

# Anytime tree search for discrete optimization

## A tutorial

---

Abdel-Malik Bouhassoun - Hadrien Cambazard - Florian Fontan  
Vincent Jost - Luc Libralesso - Aurélien Secardin

April, 28, 2020 - ROSP Seminar

G-SCOP, Grenoble, France

email: [luc.libralesso@grenoble-inp.fr](mailto:luc.libralesso@grenoble-inp.fr)

Please feel free to ask me questions at any time!

# Anytime tree search for discrete optimization

About the title

**Anytime:** provides good solutions fast and is able to improve them with more time. Similar to meta-heuristics.

# Anytime tree search for discrete optimization

About the title

**Anytime:** provides good solutions fast and is able to improve them with more time. Similar to meta-heuristics.

**Tree search:** explores a tree (more on it later)

# Anytime tree search for discrete optimization

About the title

**Anytime:** provides good solutions fast and is able to improve them with more time. Similar to meta-heuristics.

**Tree search:** explores a tree (more on it later)

**Discrete optimization:** all variables are discrete (Integer or Boolean)

# Goal of this tutorial

- Quickly present search algorithms for optimization

# Goal of this tutorial

- Quickly present search algorithms for optimization
- With a focus on anytime tree search

# Goal of this tutorial

- Quickly present search algorithms for optimization
- With a focus on anytime tree search
- Some applications (academic and industrial)



# Table of contents

1. Optimization and search
2. Tree Search
3. Sequential Ordering Problem
4. Other works
5. Take aways

# Optimization and search

---

We want to find the best possible solution out of a finite and **huge** number of solutions.

## Example: (Asymmetric) Traveling Salesman Problem

INPUT:

- graph  $G = (V, A)$
- distance function  $w : A \rightarrow \mathbb{R}$

## Example: (Asymmetric) Traveling Salesman Problem

INPUT:

- graph  $G = (V, A)$
- distance function  $w : A \rightarrow \mathbb{R}$

GOAL:

- Find a tour that visit all  $n$  cities
- Minimize the distance of selected arcs
- $n!$  possible solutions

## Resolution Methods (you may already know)

- Brute Force (very bad)

## Resolution Methods (you may already know)

- Brute Force (very bad)
- Branch and Bound (better)

## Resolution Methods (you may already know)

- Brute Force (very bad)
- Branch and Bound (better)
- Mixed Integer Programming (LP + Branch and Bound)



# Resolution Methods (you may already know)

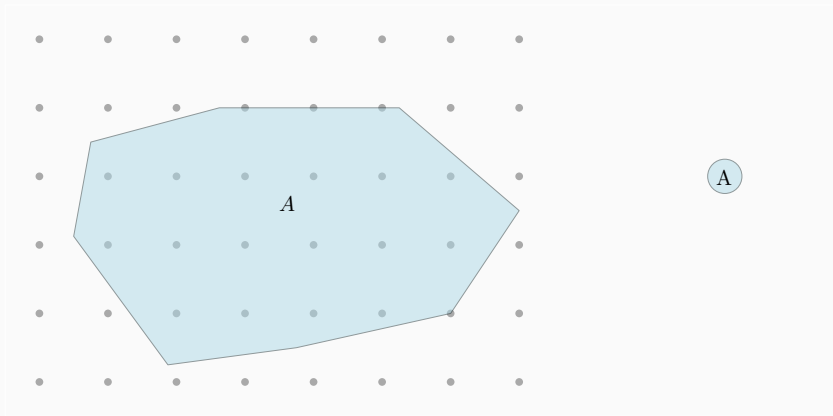
- Brute Force (very bad)
- Branch and Bound (better)
- Mixed Integer Programming (LP + Branch and Bound)
- Meta-heuristics:
  - Local Search
  - Simulated Annealing
  - Genetic Algorithms
  - Ant Colony Optimization
  - *etc.*

Search procedures are often labeled as:

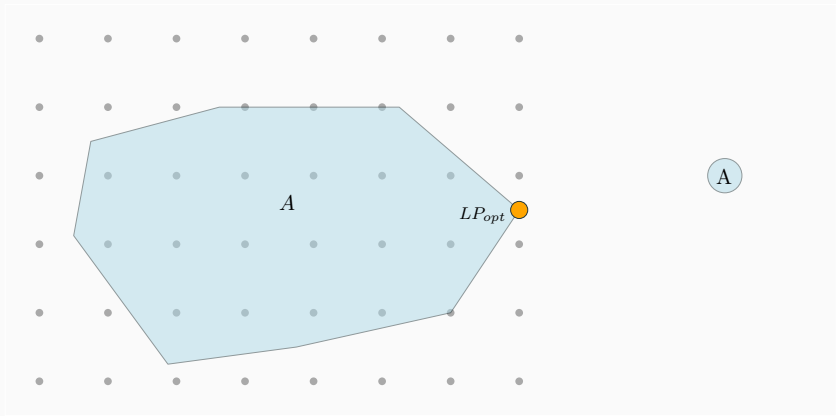
- Tree Search
- Local Search
- Population Based Search

- usually "constructs" solutions
- Models the problem as a tree
- Explores this tree

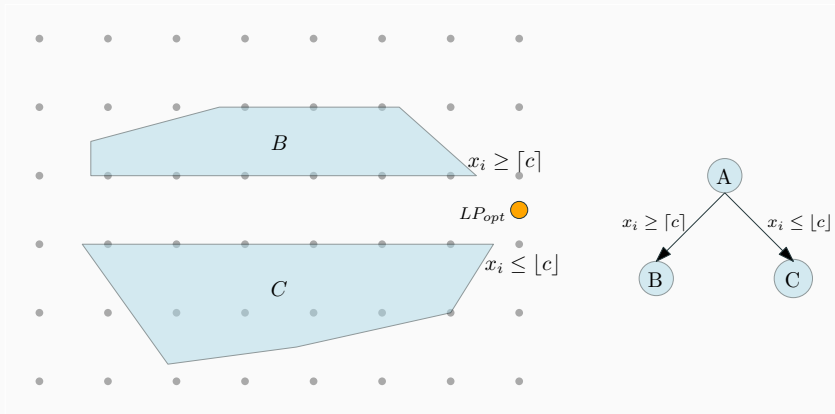
## Example: Mixed Integer Programming



# Example: Mixed Integer Programming



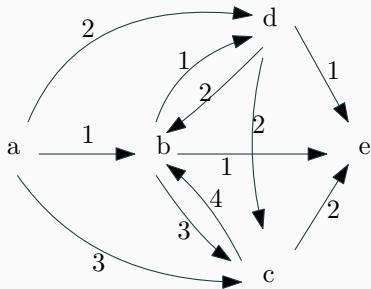
# Example: Mixed Integer Programming



## Example: Dedicated Branch and Bound

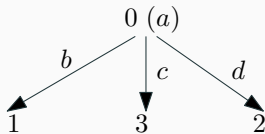
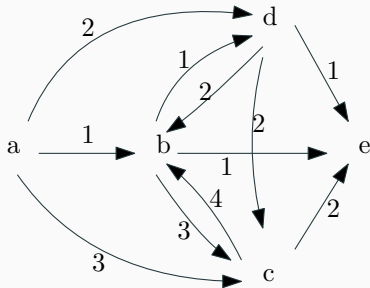
A Sequential Ordering Problem Branch and Bound (more later)

