

The Non-Neighbor Harmonic Index on Elementary Graph Operations

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Abstract—The aim of this paper is to study the behaviour of non-neighbor harmonic index of graphs with respect to the removal of pendant edge and an edge with maximal weight. The non-neighbor harmonic index for the subdivision graphs are computed and discussed in detail.

Keywords— non-neighbor harmonic index, elementary graph operations, subdivision graphs.

I-INTRODUCTION

To bring the power of mathematics to bear on real-world problems, the problem should be first modelled mathematically. Graphs, representatives of mathematics, are remarkable versatile tools for modelling. Graph theory is largely applied to the characterization of chemical structures, as well as to qualitative and quantitative structure-property (QSPR) and structure-activity (QSAR) relations by means of certain numerical characteristics, the topological indices [1]. A single number that can be used to characterize some property of the graph of a molecule is called a topological index. Many topological indices [2,3] have been introduced and studied: Randic index [4], Wiener index [5], First and Second Zagreb indices [6] are a few examples of these concepts. Many mathematical properties of these graph invariants have been studied.

In this paper we are concerned with simple graphs, having no directed or weighted edges, and no self-loops. A graph G is an ordered pair of two sets V and E . The set $V = V(G)$ is a finite non empty set and $E = E(G)$ is a binary relation defined on V . A graph can be visualized by representing the elements of V by vertices and joining the pair of vertices u, v by an edge if and only if $uv \in E(G)$. Also we denote $|V(G)| = n$ and $|E(G)| = m$. The degree of the vertex $v \in V(G)$, written $d(v)$, is the number of first neighbors of v in the underlying graph G .

Graph operations produce new graphs from initial ones. They may be classified into elementary operations or advanced operations. Elementary operations or editing operations create a new graph from initial one by a simple local change such as addition or deletion of a vertex or of an

edge, merging and splitting of vertices or edges. We define $G - uv$ to be the graph obtained from G by deleting the edge $uv \in E(G)$, and $G + uv$ to be the graph that arises from G by adding an edge uv between two non-adjacent vertices u and v of G . The subdivision graph $S(G)$ is the graph obtained from G by replacing each of its edge by a path of length 2, or equivalently by inserting an additional vertex into each edge of G . We use S_n , P_n and K_n to denote the star, path and complete graph on n vertices, respectively. For undefined terminology and notations in the paper, we refer to [7].

The paper is organized as follows, Section I contains the introduction of topological indices, graphs and elementary graph operations. Section II contain the related work of harmonic index and non-neighbor harmonic index, Section III presents the results and discussion of how the non-neighbor harmonic index of a graph G strictly increases and decreases by the removal of pendant edge [8] and an edge with maximal weight respectively. Also the non-neighbor harmonic index for the subdivision graph $S(G)$ is computed for some graphs and the results are discussed in detail. Section IV concludes the research work with the scope for future.

II-RELATED WORK

In the 1980's, Siemion Fajtlowicz created a vertex-degree-based quantity which was re-introduced by Zhong [9] in 2012 called Harmonic Index [10]. The harmonic index is one of the most important indices in chemical and mathematical fields. The harmonic index gives better correlations with physical and chemical properties of molecules. It is defined as

$$H(G) = \sum_{uv \in E(G)} \left[\frac{2}{d(u) + d(v)} \right]$$

The vertices that are not adjacent to a vertex $v \in V(G)$ are called non-neighbors of the vertex v . In this paper we define $\overline{d(v)}$ as the number of the non-neighbors of the vertex $v \in V(G)$, where $\overline{d(v)} = n - 1 - d(v)$. Based on the non-neighbors of the vertices of a graph G topological indices called Non-Neighbor Zagreb Indices and Non-Neighbor Harmonic index have been introduced [11]. The Non-Neighbor Harmonic Index is defined as

$$\overline{H(G)} = \sum_{uv \in E(G)} \left(\frac{2}{\overline{d(u)} + \overline{d(v)}} \right)$$

Non-Neighbor Harmonic Index is considered to be an important Non-Neighbor Topological Index as its values of the Path graph P_n is well correlated with the boiling point of the alkanes in Organic Chemistry.

III-RESULTS AND DISCUSSION

(A) Behaviour of non-neighbor harmonic index by the removal of an edge from the graph.

