CAIML: AI Summer School 2023

Artificial Intelligence for Optimization

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Outline

- Applications and optimization problems
- AI problem solving techniques
  - Solver-independent modelling
  - Constraint programming techniques
  - Structural decomposition methods
  - Metaheuristics
  - Hybrid techniques
- Machine learning and problem solving
  - Automated algorithm selection
  - Instance space analysis
  - Hyper-heuristics
- Case study: Test laboratory scheduling
- Conclusions

AI Fields

Problem Solving

Machine Learning

Knowledge Representation and Automated Reasoning

Natural Language Processing

Computer Vision

Robotics

...

Investigated Applications in our Lab

Rotating Workforce Scheduling

Shift Design

Break Scheduling

Nurse Rostering

Torpedo Scheduling

Electric Vehicle Charging

Tourist Trip Planning

Social Golfer Problem

High School Timetabling

Production Leveling Problem

Parallel Machine Scheduling

Industrial Oven Scheduling

Physician Scheduling During a Pandemic

Unicost Set Covering

(Hyper)tree Decomposition

Graph Coloring

Traveling Salesman Problem

Vehicle Routing

Sudoku

Bus Driver Scheduling

Test Laboratory Scheduling

Artificial Teeth Production Scheduling

Project Scheduling

Paint Shop Scheduling Problem

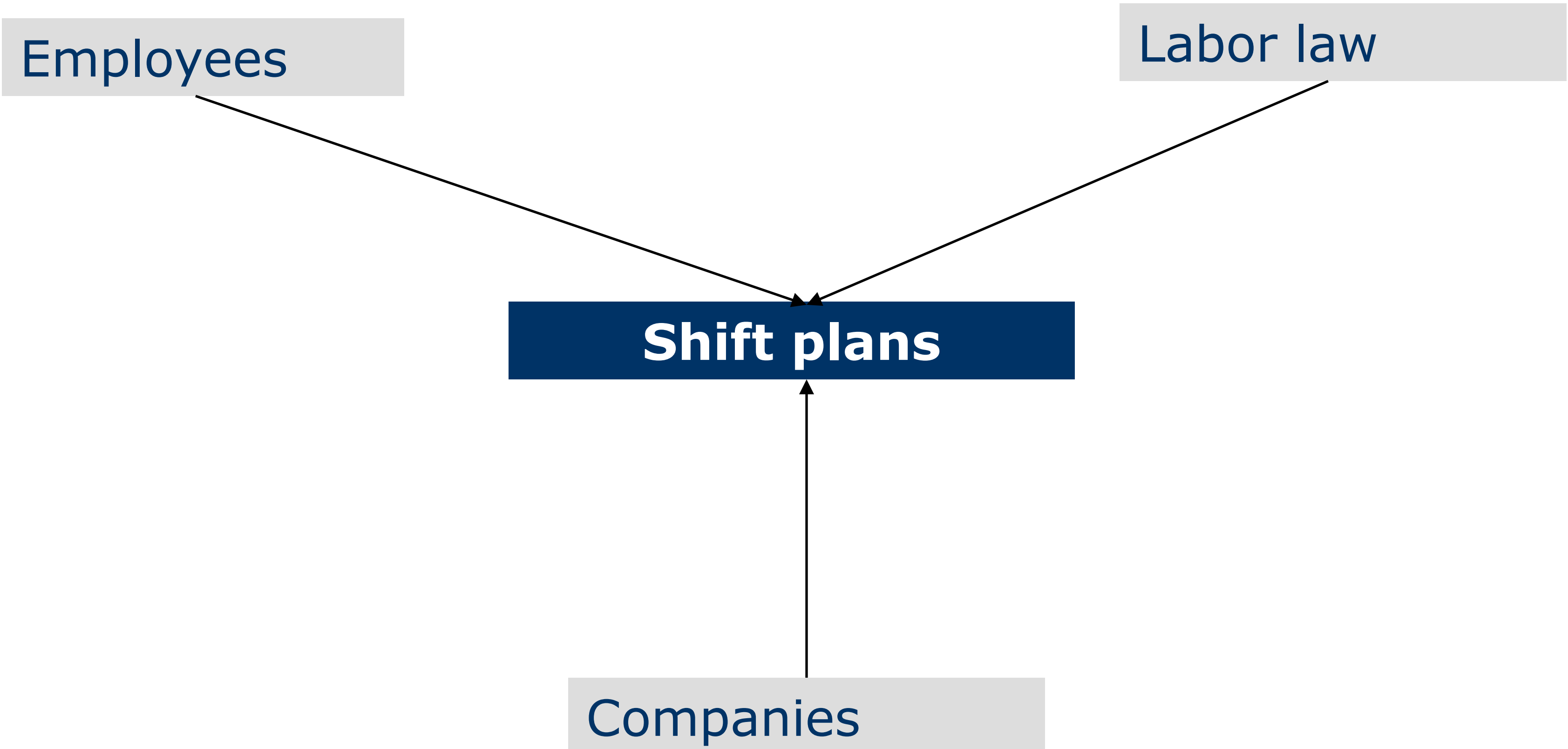
Curriculum-based Course Timetabling

...

Employee Scheduling

- Work schedules influence the lives of employees
- Unsuitable timetable can have a tremendous negative impact on one's health, social life, and motivation at work
- Organizations in the commercial and public sector must meet their workforce requirements and ensure the quality of their services and operations

