Technische
Universität
Braunschweig

Institut für Betriebssysteme
und Rechnerverbund
Algorithmik

Algorithm Engineering
Lecture 5: Optimization Fundamentals

Transition to a Different Type of Optimization

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First half: Optimize running time/CPU usage/…

Now: Solve optimization problems (different definitions of *solve*)

This lecture: Overview of techniques, applied to Knapsack

Knapsack

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Knapsack problem

Given:

Knapsack

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- n items x_i with weight w_i and price p_i,

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Goal: select which x_i to take.

maximize $\sum_{x_i \text{ taken}} p_i$ s.t.

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- capacity limit c.

Goal: select which x_i to take.

maximize $\sum_{x_i \text{ taken}} p_i$ s.t.

$$\sum_{x_i \text{ taken}} w_i \leq c.$$

Approaches

Different approaches:

- Dynamic programming
- Greedy heuristic & fractional greedy upper bound
- Backtracking & Constraint Propagation
- Branch & Bound
- Branch & Cut
- Metaheuristics

Dynamic Programming

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$c = 6$

Item	Price p	Weight w
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2	4	3
3	3	2
4	2	1

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1	0						
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3	0	0	3	4	5	7	8
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4	0	2	3	5	6	7	

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4	0	2	3	5	6	7	9

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- Know if your problem is efficiently solvable; Knapsack is the exception, not the rule!
- Sometimes a ‘recursive’ algorithm (memoization) may be better than a strict table!

Approaches

Different approaches:

- Dynamic programming
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In terms of bounds: this gives a *lower* bound!

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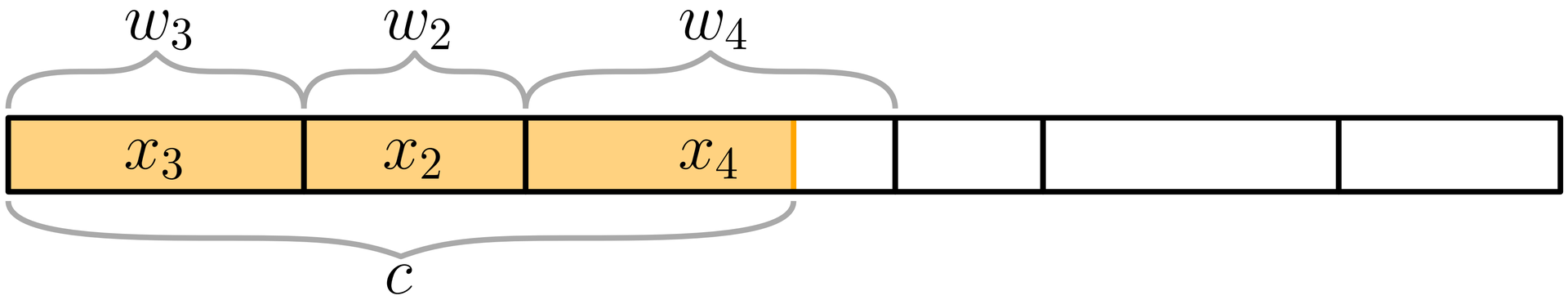

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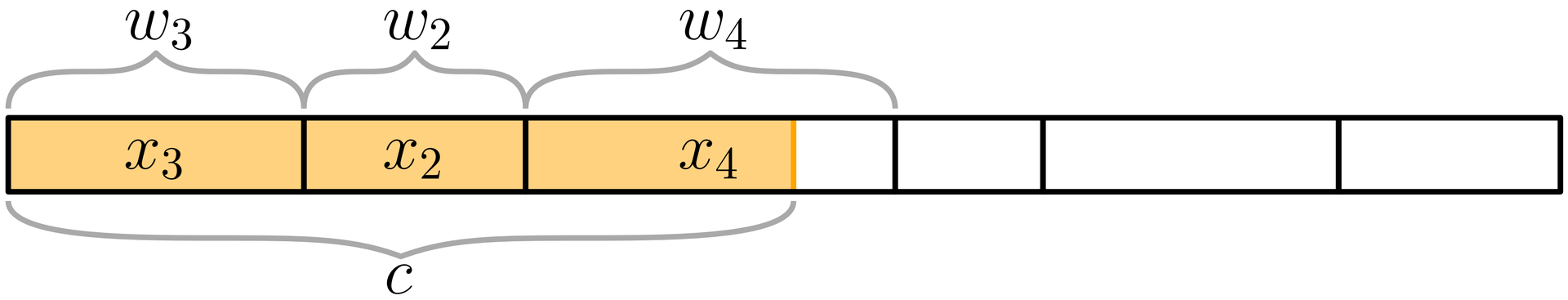

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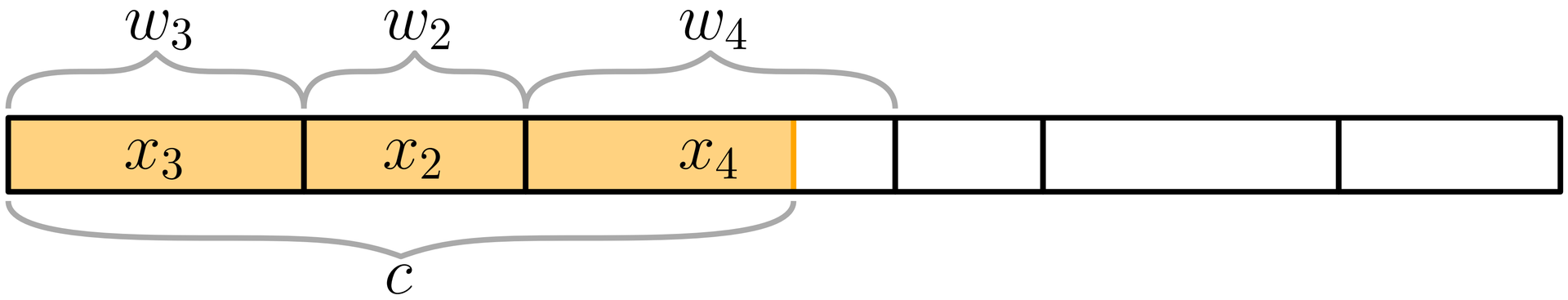

Select: $x_3 = 1, x_2 = 1, x_4 = \dfrac{c - w_3 - w_2}{w_4}$, all other $x_i = 0$.

Total price: $P = \sum_{1 \le i \le n} p_i x_i$ is an upper bound on the fractional Knapsack value.

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Price change: $\Delta P = \delta / w_i \cdot p_i - \delta / w_j \cdot p_j = \delta \cdot \left(\frac{p_i}{w_i} - \frac{p_j}{w_j} \right) \geq 0.$

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- This still holds if we fix some x_i to 0 or 1 beforehand.

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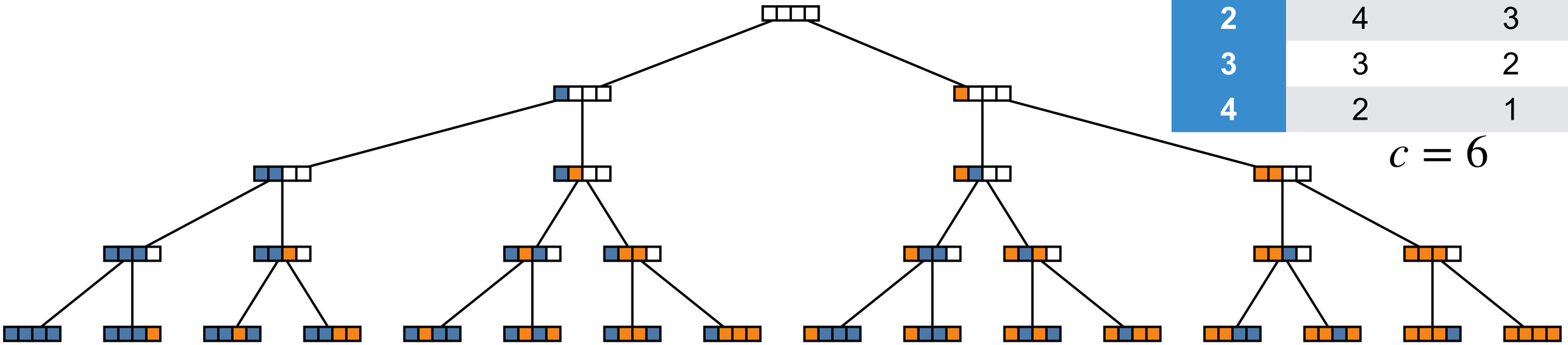

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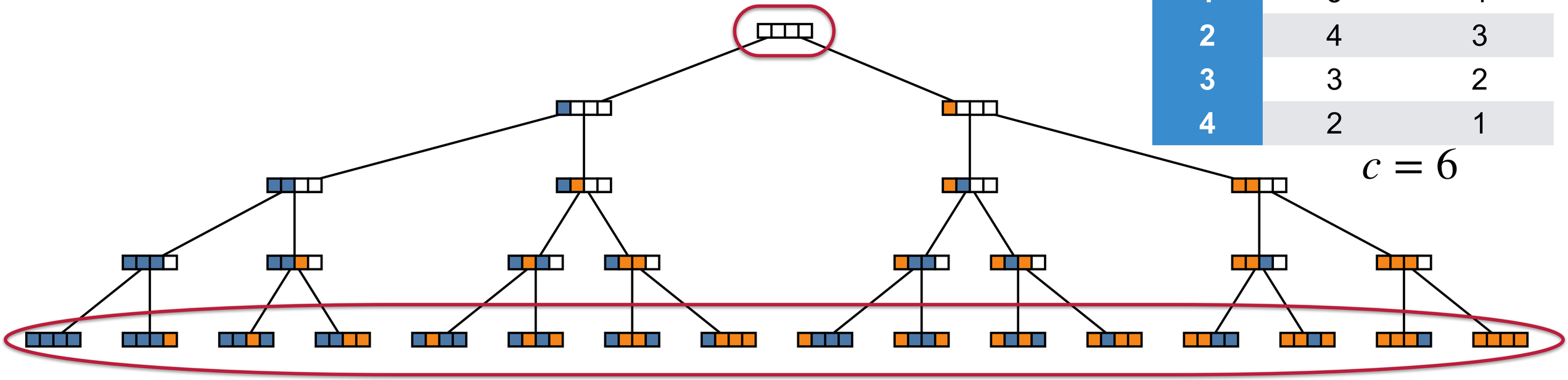