In this section, we show that the non-neighbor harmonic index strictly increases by the removal of pendant edge and strictly decreases by the removal of an edge with maximal weight. The graph $K_n + e$ is defined and its non-neighbor harmonic index is computed.

Theorem 1.1. Let G be a graph with n vertices and m edges. Removal of pendant edge strictly increases the non-neighbor harmonic index of the graph G .

Proof. Let $e = uv$ be a pendant edge of the graph G . Let $d(u) = p = 1$ and $d(v) = q$ so that $\overline{d(u)} = \overline{p} = n - 2$ and $\overline{d(v)} = \overline{q} \leq n - 3$. Let x_1, x_2, \dots, x_{q-1} be the other neighbors of the vertex v with $\overline{d(x_i)} = \overline{q_i} \leq n - 2$. Let e_1, e_2, \dots, e_{q-1} be the edges joining v to $x_i \forall i = 1, 2, \dots, q - 1$. Let e'_1, e'_2, \dots, e'_q be the remaining edges of the graph G with w_j and z_j as their end vertices. Let $\overline{d(w_j)} = \overline{r_j}$ and $\overline{d(z_j)} = \overline{s_j}$ for each $1 \leq j \leq \overline{d}$. Here $w_j = x_i$ and $z_j = w_j$ for some j . Let $G' = G - e$ be a connected graph, then

$$\begin{aligned} \overline{H(G)} - \overline{H(G')} &= \frac{2}{n - 2 + \overline{q}} + \sum_{i=1}^{q-1} \frac{2}{(\overline{q} + \overline{q_i})} - \sum_{i=1}^{q-1} \frac{2}{(\overline{q} + \overline{q_i} - 1)} \\ &\quad + \sum_{j=1}^{\overline{q}} \frac{2}{(\overline{r_j} + \overline{s_j})} - \sum_{j=1}^{\overline{q}} \frac{2}{(\overline{r_j} + \overline{s_j} - 2)} \end{aligned}$$

$$\begin{aligned} &= \frac{2}{n - 2 + \overline{q}} - \sum_{i=1}^{q-1} \frac{2}{(\overline{q} + \overline{q_i})(\overline{q} + \overline{q_i} - 1)} \\ &\quad - \sum_{j=1}^{\overline{q}} \frac{4}{(\overline{r_j} + \overline{s_j})(\overline{r_j} + \overline{s_j} - 2)} \\ &\leq \frac{2}{n - 2 + \overline{q}} - \sum_{i=1}^{q-1} \frac{2}{(\overline{q} + \overline{q_i})(\overline{q} + \overline{q_i} - 1)} \\ &\leq \frac{2}{n - 2 + \overline{q}} - \sum_{i=1}^{q-1} \frac{2}{(\overline{q} + n - 2)(\overline{q} + n - 3)} \\ &= \frac{2}{n - 2 + \overline{q}} \left[1 - \sum_{i=1}^{q-1} \frac{1}{(\overline{q} + n - 3)} \right] \\ &= \frac{2}{n - 2 + \overline{q}} \left[1 - \frac{q - 1}{(\overline{q} + n - 3)} \right] \\ &= \frac{2}{n - 2 + \overline{q}} \left[\frac{2\overline{q} - 1}{(n - 3 + \overline{q})} \right] \\ &< 0 \quad [\text{Since } \overline{q} \leq n - 3]. \end{aligned}$$

Therefore $\overline{H(G)} < \overline{H(G')}$. Hence the non-neighbor harmonic index of the graph G strictly increases by the removal of pendant edge.

Corollary 1.1.1 Let G be a graph with n vertices and m edges. Addition of a pendant edge to an arbitrary vertex of G , strictly decreases the non-neighbor harmonic index.

Definition 2.1. The graph $K_n + e$ is obtained by adding a pendant edge e to any arbitrary vertex K_n .

Definition 2.2. For any edge $e = uv$ in the graph G , Weight of the edge e is defined by the quantity $\frac{2}{\overline{d(u)} + \overline{d(v)}}$ [12].

Theorem 1.2. For the graph $K_n + e$, the non-neighbor harmonic index $\overline{H(K_n + e)} = \frac{2}{n-1} + \frac{(n-1)(n+2)}{2}$ and weight of the edge e is $\frac{2}{n-1}$.