Employee Scheduling



Employee Scheduling

Real world employee scheduling problems appear in many companies

Airports

Call centers

Air traffic control

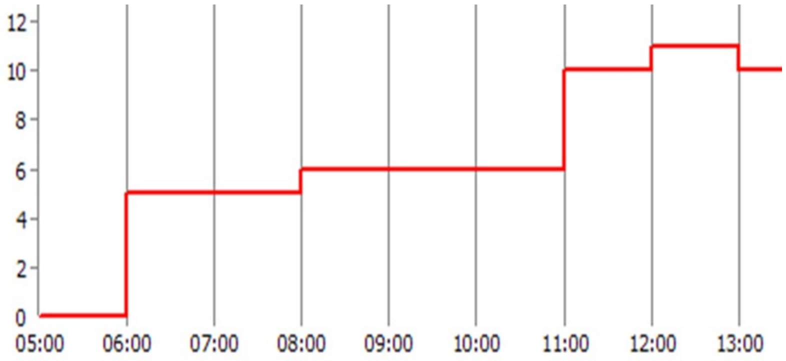
Hospitals

Public transport

Production plants

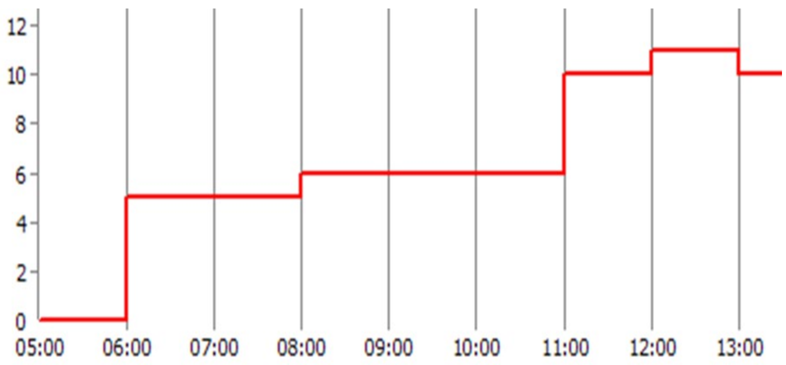
…

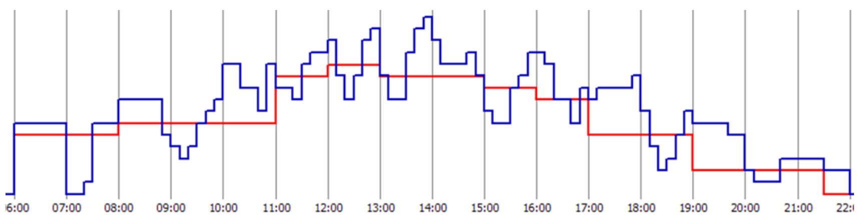
Employee Scheduling Problems

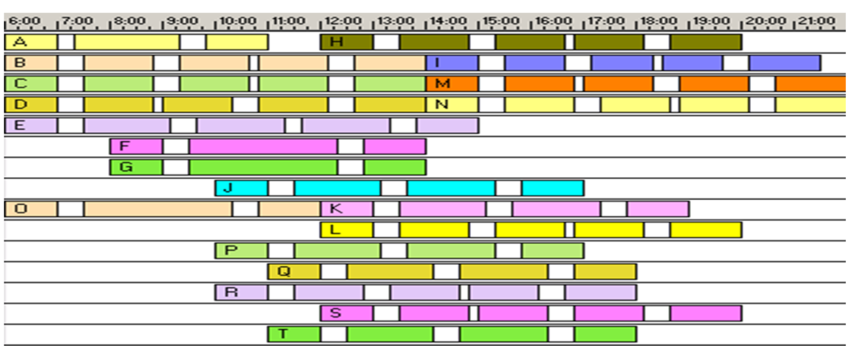


Phase 1:
Workforce requirements

Employee Scheduling Problems



