Enumeration of caterpillars

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Abstract

Frank Harary and Allen J. Schwenk have given a formula for counting the number of non-isomorphic caterpillars on n vertices with $n \geq 3$. Inspired by the formula of Frank Harary and Allen J. Schwenk, in this paper, we give a formula for counting the number of non-isomorphic caterpillars with the same degree sequence.

2010 Mathematics Subject Classification. 05A15, 05A16.

Keywords and phrases. Graph Enumeration, Tree-isomorphism, Non-isomorphic caterpillars, Degree sequence.

1 Introduction

For any tree T of order $n \geq 3$, the derived tree T' is formed by deleting all the pendant vertices of T. The tree T is called caterpillar if it's derived tree T' is a path.

In 1973, Frank Harary and Allen Schwenk [2] provided an elegant formula for counting the number of non-isomorphic caterpillars on n vertices with $n \geq 3$, to be $C_n = 2^{n-4} + 2^{\lfloor \frac{n-4}{2} \rfloor}$. Inspired by the formula of Frank Harary and Allen J. Schwenk, in this paper, we provide a formula for enumerating the number of non-isomorphic caterpillars with the given degree sequence.

2 Main Result

To prove our main result, we prove the following basic lemma which establishes the necessary and sufficient condition for given two caterpillars with their respective degree sequences to be isomorphic or not.

For the convenience, we call the derived tree T' of a caterpillar tree T as the base of T and the vertices that lie in T' are called the base vertices of the caterpillar tree T. The caterpillar tree T and its base $T' : u_0u_1u_2u_3$ are shown in Figure 1 and 2 respectively.

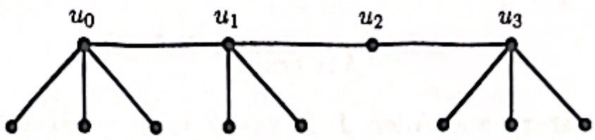

Figure 1: The caterpillar tree T

Figure 2: The derived tree(base) T' of the caterpillar tree T

Basic Lemma. *Two caterpillars T_1 and T_2 with the degree sequences $(c_0, c_1, ..., c_k, 1^{\sum_{i=0}^{k} c_i - 2k})$ and $(f_0, f_1, ..., f_k, 1^{\sum_{i=0}^{k} f_i - 2k})$ respectively (c_i and $f_i, 0 \leq i \leq k$ are the degree of the base vertices of the caterpillars T_1 and T_2, taken in the left to the right order respectively) are isomorphic if and only if either $c_i = f_i$, for each i, $0 \leq i \leq k$ or $c_i = f_{k-i}$, for each i, $0 \leq i \leq k$.*

Proof. Let T_1 and T_2 be two caterpillars having the degree sequence $(c_0, c_1, ..., c_k, 1^{\sum_{i=0}^{k} c_i - 2k})$ and $(f_0, f_1, ..., f_k, 1^{\sum_{i=0}^{k} f_i - 2k})$ respectively. Here c_i and $f_i, 0 \leq i \leq k$ are the degree of the base vertices of the caterpillars T_1 and T_2, taken in the left to the right order respectively. Let $(u_0, u_1, u_2, ..., u_k)$ and $(v_0, v_1, v_2, ..., v_k)$ be the ordered base vertices of T_1 and T_2 respectively, where the path $T_1' : u_0u_1u_2....u_k$ is the base of T_1 and the path $T_2' : v_0v_1v_2....v_k$ is the base of T_2. Here the vertices u_0 and v_0 are the left penultimate vertices of T_1 and T_2 respectively while u_k and v_k are the right penultimate vertices of T_1 and T_2 respectively, also u_i and v_i, for $1 \leq i \leq k-1$ are the internal vertices T_1 and T_2 respectively.

Suppose T_1 and T_2 are isomorphic. Then there exists a bijection $h : V(T_1) \to V(T_2)$ such that $uv \in E(T_1)$ if and only if $h(u)h(v) \in E(T_2)$. Consequently, the number of vertices and the number of edges are equal as well as the degree sequence of T_1 and T_2 are the same. In any isomorphism $h : V(T_1) \to V(T_2)$, the penultimate vertices of T_1 are mapped only to the penultimate vertices of T_2. Thus, either $h(u_0) = v_0$ and $h(u_k) = v_k$ or $h(u_0) = v_k$ and $h(u_k) = v_0$.