Proof. The number of non-neighbors of each vertex in K_n is zero. Let $e = uv$ be the pendent edge attached to the arbitrary vertex v of K_n . We have $\overline{d(u)} = n - 1$ and $\overline{d(v)} = 0$ so that the weight of the edge $e = uv$

is $\frac{2}{n-1}$. Remaining vertices v_1, v_2, \dots, v_{n-1} of K_n has $\overline{d(v_i)} = 1$. Therefore the non-neighbor harmonic index,

$$\begin{aligned} \overline{H(K_n + e)} &= \frac{2}{n-1} + 2(n-1) + \binom{n}{2} - (n-1) \\ &= \frac{2}{n-1} + 2(n-1) + \frac{n(n-1)}{2} - (n-1) \\ &= \frac{2}{n-1} + \frac{(n-1)(n+2)}{2} \end{aligned}$$

Remark 1.2.1. The non-neighbor harmonic index of the complete graph K_n is ∞ . By adding an pendant edge to K_n , the non-neighbor harmonic index can be computed easily. The quantity $\frac{(n-1)(n+2)}{2}$ is the approximate value of the non-neighbor harmonic index of the complete graph K_n .

Theorem 1.3. Let G be a weighted graph. Removal of an edge with maximal weight strictly decreases the non-neighbour harmonic index of the graph G .

Proof. Let $e = uv$ be an edge with maximal weight in G . Let $d(u) = p$ and $d(v) = q$ and hence $\overline{d(u)} = \bar{p}$ and $\overline{d(v)} = \bar{q}$ with $\bar{p}, \bar{q} \leq n - 3$. Let x_1, x_2, \dots, x_{p-1} be the neighbors of u other than v and y_1, y_2, \dots, y_{q-1} be the neighbours of v other than u . Let $G' = G - e$ be a connected graph then we have $\bar{p} + \bar{q} \leq \bar{p} + \overline{d(x_i)}$ and $\bar{p} + \bar{q} \leq \bar{q} + \overline{d(y_j)}$. Hence

$$\begin{aligned} \overline{H(G)} - \overline{H(G')} &= \frac{2}{\bar{p} + \bar{q}} + \sum_{i=1}^{p-1} \frac{2}{\bar{p} + \overline{d(x_i)}} \\ &\quad - \sum_{i=1}^{p-1} \frac{2}{\bar{p} + \overline{d(x_i)} + 1} + \sum_{j=1}^{q-1} \frac{2}{\bar{q} + \overline{d(y_j)}} \\ &\quad - \sum_{j=1}^{q-1} \frac{2}{\bar{q} + \overline{d(y_j)} + 1} \\ &= \frac{2}{\bar{p} + \bar{q}} - \sum_{i=1}^{p-1} \frac{2}{(\bar{p} + \overline{d(x_i)})(\bar{p} + \overline{d(x_i)} + 1)} \\ &\quad + \sum_{j=1}^{q-1} \frac{2}{(\bar{q} + \overline{d(y_j)})(\bar{q} + \overline{d(y_j)} + 1)} \end{aligned}$$

$$\begin{aligned} &\geq \frac{2}{\bar{p} + \bar{q}} + \sum_{i=1}^{p-1} \frac{2}{(\bar{p} + \bar{q})(\bar{p} + \bar{q} + 1)} \\ &\quad + \sum_{j=1}^{q-1} \frac{2}{(\bar{p} + \bar{q})(\bar{p} + \bar{q} + 1)} \\ &= \frac{2}{\bar{p} + \bar{q}} + \frac{2(p-1)}{(\bar{p} + \bar{q})(\bar{p} + \bar{q} + 1)} + \frac{2(q-1)}{(\bar{p} + \bar{q})(\bar{p} + \bar{q} + 1)} \\ &= \frac{2}{\bar{p} + \bar{q}} + \frac{2p + 2q - 4}{(\bar{p} + \bar{q})(\bar{p} + \bar{q} + 1)} \\ &> 0 \end{aligned}$$

Therefore $\overline{H(G)} > \overline{H(G')}$. Hence the non-neighbor harmonic index of the graph G strictly decreases by the removal of an edge with maximal weight.

Corollary 1.3.1. Let G be a weighted graph. Removal of an edge with minimal weight which is not a pendant edge, strictly decreases the non-neighbour harmonic index.

