Design and Analysis of Algorithms
Backtrack

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Outline

- **Classical examples**
- **Principles of Backtrack**
- **Loading problem**
- **Graph coloring problem**
- **Estimation of leaves**

Backtrack Paradigm

- Recurve approach is essentially travelling the whole tree defined by the recursive relation.

  The subtrees may repeat, so we need to cache intermediate results to improve efficiency. This is exactly the essence of **dynamic programming**.

- For some problems, **the subtrees will not overlap**.

  In such case, there is no better algorithm other than traveling the entire tree. But, we can travel the entire tree smartly.

  This is what **backtrack** technique concerns: *stop visiting the subtree if the solution won't appear and backtrack to the parent node.*

  \- Basic backtrack strategy: **Domino property defined by problem constraint.**

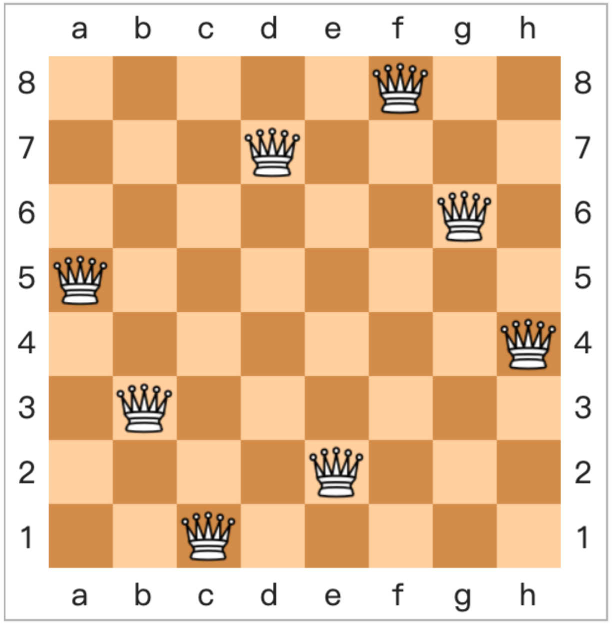
  \- Advanced backtrack strategy: ***Branch-and-bound.***

Example: 8-Queen Problems

- 8-queen puzzle. Placing eight chess queens on an 8×8 chessboard so that no two queens threaten each other.

A solution requires that no two queens share the same row, column, or diagonal.

8-queen puzzle is a special case of the more general n-queen problem: placing n non-attacking queens on an $n \times n$ chessboard.



Counting Solutions

- Solution is an n-dimension vector over $[n]$: exist for all natural numbers n with the exception of n =2,3.

  8-queen puzzle has 92 distinct solutions, the entire solution space is $C_{64}^{8} = 4{,}426{,}165{,}368$.

  If solutions that differ only by the symmetry operations of rotation and reflection of the board are counted as one, the puzzle has 12 solutions, called as **fundamental solutions**.

n	fundamental	all
8	12	92
9	46	352
10	92	724
...	...	...
26	2,789,712,466,510,289	22,317,699,616,364,044
27	29,363,495,934,315,694	234,907,967,154,122,528

Background of 8-Queen Puzzle

- Origin of 8-Queen Puzzle

  Max Bezzel first proposed this problem in 1848, Frank Nauck gave the first solution in 1850 and extended it to n-queen puzzles. Many mathematicians including Carl Gauss also studied this problem.

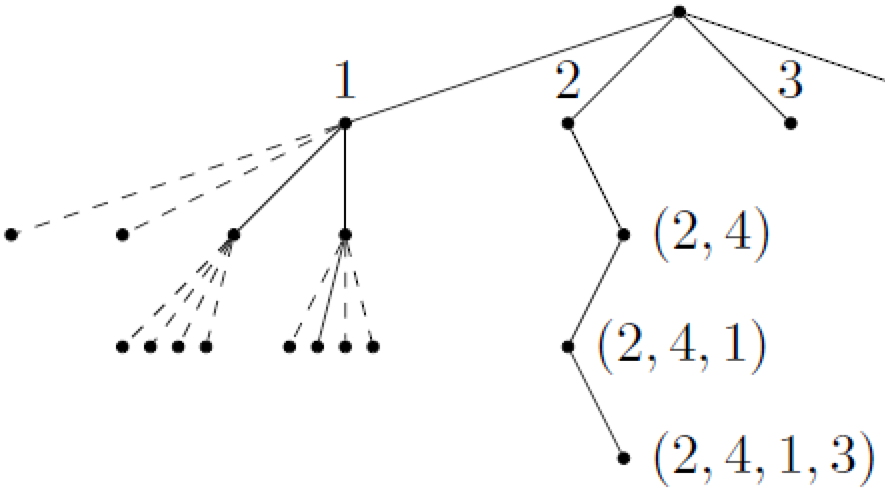
  Edsger Dijkstra exemplified the power of ***depth-first backtracking algorithm*** via this problem.

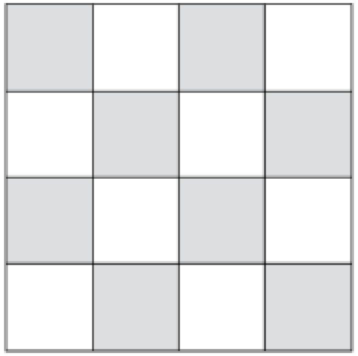
  There is no known formula for the exact number of solutions, or even for its asymptotic behavior. The 27×27 board is the highest-order board that has been completely enumerated.

