Design and Analysis of Algorithm
Backtrack (II)

Outline

Combinatorial Optimization

Combinatorial Optimization. finding an optimal solution x from a finite set of feasible/candidate solutions S.

- Constraint: $P(x) = 1 \iff x \in S$
- Optimized function $f(x) \to$ define optimal solution
  typical optimized function aims to maximize or minimize

Example of Knapsack

- $P(x) : 2x_1 + 3x_2 + 4x_3 + 7x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$
- $f(x) : \max\{x_1 + 3x_2 + 5x_3 + 9x_4\}$

W.L.O.G always assume that maximization of $f(x)$ is desired

- since one can find the minimum value of $f(x)$ by finding the maximum of $g(x) = -f(x)$

Extensively studied in operations research, applied mathematics and theoretical computer science.

- traveling salesman problem (TSP), minimum spanning tree problem (MST), knapsack problem

Motivation

Combinatorial optimization problem can always be solved via enumeration of candidate solutions and testing them all

- enumeration can be done by brute-force searching the state space tree

leaf node $\Leftrightarrow$ candidate solution

For $\mathcal{NP}$-hard problem, the state space could be exponentially large.

Can we improve on the performance of brute-force search of state space tree?

Branch-and-Bound Method

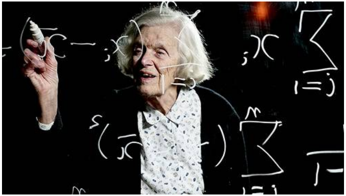
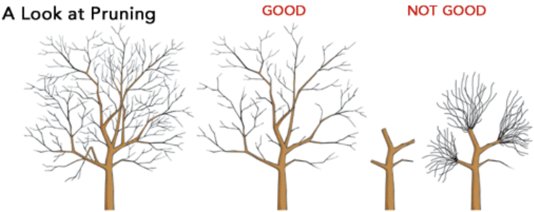


Figure: 1960, British: Ailsa Land and Alison Harcourt

the most commonly used technique for solving $\mathcal{NP}$-hard optimization problems



Key Elements of Branch-and-Bound

A B&B algorithm operates according to two principles:

- Branching. recursively split the search space into smaller spaces, then try to find maximal $f(x)$ on these smaller spaces
- Bounding. keep track of a bound value, compute an upper bound of $f(x)$ in the smaller space, and use this bound value and the upper bound to "prune" the search space, eliminate candidate solutions that will not contain an optimal solution

---

Key points of good "pruning"

- the setting of bound value
- the computing of upper bound

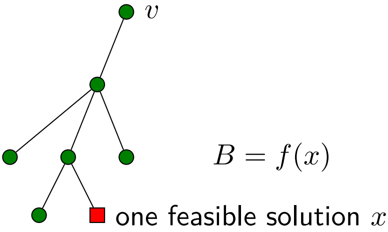
Bound Value

Meaning: maximal optimized function value of current feasible solutions

Initial Value: 0 for maximize problem and ∞ for minimize problem

Update

- when find the first solution
- when find a better solution

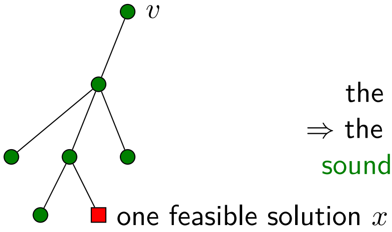


Estimate/Bound Function

Input: node of tree, say, v

Output: an upper bound of all feasible solutions in the subtree with input node as root

Soundness: let v' be a child node of v



$$E(v) \geq E(v')$$

the feasible solution set shrinks

$\Rightarrow$ the upper bound is getting smaller

soundness $\Rightarrow$ will not miss solution

The choice of estimate function is not unique, one need to make a trade-off between

- computation cost vs. accuracy

A Metaphor of Bound Function

Backtracking and Pruning

When navigating to a node v, the algorithm will stop branching and backtrack to parent node if:

- the set of feasible solutions $A(v)$ is empty: no leaf node in the subtree satisfies the constraint predicate (same as naive backtracking with default constraint)

- the estimate function value is less than current bound value

$$E(v) < B$$

simply prune this subtree and backtrack

Outline

Example from Knapsack Problem with Repetition

Example of knapsack problem (weight limit=10)

label	weight	value
1	2	1
2	3	3
3	4	5
4	7	9

Constrained predicate P:

$$2x_1 + 3x_2 + 4x_3 + 7x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$

Optimized function f: $\max\{x_1 + 3x_2 + 5x_3 + 9x_4\}$

Choice of Bound Function

For each node $v = (x_1, x_2, \ldots, x_k)$, compute the upper bound of optimized function value of feasible solutions in the subtree

- Preprocessing: sort v_i/w_i via a decreasing order, $i \in [n]$

$E(v) = K(v) + \Delta(v)$

$K(v)$: the value already loaded in the knapsack
$\Delta(v)$: the maximum value that can be further loaded

Computation of $\Delta(v)$: find the first index $j \leq (k, n]$ such that $w_j \leq$ remaining weight