(B) The non-neighbor harmonic index for the subdivision of graphs

In this section the non-neighbor harmonic index for the subdivision of some standard graphs are computed and the relation between non-neighbor harmonic index of the graph G and its subdivision graph $S(G)$ is discussed.

Theorem 2.1. For the k -regular graph G where $k \geq 2$, $\overline{H(S(G))} = \frac{2nk}{nk+2n-k-4}$

Proof. A k -regular graph has n vertices and $\frac{nk}{2}$ edges. The non-neighbors of each vertex is $(n - k - 1)$. Hence for a k -regular graph G , $\overline{H(G)} = \frac{nk}{2(n-k-1)}$. The subdivision graph $S(G)$ of a k -regular graph G has $n + \frac{nk}{2}$ vertices and nk edges. Each vertex in the k -regular graph has $(\frac{nk}{2} + n - k - 1)$ non-neighbors in $S(G)$ and each vertex obtained by subdividing the edges of G has $(\frac{nk}{2} + n - 3)$ non neighbors. Hence

$$\begin{aligned} \overline{H(S(G))} &= nk \left[\frac{2}{\frac{nk}{2} + n - k - 1 + \frac{nk}{2} + n - 3} \right] \\ &= nk \left[\frac{2}{nk + 2n - k - 4} \right] \\ &= \frac{2nk}{nk + 2n - k - 4} \end{aligned}$$

Corollary 2.1.1. For the complete graph $K_n (n \geq 2)$, $\overline{H(S(K_n))} = \frac{2n(n-1)}{n^2-3}$.

Corollary 2.1.2. For the cycle $C_n (n \geq 2)$, $\overline{H(S(C_n))} = \overline{H(C_{2n})} = \frac{2n}{2n-3}$.

Theorem 2.2. For the path $P_n (n \geq 3)$, $\overline{H(S(P_n))} = \overline{H(P_{2n-1})} = \frac{4}{4n-7} + 1$.

Proof: The non-neighbor harmonic index of the path $P_n (n \geq 4)$ is $\overline{H(P_n)} = \frac{4}{2n-5} + 1$ [13]. The subdivision of path P_n is the path with $(2n - 1)$ vertices. Hence

$$\begin{aligned} \overline{H(S(P_n))} &= \overline{H(P_{2n-1})} \\ &= \frac{4}{2(2n-1)-5} + 1. \\ &= \frac{4}{4n-7} + 1. \end{aligned}$$

Note: $\overline{H(S(P_2))} = \overline{H(P_3)} = 4$

Theorem 2.3. For the complete bipartite graph $K_{m,n}$, $\overline{H(S(K_{m,n}))} = mn \left[\frac{2}{2m(n+1)+n-4} + \frac{2}{2n(m+1)+m-4} \right] = \overline{H(K_{m,n})} \left[\frac{m+n-2}{2m(n+1)+n-4} + \frac{m+n-2}{2n(m+1)+m-4} \right]$.

Proof: The non-neighbor harmonic index of the complete bipartite graph $K_{m,n}$ is $\overline{H(K_{m,n})} = \frac{2mn}{m+n-2}$ [13]. The subdivision of a complete bipartite graph has $(m + n + mn)$ vertices and $2mn$ edges. The non-neighbors of the vertices in the vertex set V_1 is $(m - 1 + mn)$ and the non-neighbors of the vertices in the vertex set V_2 is $(n - 1 + mn)$. The vertices which subdivide the edges are of degree 2 and their number of non-neighbors is $(m + n + mn - 3)$. Hence

$$\begin{aligned} \overline{H(S(K_{m,n}))} &= mn \left[\frac{2}{m - 1 + mn + \frac{m + n + mn - 3}{2}} + \frac{2}{m + n + mn - 3 + n - 1 + mn} \right] \\ &= mn \left[\frac{2}{2m(n + 1) + n - 4} + \frac{2}{2n(m + 1) + m - 4} \right] \\ &= \frac{2mn}{m + n - 2} \left[\frac{m + n - 2}{2m(n + 1) + n - 4} + \frac{m + n - 2}{2n(m + 1) + m - 4} \right] \\ &= \overline{H(K_{m,n})} \left[\frac{m+n-2}{2m(n+1)+n-4} + \frac{m+n-2}{2n(m+1)+m-4} \right]. \end{aligned}$$