0 (a)



## Example: Dedicated Branch and Bound

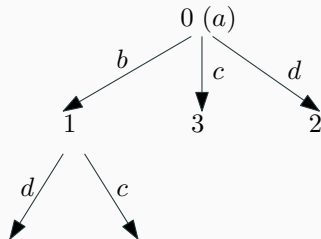
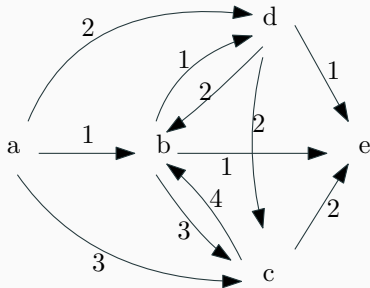
A Sequential Ordering Problem Branch and Bound (more later)





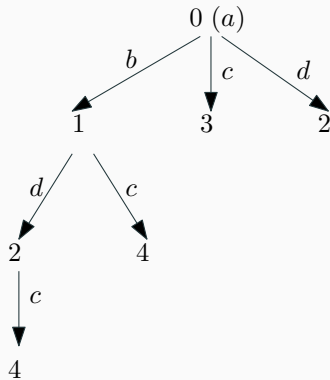
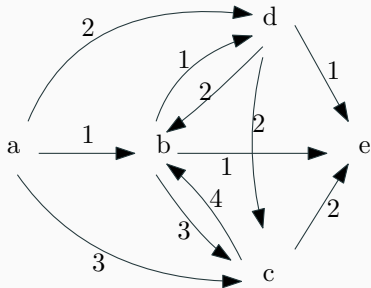
# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



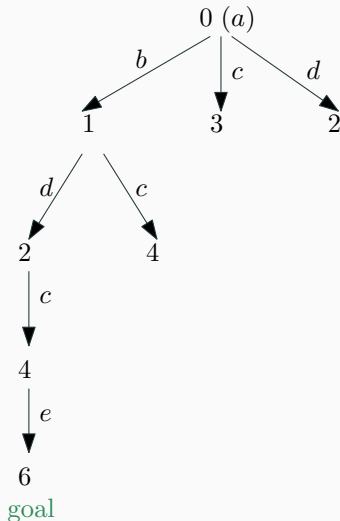
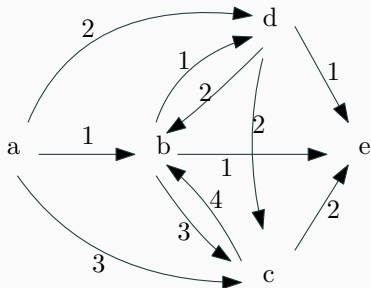
# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



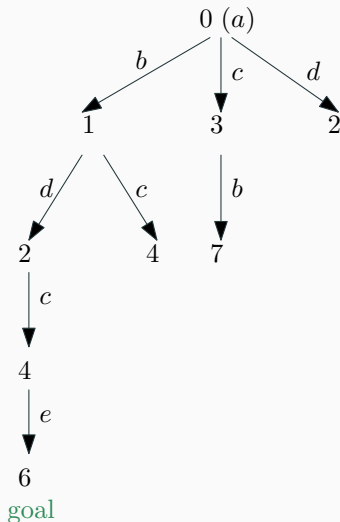
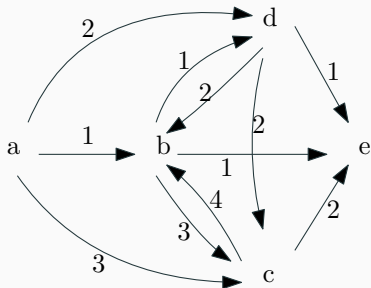
# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



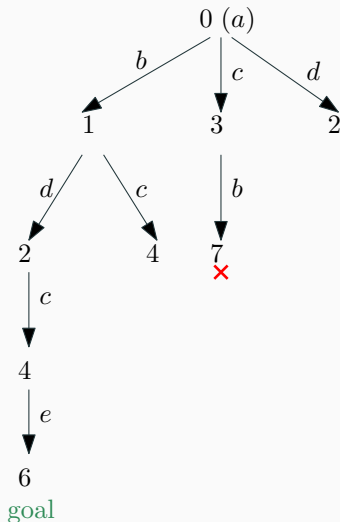
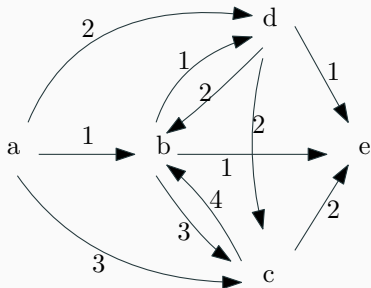
# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



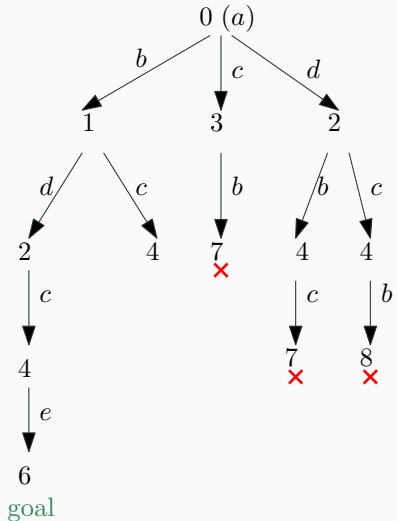
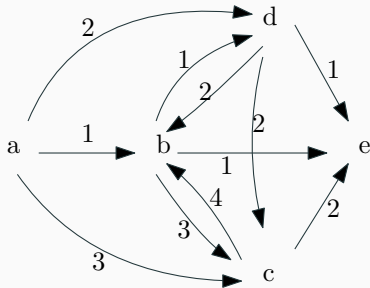
# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



# Example: Dedicated Branch and Bound

A Sequential Ordering Problem Branch and Bound (more later)



# How to improve a branch and bound

- Better bounds: MST, assignment problem, LP, *etc.* The stronger, the more prunings, but also more expensive to compute.

