Chapter 3

Backtracking

3.1 Introduction

Backtracking is a very general technique that can be used to solve a wide variety of problems in combinatorial enumeration. Many of the algorithms to be found in succeeding chapters are backtracking in various guises. It also forms the basis for other useful techniques such as branch-and-bound and alpha-beta pruning, which find wide application in operations research (and, more generally, discrete optimization) and artificial intelligence, respectively.

As an introductory problem, consider the puzzle of trying to determine all ways to place n non-taking queens on an n by n chessboard. Recall that, in the game of chess, the queen attacks any piece that is in the same row, column or either diagonal. To gain insight, we first consider the specific value of n = 4. We start with an empty chessboard and try to build up our solution column by column, starting from the left. We can keep track of the approaches that we explored so far by maintaining a *backtracking tree* whose root is the empty board and where each level of the tree corresponds to a column on the board; i.e., to the number of queens that have been places so far. Figure 3.1 shows the backtracking tree.

This tree is constructed as follows: Starting from an empty board, try to place a queen in column one. There are four positions for the queen, which correspond to the four children of the root. In column one, we first try the queen in row 1, then row 2, etc., from left to right in the tree. After successfully placing a queen in some column we then proceed to the next column and recursively try again. If we get stuck at some column k, then we *backtrack* to the previous column k - 1, where we again try to advance the queen in column k - 1from its current position. Observe that the tree is constructed in preorder. All nodes at level n represent solutions; for n = 4 there are two solutions.

Let us consider now the case of a standard 8 by 8 chessboard. Here the problem is too large to do the backtracking by hand, unless you are extremely patient. It is easier to write a program.

The backtracking process, as described above, is recursive, so it is not surprising that we can use a recursive procedure to solve the eight queens problem. A pseudo-Pascal procedure for doing this is developed next. The solution x consists of a permutation of 1 through 8, representing the row locations of the queens in successive columns. For the 4-queens problem the permutations giving solutions were x = [2, 4, 1, 3] and x = [3, 1, 4, 2]. As the algorithm is proceeding we need some way to determine whether a queen is being attacked by another queen. The easiest way to do this is to maintain three boolean arrays, call them **a**, **b**, **c**. The array **a** indicates if a row does not contain a queen. The array



Figure 3.1: The four queens backtracking tree.

b indicates if a diagonal does not contain a queen, and **c** indicates if a diagonal does not contain a queen. The sum of the row and column indices is constant along diagonals, and the difference of the row and column indices is constant along diagonals. Thus **a** is indexed 1..8, array **b** is indexed 2..16, and **c** is indexed -7..7.¹ These arrays are initialized to be **true**, and then we call **Queen(1)**. The solution is given in the global array **x**, which need not be initialized.

(Q1)	$\mathbf{procedure} \ Queen \ (\ col: \mathbb{N} \)$
(Q2)	local $row : \mathbb{N};$
(Q3)	for $row := 1$ to 8 do
(Q4)	if $a[row]$ and $b[row+col]$ and $c[row-col]$ then
(Q5)	x[col] := row;
(Q6)	a[row] := b[row+col] := c[row-col] := false ;
(Q7)	if $col < 8$ then Queen $(col + 1)$ else Printlt;
(Q8)	a[row] := b[row+col] := c[row-col] := true ;

Algorithm 3.1: Algorithm for the 8 queens problem.

It turns out that there are 92 solutions to the 8 by 8 puzzle. Only 12 of the solutions are non-isomorphic in the sense that all other solutions may be obtained from these 12 by rotating and/or flipping the board.

¹In other languages, the indexing of c may have to be offset.

3.2 Backtracking Algorithms

In the general backtracking scenario we wish to generate all strings S that satisfy some predicate P.

$$S = \{(x_1 x_2 x_3 \cdots) \in A_1 \times A_2 \times A_3 \times \cdots \mid P(x_1 x_2 x_3 \cdots)\}$$

Each A_i is a finite set. Of course, the strings must be of finite length and there must be finitely many of them. In most applications the strings will have a fixed length. In order to apply the backtracking technique the predicate P must be extended to a predicate Q defined on "prefix" strings such that the following properties hold:

$$\begin{array}{l}
P(x_1x_2x_3\cdots) \text{ implies } Q(x_1x_2x_3\cdots), \text{ and} \\
\neg Q(x_1x_2\cdots x_{k-1}) \text{ implies } \neg Q(x_1x_2\cdots x_{k-1}x) \text{ for all } x \in A_k
\end{array}$$
(3.1)