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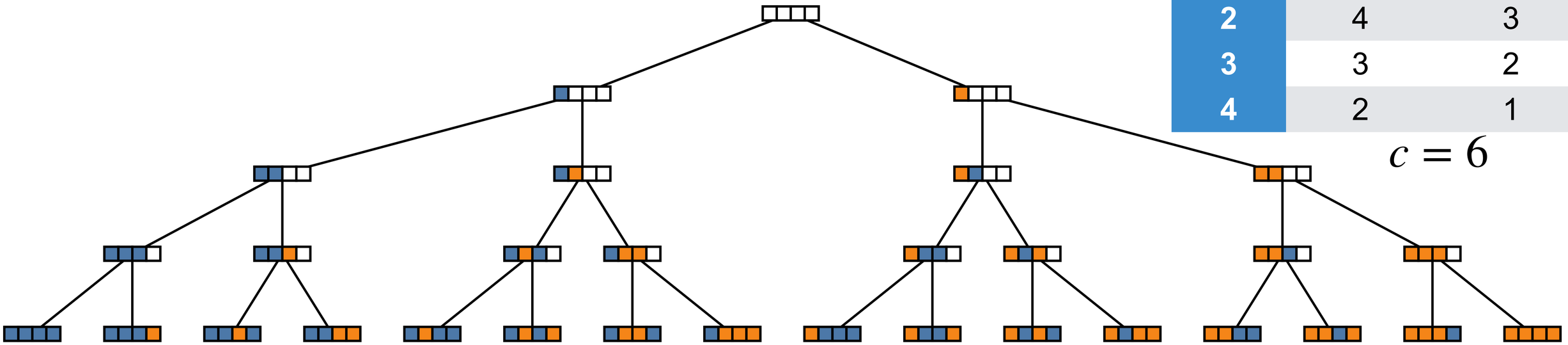

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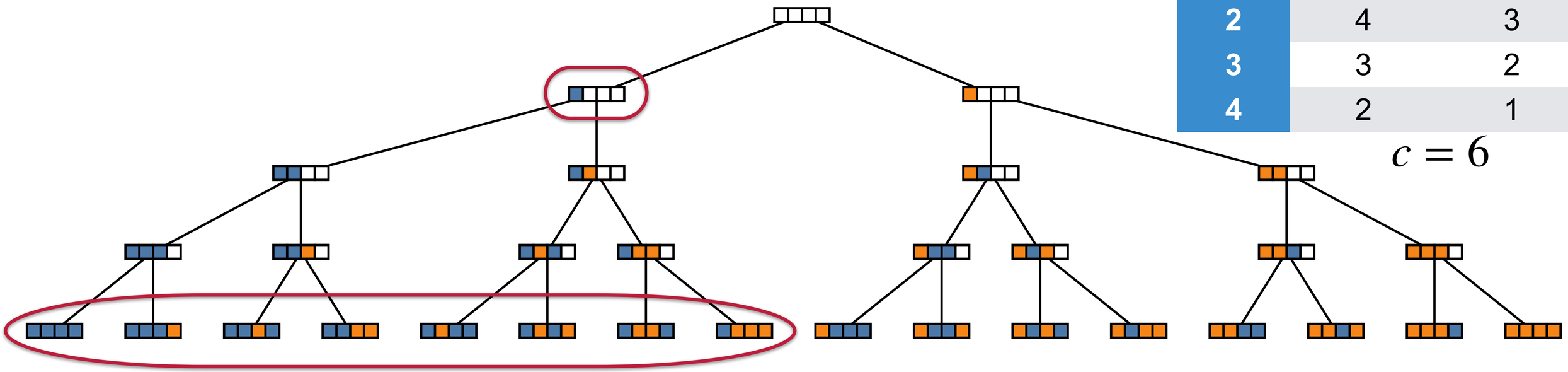

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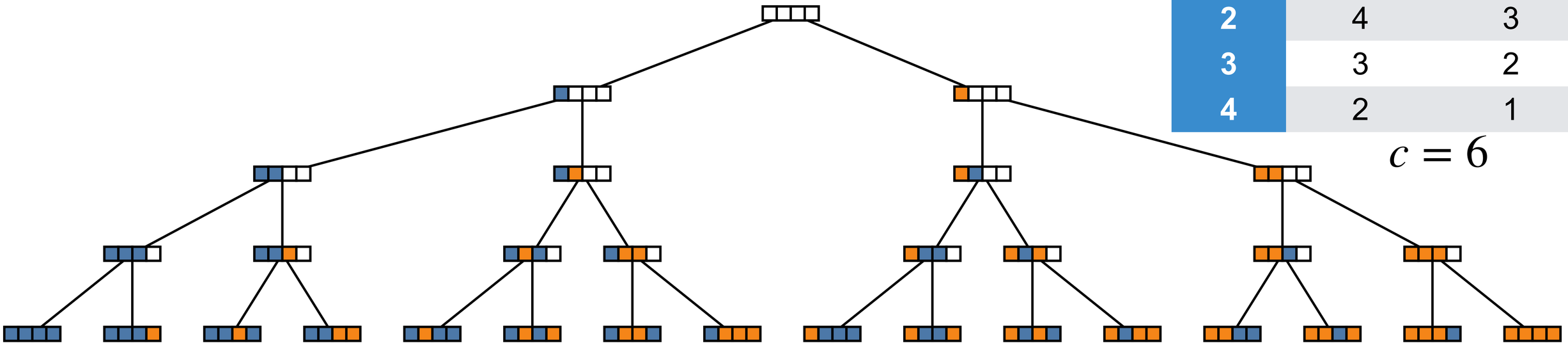

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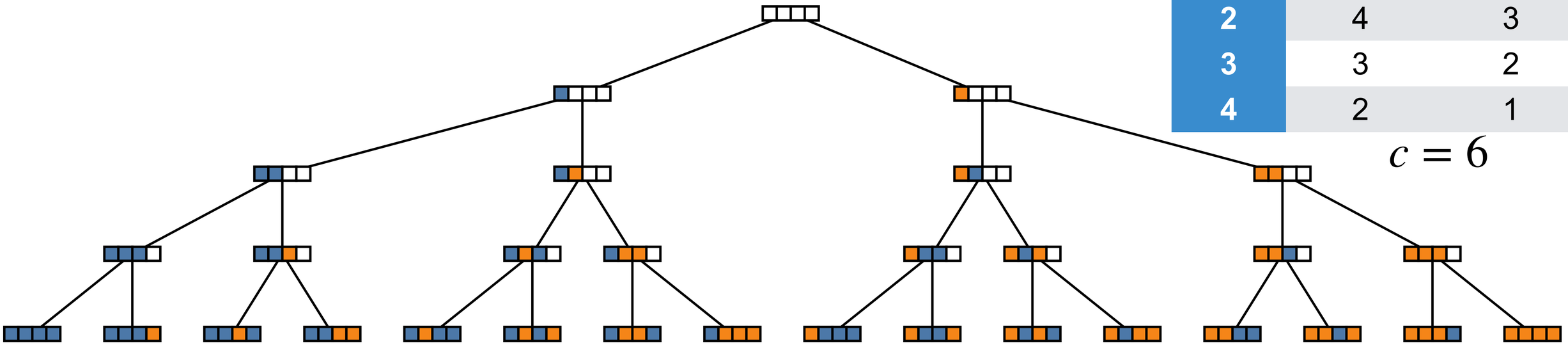

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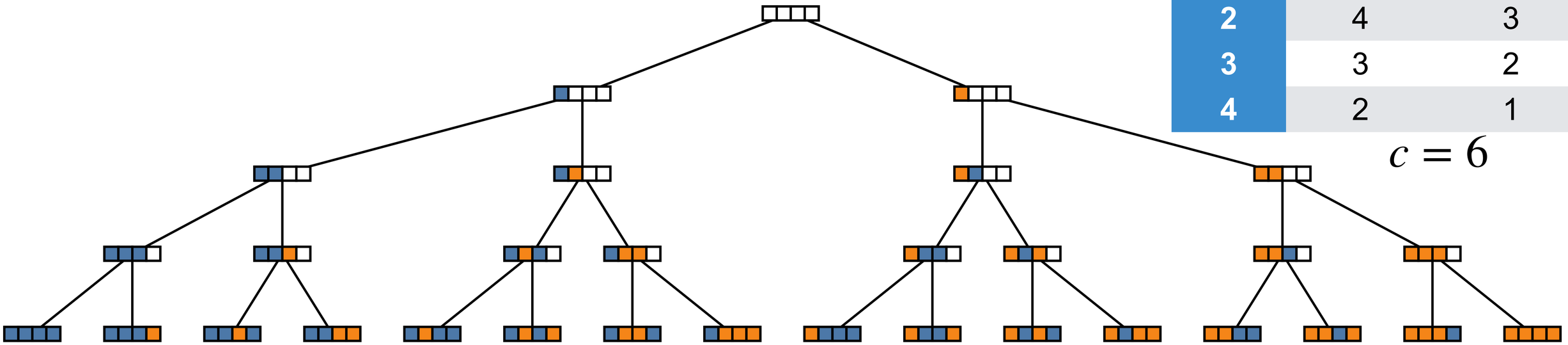