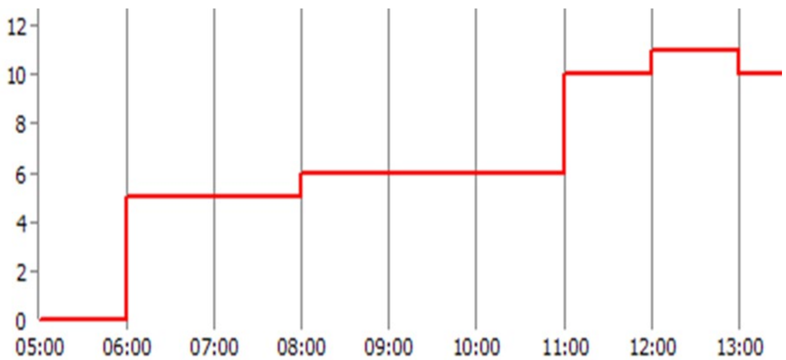




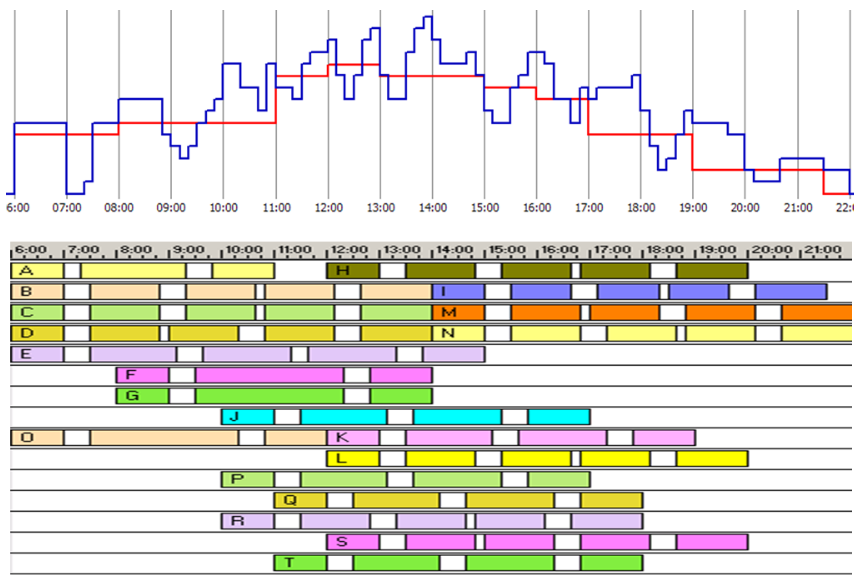
Phase 1:
Workforce requirements

Phase 2:
Shift Design/Break Scheduling

Employee Scheduling Problems



Phase 1:
Workforce requirements



Phase 2:
Shift Design/Break Scheduling

Phase 3:
Assignment of shifts

	Mo	Di	Mi	Do	Fr	Sa	So
A	F	F	F	S	S		
B		N	N	N	N		
C		F	F	N	N	N	N
D			S	S	S	N	N
E	N			F	F	S	S
F	S			F	F	F	F
G	S	S				F	F
H	F	S	S			S	S
I	N	N	N				

Selected papers: [3,4,11,12, 13]

