Design and Analysis of Algorithm
Backtrack (I)

Backtrack Paradigm

Recursive approach is essentially travelling the whole tree defined by the recusive relation.

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For some problems, the subtrees will not overlap.

- In such case, there is no better algorithm other than travelling 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

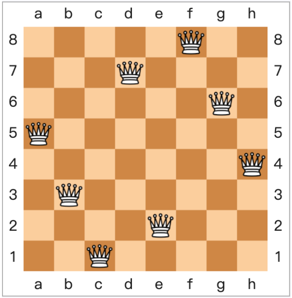
Outline

Example 1: Eight Queen Problems

Eight queens 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.

Eight queens puzzle is a special case of the more general n queens 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 $n = 2, 3$.

- Eight queens 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 Eight Queen Puzzle

Origin of Eight 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 Guass also studied this problem.

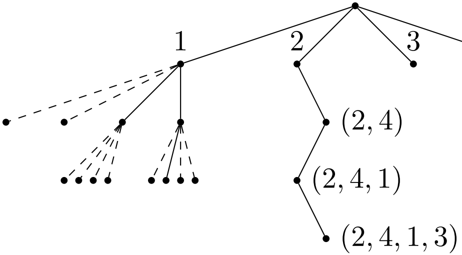
Edsger Dijkstra exemplified the power of *depth-first backtracking algorithm* via this problem.

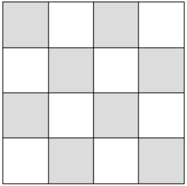
> There is no known formula for the exact number of solutions, or even for its asymptotic behavior. The 27×27 board is the highest-order board that has been completely enumerated.

How to solve?

- modeling all possible solutions as n-level leaf nodes of a tree
- traversal the solution space via travelling the tree

Demo of Quadtree for 4 Queens Puzzle





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

- i-th level node represent sub-i vector of solution vector
- in the i-th level, the branching choice is less than $n - (i - 1)$
- n-level leaf nodes correspond to solutions

Example 2: 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 maximize the value.

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

Nodes: $(x_1, x_2, \dots, x_k)$ corresponds to partial solution

Search space. In all level, the branching choice is always $2 \rightsquigarrow$ 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.

A Demo

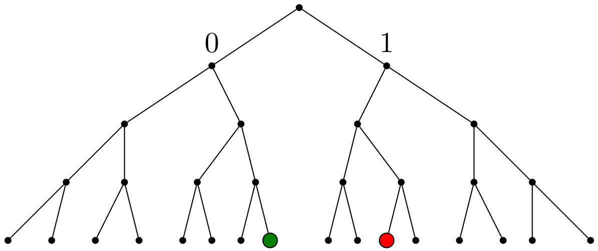
Table: $n = 4$, $W = 13$

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

Two candidate solutions

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

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

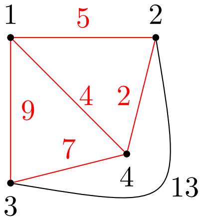


Example 3: Traversal Salesman Problem

Problem. Given n cities $C = \{c_1, c_2, \ldots, c_n\}$ and $d(c_i, c_j) \in \mathbb{Z}^+$. Find a cycle with minimal length that travels each city once.

Solution. A permutation of $(1, 2, \ldots, n)$ — $(k_1, k_2, \ldots, k_n)$ such that

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



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

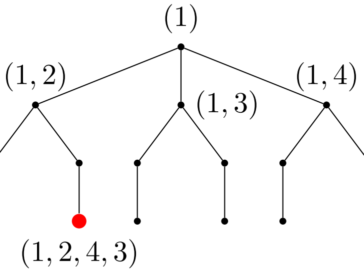
$d(1, 2) = 5$, $d(1, 3) = 9$

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

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

Solution is $(1, 2, 4, 3)$, length of cycle is $5 + 2 + 7 + 9 = 23$

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 $n - i$

- obtain a tree with $(n-1)!$ leaves $\rightsquigarrow$ number of all possible permutations over $\{1, \ldots, n\}$ under cyclic shift

Summary

Classical examples of Backtrack

- n queens 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, jump-hop

Outline

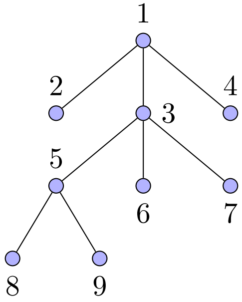
Main Idea of Backtrack

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

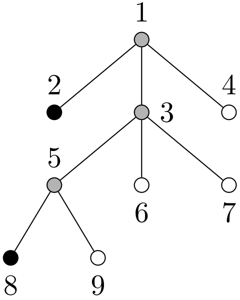
States of Nodes

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 constraint.