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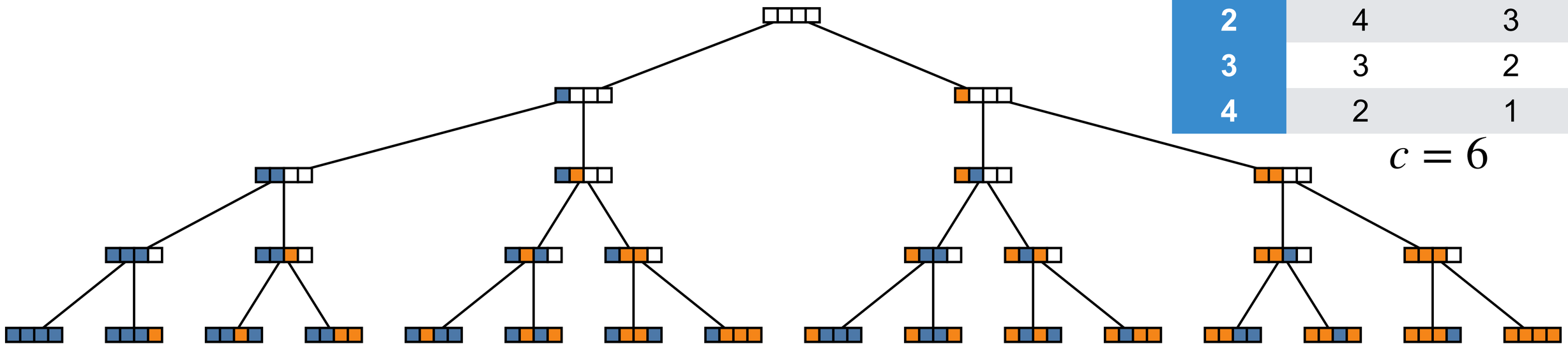

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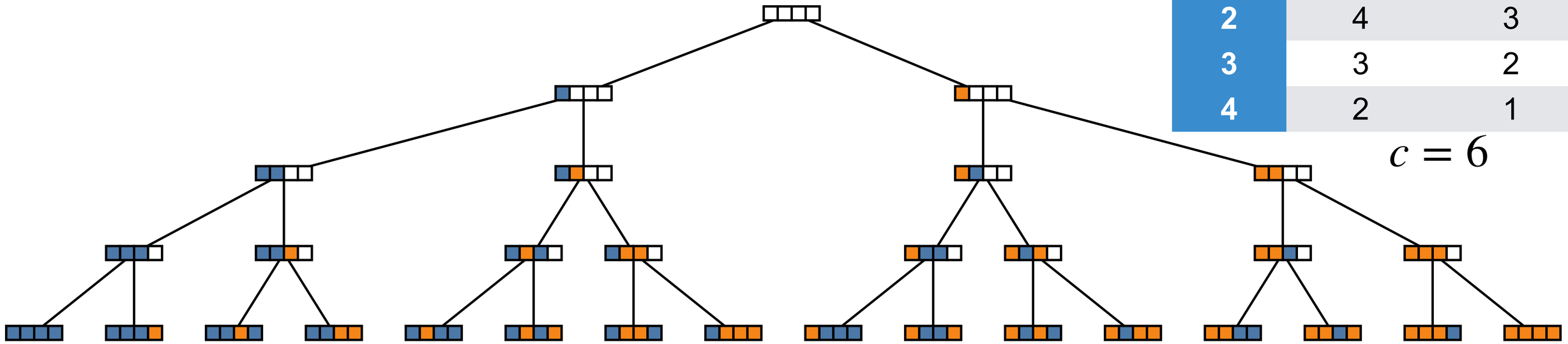

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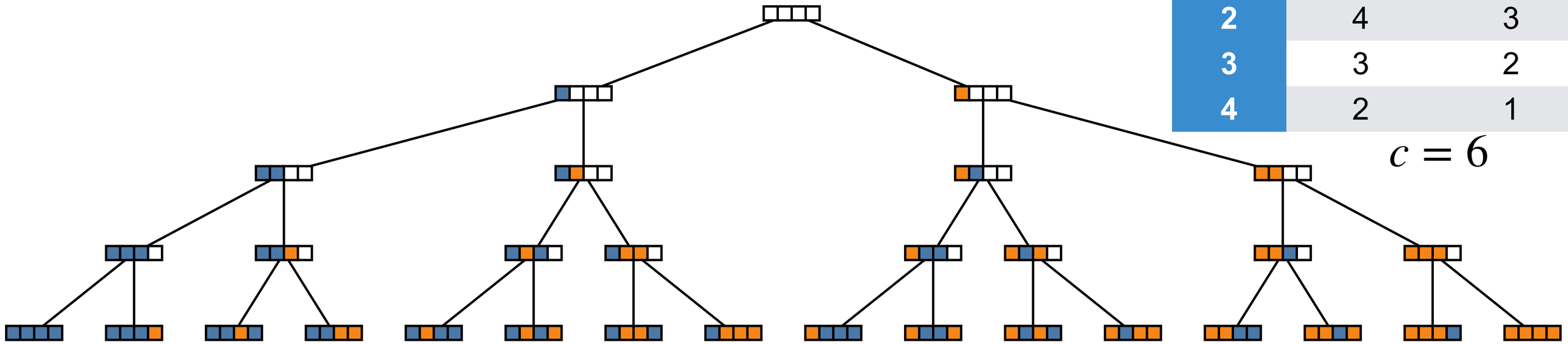

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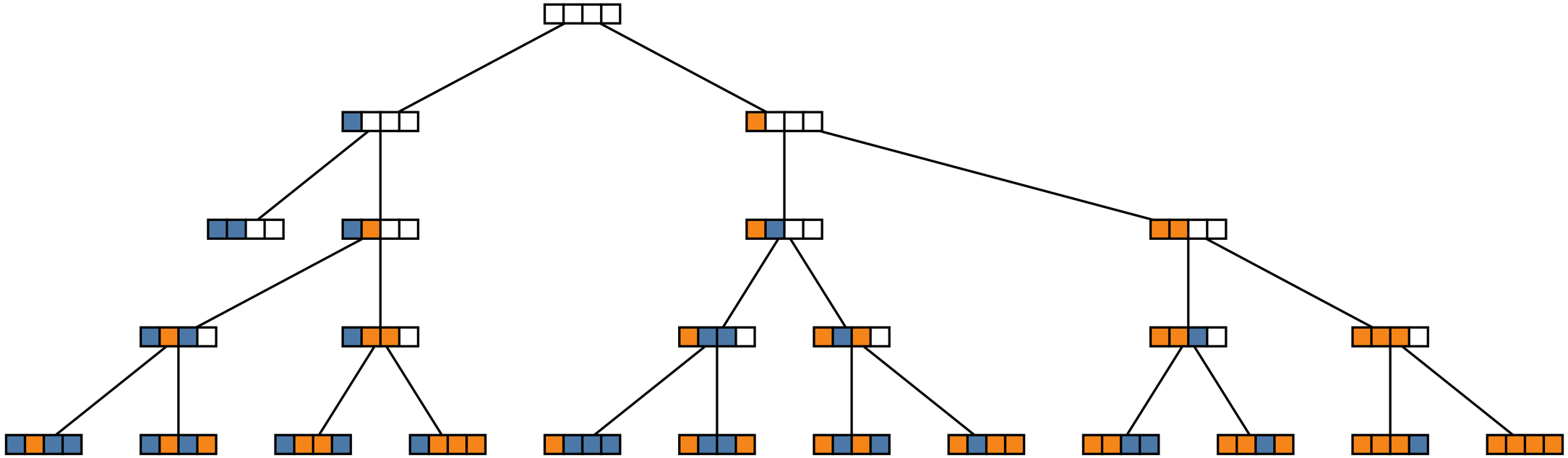