Corollary 2.3.1. For the k -regular bipartite graph, $\overline{H(S(K_{k,k}))} = \frac{4k^2}{2k^2+3k-4} = \overline{H(K_{k,k})} \left[\frac{4(k-1)}{2k^2+3k-4} \right]$

Corollary 2.3.2. For the star S_k , $\overline{H(S(S_k))} = k \left[\frac{2}{3k-2} + \frac{2}{4k-3} \right] = \overline{H(S_k)} \left[\frac{k-1}{3k-2} + \frac{k-1}{4k-3} \right]$

Theorem 2.4. For the wheel $W_n (n \geq 4)$, $\overline{H(S(W_n))} = \left[\frac{6n}{6n-5} + \frac{2n}{5n-2} \right] = \overline{H(W_n)} + \left[\frac{36n-37n^2-48n^3}{(6n-5)(5n-2)9n-3} \right]$.

Proof: The non-neighbor harmonic index of the Wheel W_n , is $\overline{H(W_n)} = \frac{3n}{n-3}$ [13]. The subdivision of wheel graph has $(3n + 1)$ vertices and $4n$ edges. The vertices which lie on the cycle C_n has $(3n - 3)$ non-neighbors and the vertices which subdivide the $2n$ edges has $(3n - 2)$ non-neighbors. The vertex at the center has $2n$ non-neighbors. Hence

$$\begin{aligned} \overline{H(S(W_n))} &= 3n \left[\frac{2}{3n - 3 + 3n - 2} \right] + n \left[\frac{2}{2n + 3n - 2} \right] \\ &= \left[\frac{6n}{6n-5} + \frac{2n}{5n-2} \right] \\ &= \frac{3n}{n-3} + \left[\frac{6n}{6n-5} + \frac{2n}{5n-2} - \frac{3n}{n-3} \right] \\ &= \overline{H(W_n)} + \left[\frac{36n-37n^2-48n^3}{(6n-5)(5n-2)9n-3} \right]. \end{aligned}$$

Note: $\overline{H(S(W_3))} = \frac{24}{13}$

(C) The Non-Neighbor Harmonic Index for the Tadpole graph, Ladder graph and their subdivision graphs.

A tadpole graph $T_{n,k}$ [14,15,16] is a graph obtained by joining a cycle $C_n (n \geq 3)$ to a path of length k and a ladder graph $L_n = K_2 \times P_n$ where P_n is a path with n vertices, K_2 is a complete graph with two vertices and \times denotes the cartesian product. When $n = 1$, L_n is a path of length 1. When $n = 2$, L_n is a cycle C_4 . The non-neighbor harmonic index for the tadpole graph $T_{n,k}$ and the ladder graph L_n together with their subdivision graphs are provided in this section.

Theorem 3.1. For the tadpole graph $T_{n,k}$, $\overline{H(T_{n,k})} = \begin{cases} \frac{1}{n-2} + \overline{H(P_n)} & \text{if } k = 1 \text{ and } n \geq 4 \\ \frac{2}{2n+2k-5} + \frac{2n+2k-8}{2n+2k-6} + \frac{6}{2n+2k-7} & \text{if } k \geq 2 \end{cases}$

Proof: A tadpole graph $T_{n,k}$ has $n + k$ vertices and $n + k$ edges.

Case(i) If $k = 1$, Then the tadpole graph $T_{n,1}$ has $(n + 1)$ vertices and $(n + 1)$ edges. The pendant vertex in $T_{n,1}$ has $(n - 1)$ non-neighbors and the vertex attached to the cycle C_n has $(n - 3)$ non-neighbors. The remaining vertices in the cycle C_n has $(n - 2)$ non-neighbors. Hence

$$\begin{aligned} \overline{H(T_{n,1})} &= \left[\frac{2}{n-1+n-3} \right] + \left[\frac{4}{n-3+n-2} \right] \\ &\quad + (n-2) \left[\frac{2}{n-2+n-2} \right] \\ &= \frac{2}{2n-4} + \frac{4}{2n-5} + 1 \\ &= \frac{1}{n-2} + \overline{H(P_n)} \end{aligned}$$