- $\Delta(v) =$ remaining weight $\times\, v_j/w_j$ (j exists – can be loaded)
- $\Delta(v) = 0$ (j does not exist – cannot be loaded anymore)

Knapsack Instance

$$\max\{x_1 + 3x_2 + 5x_3 + 9x_4\}$$
$$2x_1 + 3x_2 + 4x_3 + 7x_4 \le 10, x_i \in \mathbb{N}, i \in [4]$$

Re-arrange the label such that

$$\frac{v_i}{w_i} \ge \frac{v_{i+1}}{w_{i+1}}$$

After rearrangement

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \le 10, x_i \in \mathbb{N}, i \in [4]$$

Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$

$\frac{\text{maximum value}}{\text{current weight}}$

Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$

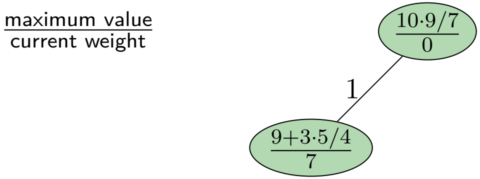
$\frac{\text{maximum value}}{\text{current weight}}$

$\frac{10 \cdot 9/7}{0}$

Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

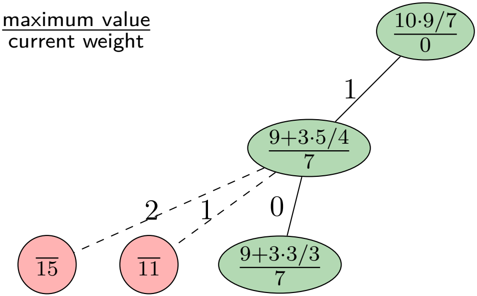
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

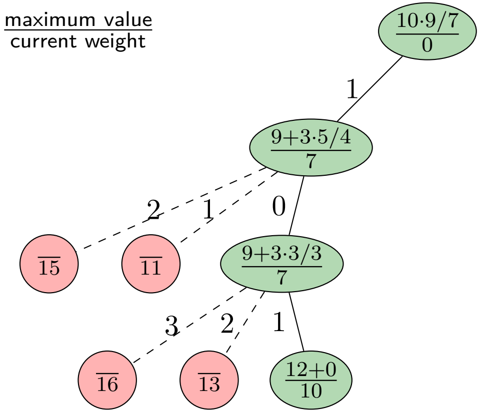
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

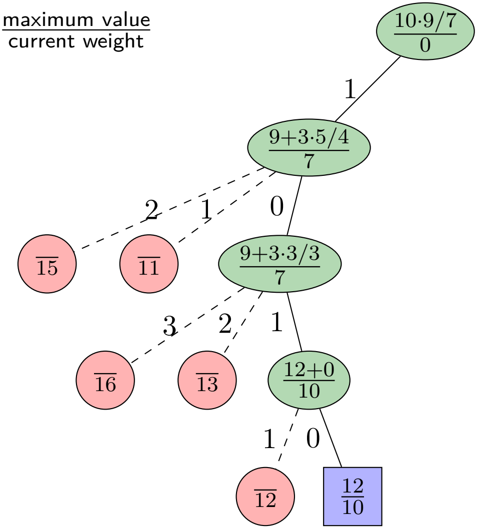
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

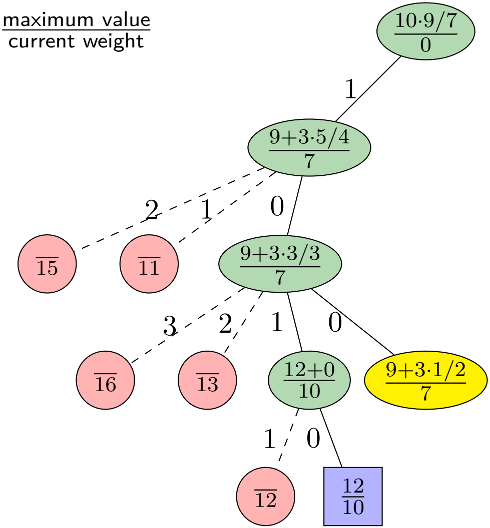
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \le 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

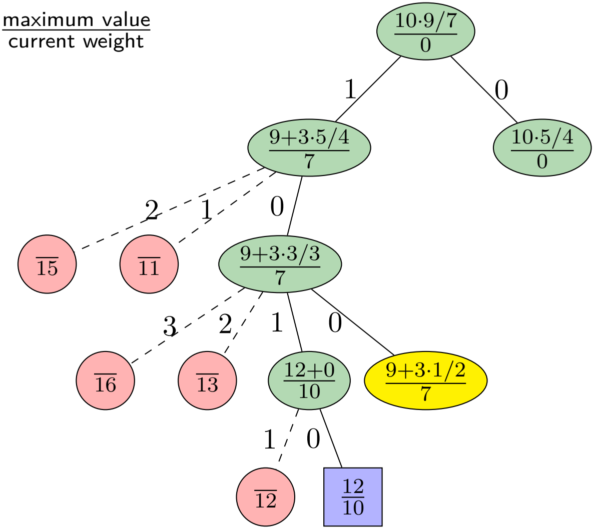
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