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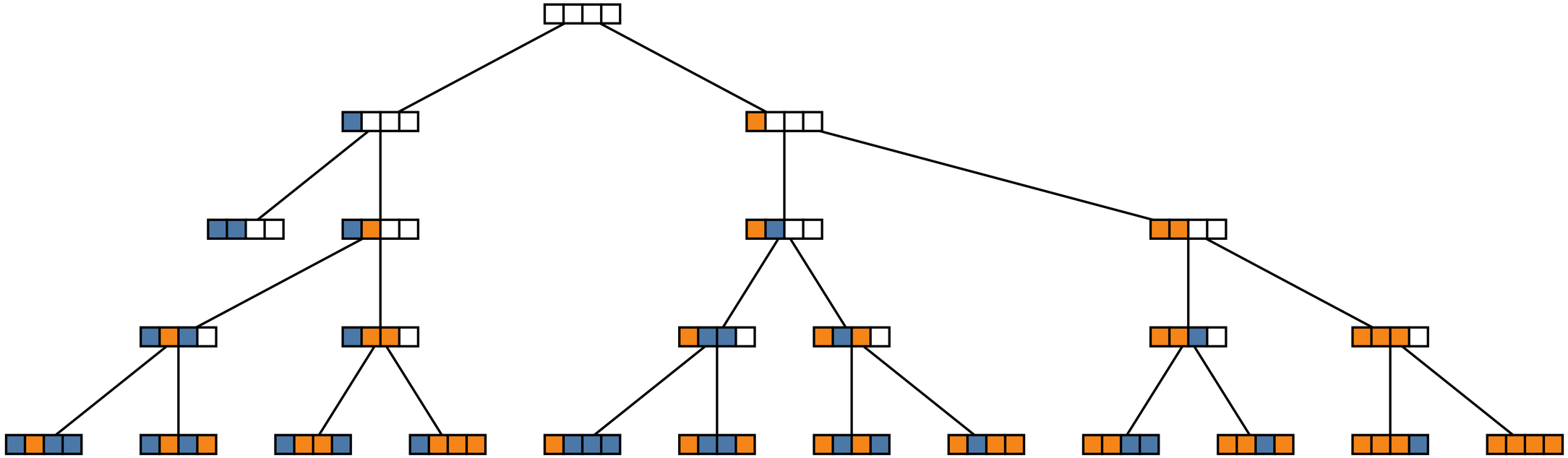

Eliminate some infeasible nodes:

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- Backtracking search tree for 4 items: 31 → 25 nodes

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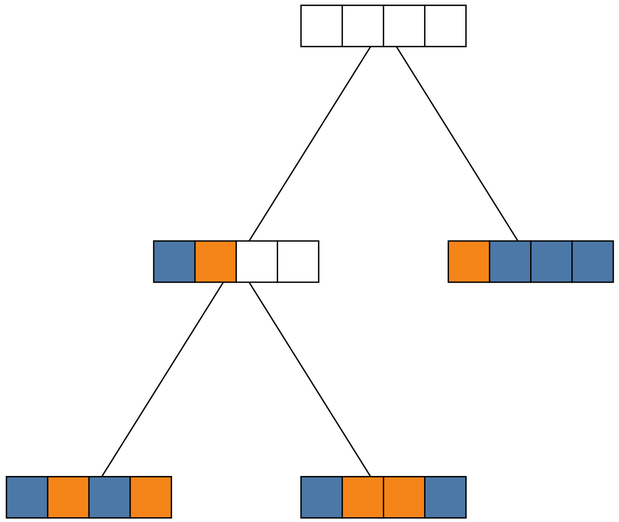
Backtracking & Constraint Propagation



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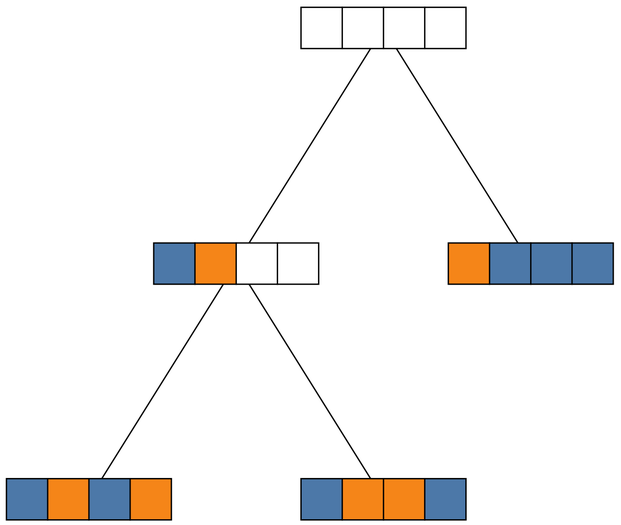

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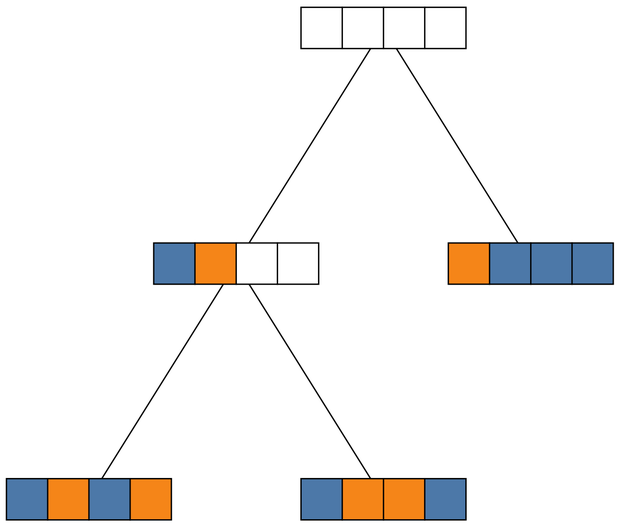

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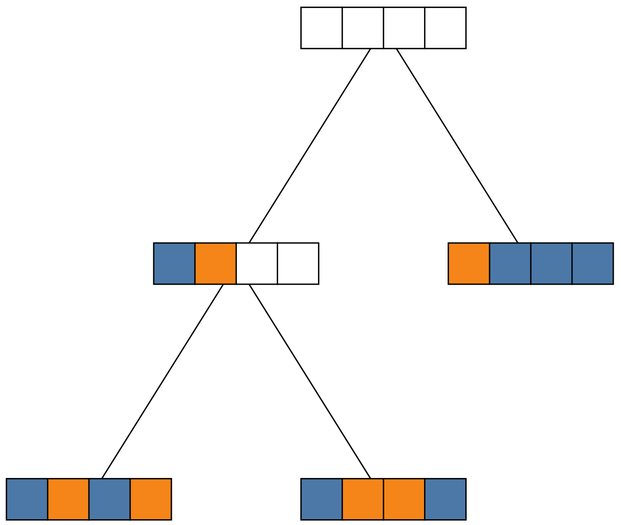

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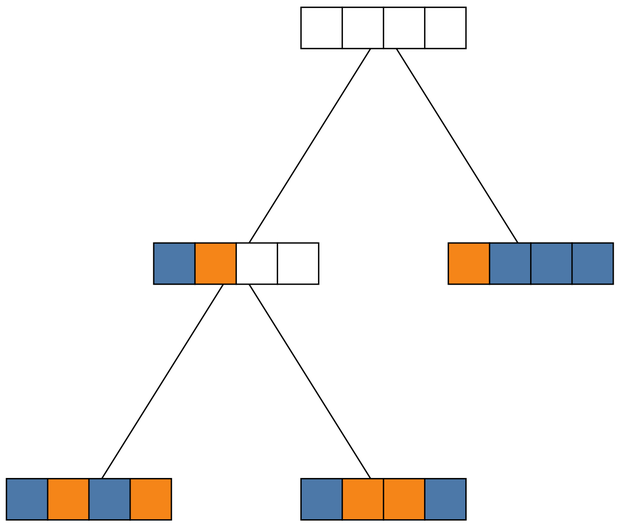
Knapsack: fix to false all items that do not fit into the container, given the items set to true.

Backtracking & Constraint Propagation



```
backtrack(partial):
  if infeasible(partial):
    return
  partial = propagate(partial)
  if index = unfixed(partial):
    partial[index] = True
    backtrack(partial)
    partial[index] = False
    backtrack(partial)
  else:
    record(partial)
```

$c = 6$

Item	Price p	Weight w
1	5	4
2	4	3
3	3	2
4	2	1

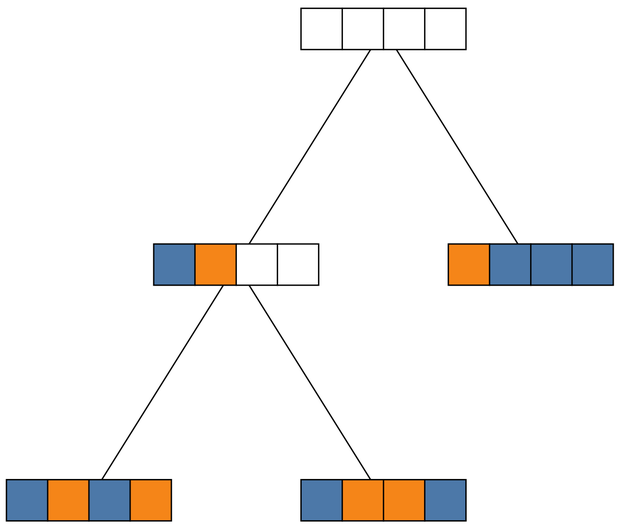
Propagation (`propagate`): Compute logical consequences of partial assignments.

Pure constraint propagation: Pure logical consequences of constraints & assignment.

Knapsack: fix to false all items that do not fit into the container, given the items set to true.

Objective-based propagation: Additionally, use the objective.

Backtracking & Constraint Propagation



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Propagation (`propagate`): Compute logical consequences of partial assignments.