How to solve?

Modeling all possible solutions as leaf nodes of a tree traversal the solution space via travelling the tree.

Demo of Quadtree for 4-Queen Puzzle





- Travel the tree via depth-first order to find all solutions.

  i-th level node represent i-th element in solution vector in the i-th level, the branching choice is less than $n-i$ leaves correspond to solutions.

Example: 0-1 Knapsack Problem

- Problem. Given n items with value v_i and weight w_i, as well as a knapsack with weight capacity W. The number of each item is 1. Find a solution that maximizes the overall value.
- Solution. n dimension vector $(x_1, x_2, \ldots, x_n) \in \{0,1\}^n$, $x_i = 1 \Leftrightarrow$ selecting item i.
- Nodes: $(x_1, x_2, \ldots, x_k)$ corresponds to partial solution.
- Search space. In all levels, the branching choice is always 2 (perfect binary tree with 2^n leaves).
- Candidate solution. Satisfy constraint $\sum_{i=1}^{n} w_i x_i \leq W$.
- Optimal solution. The candidate solutions that achieve maximal values.

Demo

- **Ex.**

Table: $n = 4$, $W = 13$

item	1	2	3	4
value	12	11	9	8
weight	8	6	4	3

Solution. n dimension vector $(x_1, x_2, \ldots, x_n) \in \{0,1\}^n$, $x_i = 1 \Leftrightarrow$ selecting item i.

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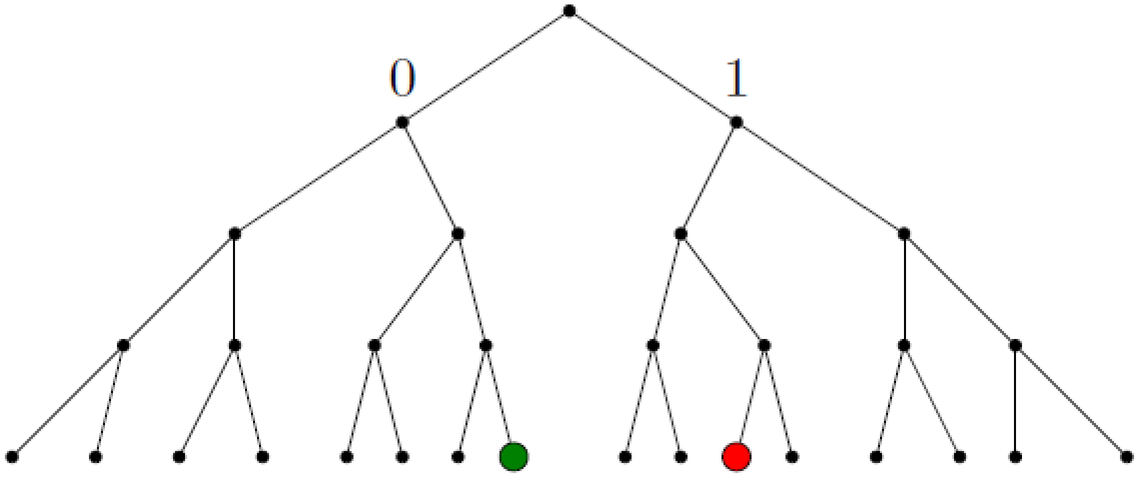
Two candidate solutions

1. $(0, 1, 1, 1)$: $v = 28,\ w = 13$
2. $(1, 0, 1, 0)$: $v = 21,\ w = 12$

Optimal solution is $(0, 1, 1, 1)$

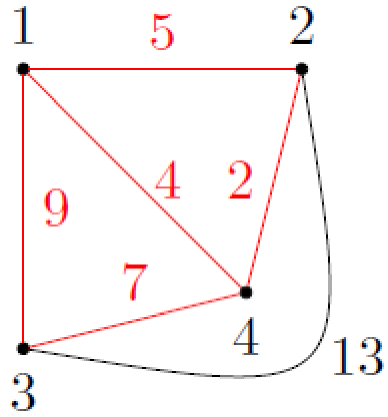


Example: Traversal Salesman Problem

- Problem. Given n cities $C = \{c_1, c_2, \dots, c_n\}$ and $d(c_i, c_j) \in Z^+$. Find a cycle with minimal length that travels each city once.
- Solution. A permutation of $(1,2,\dots,n) \Rightarrow (k_1, k_2, \dots, k_n)$ such that

$$\min\left\{\sum_{i=1}^{n-1} d\left(c_{k_i}, c_{k_i+1}\right) + d\left(c_{k_n}, c_{k_1}\right)\right\}$$

Ex.