Case(ii) Suppose $k \geq 2$, then $T_{n,k}$ has $(n+k-2)$ vertices of degree 2, one vertex of degree 3 and a pendant vertex. The pendant vertex in the path P_n has $(n+k-2)$ non-neighbors and the vertex of P_n attached to the cycle C_n has $(n+k-4)$ non-neighbors. The remaining vertices each have $(n+k-3)$ non-neighbors. Hence

$$\begin{aligned} \overline{H(T_{n,k})} &= \left[\frac{2}{n+k-2+n+k-3} \right] + (k-2) \left[\frac{2}{n+k-3+n+k-3} \right] + \\ &\quad \left[\frac{6}{n+k-4+n+k-3} \right] + (n-2) \left[\frac{2}{n+k-3+n+k-3} \right] \\ &= \frac{2}{2n+2k-5} + \frac{2n+2k-8}{2n+2k-6} + \frac{6}{2n+2k-7} \end{aligned}$$

Note: $\overline{H(T_{3,1})} = 6$

Theorem 3.2. For the tadpole graph $T_{n,k}$, $\overline{H(S(T_{n,k}))} = \overline{H(S(T_{2n,2k}))} = \frac{2}{4n+4k-5} + \frac{4n+4k-8}{4n+4k-8} + \frac{6}{4n+4k-7}$

Proof:

The subdivision of the tadpole graph $S(T_{n,k})$ is the tadpole graph with a cycle of $2n$ vertices attached to the path of length $2k$. Hence

$$\begin{aligned} \overline{H(S(T_{n,k}))} &= \overline{H(T_{2n,2k})} \\ &= \frac{2}{4n+4k-5} + \frac{4n+4k-8}{4n+4k-8} + \frac{6}{4n+4k-7} \end{aligned}$$

Theorem 3.3. For the ladder graph L_n where $n \geq 3$,

$$\overline{H(L_n)} = \frac{8}{4n-7} + \frac{3n-8}{2(n-2)} + \frac{2}{2n-3}$$

Proof. The ladder graph has $2n$ vertices and $(3n-2)$ edges among which $(2n-4)$ vertices are of degree 3 and four vertices are of degree 2. The number of non-neighbors of the 4 corner vertices is $(2n-3)$ and the remaining $(2n-4)$ vertices has $(2n-4)$ non neighbors. Hence

$$\begin{aligned} \overline{H(L_n)} &= 4 \left[\frac{2}{2n-3+2n-4} \right] \\ &\quad + 2(n-3) \left[\frac{2}{2n-4+2n-4} \right] \\ &\quad + 2 \left[\frac{2}{2n-3+2n-3} \right] \\ &\quad + (n-2) \left[\frac{2}{2n-4+2n-4} \right] \\ &= \frac{8}{4n-7} + \frac{4n-12+2n-4}{4n-8} + \frac{4}{4n-6} \\ &= \frac{8}{4n-7} + \frac{6n-16}{4(n-2)} + \frac{4}{4n-6} \\ &= \frac{8}{4n-7} + \frac{3n-8}{2(n-2)} + \frac{2}{2n-3} \end{aligned}$$

Theorem 3.4. For the ladder graph L_n where $n \geq 3$, $\overline{H(S(L_n))} = \frac{16}{10(n-1)} + \frac{12(n-2)}{10n-11}$

Proof. The subdivision of a ladder graph $S(L_n)$ has $(5n-2)$ vertices and $(6n-4)$ edges. Among the $(5n-2)$ vertices $2(n-2)$ vertices has degree 3 and the remaining vertices have degree 2. Hence the number of non-neighbors of these vertices $2(n-2)$ vertices is $(5n-6)$ and that of remaining vertices is $(5n-5)$. Hence

$$\begin{aligned} \overline{H(S(L_n))} &= 8 \left[\frac{2}{5n-5+5n-5} \right] \\ &\quad + (6n-4) \left[\frac{2}{5n-5+5n-6} \right] \\ &= \frac{16}{10(n-1)} + \frac{12(n-2)}{10n-11} \end{aligned}$$

IV. CONCLUSION AND FUTURE SCOPE

In this paper we have presented in detail the behaviour of non-neighbor harmonic index on elementary graph operations. As future work study on the behaviour of non-neighbor harmonic index on advanced graph operations could be carried out.

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