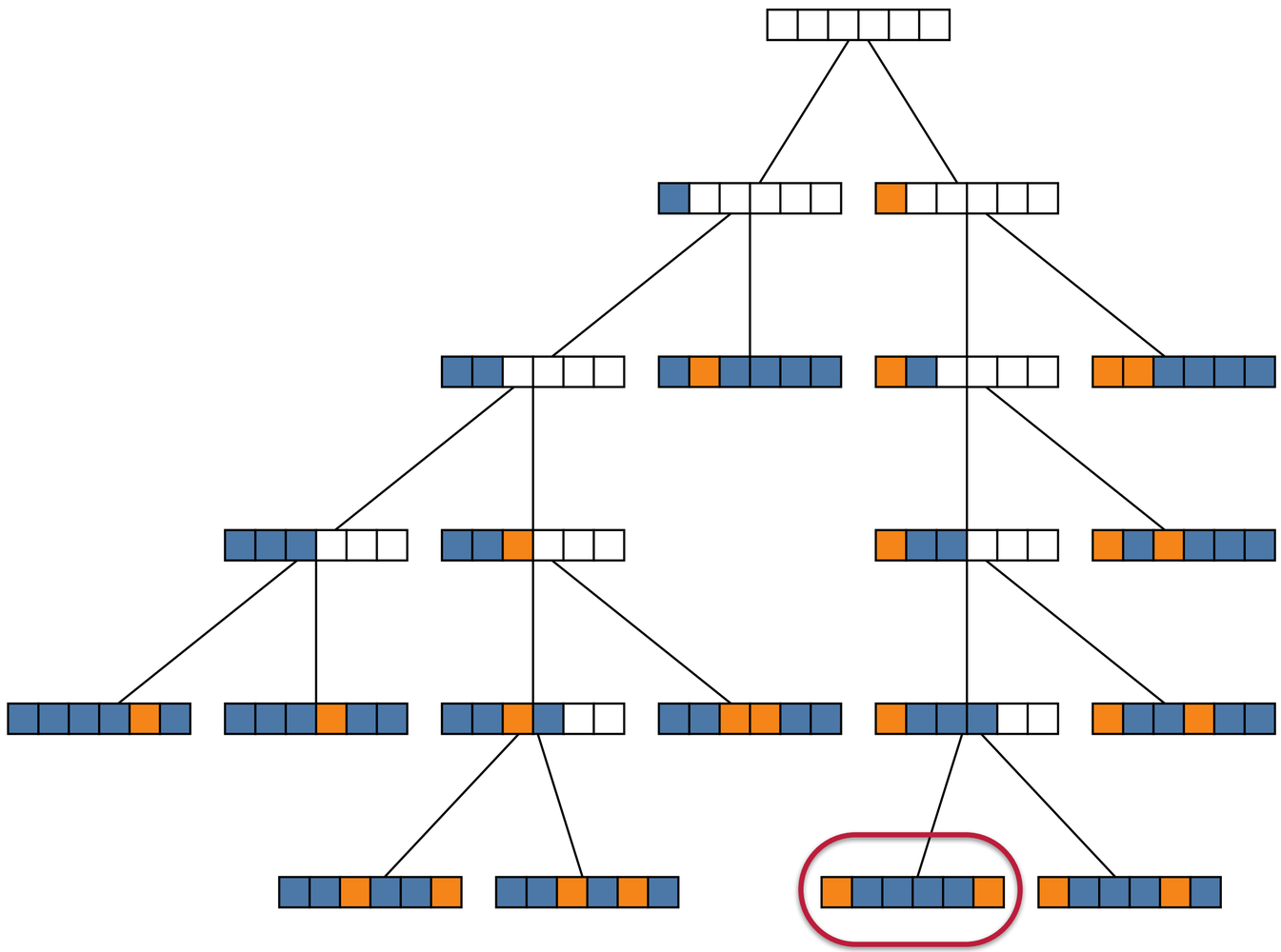
Pure constraint propagation: Pure logical consequences of constraints & assignment.

Knapsack: fix to false all items that do not fit into the container, given the items set to true.

Objective-based propagation: Additionally, use the objective.

Knapsack: fix to true all unfixed items with positive price if they all fit into the container.

Harder Instance — Backtracking & Constraint Propagation



OPT: 77 $\{2,3,4,5\}$

$$c = 19$$

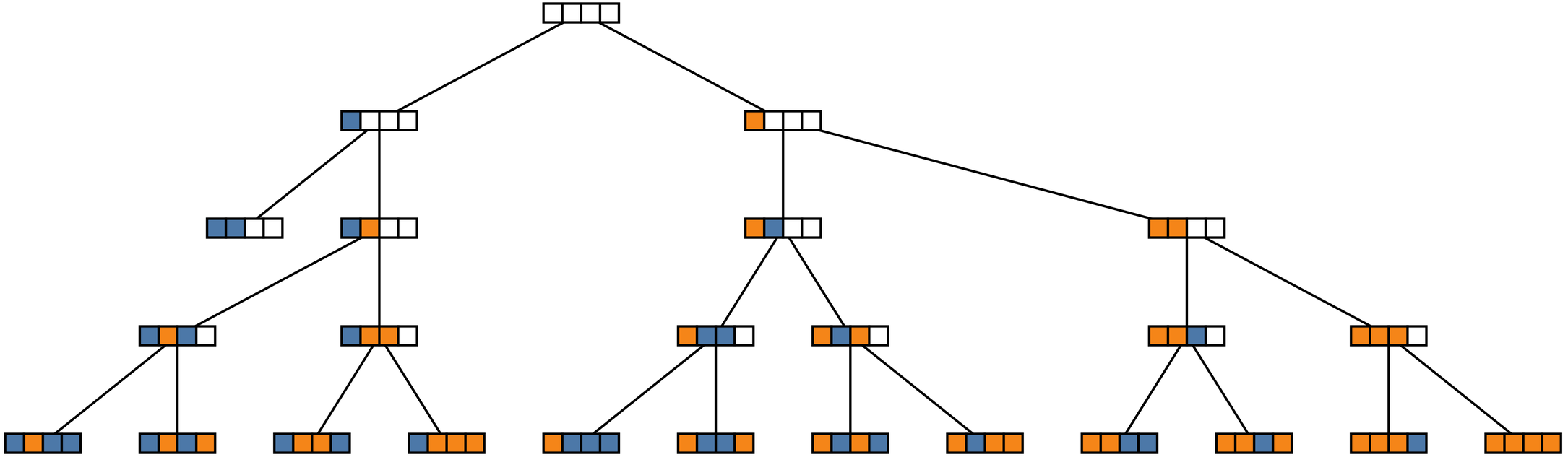
Item	Price p	Weight w
1	10	1
2	20	7
3	16	3
4	20	5
5	21	4
6	8	3

Remaining issues:
Many suboptimal nodes
Repeated subtrees

Backtracking & Constraint Propagation: Conflict Analysis

In propagation/infeasibility checking:

- Analyze *why* infeasibilities occur
- Learn more general rules than ‘that partial assignment is infeasible’
- More on that later: CDCL SAT Solvers, CP-SAT



Approaches

Different approaches:

- Dynamic programming
- Greedy heuristic & fractional greedy upper bound
- Backtracking & Constraint Propagation
- Branch & Bound
- Branch & Cut
- Metaheuristics

Branch & Bound: Key Insight

Branch & Bound: Key Insight

Backtracking:

- Throw away subtrees that cannot contain *any* valid solution

Branch & Bound: Key Insight

Backtracking:

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- Objective-based propagation: already does a little more

Branch & Bound: Key Insight

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- **Question:** When can we safely discard a whole subtree?

Branch & Bound: Key Insight

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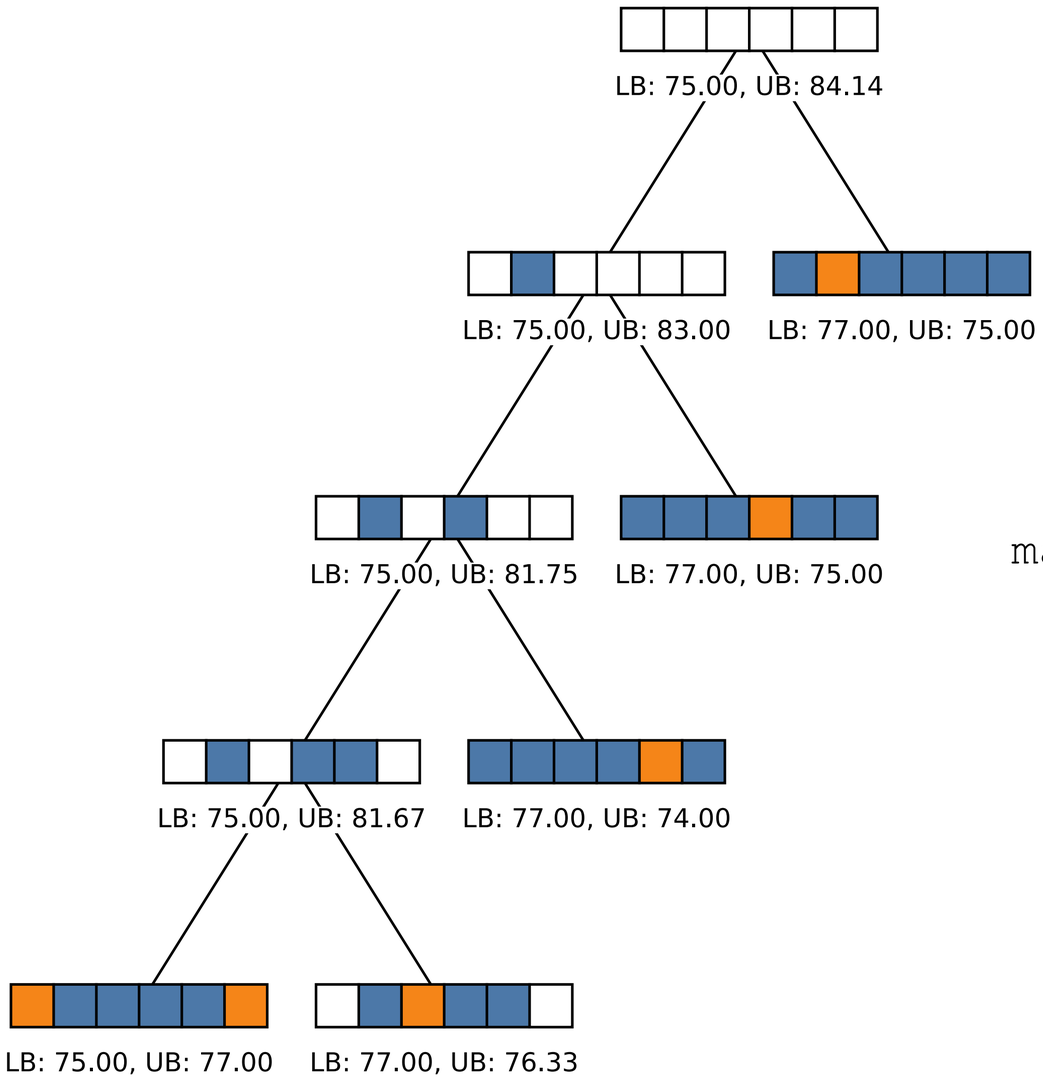
- When it cannot contain any *better* valid solution than one we already have