- $P(v) = 1 \Rightarrow$ expand
- $P(v) = 0 \Rightarrow$ backtrack to parent node

States of node

- white: unexplored
- gray: visiting its subtree
- black: finishing the traversal of this subtree



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 node $v = (x_1, \ldots, x_k)$

$$P(x_1, \ldots, x_k) = 1 \Leftrightarrow (x_1, \ldots, x_k) \text{ meet some property}$$

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

Domino property $\rightsquigarrow$ admit safe backtrack

$P(x_1, x_2, \ldots, x_{k+1}) = 1$ (cards fall) $\Rightarrow P(x_1, x_2, \ldots, x_k) = 1, 0 < k < n$

Converse-negative proposition

$$P(x_1, x_2, \ldots, x_k) = 0 \Rightarrow P(x_1, x_2, \ldots, x_{k+1}) = 0, 0 < k < n$$

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

- guarantee that backtracking will not miss any solution
- safely backtrack when $P(x_1, x_2, \ldots, x_k) = 0$

A Counterexample

Find integer solutions for inequality

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

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

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

$$5x_1 + 4x_2 + x_3' \le 13, 1 \le x_1, x_2 \le 3, 0 \le x_3' \le 2$$

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2022 级贾梦涵: 3 can be generalized to any positive integer ≥ 3.

Summary

The premise condition to use backtrack: Domino property

General steps of backtrack algorithm

- Define solution vector (include the range of every element), $(x_1, x_2, \ldots, x_n) \in X_1 \times \cdots \times X_n$
- After fixing $(x_1, x_2, \ldots, x_{k-1})$, 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 ← X_k; //initialize
ReBack(1);
```

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