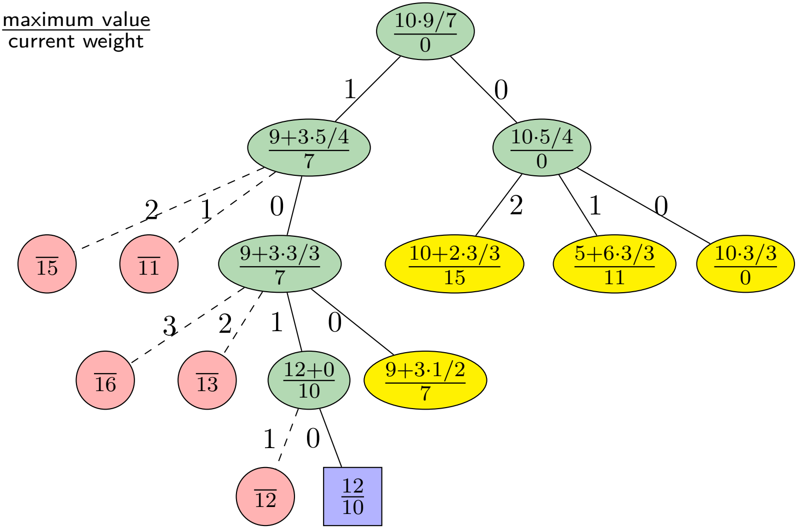
$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Branch-and-Bound Example

$$\max\{9x_1 + 5x_2 + 3x_3 + x_4\}$$

$$7x_1 + 4x_2 + 3x_3 + 2x_4 \leq 10, x_i \in \mathbb{N}, i \in [4]$$



Thinking and Summary

Q. Is the preprocessing step necessary?

A. No. But it can speed up the computation of bound function.

Q. Other possible choice of bound function?

A. Yes. But make sure it is easy to compute, hit a sweet balance between the cost and gain of pruning

---

Branch-and-Bound method $\rightsquigarrow$ Combinatorial Optimization

- bound value setting and updating
- estimate function (represent the optimistic estimation) $\Rightarrow$ guarantee that pruning will not miss solution
- pruning: compare bound value and estimate function value

Outline

Concepts of Graph

Let $G = (V, E)$ be an undirected graph

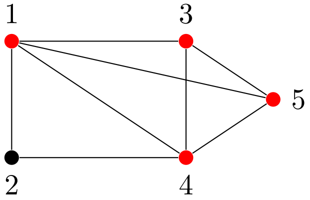
Subgraph: $G' = (V', E')$, where $V' \subseteq V$, $E' \subseteq E$

Cograph: $\overline{G} = (V, \overline{E})$, where $\overline{E}$ is the co-set of E regarding the complete graph over V

Clique: A complete subgraph of G

Maximum Clique: A clique with the largest possible number of vertices.

- MCP is a classical combinatorial optimization problem in graph theory.



maximum clique = $\{1, 3, 4, 5\}$

Independent Set and Clique (独立集与团)

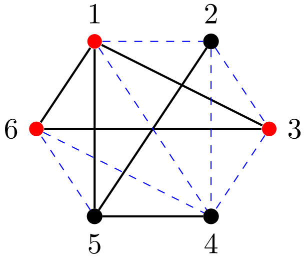
Let $G = (V, E)$ be an undirected graph

Independent Set. A subset U of V, s.t. $\forall u, v \in U$, $(u, v) \notin E$

Maximum Independent Set. An independent set of largest possible size for G.

Claim: U is the maximum clique of G if and only if U is the maximum independent set of $\overline{G}$.

independent set $\leftrightarrow$ clique in co-graph



$\{1, 3, 6\}$
maximum clique of G
maximum independent set of $\overline{G}$

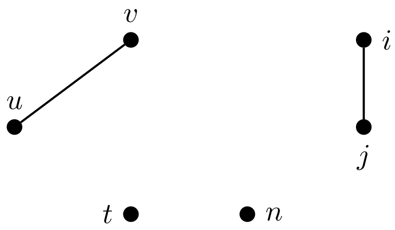
Applications of Maximum Clique

Numerous applications of MCP

- coding, cluster analysis, computer vision, economics, mobile communication, VLSI design

Example from coding. Noisy in the channel may disturb code transmission. Consider confusion graph $G = (V, E)$, V is a finite set of symbols

$$(u, v) \in E \text{ or } E(u, v) = 1 \Leftrightarrow u \text{ and } v \text{ are likely confused}$$

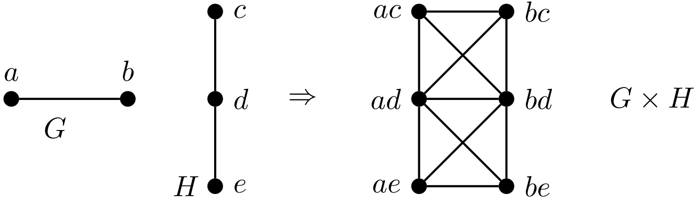


Coding Design

In coding design, we usually use a string to encode a symbol.