In other words, if a string does not satisfy the predicate Q then it cannot be extended to a string that does satisfy the predicate P. Given a partial solution $\mathbf{x} = x_1 x_2 \cdots x_{k-1}$ we let $S_k(\mathbf{x})$ denote all the valid ways of extending the string by one element. If the string \mathbf{x} is understood we simply write S_k . In other words,

$$S_k(\mathbf{x}) = \{ x \in A_k \mid Q(\mathbf{x}x) \}.$$

The vertices of the *backtracking tree* are all those strings that satisfy Q. The children of a vertex are all those sequences obtained from the parent sequence by appending a single element.

As an illustration of the preceeding definitions consider the 8 by 8 non-taking queens problem. The sets A_i are $\{1, 2, \ldots, 8\}$ for each $i = 1, 2, \ldots, 8$. The predicate Q is simply whether the queens placed so far are non-taking. An example in which the sets A_i differ for different i will be given in the next section.

A recursive procedure for the general backtracking scenario is deceptively simple. It is given in Algorithm 3.2. The initial call is $\mathsf{Back}(1,\varepsilon)$; no initialization is necessary. The call $\mathsf{Back}(k,\mathbf{x})$ generates all strings of the form \mathbf{xy} for which $\mathbf{xy} \in S$.

The parameter \mathbf{x} , representing a partial solution, is often left as a global variable, as it was in our procedure for the 8 queens problem. Another property that the 8 queens solutions have is that they are all strings of the same length. This is usually the case and results in a simplification of the algorithm. Suppose that all solutions have length n. Then Back can be modified by making lines (B5) and (B6) into the **else** clause of the **if** statement at line (B4). If, in addition, $Q(x_1x_2\cdots x_n)$ implies $P(x_1x_2\cdots x_n)$, then the test for $P(\mathbf{x})$ at line (B4) can be replace by the test "k > n". This is done in many of the procedures to be found in succeeding chapters.

```
(B1)procedure Back (k : \mathbb{N}; \mathbf{x} : \mathbf{string});(B2)local x : A_k; S_k : \mathbf{set of } A_k(B3)begin(B4)if P(\mathbf{x}) then PrintSolution(\mathbf{x});(B5)compute S_k;(B6)for x \in S_k do Back(k + 1, \mathbf{x}x);(B7)end {of Back};
```

Algorithm 3.2: Recursive backtracking algorithm.

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We also present a non-recursive version of the algorithm; see Algorithm 3.3. This version is of interest when speed is of utmost concern — for example, if the backtracking routine is being written in assembly language.

```
k := 1;

compute S_1;

while k > 0 do

while S_k \neq \emptyset do

{Advance to next position}

x_k := an element of S_k;

S_k := S_k \setminus \{x_k\};

if P(x_1x_2 \cdots x_k) then PrintSolution;

k := k + 1;

compute S_k;

{Backtrack to previous position}

k := k - 1;

end;
```

Algorithm 3.3: Non-recursive backtracking algorithm.

3.3 Solving Pentomino Problems with Backtracking.

As a somewhat more complicated problem we consider a *pentomino* problem. A pentomino is an arrangement of five unit squares joined along their edges. They were popularized by Golomb [169] ². There are 12 non-isomorphic pentominoes as shown in Figure 3.2. The pieces have been given and arbitrary numbering; traditionally letters have also been associated with the pieces and we show those as well. We will develop an algorithm to find all ways of placing the 12 pentomino pieces into a 6 by 10 rectangle. It turns out that there are 2,339 non-isomorphic ways to do this. One of the solutions is shown in Figure 3.3. Each piece can be rotated or flipped, which can give different *orientations* of a piece. Piece 1 has 1 orientation, piece 2 has two orientations, pieces 3,4,5,6,7 have 4 orientations, and pieces 8,9,10,11,12 have 8 orientations. Each solution to the problem is a member of an equivalence class of 4 other solutions, obtained by flipping and rotating the 6 by 10 board.