Case 1. When $h(u_0) = v_0$ and $h(u_k) = v_k$

Then, as h being an isomorphism, $h(u_t) = v_t$, for $1 \leq t \leq k-1$, hence $c_i = f_i$, for each $i, 0 \leq i \leq k$.

Case 2. When $h(u_0) = v_k$ and $h(u_k) = v_0$

Then, as h being an isomorphism, $h(u_t) = v_{k-t}$, for $1 \leq t \leq k-1$, hence $c_i = f_{k-i}$, for each $i, 0 \leq i \leq k$.

Thus it follows from the above two cases, either $c_i = f_i$, for each $i, 0 \leq i \leq k$ or $c_i = f_{k-i}$, for each $i, 0 \leq i \leq k$.

Conversely, suppose either $c_i = f_i$, for each $i, 0 \leq i \leq k$ or $c_i = f_{k-i}$, for each $i, 0 \leq i \leq k$, where c_i and $f_i, 0 \leq i \leq k$ are the degree of the base vertices of the caterpillars T_1 and T_2, taken in the left to the right order respectively. Then, in either case, the number of pendant vertices in T_1, $\sum_{t=0}^{k} c_i - 2k$ is equal to the number of pendant vertices in T_2, $\sum_{t=0}^{k} f_i - 2k$. This obviously implies that, the number of vertices of T_1 and that of T_2 are equal. Since $c_i = f_i$, for each $i, 0 \leq i \leq k$ or $c_i = f_{k-i}$, for each $i, 0 \leq i \leq k$, it is clear from The Handshaking Theorem [1] the number of edges of T_1 and that of T_2 are equal. Let $u_0, u_1, ..., u_k$ and $v_0, v_1, ..., v_k$ are the base vertices of T_1 and T_2 respectively with $d(u_i) = c_i$ and $d(v_i) = f_i$ for $0 \leq i \leq k$. For each $i, 1 \leq i \leq k-1$, let $u_{i_1}, u_{i_2}, ..., u_{i_{c_i-2}}$ and $v_{i_1}, v_{i_2}, ..., v_{i_{f_i-2}}$ be pendant vertices which are adjacent to the vertex u_i of T_1 and v_i of T_2 respectively. Also let $u_{i_1}, u_{i_2}, ..., u_{i_{c_i-1}}$ and $v_{i_1}, v_{i_2}, ..., v_{i_{f_i-1}}$ be the pendant vertices which are adjacent to the vertex u_i of T_1 and v_i of T_2 respectively, for $i = 0$ and k.

Case 1. When $c_i = f_i$, for each i, $0 \leq i \leq k$.

Define a map $r : V(T_1) \longrightarrow V(T_2)$ by $r(u_i) = v_i$, for each $i, 0 \leq i \leq k$. Also for each $i, 0 \leq i \leq k$, define $r(u_{i_j}) = v_{i_j}$, for each $j, 1 \leq j \leq c_i - \alpha$, where

$$\alpha = \begin{cases} 1 & \text{if } i = 0 \text{ and } k \\ 2 & \text{if } 1 \leq i \leq k-1 \end{cases}$$

It is clear that the mapping r preserves the adjacency between T_1 and T_2, Hence $T_1 \cong T_2$.

Case 2. When $c_i = f_{k-i}$, for each i, $0 \leq i \leq k$.
Define a map $g : V(T_1) \longrightarrow V(T_2)$ by $g(u_i) = v_{k-i}$, for each $i, 0 \leq i \leq k$. Also for each $i, 0 \leq i \leq k$, define $g(u_{i_j}) = v_{(k-i)_j}$, for each $j, 1 \leq j \leq c_i - \alpha$,

where

$$\alpha = \begin{cases} 1 & \text{if } i = 0 \text{ and } k \\ 2 & \text{if } 1 \leq i \leq k-1 \end{cases}$$

It is clear that the mapping g preserves the adjacency between T_1 and T_2, Hence $T_1 \cong T_2$. □

To obtain the formula for counting the number non-isomorphic caterpillars with the same degree sequence we also use the following lemmas.