Confusion of codeword. We say two strings xy and uv are likely to be confused if and only if

$$(E(x,u)=1 \wedge E(y,v)=1)\vee$$
$$(x=u \wedge E(y,v)=1) \vee (E(x,u)=1 \wedge y=v)$$



Veticies in $G \times H$ are candidate codewords

- two codewords are confused if there is an edge between them

To reduce noisy disturb, we need to find MIS in $G \times H$.

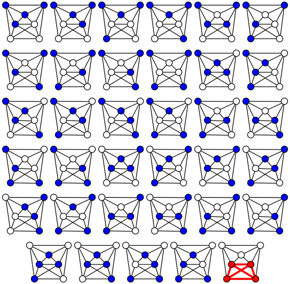
Maximum Clique Problem (最大团)

Problem. Given an undirected graph $G = (V, E)$, where $V = \{1, \ldots, n\}$, find its maximum clique.

Solution. An n-dimension vector $(x_1, x_2, \ldots, x_n) \in \{0, 1\}^n$, $x_k = 1$ if and only if k is in the maximum clique of G.

Brute Force Algorithm. For every subset of V, check if it forms a clique, i.e., a complete subgraph.

$\#$ subsets of V is $2^n \rightsquigarrow$ exponential time complexity $O(n^2) \cdot 2^n$



Branch-and-Bound Method

Search tree: Subset tree (a binary tree: the path from leaf node to root determines a subset)

Node $(x_1, x_2, \ldots, x_k)$: have checked nodes $1, 2, \ldots, k$, $x_i = 1$ denotes i belongs to the current clique, $i \in [k]$

Constraint. $x_{k+1} = 1$ if and only if it connects to all the nodes in the current clique

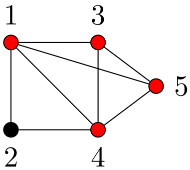
Bound value: # vertices in the current maximum clique

Estimate function: the largest number of vertices that current clique may expand to: $E(v) = C(v) + (n - k)$.

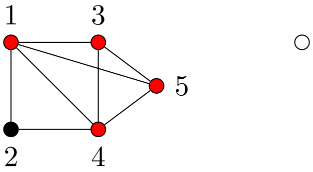
- $C(v)$: # of vertices in the current clique (initial value is 0)
- k: the depth of v

E is simple but too coarse $\rightsquigarrow$ worse-case complexity is $O(n2^n)$, asymptotically same as the brute-force algorithm