Figure 3.4 shows how the board is numbered. It also shows a particular placement of the "X" piece. This placement is represented by the set [8,13,14,15,20]. Every placement of a piece is represented by some 5-set. The *anchor* of a placement is the smallest number in the 5-set.

The backtracking algorithm successively tries to place a piece in the lowest numbered unoccupied square; call it k. Once k is determined we try to place an unused piece over it. The pieces are tried in the order 1, 2, ..., 12 as numbered in Figure 3.2. Thus we wish to know, for each piece and number k, all placements that are anchored at k. These placements are precomputed and stored in the array List from the type and variable declarations of Figure 3.4. For example, the placement of "X" in Figure 3.4 is the only set in List[1,8]. Of course, the list usually contains more than one element; List[12,8] has eight members,

²The term *pentomino*, for a 5-omino, is a registered trademark of Solomon W. Golomb (No. 1008964, U.S. Patent Office, April 15, 1975).



Figure 3.2: The 12 pentomino pieces.



Figure 3.3: A solution to the 6 by 10 pentomino problem.

0	6	12	18	24	30	36	42	48	54
1	7	13	19	25	31	37	43	49	55
2	8	14	20	26	32	38	44	50	56
3	9	15	21	27	33	39	45	51	57
4	10	16	22	28	34	40	46	52	58
5	11	17	23	29	35	41	47	53	59

Figure 3.4: Numbering the board (and the placement of a piece).

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Figure 3.5: Lists for piece 11, with those anchored at location 7 shown explicitly.

the maximum possible number. The list for List[11,7] is shown in Figure 3.5. Piece 7 has 8 orientations but only 7 of them appear on the list because one of them would extend outside of the board. The one not appearing is blank in Figure 3.5. The others show the 5 numbers that are in the set corresponding to piece 11 anchored at position 7.

\mathbf{type}	
Pie	$ceNumber = \mathbb{Z}(1\dots 12);$
Boa	$\operatorname{urdNumber} = \mathbb{Z}(0\dots 63);$
Boa	ard = word(BoardNumber);
List	Ptr = pointer to ListElement;
List	Element = node(Position : Board,Link : ListPtr);
global	
The	eBoard : Board;
List	: array [PieceNumber,BoardNumber] of ListPtr;
Pie	ceAvail : word (PieceNumber);
Sol	ntion : array [PieceNumber] of ListPtr;

Algorithm 3.4: Declarations for pentomino program.

With these global declarations the backtracking procedure is given in Figure 3.5. Intersection (\cap) is used to determine whether a piece can be placed without overlap, union (\cup) is used to add a new piece to the board, and difference (\) is used to remove a piece from the board. If the set operations are correctly implemented using AND, OR, and NOT on machine words, then this program will be quite fast.

It is natural to wonder whether the backtracking can be sped up by checking for *isolated* squares. That is to say, checking whether the unused portion of the board has a number of squares divisible by five before trying to place the next piece. This strategy will certainly cut down on the number of vertices in the backtracking tree, but now more work is done at each vertex. In the author's experience it does not pay to check for isolated squares; the extra work done at each vertex is greater than the savings obtained by having a smaller tree. Backtracking is full of such tradeoffs between the size of the tree and the amount of work done at each vertex.

The more general question that this raises is: Among two predicates Q and R both satisfying (3.1), which is better? Of course the ultimate test is in the running time of the

```
procedure BackTrack (k : BoardNumber );
local pc : PieceNumber;
     while k \in TheBoard do k := k + 1;
     for pc := 1 to 12 do
         if pc in PieceAvail then
               PieceAvail := PieceAvail \setminus [pc];
               Solution[pc] := List[pc,k];
               while Solution [pc] \neq null do
                    if TheBoard \cap Solution[pc].Position = \emptyset then
                         TheBoard := TheBoard \cup Solution[pc].Position;
                         if PieceAvail = \emptyset
                              then PrintSolution
                              else BackTrack(k + 1);
                         TheBoard := TheBoard \setminus Solution[pc].Position;
                    Solution[pc] := Solution[pc].Link;
              PieceAvail := PieceAvail \cup [pc];
end {of BackTrack}
```

Algorithm 3.5: Backtracking routine for pentomino problem.

two algorithms that arise. Two extremes are worth noting. If Q is always true then (3.1) is satisfied. No pruning of the backtracking is done; all of $A_1 \times A_2 \times \cdots$ is generated. What if Q is perfect? That is, what if $Q(\mathbf{x})$ implies that there is some \mathbf{y} such that $P(\mathbf{xy})$? Then every leaf of the backtracking tree is in S. As mentioned in Chapter 1, this is the BEST property: <u>Backtracking Ensuring Success at Terminals</u>.