Lemma 1. *Let $A = \{d_0, d_1, ..., d_k\}$ be finite multi-set contains $k+1$ non-negative integers then the number of multi-set permutations of A is $\frac{(k+1)!}{\prod_{i=0}^{p} s_i!}$, where $s_0, s_1, ..., s_p$, for some $p, 0 \leq p \leq k$ are the multiplicities of the elements of A taken in some order.*

The Lemma 1 is a well-known result, refer [3]. A permutation ϕ generated from the multi-set $A = \{d_0, d_1, ..., d_k\}$ is called palindromic if $\phi(i) = \phi(k-i)$, $0 \leq i \leq \lfloor \frac{k}{2} \rfloor$.

Lemma 2. *The number of palindromic permutations from the set of all permutations generated from the multi-set $A = \{d_0, d_1, ..., d_k\}$ is*

$$L = \begin{cases} \frac{\lceil \frac{k}{2} \rceil !}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} & \text{if } k \text{ is even and exactly one } s_i \text{ is odd} \\ & \text{or if } k \text{ is odd and each } s_i \text{ is even} \\ 0 & \text{otherwise} \end{cases}$$

where $s_0, s_1, ..., s_p$, for some $p, 0 \leq p \leq k$ are the multiplicities of the elements of A taken in some order.

Proof. Let S denote the set of all permutations generated from the multi-set $A = \{d_0, d_1, ..., d_k\}$ having the multiplicities $s_0, s_1, ..., s_p$, for some p, $0 \leq p \leq k$ of the elements of A taken in some order. Let L denote the number of palindromic permutations of the set S. We determine the L, in two cases depending on whether k is odd or even.

Case 1: k is odd

Then $|A| = k+1$ is even. By definition, any palindromic permutation $\phi \in S$ can be considered as a permutation of the form $\phi(0)\phi(1)\cdots\phi(\frac{k-1}{2})$ $\phi(\frac{k+1}{2})\cdots\phi(k)$ with $\phi(i) = \phi(k-i), 0 \leq i \leq \frac{k-1}{2}$. The part $\phi(0)\phi(1)\cdots\phi(\frac{k-1}{2})$ of ϕ is referred as the left of ϕ and the part $\phi(\frac{k+1}{2})\cdots\phi(k)$ of ϕ is referred as the right of ϕ. As $k+1$ is even, for each distinct element $x \in A$ with multiplicity $s(x) = s_i$, for some $i, 0 \leq i \leq p$, then exactly $\frac{s(x)}{2}$ times x should lie on the left of ϕ and the remaining $\frac{s(x)}{2}$ times x lie on the right of

ϕ. Therefore, $\frac{s(x)}{2}$ should be an integer. This implies that the multiplicity $s(x) = s_i$ is even for every $i, 0 \leq i \leq p$. Hence, when k is odd, the set S contains palindromic permutation only when every s_i is even for each $i, 0 \leq i \leq p$. Thus, under the case of k being odd, the set S does not have any palindromic permutation if any of the multiplicity of the elements of A is odd.

Define the multi-set $B \subseteq A$ in the following way. For each distinct element $x \in A$ with the multiplicity $s(x)$, then the set B contains the element x with the multiplicity $\frac{s(x)}{2}$. Thus $|B| = \frac{|A|}{2} = \frac{k+1}{2}$.

Then it is clear that each permutation σ generated from the multi-set B induces a unique palindromic permutation $\phi \in S$ which is defined as $\phi(i) = \phi(k-i) = \sigma(i)$, $0 \leq i \leq \frac{k-1}{2}$. Conversely, each palindromic permutation $\phi \in S$ induces a unique permutation σ on the multi-set B which is defined as $\sigma(i) = \phi(i)$, $0 \leq i \leq \frac{k-1}{2}$. Therefore the number of permutations generated from the multi-set B is equal to the number of palindromic permutation belonging to the set S. By Lemma 1, the number of permutations generated from the set B is $\frac{(\frac{k+1}{2})!}{\prod_{i=0}^{p} \frac{s_i}{2}!}$. Hence the number of palindromic permutations of the set S is $\frac{(\frac{k+1}{2})!}{\prod_{i=0}^{p} \frac{s_i}{2}!} = \frac{\lceil \frac{k}{2} \rceil !}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} = L$. Thus, it follows that if any one of the elements of A has odd multiplicity then $L = 0$.