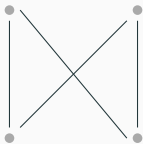
# How to improve a branch and bound

- Better bounds: MST, assignment problem, LP, *etc.* The stronger, the more prunings, but also more expensive to compute.
- Better search strategy (will be discussed in this talk)



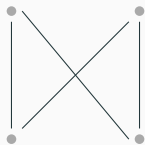
- usually improves an existing solution
- by exploring similar solutions

## Local Search Example - 2-opt for the TSP

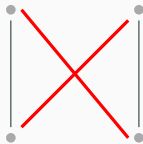


Initial solution (tour)

## Local Search Example - 2-opt for the TSP

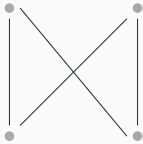


Initial solution (tour)

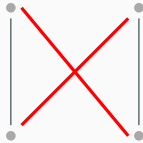


Identify edges to  
remove (in red)

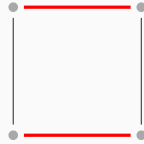
# Local Search Example - 2-opt for the TSP



Initial solution (tour)



Identify edges to remove (in red)



Replace them

# Population Based Search

- Consider a set of solutions (population)
- Combines promising solutions together (crossover)
- Possibly alter solutions (mutations)

# Recap

	Operators	Examples
Tree Search	children, bounds	MIP, CP, (more later ...)
Local Search	neighbourhood	Tabu Search, SA ...
Population Based	crossover, mutation distance from a solution	Genetic/Evolutionary

# Tree Search

---

Mathematical Programming Solver based on Local Search ([1]):

*“ Tree search approaches like branch-and-bound are in essence **designed to prove optimality** [...] Moreover, tree search has an exponential behavior which makes it **not scalable** faced with real-world combinatorial problems inducing millions of binary decisions. ”*



# Conventional wisdom - about Tree Search

Mathematical Programming Solver based on Local Search ([1]):

*“ Tree search approaches like branch-and-bound are in essence **designed to prove optimality** [...] Moreover, tree search has an exponential behavior which makes it **not scalable** faced with real-world combinatorial problems inducing millions of binary decisions. ”*

We believe it is false considering **anytime tree search algorithms**

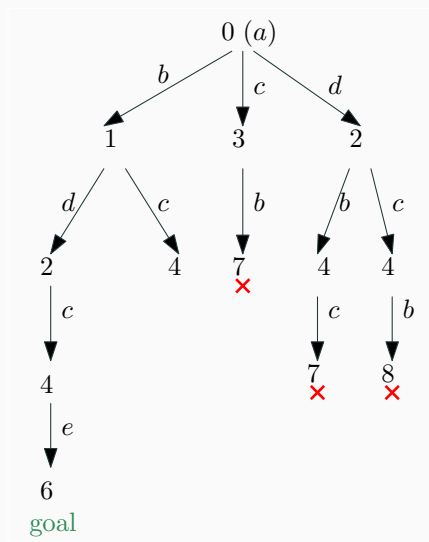
Made of two parts:

- The Implicit Tree definition:
  - root
  - children
  - bounds (optimistic estimate)
  - isGoal
  - possibly other information (*i.e.* guides, dominance prunings)

Made of two parts:

- The Implicit Tree definition:
  - root
  - children
  - bounds (optimistic estimate)
  - isGoal
  - possibly other information (*i.e.* guides, dominance prunings)
- The Search Procedure (generic):
  - Depth First Search (DFS)
  - Best First Search
  - A\*
  - Others (discussed in a few slides)

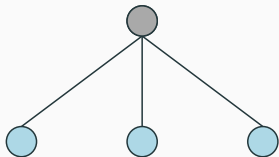
# About the Tree Search Formalism: An example