Example: Rotating Workforce Scheduling

Length of schedule: If the schedule is cyclic the total length of a planning period will be: NumberOfEmployees*7

	Mo	Tu	We	Th	Fr	Sa	Su
A	D	D	D			D	D
B	D	D	D	D			
C	A	A	A	A			A
D	A	A	A	A	A		
E	D	D	A	A	A		
F	A	A	N	N	N		
G	N	N	N	N	N		
H		N	N	N	N	N	
I			D	D	D	A	A
J				D	D	N	N
K	N				A	A	N
L	N	N			D	D	D

Number of employees

Employees working shifts:

D: Day shift ; A: Afternoon shift ,

N: Night shift; Day off

Constraints

	Mo	Tu	We	Th	Fr	Sa	Su
A	D	D	D			D	D
B	D	D	D	D			
C	A	A	A	A			A
D	A	A	A	A	A		
E	D	D	A	A	A		
F	A	A	N	N	N		
G	N	N	N	N	N		
H		N	N	N	N	N	
I			D	D	D	A	A
J				D	D	N	N
K	N				A	A	N
L	N	N			D	D	D

Not allowed sequences of shifts:

N - D
N D
A D
N A
N - A
A - D

Maximum and minimum length of periods of successive shifts.

e.g.: N: 2-5, D: 2-6

Temporal requirements: required number of employees in shift *i* during day *j*

Monday (Mo): D: 3, N: 3, A: 3

Maximum and minimum length of work days and days-off blocks

e.g.: days-off block: 2-4

work block: 2-6

Objective

Find a cyclic schedule (assignment of shifts to employees) that satisfies the temporal requirement, and all other constraints

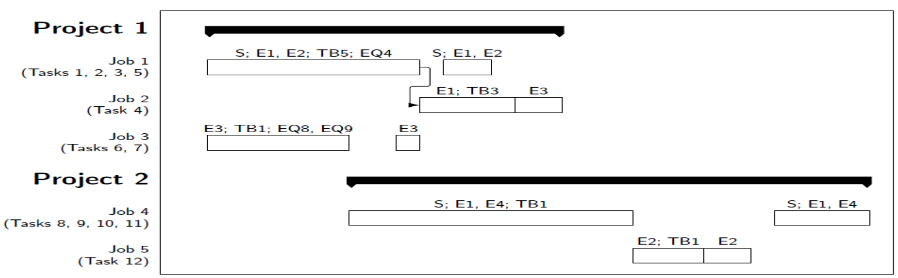
Possible soft constraints:

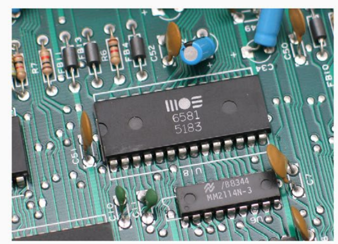
- Optimization of free weekends (weekends off)
- …

Production Planning and Scheduling/Project Scheduling

- In these applications it is important to
  - Reduce resource consumption, including energy
  - Increase production efficiency