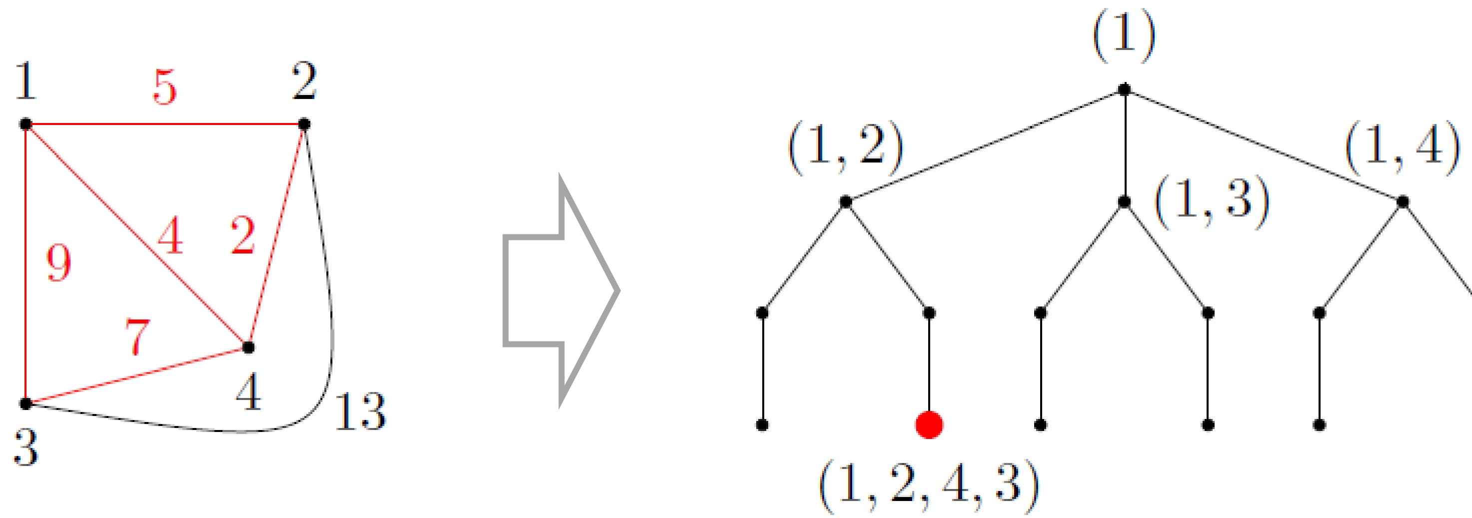
$C = \{1, 2, 3, 4\}$

$d(1,2) = 5,\ d(1,3) = 9$

$d(1,4) = 4,\ d(2,3) = 13$

$d(2,4) = 2,\ d(3,4) = 7$

Search Space of TSP



- Any node can serve as the root, cause TSP is defined over an undirected graph.
- Search space. In the i-th level, the branching choice is always $n - i \Longrightarrow$ obtain a tree with $(n-1)!$ leaves (number of all possible permutations over $\{1,2, \ldots, n\}$.
- Solution is (1,2,4,3), length of cycle is 5+2+7+9=23.

Classical Examples of Backtrack

- Problem: n-Queen Puzzle, 0-1 Knapsack, TSP
- Solution: Vector
- Search space: Tree

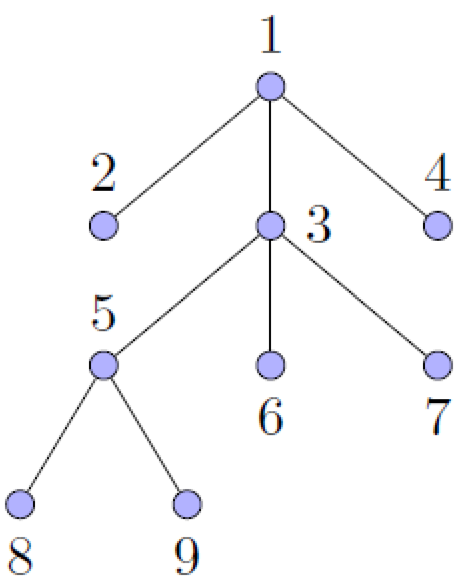
  Nodes correspond to partial solutions, leaves correspond to candidate solutions.
- Search order: Depth-first, Breadth-first,…

Main Idea of Backtrack

- Scope of application. Search or optimization problem
- Search space. Tree

  Leaves: candidate solution

  Nodes: partial solution
- How to search. Systematically traversal the tree: DFS, BFS, …



DFS: $1 \to 2 \to 3 \to 5 \to 8 \to 9 \to 6 \to 7 \to 4$

BFS: $1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 7 \to 8 \to 9$

States of Nodes

- The tree is explored dynamically. Let v be the candidate node (corresponding to partial solution) and P be the predicate that checks if v satisfies the constraint.

  $P(v) = 1 \Rightarrow$ expand

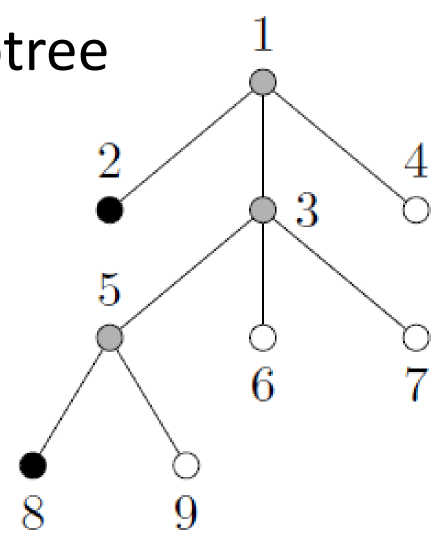
  $P(v) = 0 \Rightarrow$ backtrack to the parent node

- States of node

  Black: finishing the traversal of this subtree

  Gray: visiting its subtree

  White: unexplored



DFS: $1 \to 2 \to 3 \to 5 \to 8$

finished visiting: $2, 8$

being visited: $1, 3, 5$

unexplored: $9, 6, 7, 4$

Basic Backtrack Technique: Domino Property

- At note $v = (x_1, \dots, x_k)$,

  $P(x_1, \dots, x_k) = 1 \Rightarrow (x_1, \dots, x_k)$ meet some property.