Case 2: k is even

Then $|A| = k+1$ is odd. By the definition of palindromic permutation, any palindromic permutation $\phi \in S$ can be considered a permutation of the form $\phi(0)\phi(1)\cdots\phi(\frac{k-2}{2})\phi(\frac{k}{2})\phi(\frac{k+2}{2})\cdots\phi(k)$, with $\phi(i) = \phi(k-i)$, $0 \leq i \leq \frac{k-2}{2}$. The part $\phi(0)\phi(1)\cdots\phi(\frac{k-2}{2})$ of ϕ is referred as the left of ϕ; the part $\phi(\frac{k+2}{2})\cdots\phi(k)$ of ϕ is referred as the right of ϕ and $\phi(\frac{k}{2})$ of ϕ is the middle of ϕ. As $k+1$ is odd, alteast one distinct element $x \in A$ should have an odd multiplicity.

Claim: Exactly one distinct element of the set A has odd multiplicity

Let $x \in A$ having odd multiplicity $s(x)$, in any palindromic permutation $\phi \in S$, exactly $\frac{s(x)-1}{2}$ times of x lying on the left of ϕ, $\frac{s(x)-1}{2}$ times of x lying on the right of ϕ and the middle of ϕ, $\phi(\frac{k}{2}) = x$. Suppose that if there exist another distinct element $y \in A$, $y \neq x$ which also has odd multiplicity $s(y)$, in any palindromic permutation $\phi \in S$, there are exactly $\frac{s(y)-1}{2}$ times of y lying on the left of ϕ, $\frac{s(y)-1}{2}$ times of y lying on the right of ϕ and the middle of ϕ, $\phi(\frac{k}{2}) = y$. This would imply that $y = x$, which is a contradiction to our assumption that $x \neq y$. Hence there is exactly one distinct element say $x^* \in A$ having odd multiplicity while all the other distinct element of A have even multiplicity.

Hence, when k is even, the set S contains a palindromic permutation only when all the multiplicity $s_i, 0 \le i \le p$ are even with the exception of exactly one multiplicity s_i being odd. It is clear that for all the other cases which are based on the nature of the multiplicity of $s_i's$ the set S does not have any palindromic permutation.

Define the multi-set $C \subseteq A$ in the following way. For each distinct element $x \neq x^* \in A$ with the multiplicity $s(x)$, the set C contains the element x with multiplicity $\frac{s(x)}{2}$ and C also contains the element $x^* \in A$ with multiplicity $\frac{s(x^*)-1}{2}$. Thus $|C| = \frac{|A|-1}{2} = \frac{k}{2}$.

It is clear that each permutation σ generated from the multi-set C induces a unique palindromic permutation $\phi \in S$ which is defined as $\phi(i) = \phi(k-i) = \sigma(i)$, $0 \le i \le \frac{k-2}{2}$ and $\phi(\frac{k}{2}) = x^*$. Conversely, each palindromic permutation $\phi \in S$ induces a unique permutation σ on the multi-set C which is defined as $\sigma(i) = \phi(i)$, $0 \le i \le \frac{k-2}{2}$. Therefore, the number of permutations generated on the multi-set C is equal to the number of palindromic permutations that belong to the set S. By Lemma 1, the number of permutations generated from the set multi-set C is $\frac{(\frac{k}{2})!}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !}$. Hence the number of palindromic permutations from the set S is $\frac{(\frac{k}{2})!}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} = \frac{\lceil \frac{k}{2} \rceil !}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} = L$. Thus, it follows that either if A has two or more distinct elements with odd multiplicity or all the distinct elements of A have even multiplicities, then $L = 0$. □

The following theorem provides a formula for counting the number of non-isomorphic caterpillars with the same degree sequence.