…



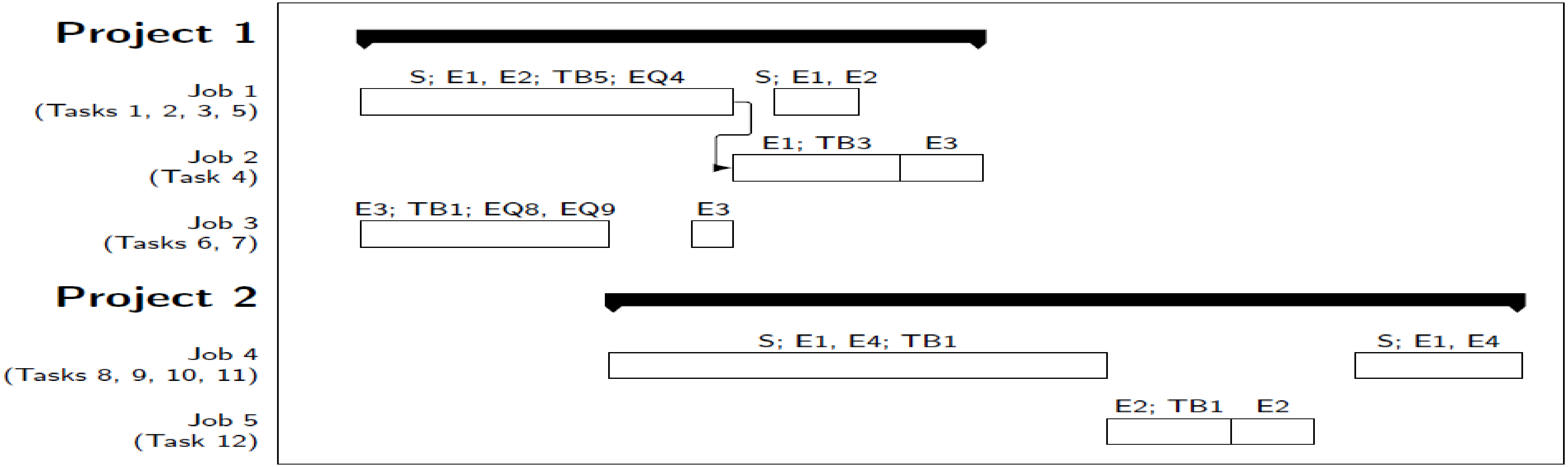


https://commons.wikimedia.org/wiki/File: MOS6581_chtaube061229.jpg, Christian Taube

https://commons.wikimedia.org/wiki/File: Reflow_oven.jpg, Nelatan

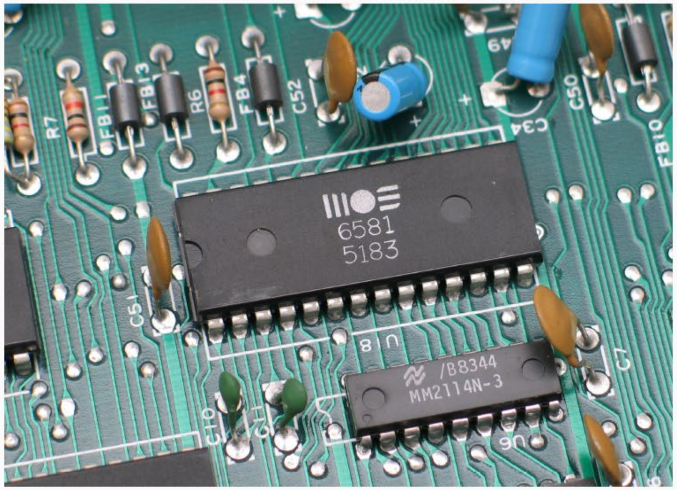
	R1	*R2*	*R3*	...
1	A	A	C	...
2	A	A	C	...
3	A	C	C	...
4	B	B	B	...
5	B	B	B	...

Test Laboratory Scheduling



Selected papers: [1,5]

Industrial Oven Scheduling



https://commons.wikimedia.org/wiki/File:
MOS6581_chtaube061229.jpg, Christian Taube
CC BY-SA 2.5

https://commons.wikimedia.org/wiki/File:
Reflow_oven.jpg, Nelatan
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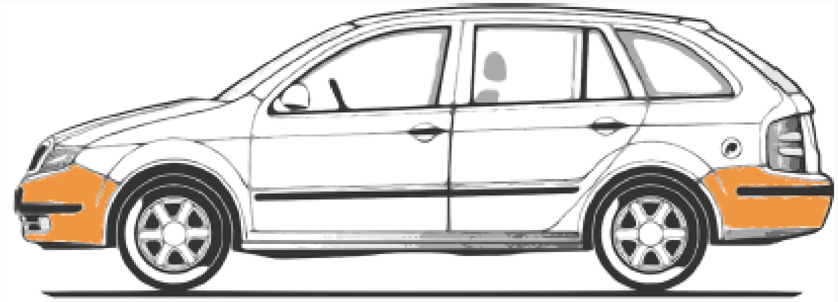
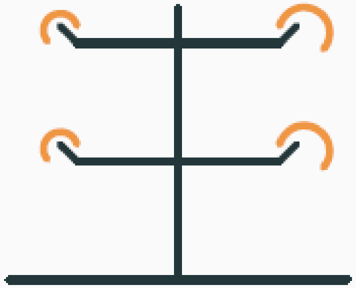
Task: Jobs need to be scheduled and batched efficiently for processing in ovens