Example. n-queen puzzle, placing k queens in positions without attacking each other.

Domino property (admit safe backtrack)

$$P(x_1, \dots, x_{k+1}) = 1 \Rightarrow P(x_1, \dots, x_k) = 1, 0 < k < n$$

Converse-negative proposition

$$P(x_1, \dots, x_k) = 0 \Rightarrow P(x_1, \dots, x_{k+1}) = 0, 0 < k < n$$

k-dimension vector does not satisfy constrain $\Rightarrow$ its k+1-dimension extension does not satisfy constraint either

This property guarantees that backtracking will not miss any solution. Safely backtrack when $P(x_1, \dots, x_k) = 0$

Counterexample

- Find integer solutions for inequality

$$5x_1 + 4x_2 - x_3 \le 10$$
$$1 \le x_k \le 3, k = 1,2,3$$

$P(x_1, \ldots, x_k) = 1$ iff $\sum_{i=1}^{k} a_i x_i \le 10$

Does not satisfy Domino property

$$5x_1 + 4x_2 - x_3 \le 10 \;\not\Rightarrow 5x_1 + 4x_2 \le 10$$

Modification to satisfy Domino property: set $x_3' = 3 - x_3$

$$5x_1 + 4x_2 + x_3' \le 13$$

$$1 \le x_1, x_2 \le 3, 0 \le x_3' \le 2$$

Domino Property

- The premise condition to use backtrack: Domino Property.

- General steps of backtrack algorithm:

  Define solution vector (include the range of every element),
  $$(x_1, \dots, x_n) \in X_1 \times \cdots \times X_n$$

  After fixing $(x_1, \dots, x_{k-1})$, update admissible range of x_k as $A_k \subseteq X_k$ using predicate P.

  Decide if Domino property is satisfied.

  Decide the search strategy: DFS, BFS.

  Decide the data structure to store the search path.

Backtrack Recursive Template

Algorithm 1: BackTrack(n) // output all solutions

for $k = 1\ to\ n$ do $A_k \leftarrow X_k$; // initialize

ReBack(1);

Algorithm 2: ReBack(k) // k is the current depth of recursion

if $k = n$ then return solution $(x_1, \ldots, x_n)$;

else

  while $A_k \neq \emptyset$ do

    $x_k \leftarrow A_k$ // according to some order;

    $A_k \leftarrow A_k - \{x_k\}$;

    update A_{k+1}, ReBack(k+1)

  end

end

The above is the oversimplified pseudocode. One must be careful when dealing with domains A_k and solution vector x when coding.

Backtrack Iterative Template

Algorithm 3: BackTrack(n) // all solutions

1: for $k = 1\ to\ n$ do $A_k \leftarrow X_k$; // initialize

2: $k \leftarrow 1$;

3: while $A_k \neq \emptyset$ do

4: $\quad x_k \leftarrow A_k; A_k \leftarrow A_k - \{x_k\}$;

5: $\quad$ if $k < n$ then $k \leftarrow k + 1$;

6: $\quad$ else $(x_1, \ldots, x_n)$ is solution;

7: end

8: if $k > 1$ then $k \leftarrow k + 1$; goto 3;

A_k is determined by $(x_1, \ldots, x_{k-1})$. The algorithm terminates when all A_i are empty. Otherwise, it will backtrack (line 8).

Loading Problem

- Problem. Given n containers with weight w_i, two boats with weight capacity W_1 and W_2 s.t. $w_1 + \cdots + w_n \leq W_1 + W_2$.
- Goal. If there exists a scheme to load the n containers on two boats. Please give a scheme if it is solvable.

Ex.

$$w_1 = 90, w_2 = 80, w_3 = 40, w_4 = 30, w_5 = 20, w_6 = 12,$$
$$w_7 = 10, W_1 = 152, W_2 = 130$$

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Main idea: Let the total weights be W.

Load on boat 1 first. Using backtrack to find a solution that maximizes W_1^*, where W_1^* is the real capacity.

Then check if $W - W_1^* \leq W_2$. Return "yes" if true and "no" otherwise.

Solution: load 1, 3, 6, 7 on boat 1 and the rest on boat 2.

Pseudocode

Algorithm 4: Loading(W_1)

1: $W_1^* \leftarrow 0; C \leftarrow 0; i \leftarrow 1;$

2: while $i \leq n$ do // line 3-4: whether to load container i

3: if $C + w_i \leq W_1$ then $C \leftarrow C + w_i, x[i] \leftarrow 1, i = i + 1;$

4: else $x[i] \leftarrow 0, i = i + 1;$

5: end

6: if $W_1^* < C$ then record solution, $W_1^* \leftarrow C;$

7: while $i > 1$ and $x[i] = 0$ do $i - 1;$ // find a backtrack node

8: if $i = 1$ then return optimal solution; // backtrack to root

9: else $x[i] \leftarrow 0; C \leftarrow C - w_i; i = i + 1,$ goto 2; // continue to search

Line 7-9: find a backtrack point.