```
if k = n then return solution (x_1, ..., x_n);
else
    while A_k ≠ ∅ do
        x_k ← A_k //according to some order;
        A_k ← A_k − {x_k};
        update A_{k+1}, ReBack(k + 1);
    end
```

- The above is the oversimplified pseudocode.
- One must be careful when dealing with domains A_k and solution vector x when coding (value transfer vs. reference transfer)

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:     $x_k \leftarrow A_k$; $A_k \leftarrow A_k - \{x_k\}$;
5:     **if** $k < n$ **then** $k \leftarrow k + 1$;
6:     **else** $(x_1, x_2, \ldots, x_n)$ 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).

Outline

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.

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Example

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

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

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Main idea: Let the total weights be W.

1. Load on boat 1 first. Using backtrack to find a solution that maximizes W_1^*, where W_1^* is the real capacity.
2. Then check if $W - W_1^* \leq W_2$. Return "yes" if true and "no" otherwise.

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** $x[i] \leftarrow 0$, $i \leftarrow i + 1$;
5: **end**
6: **if** $W_1^* < C$ **then** record solution, $W_1^* \leftarrow C$;
7: **while** $i > 1$ *and* $x[i] = 0$ **do** $i = i - 1$; //find a backtrack node
8: **if** $i = 0$ **then return** optimal solution; //backtrack to root
9: **else** $x[i] \leftarrow 0$; $C \leftarrow C - w_i$; $i = i + 1$, goto 2 ; //$x[i] = 1$: continue to search

line 7-9: find a backtrack point

1. line 8: have travelled all the tree and back to the root
2. line 9: find a left branch, means there still exist unexplored right branch $\rightsquigarrow$ change it to right branch

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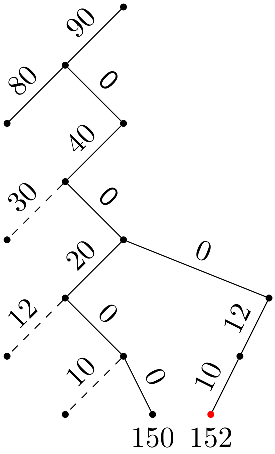

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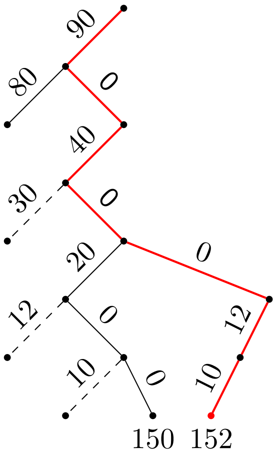

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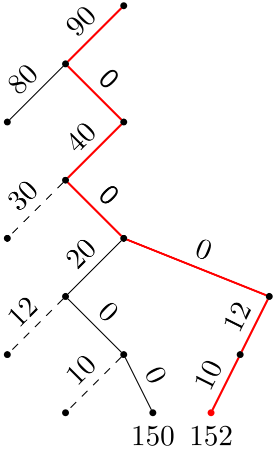

it is loadable

- $1, 3, 6, 7$ on boat 1
- $2, 4, 5$ on boat 2

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

Outline

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.