Challenge: Many constraints and solution objectives need to be considered

Selected papers: [8]

Paint Shop Scheduling

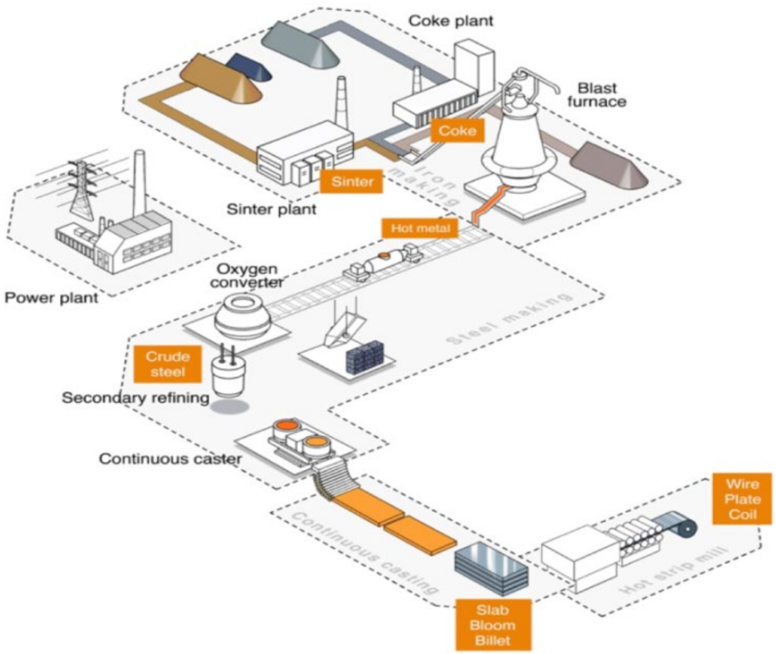




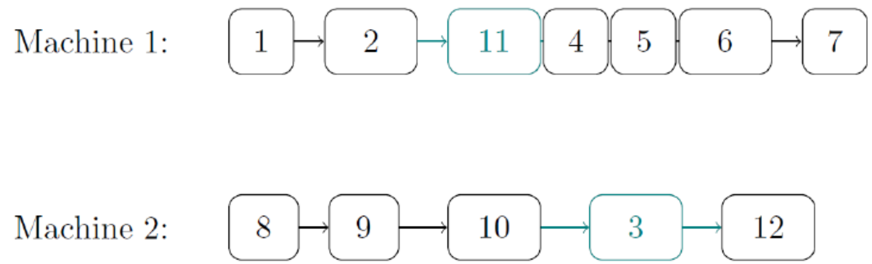
	R1	R2	R3	...
1	A	A	C	...
2	A	A	C	...
3	A	C	C	...
4	B	B	B	...
5	B	B	B	...

Selected papers: [6,7]

Other real-world problems…



Torpedo Scheduling, ACP Challenge, 2016



Parallel Machine Scheduling

Selected papers: [9,10]

...

Other problems…

Time	Monday	Tuesday	Wednesday	Thursday
8:00-9:00	Math	Biology	Math	Math
9:00-10:00	Math	Chemistry	Biology	
10:00-11:00	Physics	Physics		