Line 8: have travelled all the tree and back to the root.

Line 9: find a left branch, means there still exist unexplored right branch

Demo

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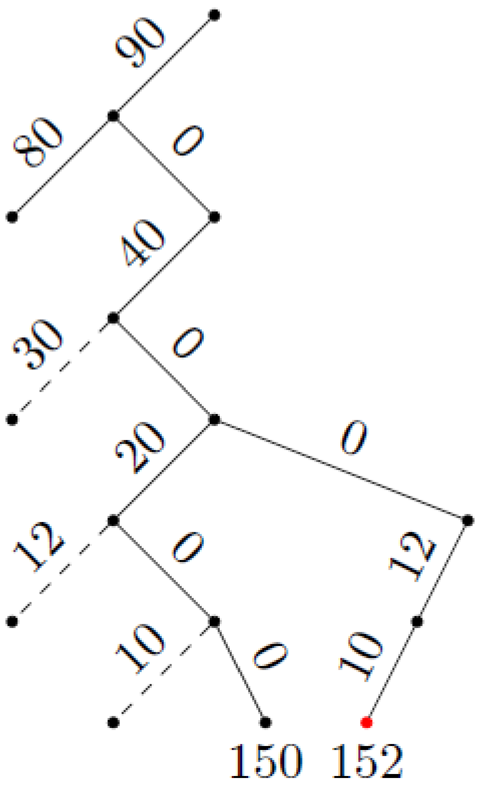

Demo

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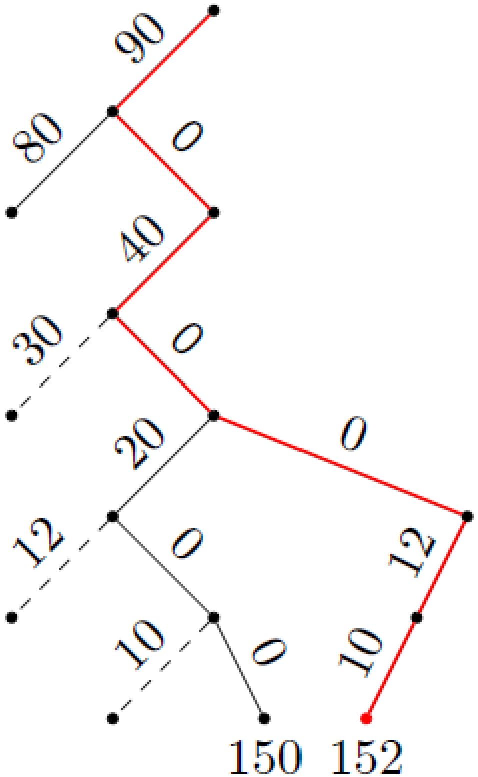


it is loadable

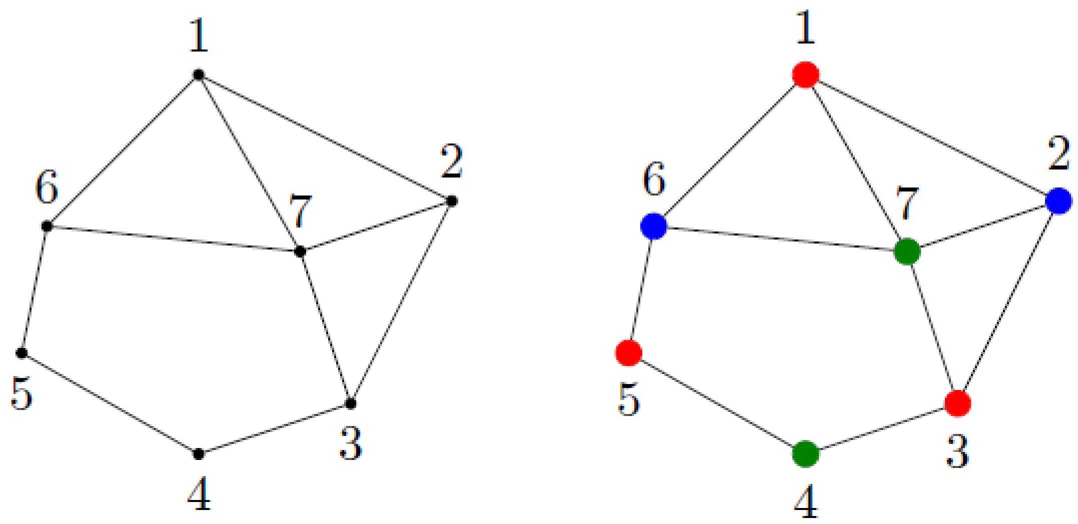
1, 3, 6, 7 on boat 1

2, 4, 5 on boat 2

time complexity $W(n) = O(2^n)$

Graph Coloring Problem

- Problem. Undirected graph G and m colors. Coloring the vertices to ensure the connected two vertices with different color.
- Goal. Output all possible coloring schemes. Output “no” if there is none.