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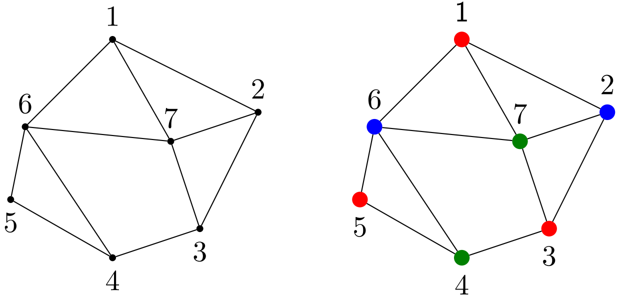


$$n = 7, m = 3$$

Algorithm Design

Input. $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, color set $\{1, 2, \ldots, m\}$

Solution vector. $(x_1, x_2, \ldots, x_n)$, $x_i \in [m]$

$(x_1, \ldots, x_k)$ gives partial solution for vertice set $\{1, 2, \ldots, k\}$

Search tree. m-fork tree

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

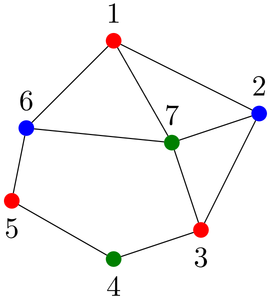
- If the nodes in adjacent list have used up m colors, then node $k + 1$ is not colorable. In this case, back to parent node. (Domino property obviously holds)

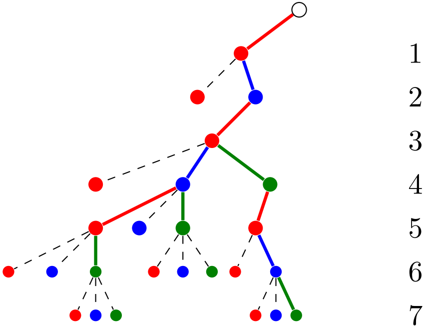
Search strategy: DFS

Time complexity: $O(nm^n)$

- the depth of tree is $n \Rightarrow$ totally at most m^n nodes
- every step need to find usable colors $\Rightarrow$ require $O(n)$ cost

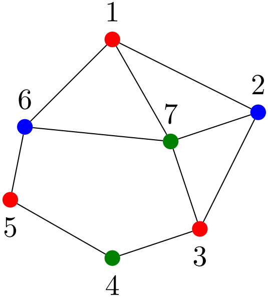
Demo

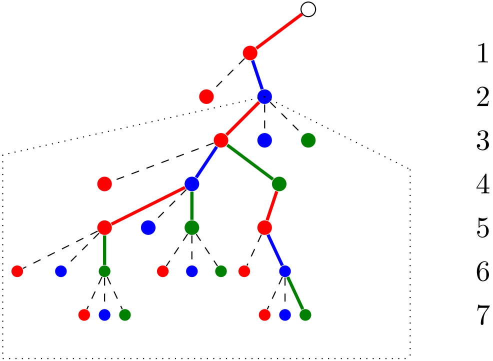




the first solution vector: $(1, 2, 1, 3, 1, 2, 3)$

The Structure of Search Tree





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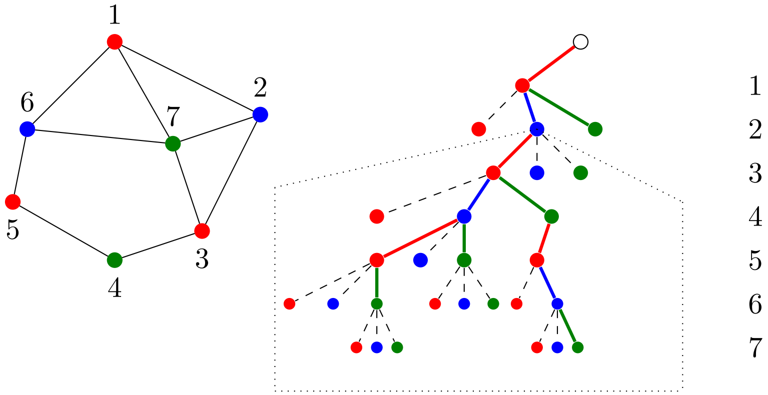

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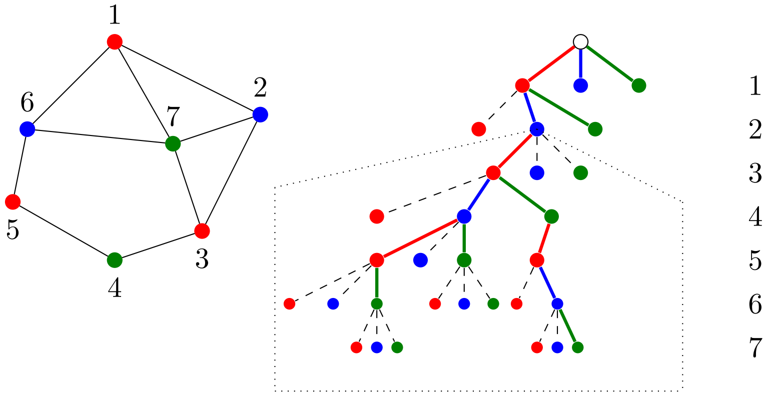

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Complexity Analysis

Time complexity: $O(nm^n)$

Symmetry $\rightsquigarrow$ only need to search at most $1/6$ solution space

- the permutation over $(1, 2, 3)$ is $6 \rightsquigarrow$ 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.

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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 $1, 2, 3 \rightsquigarrow$ 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?

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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 to finding a coloring scheme with smallest colors.

Outline

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

1. Choose a random path from root until there is no more branching, i.e., randomly and sequentially assign values to $x_1, x_2, \ldots,$ until the vector cannot be further expanded.
2. Assume other $|A_i| - 1$ branches has the same path as selected one, calculate the nodes of search tree
3. Repeat step 1 and 2, 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 node of t times sampling