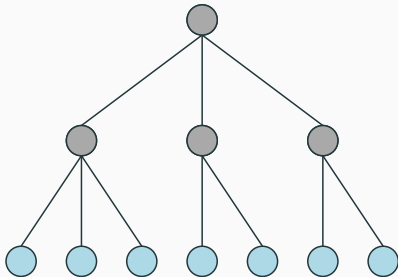
# Breadth First Search



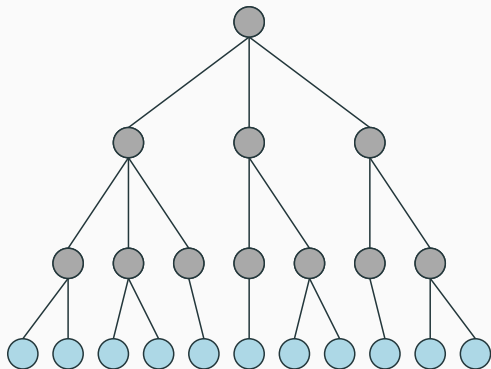
# Breadth First Search



# Breadth First Search



# Breadth First Search

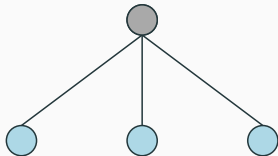




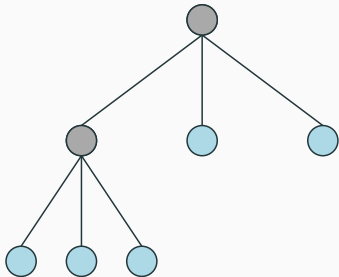
# Depth First Search



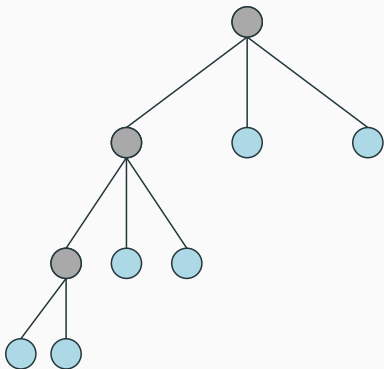
# Depth First Search



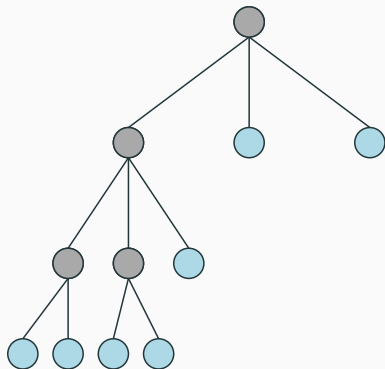
# Depth First Search



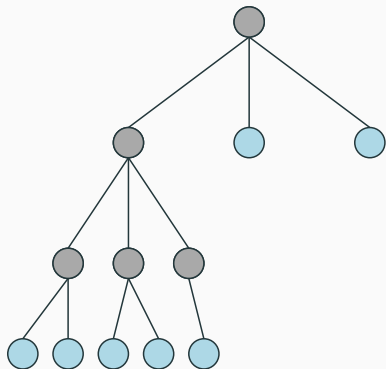
# Depth First Search

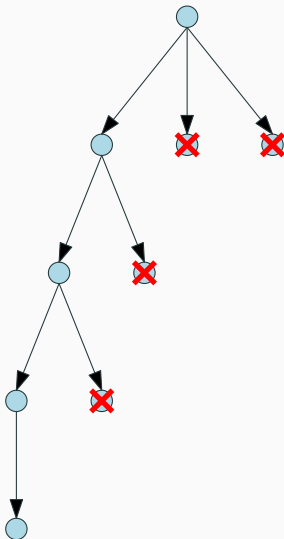


# Depth First Search



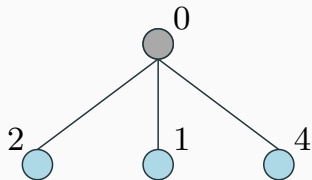
# Depth First Search

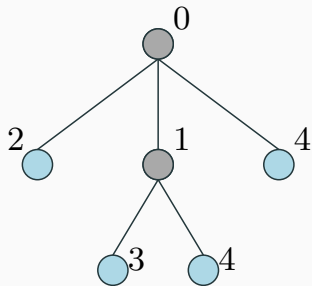




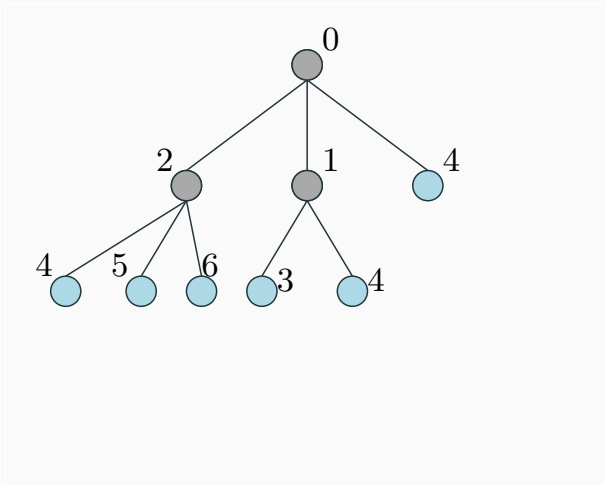




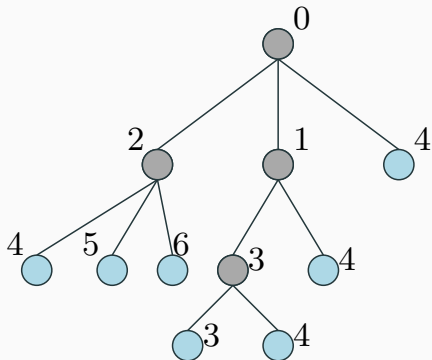




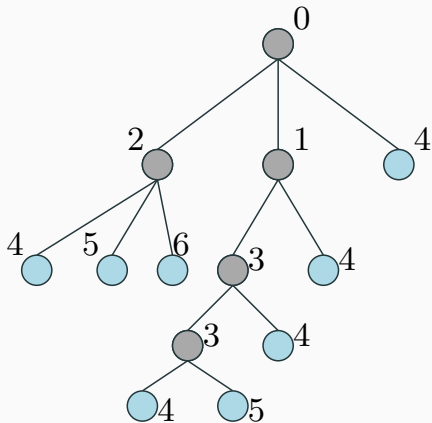
## Best (bound) First / A\*



## Best (bound) First / A\*



## Best (bound) First / A\*



## Exercise 1 : Advantages and Drawbacks

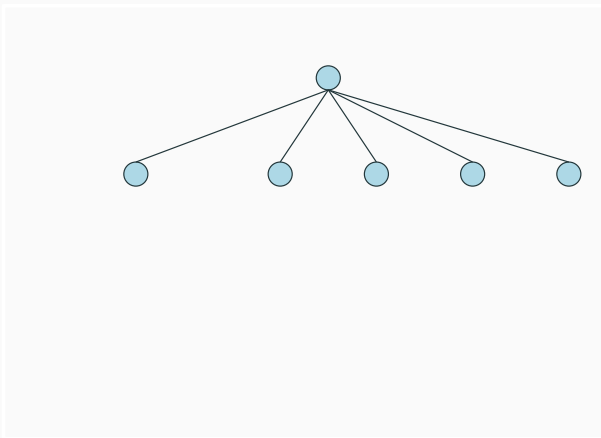
Depth First Search	A*/Best First
--------------------	---------------

## Exercise 1 : Advantages and Drawbacks

	Depth First Search	A*/Best First
Pros	<ol style="list-style-type: none"><li>1. Anytime</li><li>2. Memory Bounded</li></ol>	<ol style="list-style-type: none"><li>1. less nodes to close the instance</li><li>2. no need of good solutions</li></ol>
Cons	<ol style="list-style-type: none"><li>1. requires good solutions</li><li>2. suffers from early bad decisions</li></ol>	<ol style="list-style-type: none"><li>1. not anytime</li><li>2. Can use too much memory</li></ol>

# Limited Discrepancy Search (LDS) - key idea

Correct DFS drawback: early bad decisions

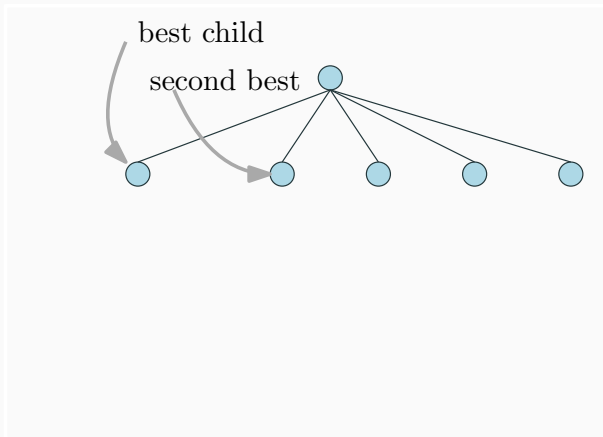


Explore more the most promising but still keep exploring others



# Limited Discrepancy Search (LDS) - key idea

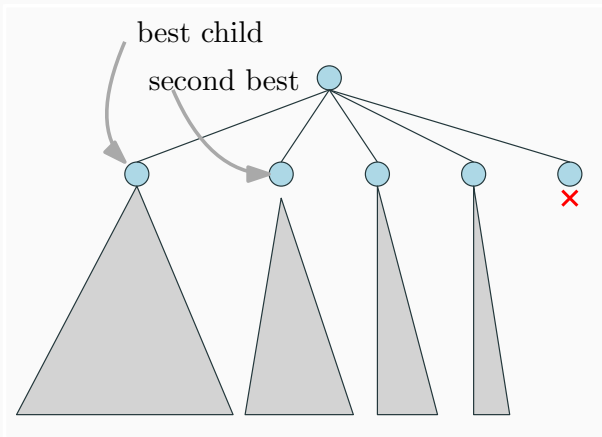
Correct DFS drawback: early bad decisions



