Übungen zu Algorithmen und Programmentwicklung für die Biologische Chemie

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Sommersemester 2025

Optimization

Optimization problems

Definition: A ***combinatorial*** **optimization problem** consists of

- an arbitrary ***finite*** set X: the **solution space**
- a **cost function** $f : X \to \mathbb{R}$,
  which assigns the cost $f(x)$ to each $x \in X$.

Task: Find a solution.

Def.: A **solution** of the COP (X, f) is an $x_0 \in X$ with minimal cost, i.e.

$$f(x_0) = \min_{x \in X} f(x)$$

Optimization problems: Examples

Example 1:

- $X = \{1, \ldots, 100\}$
- $f : X \to \mathbb{R}$, $x \mapsto |x - 42|$

optimal solution is 42 at minimum cost $f(42) = 0$.

Example 2: Travelling Salesperson Problem.

- Input: distances between n cities.
- The solution set X consists of all tours.
  (a tour visits every city exactly once and returns to the start city)
- Cost function f yields the length of the tour.

Example disctances:

	A	B	C	D
A	-	2	4	2
B	2	-	3	3
C	4	3	-	1
D	2	3	1	-

Brute force—Generate and minimize

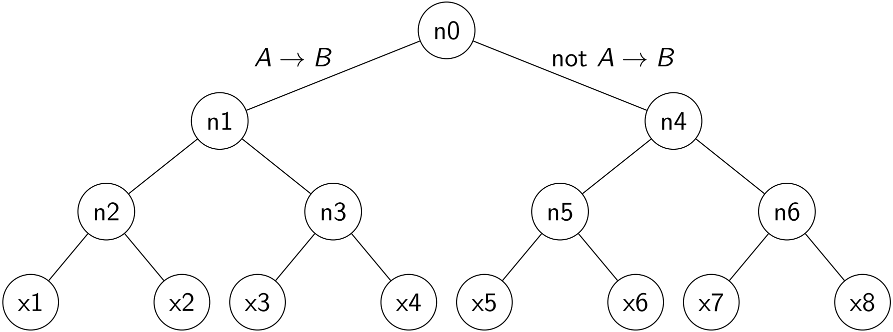
Algorithmic "strategy" that works without any knowledge of the problem's structure

$best \leftarrow +\infty$;
$x_0 = \varnothing$;
for $x \in X$ **do**
    $cost \leftarrow f(x)$;
    if $cost < best$ **then**
        $best \leftarrow cost$;
        $x_0 \leftarrow x$;
    end
end

Branch and Bound

Systematic enumeration of the solution space

- **Enumerate** solutions by systematically deciding on features of the solutions $\Rightarrow$ search tree
  Example: Salesperson travels **A**$\rightarrow$**B** vs. **not A**$\rightarrow$**B**.
- Each **leaf** represents a **solution**
- Each **inner node** represents a **partial solution**
- Each **subtree** represents a sub-space of the **solution space**



Exploration of the solution space

Depth First Search

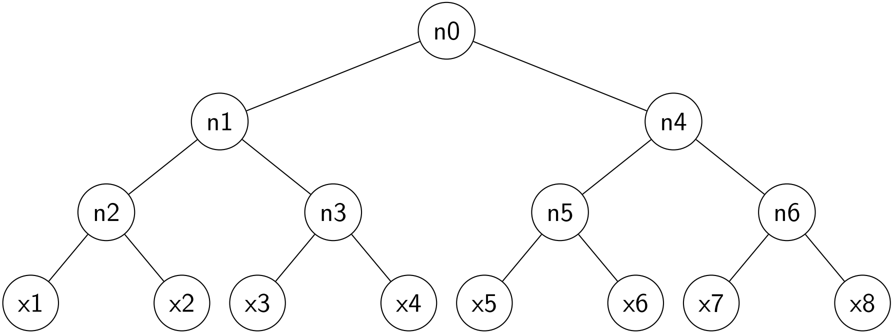
At inner node, generate all children and push them onto a **stack**.

Continue with node on top of stack (**LIFO**).

Breadth First Search

At inner node, generate all children and add them to a **queue**.

Continue with first node in the queue (**FIFO**).



Branch and Bound optimization

Idea:

- systematically search through the search tree, depth-first
- skip subtrees that cannot improve the currently best solution

Ingredients:

- **Enumeration strategy** (how to generate search tree)
- **Lower bound cost function** g on partial solutions at inner nodes. Bounds cost of all possible solutions of the subtree.

For example: TSP. g yields the length of the beginning of a tour: a lower bound for the possible total length.

Branch and Bound, basic algorithm

```
best ← +∞; INIT(S);
PUSH(S,X);
while not EMPTY(S) do
    A=POP(S);
    if A is consistent then
        if g(A) < best then
            if A is a solution then
                best ← g(A);
            else
                (B, C)=Split(A);
                PUSH(S,B) ;
                PUSH(S,C) ;
            end
        end
    end
end
```

Branch and Bound, recursive formulation

```
bound = infty

def BAB( A ):
    if A is consistent and g(A) < bound :
        if A is a solution :
            bound = f( A )
        else:
            (B,C) = Split( A )
            BAB( B )
            BAB( C )

BAB( S )
```

In general, recursion...

means that a function calls itself (directly or indirectly)

```
fac :: Int -> Int
fac 0 = 1
fac n = n * fac (n-1)

Example:
 (fac 4) --> 24
  | ^
  | | 24
  V |
 (4 * (fac 3))
       | ^
       | | 6
       V |
      (3 * (fac 2)
            | ^
            | | 2
            V |
           (2 * (fac 1))
                 | ^
                 | | 1
                 V |
                (1 * (fac 0))
                      | ^
                      | | 1
                      V |
                       1
```

Assignment 2: Optimal Distribution of Authorities

Go to:

`https://github.com/TBIAPBC/APBC2025/tree/master/A2`

This assignment is due on 28 April 10:00 AM

(GitHub pull request must be placed by this time at latest)

Happy Hacking!

Next meeting: 29 April 2025