splice of G and H by vertices v_n and u_1 , $(G \bullet H)(v_n, u_1)$, is defined by identifying the vertices v_n and u_1 in the union of G and H . Also we construct the vector $s = [x_1, \dots, x_{n-1}, x_n + y_1, y_2, \dots, y_m]$ from the vectors x and y to associate it to graph $(G \bullet H)(v_n, u_1)$. Similarly, a link of G and H by vertices v_n and u_1 is defined as the graph $(G \sim H)(v_n, u_1)$ obtained by joining v_n and u_1 by an edge in the union of these graphs [4]. Also we associate the vector $l = [x_1, \dots, x_n, y_1, y_2, \dots, y_m]$ to the graph $(G \sim H)(v_n, u_1)$. In Theorem 2.5, we generalize the Theorem 2 and the Theorem 3 in [6].

Theorem 2.4 *If G and H are two graphs with n and m number of vertices, respectively, then*

$$\begin{aligned} &GNK((G \bullet H)(v_n, u_1), s) \\ &= \frac{(d_G(v_n) + d_H(u_1))^{x_n + y_1}}{(d_G(v_n))^{x_n} (d_H(u_1))^{y_1}} \\ &\times GNK(G, x) GNK(H, y). \\ &GNK((G \sim H)(v_n, u_1), l) \\ &= \frac{(d_G(v_n) + 1)^{x_n} (d_H(u_1) + 1)^{y_1}}{(d_G(v_n))^{x_n} (d_H(u_1))^{y_1}} \\ &GNK(G, x) GNK(H, y). \end{aligned}$$

Let G and H be two graphs such that $V(G) = \{v_1, \dots, v_n\}$ and $V(H) = \{u_1, \dots, u_m\}$. We have

$$\begin{aligned} &GNK((G \bullet H)(v_n, u_1), s) \\ &= \prod_{i=1}^{n-1} (d_{(G \bullet H)(v_n, u_1)}(v_i))^{x_i} \\ &\times \prod_{j=2}^m (d_{(G \bullet H)(v_n, u_1)}(u_j))^{y_j} \\ &\times (d_G(v_n) + d_H(u_1))^{x_n + y_1} \\ &= \prod_{i=1}^{n-1} (d_G(v_i))^{x_i} \prod_{j=2}^m (d_H(u_j))^{y_j} \\ &\times (d_G(v_n) + d_H(u_1))^{x_n + y_1} \\ &= \frac{(d_G(v_n) + d_H(u_1))^{x_n + y_1}}{(d_G(v_n))^{x_n} (d_H(u_1))^{y_1}} \\ &\times GNK(G, x) GNK(H, y) \end{aligned}$$

Similarly,

$$\begin{aligned}
 &GNK((G \sim H)(v_n, u_1), l) \\
 &= \prod_{i=1}^n (d_{(G \sim H)(v_n, u_1)}(v_i))^{x_i} \\
 &\times \prod_{j=1}^m (d_{(G \sim H)(v_n, u_1)}(u_j))^{y_j} \\
 &= \prod_{i=1}^{n-1} (d_G(v_i))^{x_i} \prod_{j=2}^m (d_H(u_j))^{y_j} \\
 &\times (d_G(v_n) + 1)^{x_n} (d_H(u_1) + 1)^{y_1} \\
 &= \frac{(d_G(v_n) + 1)^{x_n} (d_H(u_1) + 1)^{y_1}}{(d_G(v_n))^{x_n} (d_H(u_1))^{y_1}} \\
 &\times GNK(G, x) GNK(H, y).
 \end{aligned}$$

3 GNK Index of a Class of Dendrimers

In this section we use some of our results in Section 2 to compute the general Narumi-Katayama index of some dendrimer nanostars. To do this, we start with a class of dendrimers such that they have an inductive structure and are denoted by $D'_1[n]$, (see [1]). In computer science, a binary tree is a tree data structure in which each node has at most two child nodes, usually distinguished as left and right. Nodes with children are parent nodes, and child nodes may contain references to their parents. Outside the tree, there is often a reference to the root node (the ancestor of all nodes), if it exists. Any node in the data structure can be reached by starting at root node and repeatedly following references to either the left or right child. The graph $D'_1[3]$ is shown in Figure 1.

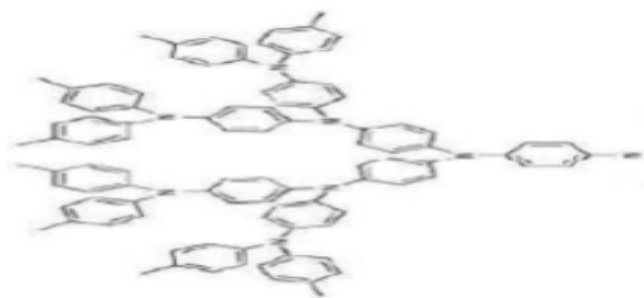


Figure 1: The graph $D'_1[3]$.