$n = 7, m = 3$

Algorithm Design

- Input. $G = (V, E), V = \{1,2, \dots, n\}$, color set $= \{1,2, \dots, m\}$
- Solution vector. $(x_1, x_2, \dots, x_n), x_i \in [m]$

  $(x_1, x_2, \dots, x_k)$ gives partial solution for vertex set $\{1,2, \dots, k\}$

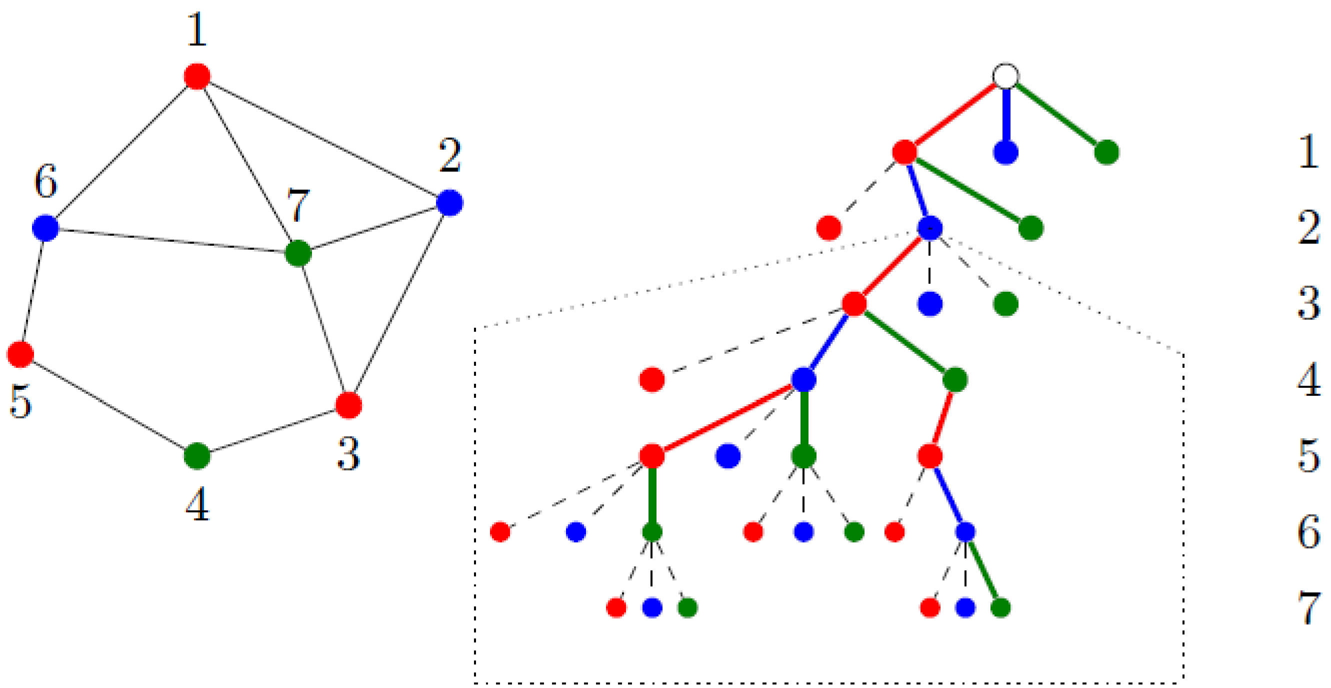
Search tree. m-fork tree

Constraint. At node $(x_1, x_2, \dots, x_k)$, the set of available colors for node $k+1$ is not empty.

  If the nodes in adjacent list have used up m colors, then node $k+1$ is not colorable. In this case, back to parent node.

Search strategy: DFS

Demo



The first solution vector: $(1, 2, 1, 3, 1, 2, 3)$

Reduce Search Scope

- Symmetry (only need to search at most 1/6 solution space).

  The permutation over (1,2,3) is 6. For any specific solution, there exist 6 homogeneous solution.

  Level-2 has 2-fold solution (e.g. color blue and green are exchangeable), level-1 has 3-fold solution (node 1 can pick red, green or blue); the closer to the root, the more choice of replacement.

- Additional reasoning also helps to reduce search scope.

  Example: if node 1,2,3 have been colored differently, then node 7 is definitely non-colorable because it connects with node 1,2,3 (backtrack from this node)

  Need trade-off between search and decide.

Applications of Graph Coloring

- Arrangement of meeting room

  There are n events to be arranged, if the slots of event i and event j overlap, we say i and j are not compatible. How to arrange these events with smallest number of meeting rooms?

- Modeling

  Treat event as node, if i, j are not compatible, then add an edge between i and j.

  Treat meeting rooms as colors.

The arrangement problem is transformed into finding a coloring scheme with smallest colors.

Estimation of Leaves

Sometimes, we need to know the size of problems (captured by the number of nodes)

Finding the exact number may require to travel the whole tree exhaustively, which is equivalent to solve the problem.

Monte Carlo method

- Step 1: Choose a random path from root until there is no more branching, i.e., randomly and sequentially assign values to $x_1, x_2, \dots$, until the vector cannot be further expanded.
- Step 2: Assume other $|A_i| - 1$ branches has the same path as selected one, calculate the nodes of search tree.
- Repeat Steps 1-2, and compute the average number of nodes.