Branch & Bound: Key Insight

Backtracking:

- Throw away subtrees that cannot contain *any* valid solution
- Objective-based propagation: already does a little more
- **Question:** When can we safely discard a whole subtree?
- When it cannot contain any *better* valid solution than one we already have
- Try and track (at sustainable effort) whether each subtree can still have a better solution!

Branch & Bound: Pruning



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```
max_bnb(problem):
  lb = heuristic_solution(problem)
  open_nodes = [empty_partial(problem)]
  while node = select_and_pop(open_nodes):
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      continue  # infeasible
    node_lb, node_ub = bound(partial)
    if node_lb and node_lb > lb:
      lb = node_lb
    if node_ub <= lb:
      continue  # prune
    open_nodes += branch(partial)
```

Branch & Bound: Open Factors

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Exploration order:

Branch & Bound: Open Factors

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Exploration order:

- Depth first: memory efficient

Branch & Bound: Open Factors

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Exploration order:

- Depth first: memory efficient
- Best first: UB focus

Branch & Bound: Open Factors

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Exploration order:

- Depth first: memory efficient
- Best first: UB focus
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- Problem-specific

Branch & Bound: Open Factors

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Exploration order:

- Depth first: memory efficient
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- Problem-specific
- UB always needed

Branch & Bound: Open Factors

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Exploration order:

- Depth first: memory efficient
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- Problem-specific
- UB always needed
- LB = UB for full solutions

Branch & Bound: Open Factors

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Branch (variable) selection: Only one reasonable choice in KP

Branch & Bound: Open Factors

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- Dep
- Bes
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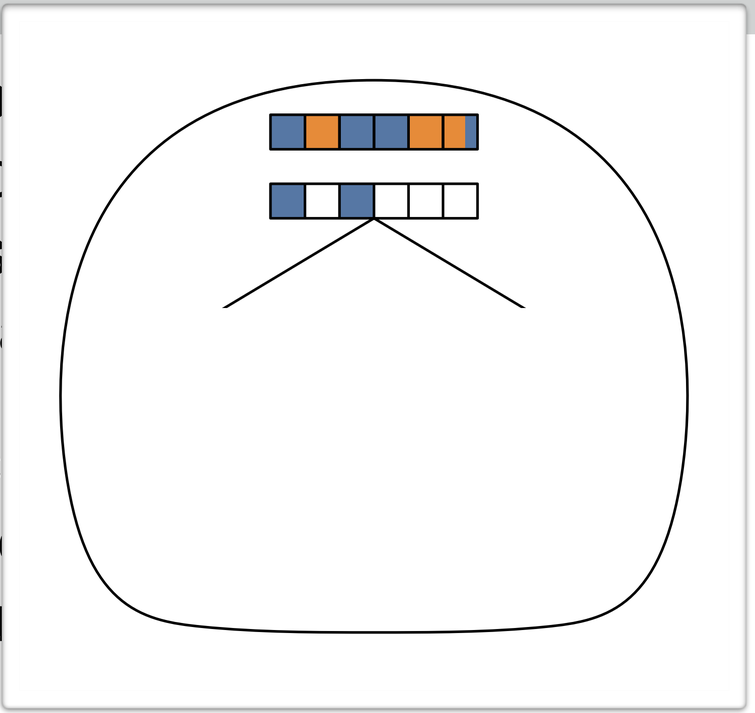

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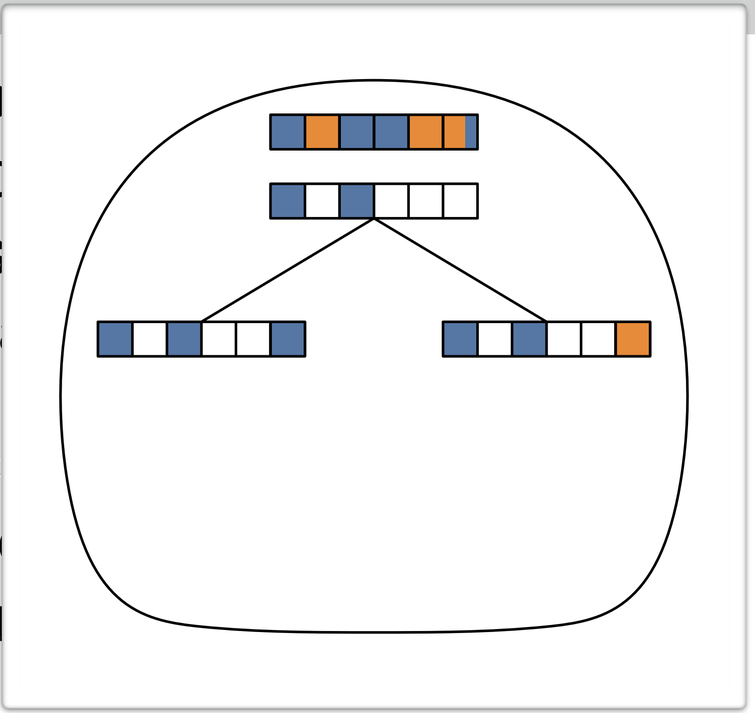

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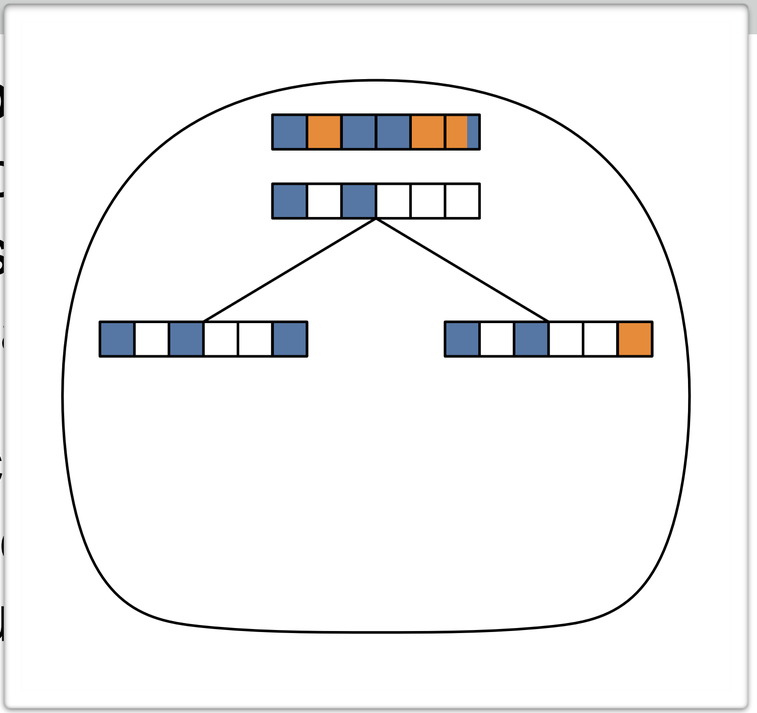

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- Which reduces the tree most? → we cannot know; heuristic choice