Theorem 1. *The number of non-isomorphic caterpillars on $n \ge 3$ vertices having the degree sequence $d_0, d_1, ..., d_k, 1^{n-k-1}, d_i \ge 2$, for $0 \le i \le k$ is* $\frac{1}{2}\left(\frac{(k+1)!}{\prod_{i=0}^{p} s_i!} + L\right)$, *where*

$$L = \begin{cases} \frac{\lceil \frac{k}{2} \rceil !}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} & \text{if } k \text{ is even and exactly one } s_i \text{ is odd} \\ & \text{or if } k \text{ is odd and each } s_i \text{ is even} \\ 0 & \text{otherwise} \end{cases}$$

and s_i, for $i, 0 \le i \le p$ are the multiplicities of the elements of the multi-set $A = \{d_0, d_1, ..., d_k\}$.

Proof. Let $(d_0, d_1, ..., d_k, 1^{n-k-1}), d_i \ge 2$, for $0 \le i \le k$ be the degree sequence of a caterpillar with $n \ge 3$ vertices. By the definition of caterpillar, a vertex v has degree ≥ 2 if and only if v should be a base vertex. This implies that the terms $d_0, d_1, ..., d_k$ of the degree sequence $d_0, d_1, ..., d_k, 1^{n-k-1}$ are the degree of the $k+1$ base vertices of the caterpillar.

Let $u_0 u_1 u_2 .... u_k$ be the base of such caterpillar having the degree sequence $d_0, d_1, ..., d_k, 1^{n-k-1}, d_i \geq 2$, for $0 \leq i \leq k$. Then the degrees $d(u_0), d(u_1), \ldots, d(u_k)$ should satisfy $d(u_0) = d_{\alpha_0}, d(u_1) = d_{\alpha_1}, \ldots d(u_k) = d_{\alpha_k}$, where $\{d_{\alpha_0}, d_{\alpha_1}, \ldots d_{\alpha_k}\} = \{d_0, d_1, ..., d_k\}$. Therefore $(d(u_0), d(u_1), ..., d(u_k))$ is nothing but some arrangement of the elements of the multi-set $A = \{d_0, d_1, ..., d_k\}$. Conversely, for each arrangement $(d_{\alpha_0}, d_{\alpha_1}, \ldots d_{\alpha_k})$ on the elements of the multi-set A induces a caterpillar having the degree sequence $(d_0, d_1, ..., d_k, 1^{n-k-1})$ with the base $u_0 u_1 u_2 .... u_k$, such that $d(u_i) = d_{\alpha_i}, 0 \leq i \leq k$. Therefore the number of all possible caterpillar with $(d_0, d_1, ..., d_k, 1^{n-k-1})$ as the degree sequence is equal to the number of all possible arrangements on the elements of the multi-set A.

It is clear that an arrangement $(d_{\alpha_0}, d_{\alpha_1}, \ldots d_{\alpha_k})$ of the multi-set A is essentially a permutation ϕ, generated on the multi-set A such $\phi(i) = d_{\alpha_i}$, for $0 \leq i \leq k$. By Lemma 1, the number of all possible permutations generated on the multi-set A is $\frac{(k+1)!}{\prod_{i=0}^{p} s_i!} = R$, where $s_0, s_1, \cdots s_p$ denotes the multiplicities of the elements of the set A taken in some order. Hence there are R caterpillars each having the degree sequence $(d_0, d_1, ..., d_k, 1^{n-k-1})$. As non-isomorphic caterpillars can also have the same degree sequence, all the R caterpillars generated here need not be non-isomorphic.

Let S denote the set of all permutation ϕ, generated on the multi-set A. Note that for a member $\phi = \binom{0 \ 1 \ \ldots \ k}{\phi(0)\phi(1)\ldots\phi(k)} \in S$ the reverse permutation of ϕ denoted $\phi^R = \binom{0 \ 1 \ \ldots \ k}{\phi(k)\phi(k-1)\ldots\phi(0)}$ also belongs to S.

Define a subset S_1 of the set S by $S_1 = \{\phi \in S : \phi^R = \phi\}$. Let $S_2 = S - S_1$. Then it is clear that $S = S_1 \cup S_2$ and $S_1 \cap S_2 = \phi$. Thus $|S| = |S_1| + |S_2|$.