3.3.1 Eliminating Isomorphic Solutions

Reject isomorphs! The is no reason to generate isomorphic solutions when generating all solutions to pentomino and other "space-filling" puzzles. In particular, for the 6 by 10 pentomino puzzle, each solution has four equivalent solutions (including itself) in the equivalence class obtained by rotating and flipping. Thus, even if we wanted all solutions, isomorphic or not, we could generate the non-isomorphic ones and then flip and rotate to get the others. As we will see, there is absolutely no computational overhead in rejecting isomorphic solutions in the 6 by 10 case, so that we save a factor of 4 in the running time.

In general, the basic idea is to fix the positions and orientations of some selected piece (or pieces). Two properties are necessary: (a) Each equivalence class must have a member with the selected piece in the one of the fixed positions and orientations, and (b) each of the symmetries of the board must move the piece out of the set of fixed positions and orientations.

For the 6 by 10 pentomino problem we will fix the center square of the "X" shaped piece so that it lies in the upper quadrant (thinking of the board as being centered at its center). See Figure 3.6.

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Figure 3.6: Eliminating isomorphs in the 6 by 10 pentomino puzzle.

3.4 Estimating the Running Time of Backtracking.

In many instances it is useful to obtain an estimate of the number of vertices that will occur in a backtracking tree, before the actual algorithm is run. The estimate presented in this section only applies in those instances when we are searching for all possible solutions (i.e. the entire tree is being examined).

The basic idea is to run an experiment in which we follow a random path in the tree from the root to a leaf, and then assume that the entire tree has a similar "parent" – "number of children relationship" as the vertices on this path. The random path is chosen by successively picking a random child of the current vertex to be included next in the path. Each child is regarded as being equally likely. For example, consider the tree shown in Figure 3.7(a) where the thickened edges indicates the random path.

In the experiment the root had three children, the root's child on the thickened path had two children, and so on. Thus we assume that the root has three children, all children of the root have two children, etc. This gives rise to the tree of Figure 3.7(b). This tree has $1 + 3 + 3 \cdot 2 + 3 \cdot 2 \cdot 1 + 3 \cdot 2 \cdot 1 \cdot 2 + 3 \cdot 2 \cdot 1 \cdot 2 \cdot 1 = 40$ vertices. In general, let n_k denote the degree of the (k - 1)st vertex along the experimental path. There are $n_1n_2 \cdots n_k$ vertices at level k in the assumed tree. Thus the estimate is the (finite) sum

 $X = 1 + n_1 + n_1 n_2 + n_1 n_2 n_3 + \cdots$

A procedure to compute the estimate is given in Algorithm 3.6. A recursive version can also be easily derived.

For any probabilistic estimate a desirable property is that the expected value of the estimate is equal to the quantity being estimated. In probability theory such an estimator



Figure 3.7: (a) True backtracking tree with random root-to-leaf path shown. (b) Assumed tree from that random path.

```
\begin{array}{l} estimate := product := 1;\\ k := 1;\\ \text{compute } S_1;\\ \textbf{while } S_k \neq \emptyset \ \textbf{do} \\ \{\text{Advance}\}\\ n_k := |S_k|;\\ product := n_k \cdot product;\\ estimate := estimate + product;\\ x_k := \text{an element of } S_k, \text{ chosen at random;}\\ k := k + 1;\\ \text{compute } S_k; \end{array}
```

Algorithm 3.6: Estimation algorithm.

is referred to as being *unbiased*. Let T be the tree whose size |T| is being estimated. Intuitively, the reason that the estimate is unbiased is that the probability of reaching a vertex x in the tree whose ancestors have degrees n_1, n_2, \ldots, n_t is equal to $1/(n_1n_2\cdots n_t)$, which is the inverse of the weight assigned to that vertex by X. We will now give a more formal argument. Define two functions on the vertices v of the backtracking tree:

$$\tau(v) = \begin{cases} 1 & \text{if } v \text{ is the root} \\ deg(\bar{v}) \cdot \tau(\bar{v}) & \text{if } v \text{ has parent } \bar{v} \end{cases}$$

and

I(v) = [vertex v is visited in the experiment].