Theorem 3.1 If $x = k_j$, $k \in \mathbb{N}$ and $j = [1, \dots, 1]$, then

$$GNK(D'_1[n], x) = 2^{k(2^{n+3}-4)} 3^{k(5(2^n-2)+7)}$$

To prove the theorem, we apply induction on n . If $n = 1$, then $GNK(D'_1[1], x) = 2^{12k} 3^{7k}$ and the assertion holds. Therefore, let $n > 1$. By construction of dendrimer $D'_1[n]$, one can see that $D'_1[n]$ is obtained from the splice of $D'_1[n]$ and 2^{n-1} copies of the graph H in Figure 2. Thus,

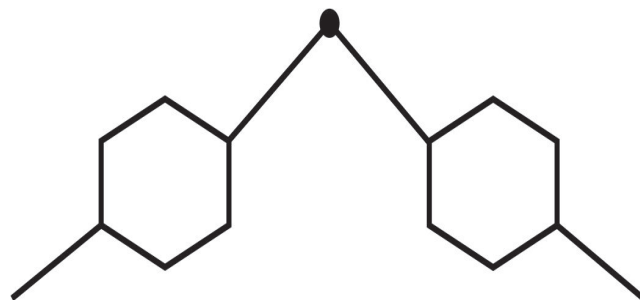


Figure 2: The graph H .

by Theorem 2.3, we have

$$\begin{aligned}
 &GNK(D'_1[n], x) \\
 &= GNK(D'_1[n-1], x) 3^{5k2^{n-1}} 2^{k2^{n+2}} \\
 &= 2^{k(2^{n+2}-4)} 3^{k(5(2^{n-1}-2)+7)} \\
 &\times 3^{5k2^{n-1}} 2^{k2^{n+2}} \\
 &= 2^{k(2^{n+3}-4)} 3^{k(5(2^n-2)+7)}.
 \end{aligned}$$

Now, we apply our results to compute the general Narumi-Katayama index of a dendrimer nanostar. We consider the first kind of dendrimer which has grown n steps denoted $D_3[n]$, [1]. The dendrimer $D_3[n]$ is depicted in Figure 3. First

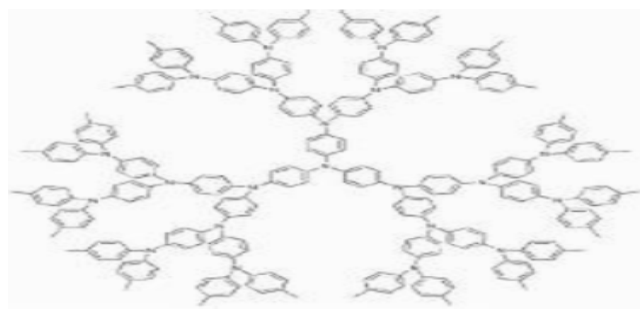


Figure 3: The first kind of dendrimer of generation 1-3 has grown 3 stages.

we construct $D_3[n]$ from $D'_1[n]$. Consider three

copies of $D'_1[n]$ with roots O , P and Q . The dendrimer $D_3[n]$ is obtained by identifying the vertex O of one copy of $D'_1[n]$ with two vertices P and Q of two another copy of $D'_1[n]$. We have the following theorem:

Theorem 3.2 *If $x = k_j$, $k \in \mathbb{N}$ and $j = [1, \dots, 1]$, then*

$$GNK(D_3[n], x) = 2^{3k(2^{n+3}-4)} 3^{3k(5(2^n-2)+7)}$$

By definition of $D_3[n]$, one can see that if we consider the splice of two copies of $D'_1[n]$ by vertices O and P , then the splice of the resulting graph with another copy of $D'_1[n]$ by vertex Q will be the graph $D_3[n]$. So, using the Theorem 2.3 and Theorem 2.4, we have

$$\begin{aligned} & GNK((D'_1[n] \bullet D'_1[n])(O, P), x) \\ &= 2^{k(2^{n+3}-4)} 3^{k(5(2^n-2)+7)} \\ &\times 2^{k(2^{n+3}-4)} 3^{k(5(2^n-2)+7)} \times 2 \\ &= 2^{2k(2^{n+3}-4)} 3^{2k(5(2^n-2)+7)} \times 2^k. \end{aligned}$$

Therefore,

$$\begin{aligned} & GNK(D_3[n], x) \\ &= 2^{2k(2^{n+3}-4)} 3^{2k(5(2^n-2)+7)} \\ &\times 2^{k(2^{n+3}-4)} 3^{k(5(2^n-2)+7)} \times 3^k \\ &= 2^{3k(2^{n+3}-4)} 3^{k(15(2^n-2)+22)}. \end{aligned}$$

4 Conclusions

In this paper, we introduced the general Narumi-Katayama index, GNK , of a graph. This index is a generalization of Narumi-Katayama index, the first multiplicative Zagreb index and the second multiplicative Zagreb index. Then, some graph theoretical properties of this index is computed. As instance, we compute the GNK index of the sun graph. Also, we obtain some bounds for this index by terms of clique number and independent number of a graph. In continue, we compute the GNK index of some graph operations such as splice and link of two graphs. Finally, we applied our results on these graph operations to compute GNK index of a class of dendrimers. By this method, the GNK index of many families of dendrimers can be computed.

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