Demo of Search

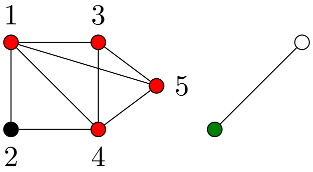


Demo of Search



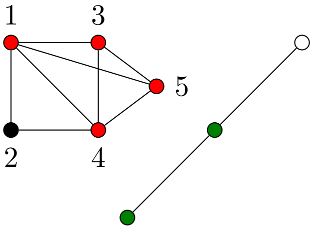
initial value $B = 0$

Demo of Search



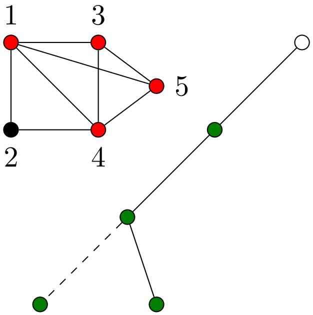
initial value $B = 0$

Demo of Search



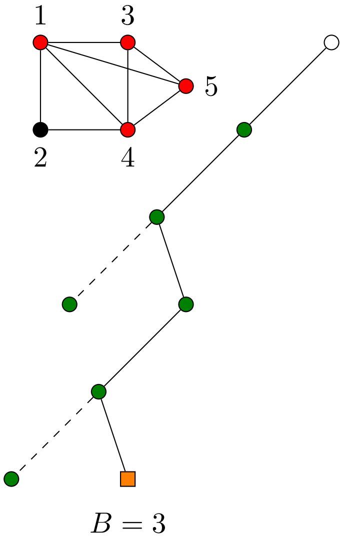
initial value $B = 0$

Demo of Search



initial value $B = 0$

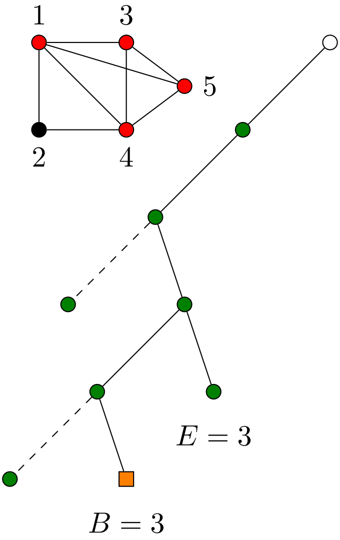
Demo of Search



initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

Demo of Search

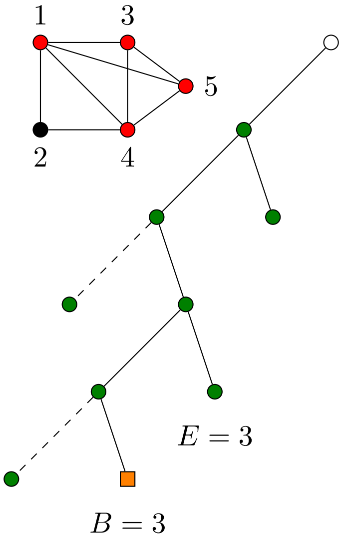


initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

$E = 3 \leq B$, backtrack

Demo of Search

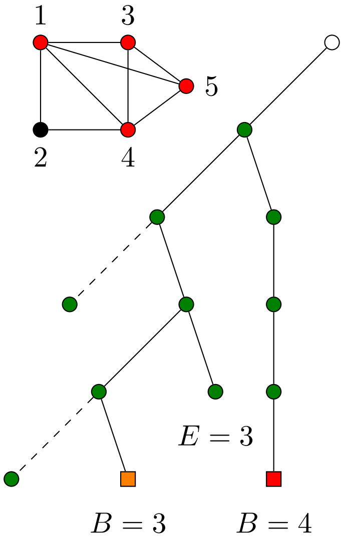


initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

$E = 3 \leq B$, backtrack

Demo of Search



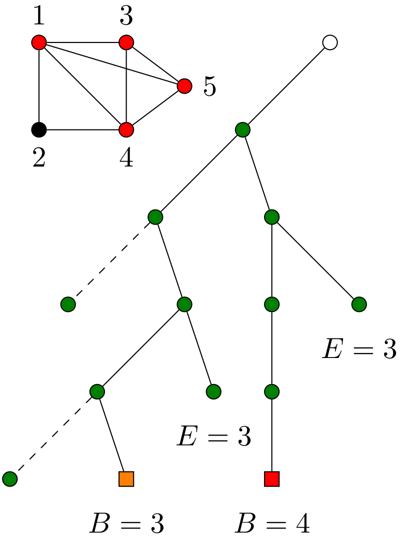
initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

$E = 3 \leq B$, backtrack

MC $= \{1, 3, 4, 5\}$, $B = 4$

Demo of Search



initial value $B = 0$

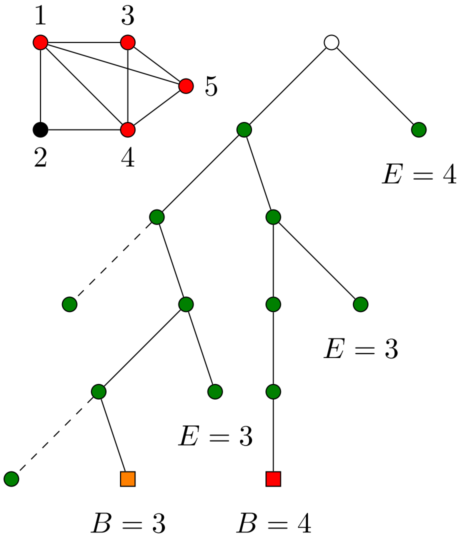
MC $= \{1, 2, 4\}$, $B = 3$

$E = 3 \leq B$, backtrack

MC $= \{1, 3, 4, 5\}$, $B = 4$

$E = 3 < B$, backtrack

Demo of Search



initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

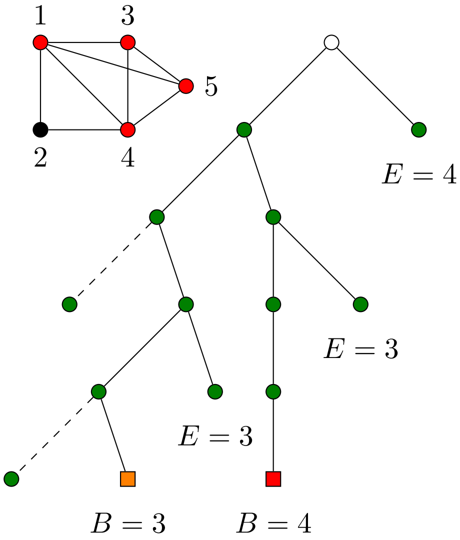
$E = 3 \leq B$, backtrack

MC $= \{1, 3, 4, 5\}$, $B = 4$

$E = 3 < B$, backtrack

$E = 4 \leq B$, backtrack

Demo of Search



initial value $B = 0$

MC $= \{1, 2, 4\}$, $B = 3$

$E = 3 \leq B$, backtrack

MC $= \{1, 3, 4, 5\}$, $B = 4$

$E = 3 < B$, backtrack

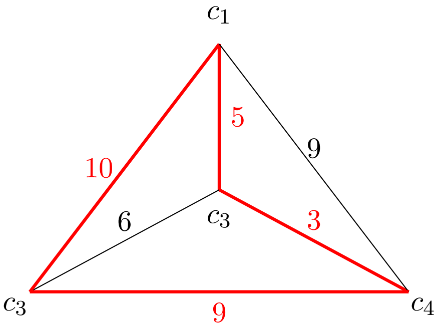
$E = 4 \leq B$, backtrack

MC $= \{1, 3, 4, 5\}$

Outline

Traveling Salesman Problem (TSP)

Problem. Given n cities and the distances between each pair of cities, what is the shortest possible route that visits each city and returns to the origin city?