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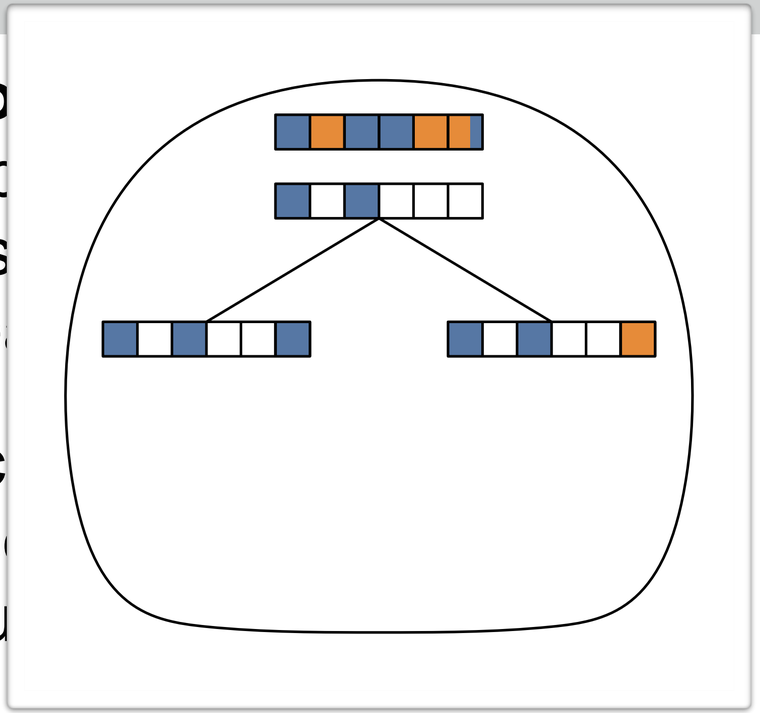

- Problem-spec
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Branch (variable) selection: Only one reasonable choice in KP

- Which reduces the tree most? → we cannot know; heuristic choice
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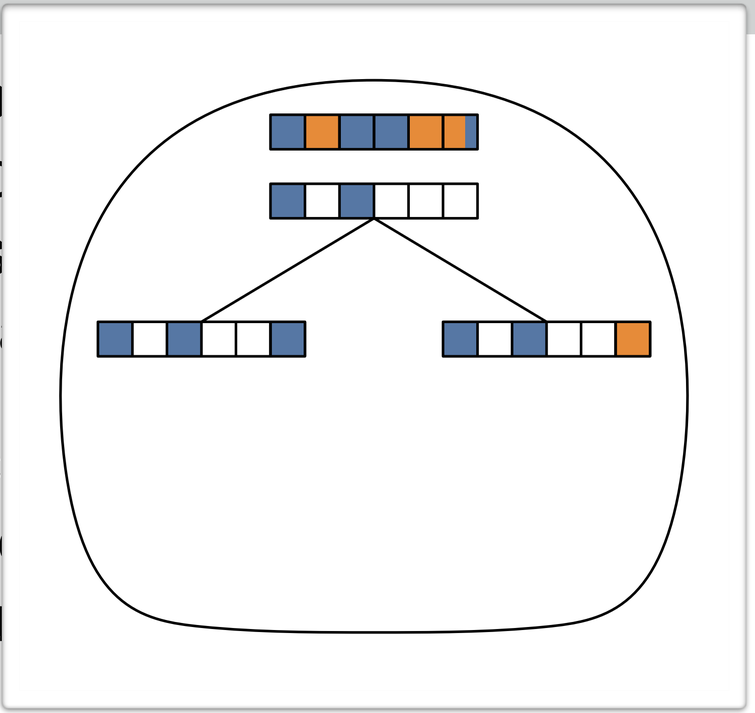

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Branch (variable) selection: Only one reasonable choice in KP

- Which reduces the tree most? → we cannot know; heuristic choice
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- Pseudocost branching (average bound improvement per unit change)

Branch & Bound: Open Factors

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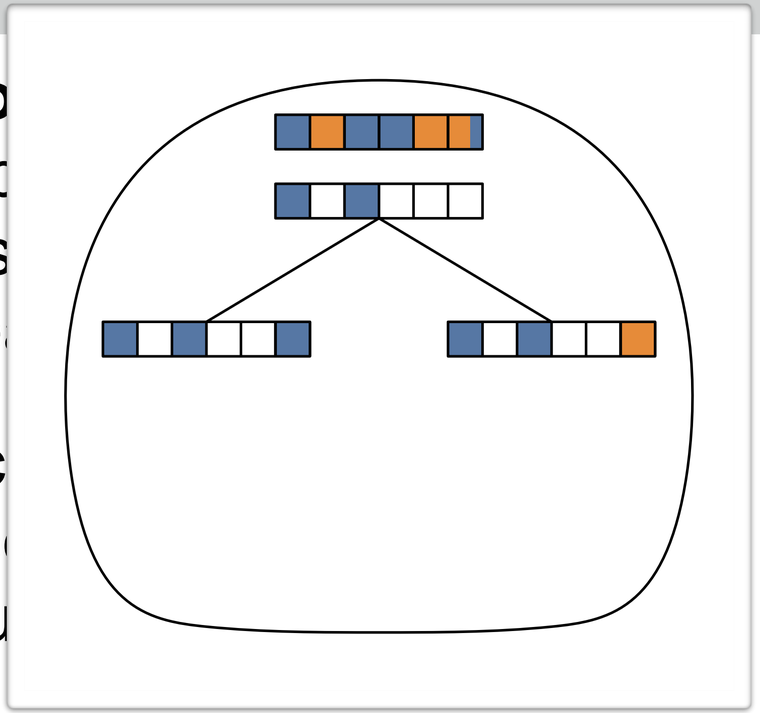

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- Reliability branching

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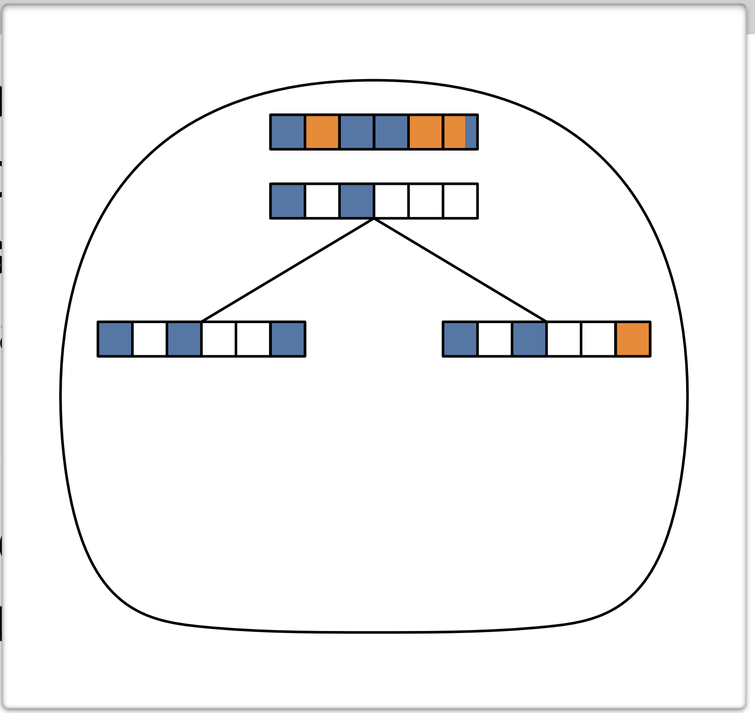

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- Which reduces the tree most? → we cannot know; heuristic choice
- Strong branching: try multiple variables, compute bounds on both sides
- Pseudocost branching (average bound improvement per unit change)
- Reliability branching
- Simple scores (distance to integrality), Hybrid, ML, conflict-based, …

Approaches

Different approaches:

- Dynamic programming
- Greedy heuristic & fractional greedy upper bound
- Backtracking & Constraint Propagation
- Branch & Bound
- Branch & Cut
- Metaheuristics

Extension: Branch & Cut

Linear program

$$\max \sum_i c_i x_i \text{ s.t.}$$

$$1 \leq j \leq m : \sum_i a_{ji} x_i \leq b_j$$

$$\in P$$

Extension: Branch & Cut

Linear program

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Binary program

$$\max \sum_i c_i x_i \text{ s.t.}$$

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$$x_i \in \{0,1\}$$

NP-complete

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Mixed Integer Program (MIP): mixing integer/real variables

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NP-complete

Mixed Integer Program (MIP): mixing integer/real variables

Most common implementation of `bound`**:**

Solve the linear relaxation (drop $x_i \in \mathbb{Z}$, $x_i \in \{0,1\} \rightarrow x_i \in [0,1]$; turns MIP into LP)

Extension: Branch & Cut

Extension: Branch & Cut

Knapsack (Bin. Program)

$$\max \sum_i p_i x_i \text{ s.t.}$$

Extension: Branch & Cut

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$$\max \sum_i p_i x_i \text{ s.t.}$$

$$\sum_i w_i x_i \leq c$$

Extension: Branch & Cut

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NP-complete

Extension: Branch & Cut

Knapsack (Bin. Program)