Recall the [] notation, defined the previous chapter: [P] is 1 if P is true and is 0 if P is false. Note that τ depends only on the tree and not the experiment. The random variable X may be rewritten as

$$X = \sum_{v \in T} \tau(v) \cdot I(v).$$

Now take the expected value of the random variable X and use linearity of expectation to obtain

$$E(X) = \sum_{v \in T} \tau(v) \cdot E(I(v)) = \sum_{v \in T} \tau(v) \cdot \frac{1}{\tau(v)}$$
$$= \sum_{v \in T} 1 = |T|.$$

The estimator is therefore unbiased.

Some care should be exercised in applying this estimate. Backtracking trees tend to vary wildly in their structure and subtrees with many vertices may be well hidden in the sense that they are accessed only through paths from the root with vertices of low degree. It is essential in applying the test that a large number of trials are used. Once this is done, however, the test is remarkably effective.

3.5 Exercises.

- 1. [1+] Use backtracking by hand to determine the number of solutions to the 5 by 5 queens problem. How many of the solutions are non-isomorphic?
- 2. [1] Generate an estimate of the number of vertices in the backtracking tree for the 8 by 8 queens problem. In picking your "random" row positions, simply use the lowest numbered valid row.
- 3. [1+] Show that the number of solutions to the *n* by *n* Queens problem is less than or equal to $n(n-4) \cdot (n-2)!$. Can you derive a better bound?
- 4. The following 150 characters of C code outputs the number of solutions to the *n*-Queens problem. Explain how the code works. What's the largest value of n for which it will produce a correct answer (after a potentially very long wait) on your machine?



Figure 3.8: The Soma cube pieces.

t(a,b,c){int d=0,e=a&~b&~c,f=1;if(a)for(f=0;d=(e&=~d)&-e;f+=t(a&~d,(b|d)<<1, (c|d)>>1));return f;}main(q){scanf("%d",&q);printf("%d\n",t(~(~0<<q),0,0));}</pre>

- 5. [2] Write a backtracking program to determine a configuration containing the smallest number of queens on a n by n board so that every square of the board is under attack. Is the problem easier if the queens are specified to be non-taking? Give explicit solutions for $1 \le n \le 8$.
- 6. [1+] How many hexominoes (6-ominoes) are there? [2] Prove that the set of all hexominoes cannot be placed in a rectangular configuration without holes.
- 7. [3-] Define the *order* of a polyomino to be the smallest number of copies of P that will fit perfectly into a rectangle, where rotations and reflections of P are allowed. The figure below shows that the pentomino \square has order at most 10. Show that its order is exactly 10. What are the orders of the other two polyomino shapes shown below?



8. [2] A polyomino puzzle with the following pieces has been marketed.



The puzzle is to place the pieces on an 8 by 8 board. Write a backtracking program to determine the number of different non-isomorphic solutions.

- 9. [2] The Soma Cube puzzle is to fit the seven pieces listed in Figure 3.8 into a 3 by 3 by 3 cube. Write a backtracking program to generate all 240 non-isomorphic solutions to the Soma Cube puzzle.
- 10. [2] Snake-in-a-cube puzzle: A snake consists of 27 unit cubes arranged in order. They are held together by a shock-cord, but can be rotated around the cord. Each unit cube is either "straight-through" (the cord passed through one face of the cube and exits



Figure 3.9: A 6 by 6 knight's tour.