Estimate n-Queen Puzzle

Algorithm 5: MonteCarlo(n, t)

Input: $n =$ # number of queens, $t =$ # number of sampling

Output: l average number of nodes for t times sampling

1: $l \leftarrow 0;$

2: for $i = 0$ to t do // sampling time is t

3: $m \leftarrow$ Estimate(n); // number of nodes

4: $l \leftarrow l + m;$

5: end

6: $l \leftarrow l/t;$

One Sampling

- Parameter

  l is the total number of nodes

  k is the current depth

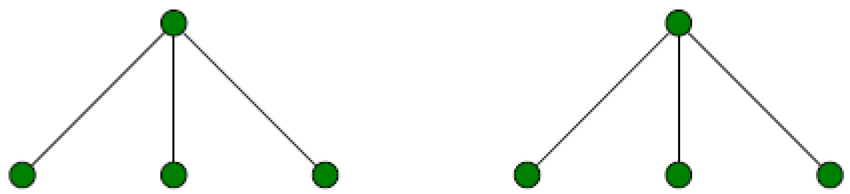
  r_{prev}: # nodes on the previous level

  $r_{current}$: # nodes on the current level

  $r_{current} = r_{prev} \times$ # branches

  n is the depth of tree

- Computation order: randomly select until reaching the leaves



$$r_{\text{prev}} = 2,\ r_{\text{current}} = r_{\text{prev}} \cdot 3 = 6$$

Pseudocode

Algorithm 6: Estimate(n)

$l \leftarrow 1$; $r_{prev} \leftarrow 1$; $k \leftarrow 1$; // the root node

while $k \leq n$ do

    if $A_k = \emptyset$ then return l; // no more branch

    $x_k \leftarrow A_k$ // randomly select a branch

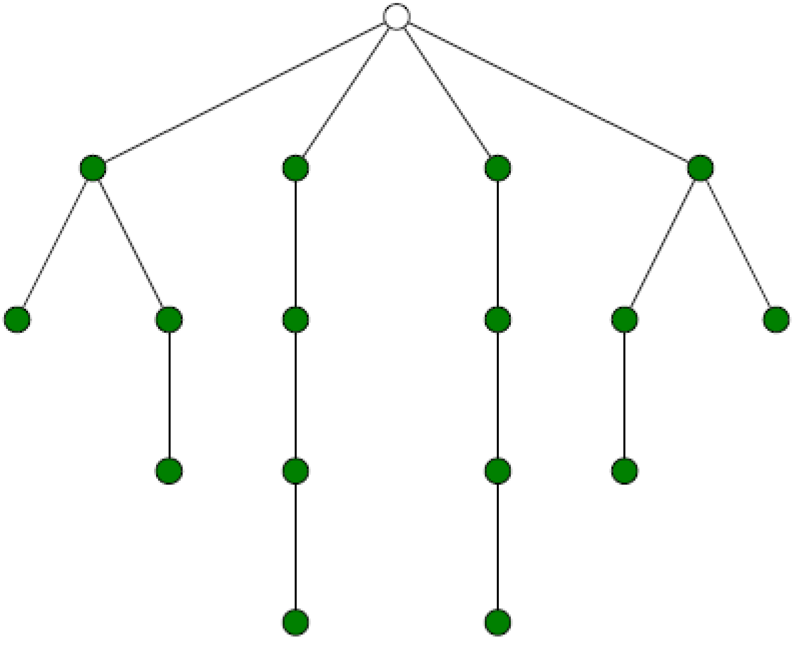
    $r_{current} \leftarrow r_{prev} \times |A_k|$ // number of nodes on k level

    $l \leftarrow l + r_{current}$;

    $k \leftarrow k + 1$;