Explore more the most promising but still keep exploring others

# Limited Discrepancy Search (LDS) - key idea

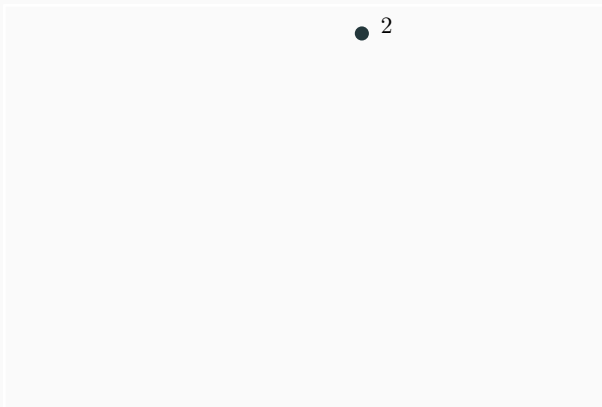
Correct DFS drawback: early bad decisions



Explore more the most promising but still keep exploring others

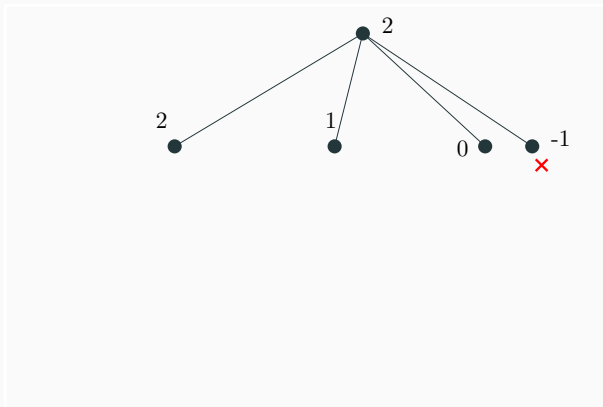
## Limited Discrepancy Search (LDS) - An example: $D=2$

Count the number of deviations from the best child (discrepancies)



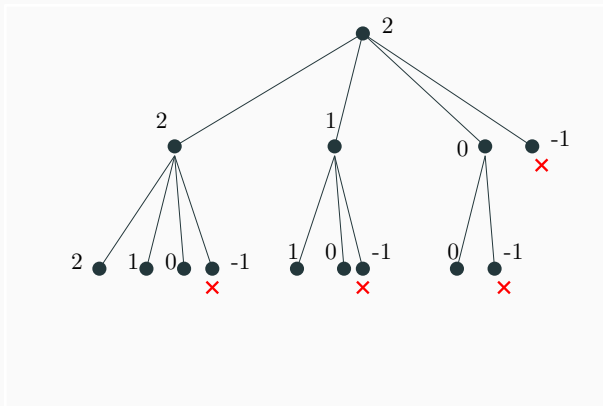
## Limited Discrepancy Search (LDS) - An example: $D=2$

Count the number of deviations from the best child (discrepancies)



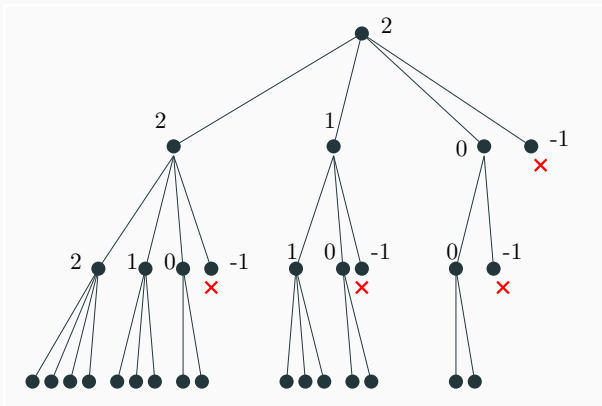
## Limited Discrepancy Search (LDS) - An example: $D=2$

Count the number of deviations from the best child (discrepancies)



## Limited Discrepancy Search (LDS) - An example: $D=2$

Count the number of deviations from the best child (discrepancies)

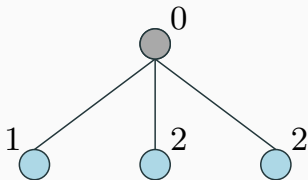


## Beam Search (D=3)



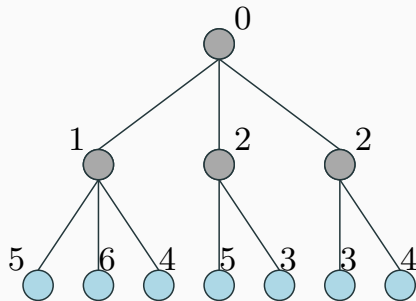
0

## Beam Search (D=3)

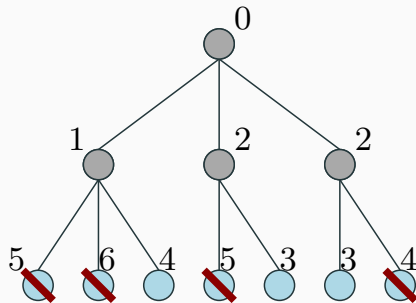




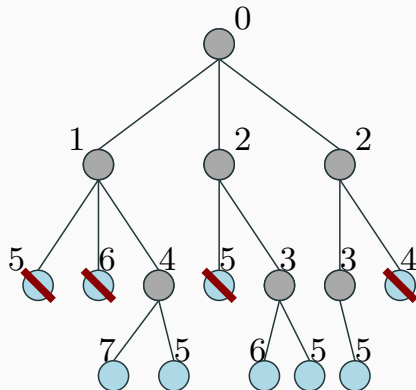
## Beam Search (D=3)