```python
def solve_knapsack_gurobi(instance: KnapsackProblem):
    model = grb.Model()
    n = instance.item_count
    p = instance.prices
    w = instance.weights
    c = instance.capacity
    x = [model.addVar(vtype=grb.GRB.BINARY, obj=p[i])
         for i in range(n)]
    model.ModelSense = grb.GRB.MAXIMIZE
    model.addConstr(grb.quicksum(x[i] * w[i] for i in range(n)) <= c)
    model.optimize()
    values = [x_i.X for x_i in x]
    return KnapsackSolution(
        items_included=[i for i in range(n) if values[i] > 0.5],
        total_price=model.ObjVal
    )
```

Extension: Branch & Cut

Knapsack (Bin. Program)

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$$\sum_i w_i x_i \leq c$$

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NP-complete

Extension: Branch & Cut

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NP-complete

Linear Relaxation

$$\max \sum_i p_i x_i \text{ s.t.}$$

$$\sum_i w_i x_i \leq c$$

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Extension: Branch & Cut

Knapsack (Bin. Program)

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$$\sum_i w_i x_i \leq c$$

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BP formulation of Knapsack: equivalent to Knapsack (*Formulation* of Knapsack as BP)

Extension: Branch & Cut

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LP relaxation: equivalent to fractional greedy Knapsack

Extension: Branch & Cut

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$$\sum_i w_i x_i \leq c$$

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NP-complete

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Possible cuts: $\sum_{i \in C} x_i \leq |C| - 1$ for some C that does not fit into the Knapsack

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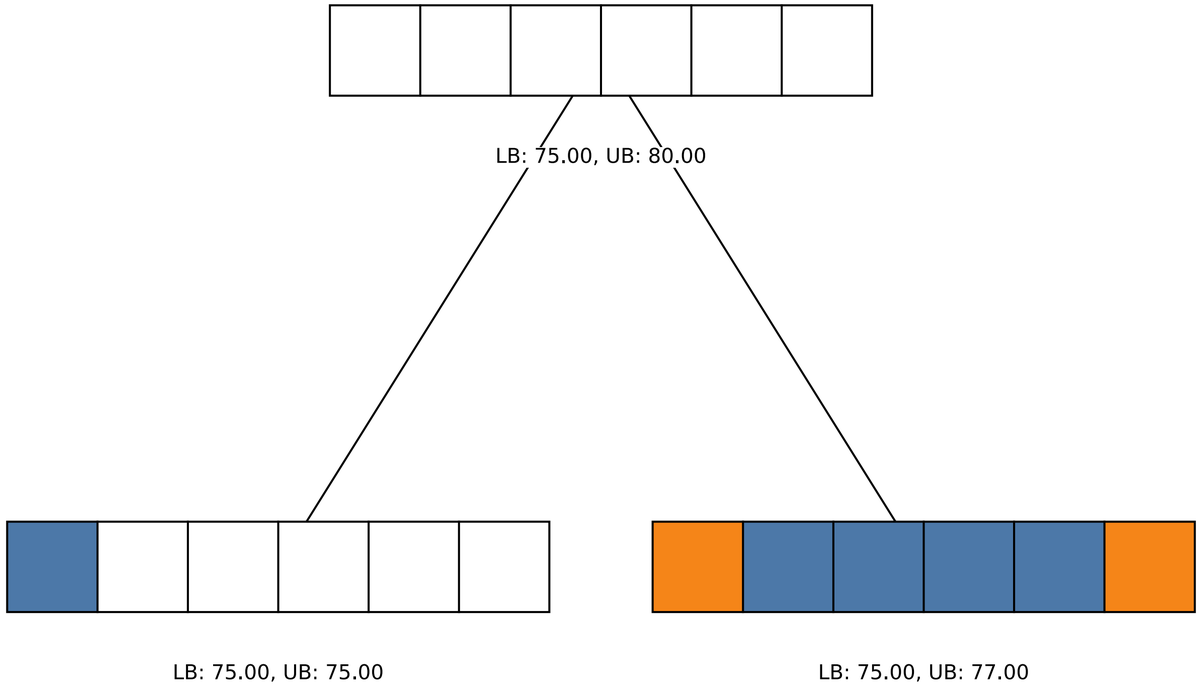

Approaches

Different approaches:

- Dynamic programming
- Greedy heuristic & fractional greedy upper bound
- Backtracking & Constraint Propagation
- Branch & Bound
- Branch & Cut
- Metaheuristics

Metaheuristics

Why heuristics?

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High Level Types of Metaheuristics

- Constructive heuristics
- Local search and variants
- Population-based algorithms
- These cover most (meta)heuristics, but there are other approaches

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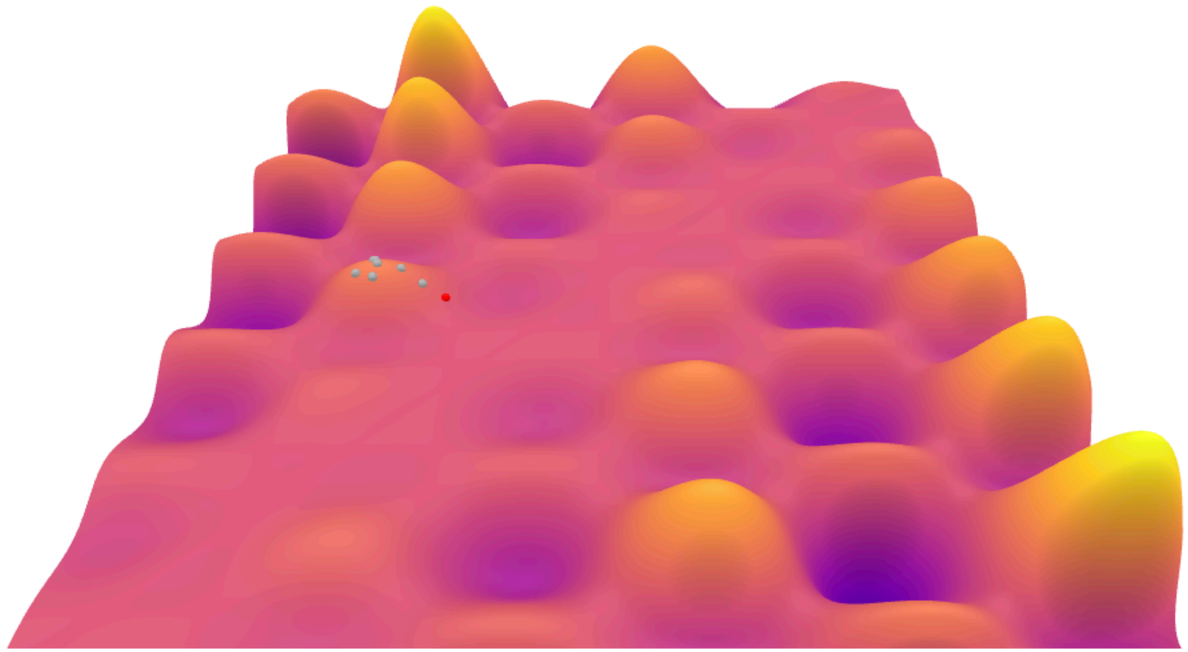
- Possibly enhanced by local search
- Typically fast; trade-off between number of solutions and chance of good solution

Local Search



General idea:

- Starting from a solution S
- Consider neighboring solutions S'
- Stay at S or move to some neighbor S'
- Repeat until some termination criterion

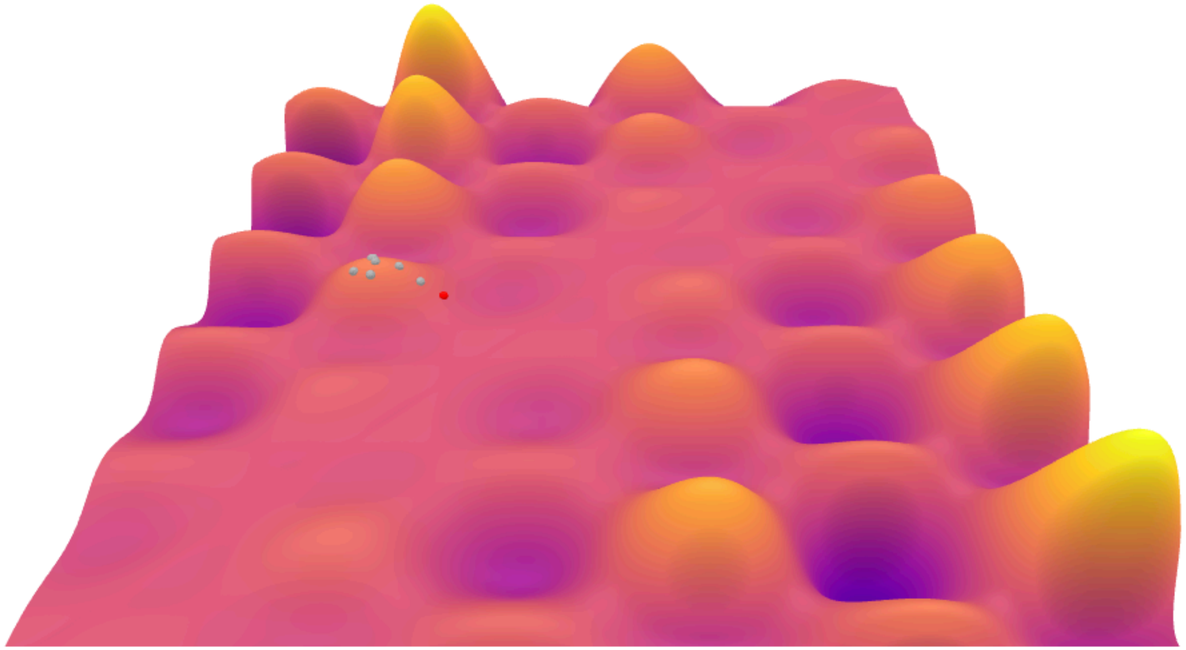
Main issue:

- Local optima

Examples:

- 2-OPT and other simple improvements
- Simulated annealing
- Large Neighborhood Search (LNS)
- Limited Discrepancy Search
- …

Exploration vs. Exploitation



Exploration:

- How good are we at exploring all relevant parts of the search space?

Exploitation:

- How good are we at improving solutions to a local optimum?

Balance: usually start more explorative/broad/diverse, then focus/intensify

Population-based Heuristics

General idea:

- Do not maintain a single solution
- Instead, maintain a population of solutions
- In each iteration (generation), create a new population from the old
- Typically involves combining solutions
- Typically, prefer better solutions
- Typically, some mechanism encourages diversity

Examples:

- Genetic algorithms
- Memetic algorithms
- Particle swarms
- …

Key Ideas

- Tree search idea (partial assignments, connection to solution space)
- Relaxation
- Constraint propagation
- Eliminate nodes/branches that have no solution (backtracking)
- Eliminate nodes/branches that cannot have a better solution (branch & bound)
- Heuristic initial solutions can be worthwhile (better pruning)
- Strengthening bounds can be worthwhile (branch & cut)
- Metaheuristics often are the best practical approach (scalability)
- They can still use exact methods (we will see this later)