Modeling

Input. A finite set of cities $C = \{c_1, c_2, \ldots, c_n\}$, distance $e(c_i, c_j) = e(c_j, c_i) \in \mathbb{Z}^+$, $1 \leq i < j \leq n$.

Solution. A permutation of $(1, 2, \ldots, n)$ — $(i_1, i_2, \ldots, i_n)$ such that:

$$\min \left\{ \sum_{i=1}^{n} e(c_{k_{i \bmod n}}, c_{k_{i+1 \bmod n}}) \right\}$$

State space. Permutation tree, node $(i_1, i_2, \ldots, i_k)$ represents route up to k steps

Constraint. Let $S = \{i_1, i_2, \ldots, i_k\}$, then $i_{k+1} \in V - S$, cause every node can be visited once and only once.

Bound Value and Estimate Function

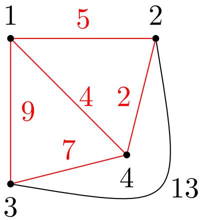
Bound Value: the length of current shortest route

Estimate Function: let the length of shortest edge connected to c_i is ℓ_i, d_j is the j-th length in the current route

$$E([i_1, \ldots, i_k]) = \sum_{j=1}^{k-1} d_j + \ell_{i_k} + \sum_{i_j \notin S} \ell_{i_j}$$

- the first part: length of traveled route
- the second part: lower bound of rest route

Example of Bound Function

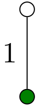


$$E([i_1, \ldots, i_k]) = \sum_{j=1}^{k-1} d_j + \ell_{i_k} + \sum_{i_j \in V-S} \ell_{i_j}$$

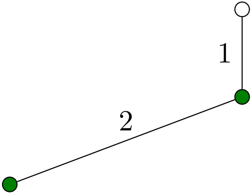
Partial route: $(1, 3, 2)$, $E([1, 3, 2]) = (9 + 13) + 2 + 2 = 26$,
$S = \{1, 3, 2\}$, $V - S = \{4\}$

- $9 + 13$: length of traveled route
- 2: length of shortest edge connected to node 2
- 2: length of shortest edge connected to node 4