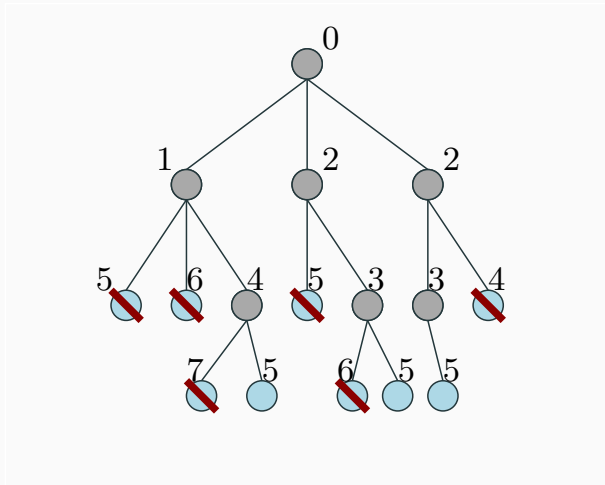
## Beam Search (D=3)



## Beam Search (D=3)



## Beam Search (D=3)



# Iterative Beam Search

- Start a beam search of size  $D = 1$  (greedy)
- Then a beam search of size  $D = 2$
- Then 4, 8, *etc.*

# Iterative Beam Search

- Start a beam search of size  $D = 1$  (greedy)
- Then a beam search of size  $D = 2$
- Then 4, 8, *etc.*

A few properties:

- A **complete/exact** algorithm. When the beam is wide enough, no “heuristic” fathoming.

# Iterative Beam Search

- Start a beam search of size  $D = 1$  (greedy)
- Then a beam search of size  $D = 2$
- Then 4, 8, *etc.*

A few properties:

- A **complete/exact** algorithm. When the beam is wide enough, no “heuristic” fathoming.
- The algorithm may open a node multiple times

# Iterative Beam Search

- Start a beam search of size  $D = 1$  (greedy)
- Then a beam search of size  $D = 2$
- Then 4, 8, *etc.*

A few properties:

- A **complete/exact** algorithm. When the beam is wide enough, no “heuristic” fathoming.
- The algorithm may open a node multiple times

**Theorem:** Because of the exponential growth, no more than 2 times in average.



# Sequential Ordering Problem

---

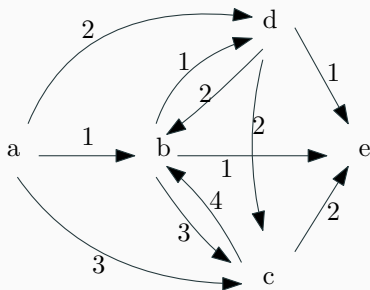
# Sequential Ordering Problem (SOP)

Collaboration with

Abdel-Malik Bouhassoun, Hadrien Cambazard and Vincent Jost

# SOP - problem definition

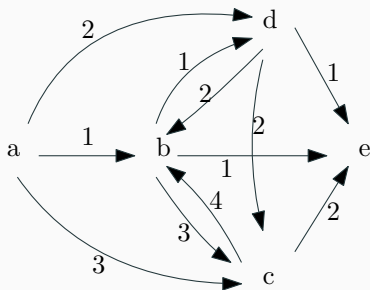
Asymmetric Traveling Salesman Problem with precedence constraints



- *a* before *b, c, d, e*
- *a, b, c, d* before *e*
- *d* before *c*

# SOP - problem definition

## Asymmetric Traveling Salesman Problem with precedence constraints

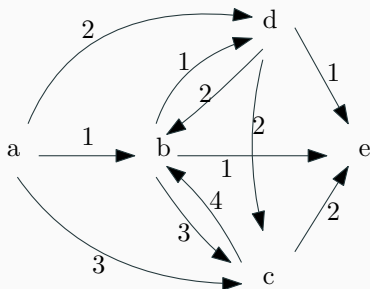


- $a$  before  $b, c, d, e$
- $a, b, c, d$  before  $e$
- $d$  before  $c$

- $a, d, c, b, e$  is a feasible and costs 10

# SOP - problem definition

## Asymmetric Traveling Salesman Problem with precedence constraints

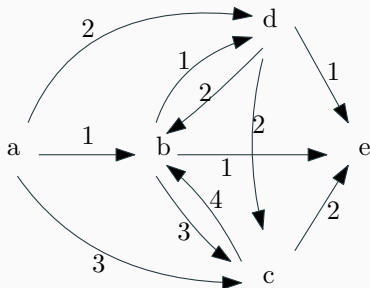


- $a$  before  $b, c, d, e$
- $a, b, c, d$  before  $e$
- $d$  before  $c$

- $a, d, c, b, e$  is a feasible and costs 10
- $a, b, c, d, e$  is not feasible

# SOP - problem definition

## Asymmetric Traveling Salesman Problem with precedence constraints



- $a$  before  $b, c, d, e$
- $a, b, c, d$  before  $e$
- $d$  before  $c$

- $a, d, c, b, e$  is a feasible and costs 10
- $a, b, c, d, e$  is not feasible
- $a, b, d, c, e$  is optimal and costs 6

# The benchmark: SOPLIB

- proposed in 2006
- Standard for meta-heuristics
- “large” instances (200 to 700 cities)
- different densities (1, 15, 30, 60) % precedence constraints
- 15% precedence-dense instances remain open (7 instances)

# The benchmark: SOPLIB

- proposed in 2006
  - Standard for meta-heuristics
  - “large” instances (200 to 700 cities)
  - different densities (1, 15, 30, 60) % precedence constraints
  - 15% precedence-dense instances remain open (7 instances)
- 
- **1% precedences** are easy (using MIP + lazy constraints)
  - **15% precedences** are “hard”
  - **30% and 60% precedences** are easy (solved by dynamic programming)



Many methods implemented during the 30 last years to solve SOP

**Exact methods:**

- Branch and cuts
- Decision diagrams + CP
- Branch & Bounds with advanced bounds/fathomings

Many methods implemented during the 30 last years to solve SOP

**Exact methods:**

- Branch and cuts
- Decision diagrams + CP
- Branch & Bounds with advanced bounds/fathomings

**Meta-heuristics:**

- Local search (3-opt)
- Ant Colony Optimization
- Various searches (GA, ABC, parallel roll-out, LKH ...)

Many methods implemented during the 30 last years to solve SOP

**Exact methods:**

- Branch and cuts
- Decision diagrams + CP
- Branch & Bounds with advanced bounds/fathomings

**Meta-heuristics:**

- Local search (3-opt)
- Ant Colony Optimization
- Various searches (GA, ABC, parallel roll-out, LKH ...)