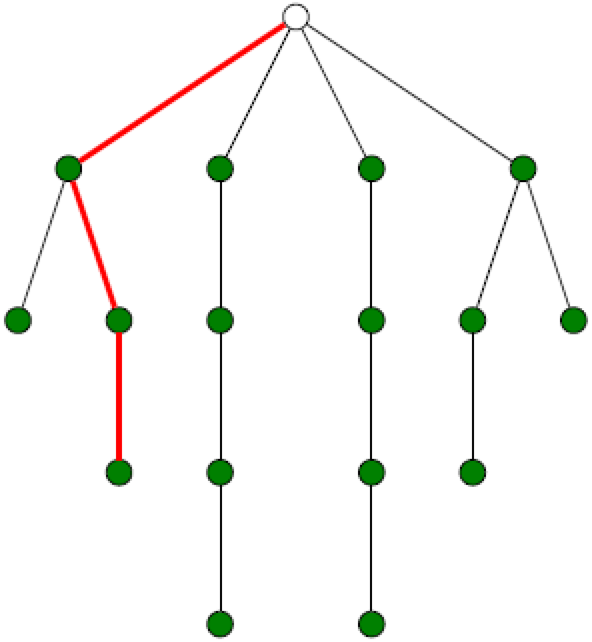
end

Real Case: 4-Queen Puzzle

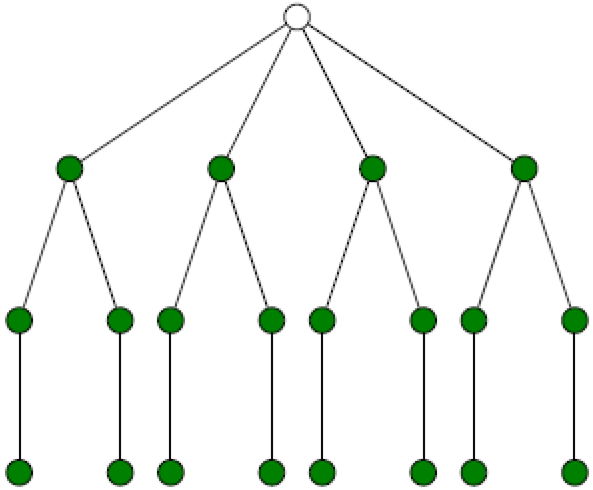


17 nodes

Random Selected Path 1

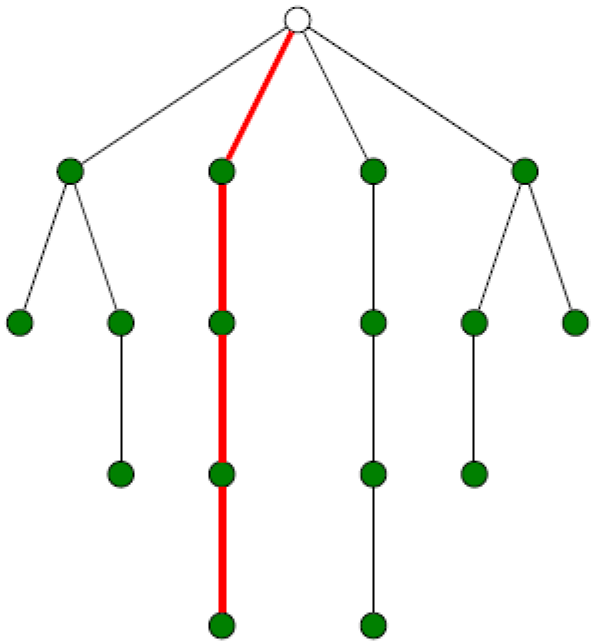


case 1: $(1, 4, 2)$

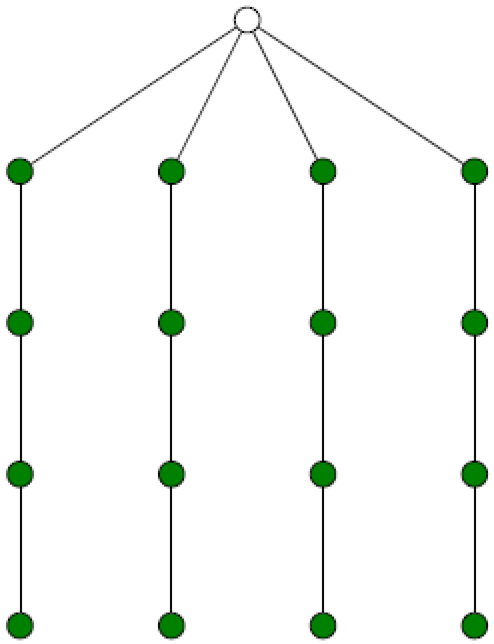


21 nodes

Random Selected Path 2

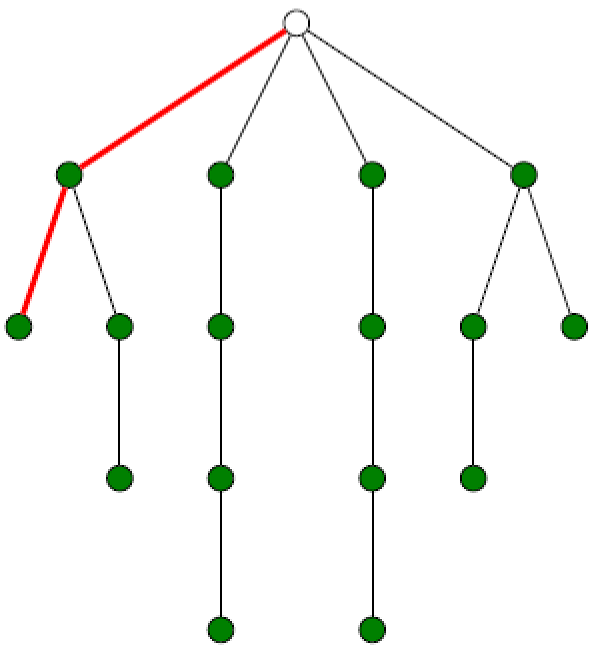


case 2: $(2, 4, 1, 3)$

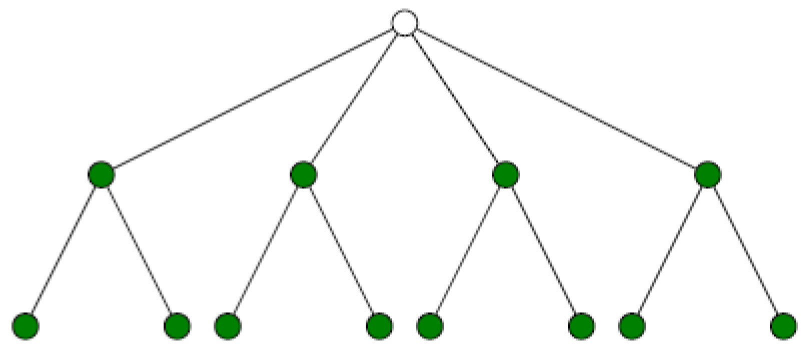


17 nodes

Random Selected Path 3



case 3: $(1, 3)$



13 nodes

Estimate Result

Suppose sampling four times:

Case 1: 1

Case 2: 1

Case 3: 2

Average number of nodes: $\frac{21+17+13+13}{4} = 16$

The real number of nodes: 17

More samplings will make the estimation approaches the real number