```
ℓ ← 0;
for i = 1 to t do                    //sampling t times
    m ← Estimate(n);                 //number of nodes;
    ℓ ← ℓ + m;
end
ℓ ← ℓ/t;
```

One Sampling

Parameter

- ℓ is the total number of nodes
- k is the depth
- r_{prev}: # (nodes on the previous level)
- r_{current}: # (nodes on the current level)
- $r_{\text{current}} = r_{\text{prev}} \times \#(\text{branches})$
- n is the depth of tree

Computation oder: randomly select until reaching the leaves

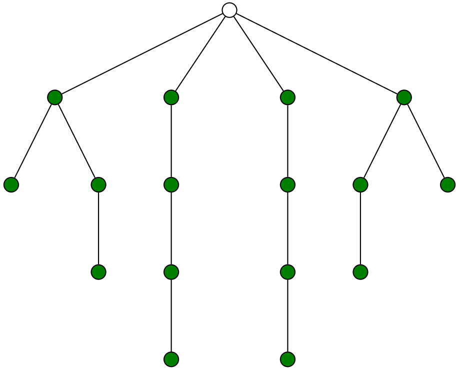
$$r_{\text{prev}} = 2,\ r_{\text{current}} = r_{\text{prev}} \cdot 3 = 6$$

Pseudocode

Algorithm 6: Estimate(n)

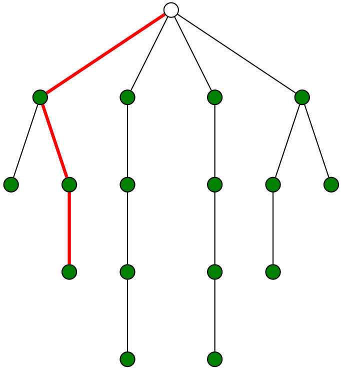
$\ell \leftarrow 1$; $r_{\text{prev}} \leftarrow 1$; $k \leftarrow 1$; //the root node;
while $k \leq n$ **do**
    if $A_k = \emptyset$ **then return** ℓ; //no more branch
    $x_k \overset{R}{\leftarrow} A_k$ //randomly select a branch;
    $r_{\text{current}} \leftarrow r_{\text{prev}} \times |A_k|$ //number of nodes on k level;
    $\ell \leftarrow \ell + r_{\text{current}}$;
    $r_{\text{prev}} \leftarrow r_{\text{current}}$;
    $k \leftarrow k + 1$;
end

Real Case: 4-Queens Puzzle

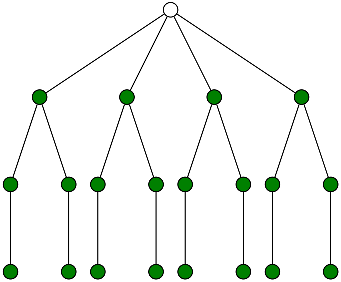


17 nodes

Random Selected Path 1

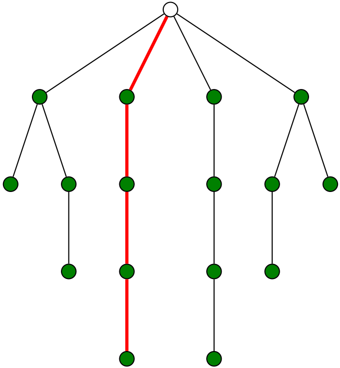


case 1: $(1, 4, 2)$

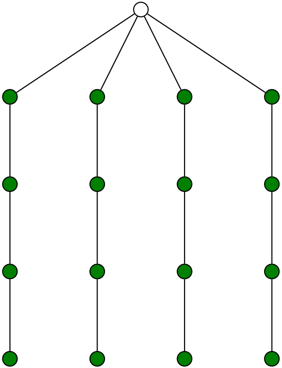


21 nodes

Randomly Selected Path 2

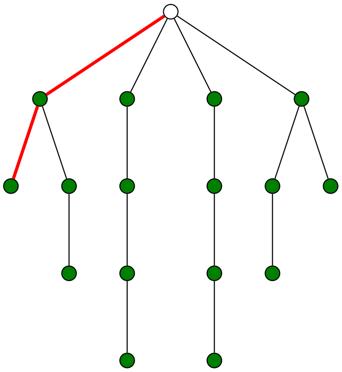


case 2: $(2, 4, 1, 3)$

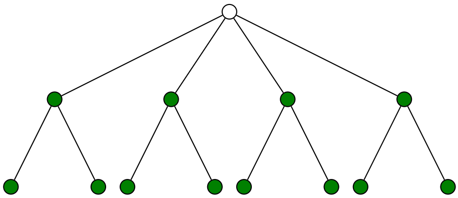


17 nodes

Randomly Selected Path 3



case 3: $(1, 3)$



13 nodes

Estimation Result

Suppose sampling four times

- case 1: 1
- case 2: 1
- case 3: 2

Average number of nodes: $(21 \times 1 + 17 \times 1 + 13 \times 2)/4 = 16$

The real number of nodes: 17

- more samplings will make the estimation approaches the real number