- Exact methods tend to build stronger bounds
- meta-heuristics strongly rely on 3-opt (local search)

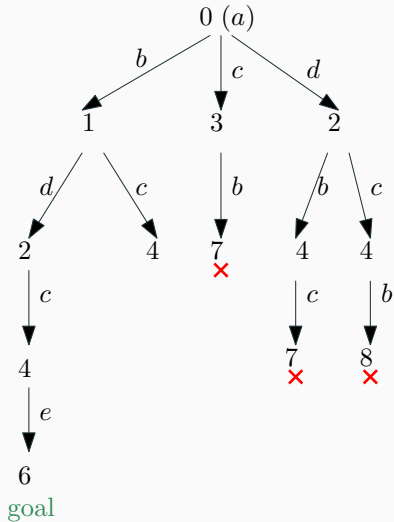
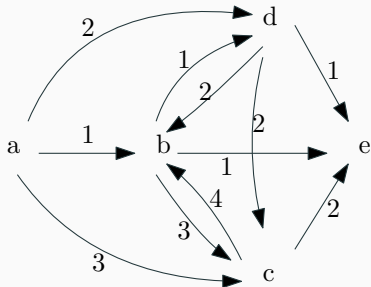
Two parts:

**Implicit tree:** how to branch, bounds ...

**Search strategy:** DFS, best-first, Beam Search ...

# Implicit tree - Branching

Forward branching



We consider 3 (simple) bounds:

**Prefix bound:** only arcs between selected vertices (previous example)

**ingoing/outgoing:** adding minimum ingoing/outgoing arc for not-selected vertices

We consider 3 (simple) bounds:

**Prefix bound:** only arcs between selected vertices (previous example)

**ingoing/outgoing:** adding minimum ingoing/outgoing arc for not-selected vertices

**MST:** compute a MST using remaining vertices

We consider 3 (simple) bounds:

**Prefix bound:** only arcs between selected vertices (previous example)

**ingoing/outgoing:** adding minimum ingoing/outgoing arc for not-selected vertices

**MST:** compute a MST using remaining vertices



We consider 3 (simple) bounds:

**Prefix bound:** only arcs between selected vertices (previous example)

**ingoing/outgoing:** adding minimum ingoing/outgoing arc for not-selected vertices

**MST:** compute a MST using remaining vertices

Out of our experiments, the prefix bound (despite its simplicity) provides the same guiding quality as other bounds. For simplicity, we only show results using it.

# Prefix equivalence fathomings

Inspired from dynamic programming

Example, two partial equivalent<sup>1</sup> solutions:

1. **a,b,c,d** cost 10
2. **a,c,b,d** cost 12

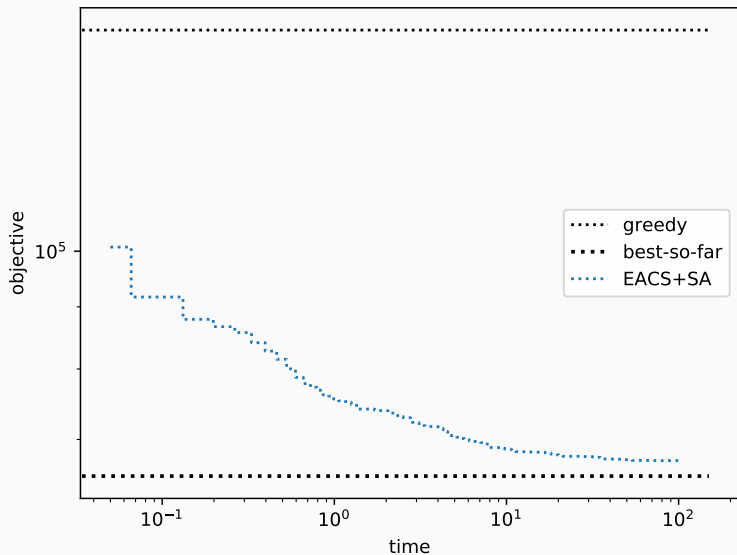
Discard (2) as it is “dominated” by (1).

---

<sup>1</sup>have the same sub-trees. The node contains the same subset of visited nodes and the same last vertex

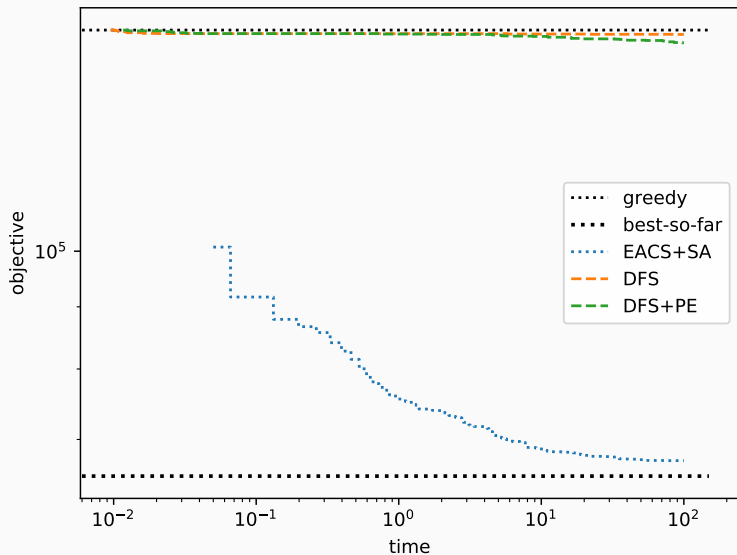
# Results - Performance profiles on R.700.1000.15

best-so-far LKH3 with 100.000 seconds run ( $\approx 27\text{h}$ )



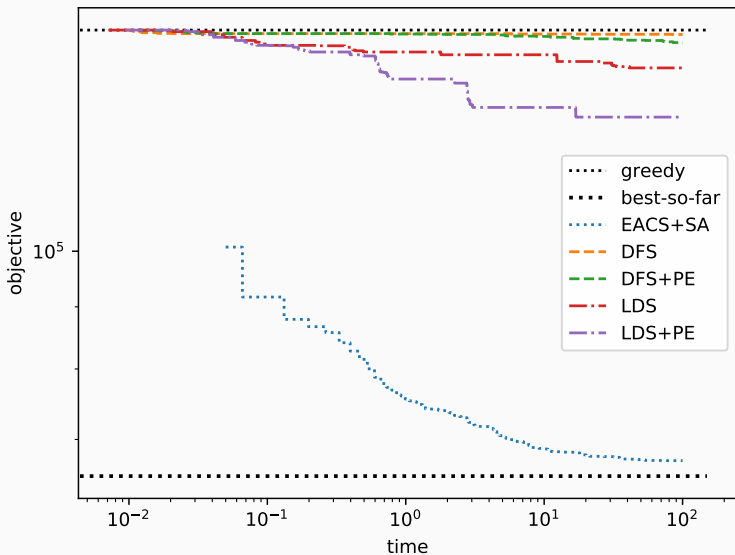
# Results - Performance profiles on R.700.1000.15

best-so-far LKH3 with 100.000 seconds run ( $\approx 27\text{h}$ )