The number of non-isomorphic caterpillars defined from all permutations belonging to S is nothing but the number of non-isomorphic caterpillars defined from all permutations belonging to S_1 plus the number of non-isomorphic caterpillars defined from all permutations belonging to S_2.

Claim.1 : The set of all caterpillars, which are defined from the permutations belonging to S_1 are mutually non-isomorphic

Observe that any two members $\phi, \mu \in S_1$ with $\phi \neq \mu$ then $\phi \neq \mu^R$ and $\phi^R \neq \mu$, then by Basic Lemma, the caterpillars T_ϕ, defined from the permutation ϕ and the caterpillar T_μ, defined from the permutation μ are non-isomorphic. This implies that all the caterpillars that are generated from the permutations belonging to S_1 are mutually non-isomorphic.

In order to determine all the non-isomorphic caterpillar that are generated from the permutations belonging to S_2 we define two subsets S_2' and S_2'' of the set S_2 in the following way. Take a member $\phi \in S_2$, then assign ϕ in S_2' and assign its unique reverse ϕ^R in S_2''. It is clear that $S_2 = S_2' \cup S_2''$ and $S_2' \cap S_2'' = \phi$, thus $|S_2| = |S_2'| + |S_2''|$. By the definition of the sets, S_2' and S_2'', $|S_2'| = |S_2''| = \frac{|S_2|}{2}$.

Observation.1 : By Basic Lemma, for each $\phi \in S_2'$ the caterpillar defined from ϕ, T_ϕ is isomorphic to the caterpillar T_{ϕ^R} defined from the corresponding permutation $\phi^R \in S_2''$ and conversely. Thus the set of caterpillars defined from the permutations of the set S_2' and that of S_2'' are identical.

Claim.2: The set of all caterpillars, which are defined from the permutations belonging to S_2' are mutually non-isomorphic

By the definition of S_2', any two members $\phi, \mu \in S_2'$ with $\phi \neq \mu$ then $\phi \neq \mu^R$ or $\phi^R \neq \mu$. By Basic Lemma, the caterpillars T_ϕ, defined from the permutation ϕ and the caterpillar T_μ, defined from the permutation μ are non-isomorphic. This implies that all caterpillars defined from the permutations belonging to S_2' are mutually non-isomorphic.

By Claim 1, Observation 1, Claim 2 and from the fact that $S_1 \cap S_2' = \phi$ and $S_1 \cap S_2'' = \phi$, [since S_2' and S_2'' are the subsets of S_2 and $S_1 \cap S_2 = \phi$], it follows that the number of non-isomorphic caterpillars defined from all permutations belonging to S is nothing but the number of caterpillars defined from all the permutations belonging to S_1 plus the number of caterpillars defined from all the permutations contained exclusively in S_2' [or exclusively in S_2'']. Thus, the number of non-isomorphic caterpillars having the degree sequence $(d_0, d_1, ..., d_k, 1^{n-k-1})$ is equal to $|S_1| + |S_2'|$. Since the set S_1 contains all the palindromic permutations generated on the set A, By Lemma 1, the number of palindromic permutation,

$$|S_1| = L = \begin{cases} \frac{\lceil \frac{k}{2} \rceil !}{\prod_{i=0}^{p} \lfloor \frac{s_i}{2} \rfloor !} & \text{if } k \text{ is even and exactly one } s_i \text{ is odd} \\ & \text{or if } k \text{ is odd and each } s_i \text{ is even} \\ 0 & \text{otherwise} \end{cases}$$

Hence the total number of caterpillars on $n \geq 3$ vertices having the degree sequence $d_0, d_1, ..., d_k, 1^{n-k-1}$ is $= |S_1| + |S_2'| = L + \frac{|S| - |S_1|}{2} = L + \frac{|S| - L}{2} = \frac{|S| + L}{2} = \frac{1}{2} \left(\frac{(k+1)!}{\prod_{i=0}^{p} s_i !} + L \right)$. □

Acknowledgment

The authors are grateful to Dr. Aravind, Professor at IMSc Chennai, India, for his valuable suggestions and comments. The first author gratefully acknowledges Centre for Research, Anna University, Chennai for the financial support through the Anna Centenary Research Fellowship under the grant Ref:CR/ACRF/2014/40, Dated: 28.12.2013.

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