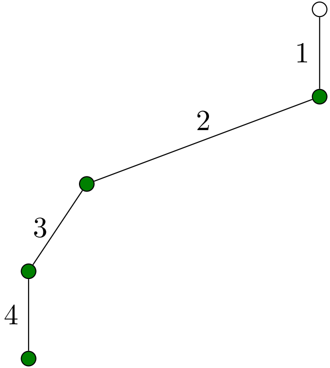
Demo of Search



Demo of Search

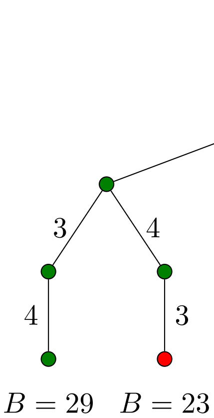


Demo of Search

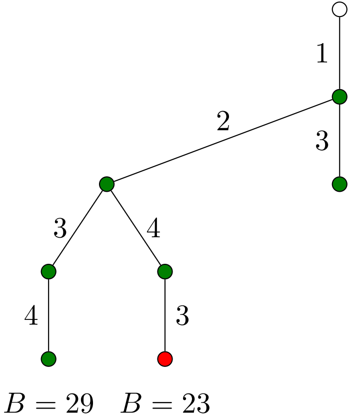


$B = 29$

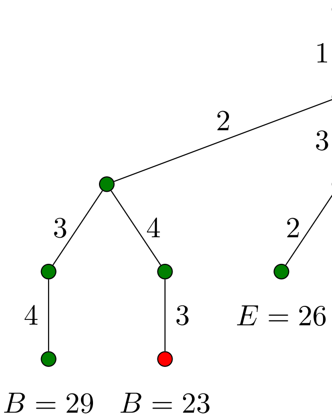
Demo of Search



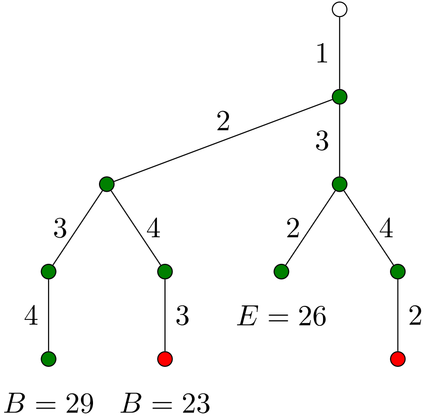
Demo of Search



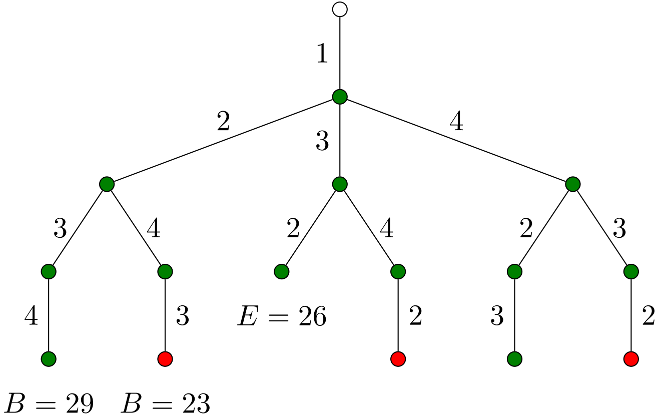
Demo of Search



Demo of Search



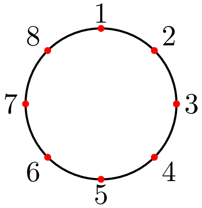
Demo of Search



Complexity Analysis (1/2)

leaf nodes: $(n-1)!$

- each leaf node corresponds to a route
- each route (actually a circle) has n cities $\rightsquigarrow$ equivalence under shift $\rightsquigarrow$ at most $(n-1)!$ different routes

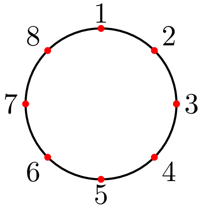


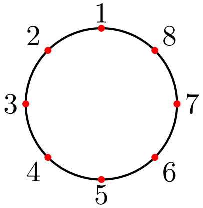
Complexity Analysis (1/2)

leaf nodes: $(n-1)!$

- each leaf node corresponds to a route
- each route (actually a circle) has n cities $\rightsquigarrow$ equivalence under shift $\rightsquigarrow$ at most $(n-1)!$ different routes

Further observation: solution is a cycle in undirected graph $\rightsquigarrow$ clockwise and counter-clockwise are symmetric $\rightsquigarrow$ at most $(n-1)!/2$ different routes (two equivalences do not overlap)





Complexity Analysis (2/2)

Complexity of $E(\cdot)$ is $O(1) \rightsquigarrow$ traveling each route requires $O(n)$

$$E(i_1, \ldots, i_k) = \sum_{j=1}^{k-1} d_j + \ell_{i_k} + \sum_{i_j \in V-S} \ell_{i_j}$$

Complexity Analysis (2/2)

Complexity of $E(\cdot)$ is $O(1)$ $\rightsquigarrow$ traveling each route requires $O(n)$

$$E(i_1, \ldots, i_k) = \sum_{j=1}^{k-1} d_j + \ell_{i_k} + \sum_{i_j \in V-S} \ell_{i_j}$$

- update when move to its child node i_{k+1} (add $d_k - \ell_{i_k}$), where $d_k = e(i_k, i_{k+1})$

$$E(i_1, \ldots, i_k, i_{k+1}) = \sum_{j=1}^{k} d_j + \ell_{i_{k+1}} + \sum_{i_j \in V-(S+i_{k+1})} \ell_{i_j}$$

$$= \sum_{j=1}^{k} d_j + \sum_{i_j \in V-S} \ell_{i_j}$$

- the initial value is $E([i_1]) = \sum_{j=1}^{k} \ell_{i_j}$

Complexity Analysis (2/2)

Complexity of $E(\cdot)$ is $O(1) \rightsquigarrow$ traveling each route requires $O(n)$

$$E(i_1, \ldots, i_k) = \sum_{j=1}^{k-1} d_j + \ell_{i_k} + \sum_{i_j \in V-S} \ell_{i_j}$$

- update when move to its child node i_{k+1} (add $\underline{d_k - \ell_{i_k}}$), where $d_k = e(i_k, i_{k+1})$

$$E(i_1, \ldots, i_k, i_{k+1}) = \sum_{j=1}^{k} d_j + \ell_{i_{k+1}} + \sum_{i_j \in V-(S+i_{k+1})} \ell_{i_j}$$

$$= \sum_{j=1}^{k} d_j + \sum_{i_j \in V-S} \ell_{i_j}$$

- the initial value is $E([i_1]) = \sum_{j=1}^{k} \ell_{i_j}$

The overall worse case complexity is $O(n!)$

Outline

Continuous Postage Problem

Problem. Suppose a country issues stamps of n different denominations, and requires a maximum of m sheets per envelope.


Goal. For a given value of n and m, find the best design for the face value of the stamp so that the maximum continuous postage interval starting from postage 1 can be posted on an envelope.

Example: $n = 5$, $m = 4$

- design 1: $V = (1, 3, 11, 15, 32) \Rightarrow$ continuous range $[1, \ldots, 70]$
- design 2: $V = (1, 6, 10, 20, 30) \Rightarrow$ continuous range $[1, 2, 3, 4]$

Feasible solution. $(x_1, x_2, \ldots, x_n)$, $x_1 = 1$, $x_1 < x_2 < \cdots < x_n$

Search strategy. DFS

Branching Constraint. At node $v = (x_1, x_2, \ldots, x_k)$, the largest continuous range is $[1, \ldots, r_k]$, then $x_{k+1} \in [x_k + 1, \ldots, r_k + 1]$

- left boundary: the denomination is of ascending order
- right boundary: otherwise, if $x_{k+1} > r_k + 1$, $r_k + 1$ can not be expressed $\rightsquigarrow$ a breakpoint

How to compute r_k?