- 11. [2] A knight's tour of an n by n chessboard is a sequence of moves of the knight on the chessboard so that each of the n^2 squares is visited exactly once. Shown in Figure 3.9 is a knight's tour of a 6 by 6 chessboard. Write a backtracking program to find a single knight's tour on an 8 by 8 chessboard starting from the upper left corner. A knight's tour that returns to the square upon which it started is said to be *re-entrant*. Modify your program from so that it finds a re-entrant knight's tour. Estimate the time that it would take to explore the entire backtracking tree assuming that it takes a millisecond to process one vertex in the tree. Prove that no Knight's tour can exist if n is odd.
- 12. [1+] Draw a graph representing the possible moves of a knight on a 4 by 4 chessboard. Use this graph to prove that there is no knight's tour on a 4 by 4 board.
- 13. [2] In a noncrossing Knight's tour the lines drawn for each move of the knight do not cross. The tour shown in Figure 3.9 has many crossings, and in general, a non-crossing tour cannot visit every square of the board. Determine the longest possible non-crossing knight's tour on an 8 by 8 board.
- 14. [2] Write a backtracking program to determine the number of ways to color the vertices of a graph with k colors for k = 1, 2, ..., n where n is the number of vertices in the graph. In any such coloring adjacent vertices must receive distinct colors. Deciding whether a graph can be colored with k colors is a well-known NP-complete problem.
- 15. [2] Write a backtracking program to count the number of topological sortings (linear extensions) of a directed acyclic graph (partially ordered set).

3.6. BIBLIOGRAPHIC REMARKS

- 16. [2] Write a backtracking program to list all Hamilton cycles (if any) in a graph. Use your program to determine the number of Hamilton cycles in the tesseract.
- 17. [2] For given k, a subset $K \subseteq [k]$, is said to represent k if there is some unique $I \subseteq K$ such that $\sum_{x \in I} x = k$. For given n, a pair of subsets $P, Q \subseteq [n]$ is said to dichotomize [n] if, for each $k \in [n]$, the number k is representable by P or by Q, but not by both. For example $\{1, 2, 6\}, \{4, 5\}$ dichotomizes [9], but [12] is not dichotomized by $\{1, 2, 9\}, \{3, 4, 5\}$ since 3 and 9 are represented twice and 6 is not represented. Write a backtracking program that takes as input n and outputs all pairs of subsets of [n] that dichotomize it. How many solutions are there for n = 17?
- 18. [3] Let $\tau = (1 \ 2)$ and $\sigma = (1 \ 2 \ \cdots \ n)$. Write a backtracking program to find a Hamilton cycle in the directed Cayley graph $Cay(S_n : \{\sigma, \tau\})$ when n = 5. Can you find a Hamilton path for n = 6? $[\mathbf{R}-]$ Find a Hamilton cycle for n = 7. It is known that there is no Hamilton cycle for n = 6.
- 19. There is a large family of combinatorial questions involving the packing of squares into squares. [2+] For $n \leq 13$ determine the least number of smaller squares that will tile a n by n square. [2+] The sum $1^2 + 2^2 + \cdots + 24^2 = 70^2$ suggests that it might be possible to tile a 70 by 70 square with squares of sizes $1, 2, \ldots, 24$. Show that this is impossible.
- 20. [1] Write Algorithm 3.6 as a recursive procedure.
- 21. [3] Extend the unbiased procedure for estimating the size of a backtracking tree to that of estimating the size of a directed acyclic graph that is rooted at r (all vertices are reachable from r).

3.6 Bibliographic Remarks

Perhaps the first description of the general backtracking technique is in Walker [474]. Early papers about backtracking include Golomb and Baumert [171].

The eight queens problem is attributed to Nauck (1850) by Schuh [409]. It is said that Gauss worked on the problem and obtained the wrong answer! Sosic and Gu [430] analyze programs for the 8-queens problem.

A paper of Bitner and Reingold [43] discusses a number of interesting ways to speed up backtracking programs and contains some applications to polyomino problems.

A (very ugly) program for generating all solutions to the Soma cube problem may be found in Peter-Orth [335].

The book that really popularized polyominoes, and pentominoes in particular, is "Polyominoes" by Golomb [169]. The book by Martin [290] contains much interesting material about polyominoes and contains further references on the topic. The two volume book by Berlekamp, Conway and Guy [38] on mathematical games contains interesting chapters about the Soma cube (including a map of all solutions!) as well as scattered references to polyominoes.

The method for estimating the size of the backtracking tree comes from Hall and Knuth [184] and further analysis is carried out in Knuth [240]. The efficiency of the method has been improved by Purdom [353]. The estimation method can be extended from rooted trees to directed acyclic graphs; see Pitt [340].

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