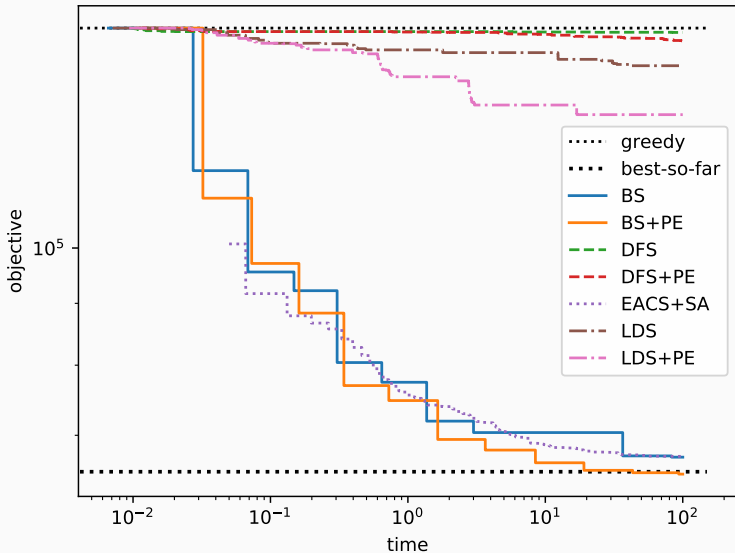
# Results - Performance profiles on R.700.1000.15

best-so-far LKH3 with 100.000 seconds run ( $\approx 27\text{h}$ )



# Results - Performance profiles on R.700.1000.15

best-so-far LKH3 with 100.000 seconds run ( $\approx 27\text{h}$ )



## Results - New best-so-far solutions

6 over 7 new-best-so-far solutions  
(the other one is probably optimal)

Instance	best known	BS+PE (600s)
R.500.100.15	5.284	5.261
R.500.1000.15	49.504	49.366
R.600.100.15	5.472	5.469
R.600.1000.15	55.213	54.994
R.700.100.15	7.021	7.020
R.700.1000.15	65.305	64.777

## Results - Overview

How this simple tree search behaves on the SOPLIB:

**1% precedence constraints:** poor results. too many choices and too simple guides



## Results - Overview

How this simple tree search behaves on the SOPLIB:

**1% precedence constraints:** poor results. too many choices and too simple guides

**15% precedence constraints:** state of the art. small number of choices (5 children per node in average)

## Results - Overview

How this simple tree search behaves on the SOPLIB:

- 1% precedence constraints:** poor results. too many choices and too simple guides
- 15% precedence constraints:** state of the art. small number of choices (5 children per node in average)
- 30,60% precedence constraints:** depletes the search tree (proves optimality) in a few seconds. 10 to 100 faster than other exact methods.

# Results - Overview

How this simple tree search behaves on the SOPLIB:

**1% precedence constraints:** poor results. too many choices and too simple guides

**15% precedence constraints:** state of the art. small number of choices (5 children per node in average)

**30,60% precedence constraints:** depletes the search tree (proves optimality) in a few seconds. 10 to 100 faster than other exact methods.

The SOPLIB mainly contains heavily constrained instances:

- hard for MIPs and local search
- but (relatively) easy for constructive algorithms

# Results - Overview

How this simple tree search behaves on the SOPLIB:

- 1% precedence constraints:** poor results. too many choices and too simple guides
- 15% precedence constraints:** state of the art. small number of choices (5 children per node in average)
- 30,60% precedence constraints:** depletes the search tree (proves optimality) in a few seconds. 10 to 100 faster than other exact methods.

The SOPLIB mainly contains heavily constrained instances:

- hard for MIPs and local search
- but (relatively) easy for constructive algorithms
- thus the need to consider anytime tree search

## Other works

---

## Collaboration with Florian Fontan

- Every two years, the french OR society organizes an optimization challenge in collaboration with a company.

## Collaboration with Florian Fontan

- Every two years, the french OR society organizes an optimization challenge in collaboration with a company.
- last year's challenge was about optimizing *Saint Gobain's* glass cutting process

## Collaboration with Florian Fontan

- Every two years, the french OR society organizes an optimization challenge in collaboration with a company.
- last year's challenge was about optimizing *Saint Gobain's* glass cutting process
- We won the 3 final phase's prizes with a tree search algorithm



## Collaboration with Florian Fontan

- Every two years, the french OR society organizes an optimization challenge in collaboration with a company.
- last year's challenge was about optimizing *Saint Gobain's* glass cutting process
- We won the 3 final phase's prizes with a tree search algorithm
- We later generalized our algorithm on multiple variants and obtained excellent results.

## Collaboration with Vincent Jost and Aurélien Secardin

- large application range. For instance in molecular biology, gene recognition, pattern matching, *etc.*

## Collaboration with Vincent Jost and Aurélien Secardin

- large application range. For instance in molecular biology, gene recognition, pattern matching, *etc.*
- many tree search algorithms in the literature to solve this problem

## Collaboration with Vincent Jost and Aurélien Secardin

- large application range. For instance in molecular biology, gene recognition, pattern matching, *etc.*
- many tree search algorithms in the literature to solve this problem
- We show that the (simple) Iterative Beam Search obtains state-of-the-art performance compared to more intricate methods

## Take aways

---

- Model the implicit search tree
- Then, perform some tree search algorithm

## Are tree suited on large instances?

YES!

- If the tree size is (relatively) small

# Are tree suited on large instances?

YES!

- If the tree size is (relatively) small
- Some constraints favor tree search (for instance precedences)



# Are tree suited on large instances?

YES!

- If the tree size is (relatively) small
- Some constraints favor tree search (for instance precedences)
- Good greedy guides

The choice is crucial

- **Iterative beam search** seems to work well in most scenarios

## References

---

- [1] Frédéric Gardi, Thierry Benoist, Julien Darlay, Bertrand Estellon, and Romain Megel. *Mathematical programming solver based on local search*. Wiley Online Library, 2014.

# Anytime tree search for discrete optimization

## A tutorial

---

Abdel-Malik Bouhassoun - Hadrien Cambazard - Florian Fontan  
Vincent Jost - [Luc Libralesso](#) - Aurélien Secardin

April, 28, 2020 - ROSP Seminar

G-SCOP, Grenoble, France

email: [luc.libralesso@grenoble-inp.fr](mailto:luc.libralesso@grenoble-inp.fr)