Computation of r_k

According to the definition, the largest continuous range $[1, r_k]$ derived from (k, m)-combination implies r_k requires at most m stamps while $r_k + 1$ requires at least $m + 1$ stamps.

We will use the above observation to compute r_k.

- Define a function $h_k(v)$ that computes minimal number of stamps for value v using the first k-types of stamps with face value $(x_1, \ldots, x_k)$:
- Now, we can compute r_k via

$$r_k = \min\{v | h_k(v) \leq m, h_k(v+1) > m\}$$

Such value (breakpoint) may not be unique, we have to compute the min. Consider the instance $(1, 5, 20)$, $m = 3$.

1. $h_3(3) = 3$, $h_3(4) = \infty$: the first breakpoint is 4
2. $h_3(22) = 3$, $h_3(23) = \infty$: the second breakpoint is 23

Computation of h_k

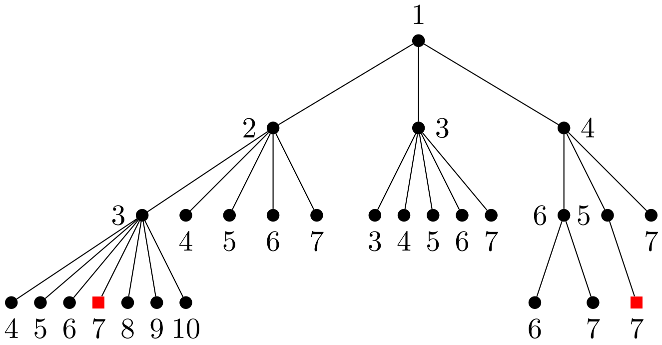
$h_k(v)$: the minimal number of stamps that yields value v using the first k types of stamps

$$h_k(v) = \begin{cases} \min_{0 \le t \le m}\{t + h_{k-1}(v - tx_k)\} & \text{if } k > 1 \\ v & \text{if } k = 1 \\ +\infty & \text{if } v > mv_k \end{cases}$$

Demo of $n = 4$, $m = 3$

- $(x_1 = 1)$
  $h_1(0) = 0$, $h_1(1) = 1$, $h_1(2) = 2$, $h_1(3) = 3$, $h_1(4) = +\infty$, $r_1 = 3 \rightsquigarrow$ range of 2rd stamp is $[2, 4]$
- $(x_1 = 1, x_2 = 2)$
  $h_2(0) = 0$, $h_2(1) = 1$, $h_2(2) = 1$, $h_2(3) = 2$, $h_2(4) = 2$, $h_2(5) = 3$, $h_2(6) = 3$, $h_2(7) = 4$, $r_2 = 6 \rightsquigarrow$ range of 3st stamp is $[3, 7]$
- $(x_1 = 1, x_2 = 2, x_3 = 3)$
  $h_3(0) = 0$, $h_3(1) = 1$, $h_3(2) = 1$, $h_3(3) = 1$, $h_3(4) = 2$, $h_3(5) = 2$, $h_3(6) = 2$, $h_3(7) = 3$, $h_3(8) = 3$, $h_3(9) = 3$, $h_3(10) = 4$, $r_3 = 9 \rightsquigarrow$ range of 4th stamp is $[4, 10]$

Part of the Search Tree: $n = 4$, $m = 3$



Best design is $(1, 4, 6, 7) \Rightarrow h_4(21) = 3,\ h_4(22) = 4 \rightsquigarrow$ largest continuous range $[1, \ldots, 21]$

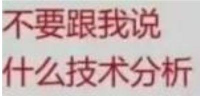
branching is not fixed at the very beginning, need dynamic programming to compute the possible branches

Summary (1/3)

General steps for solving combinatorial optimization problem

- solution $\rightsquigarrow$ vector
- state space $\rightsquigarrow$ search tree (partial vector is inner node, vector is leaf node)
- searching order (DFS, BFS)

Brute-force algorithm: travel the entire tree (recall the integer solution for inequality problem)



Can we implement the brute-force algorithm smartly?

Summary (2/3)

Yes. The backtracking technique! Backtracking need criteria

Basic backtracking

- Derive the criteria from the default constraint: ensure that the Domino property holds

Additional optimization trick

- It is possible to explore symmetric property to reduce the size the search tree

Example: loading problem, graph coloring problem

Summary (3/3)

Advanced backtracking

- Branch-and-bound method: in addition to default criteria, introduce bound value and estimate function to prune the search tree $\rightsquigarrow$ further reduce the complexity $\rightsquigarrow$ fine-grained criteria

Example: MCP, TSP

When applying the branch-and-bound method, one need to find a trade-off between the gain and cost