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

Week 1

6	10	12
13	3	4
15	5	1
11	14	7
8	9	2

Week 2

8	4	6
12	3	7
10	11	5
13	15	2
9	14	1

Week 3

1	4	2
11	6	15
7	13	9
12	8	5
14	10	3

Week 4

6	5	14
2	10	7
4	9	11
3	15	8
12	1	13

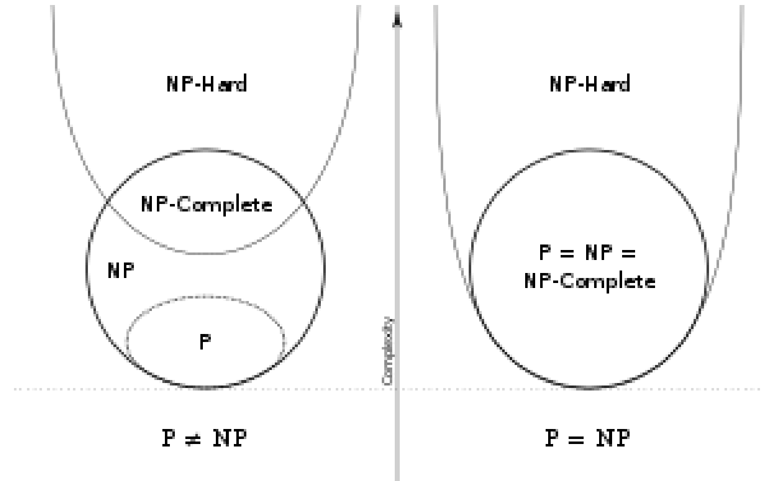
8	14	13
1	6	3
15	10	9
12	2	11
5	4	7

Selected papers: [24, 25, 26]

https://www.un.org/en/sustainable-development-goals

The General Obstacle

- NP-hard (intractable) problems
- No efficient algorithms could be found yet
- P problems can be solved efficiently (in polynomial time)
- P ≠ NP ? **(Millennium Prize Problem)**



https://en.wikipedia.org/wiki/NP-hardness

Tremendous size of the search space of possible solutions

Example: 12 employees, 1 week, 4 shifts

4^{84}

	Mo	Di	Mi	Do	Fr	Sa	So
A	F	F	F	S	S		
B		N	N	N	N		
C		F	F	N	N	N	N
D			S	S	S	N	N
E	N			F	F	S	S
F	S			F	F	F	F
G	S	S				F	F
H	F	S	S			S	S
I	N	N	N				

AI problem solving techniques

Research work in the CD-Lab Artis

Existing problems

New challenging problems provided by the industry

- Formal mathematical formulations
- Identification of related problems in the literature
- Complexity analysis
- General variants of problems
- New problem instances provided to the literature

- Modelling techniques
- AI/Optimization solving techniques
- Meta/Hyper-heuristics
- Hybrid algorithms
- Algorithm selection and instance space analysis

AI and optimization methods

Complete approaches

Constraint programming
Answer set programming
SAT/SMT
Mathematical programming
…

Metaheuristic techniques

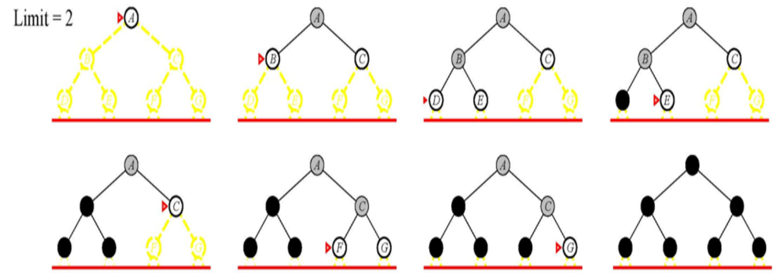
Tabu search
Simulated annealing
Evolutionary strategies
Memetic algorithms
…

Hybrid methods

Large neighborhood search
Hyper-heuristics
Machine learning based approaches
…

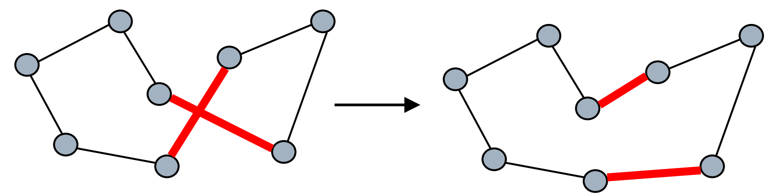
Automated Problem Solving: Techniques

Constraint Satisfaction

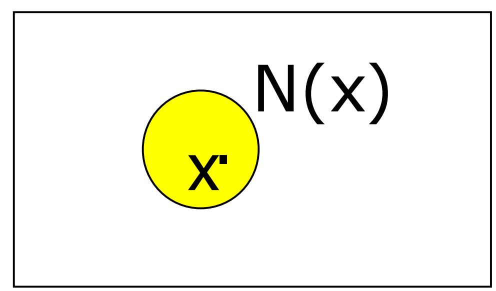


Artificial Intelligence: A Modern Approach. Norvig and Russell

Heuristic Search



SAT Solving



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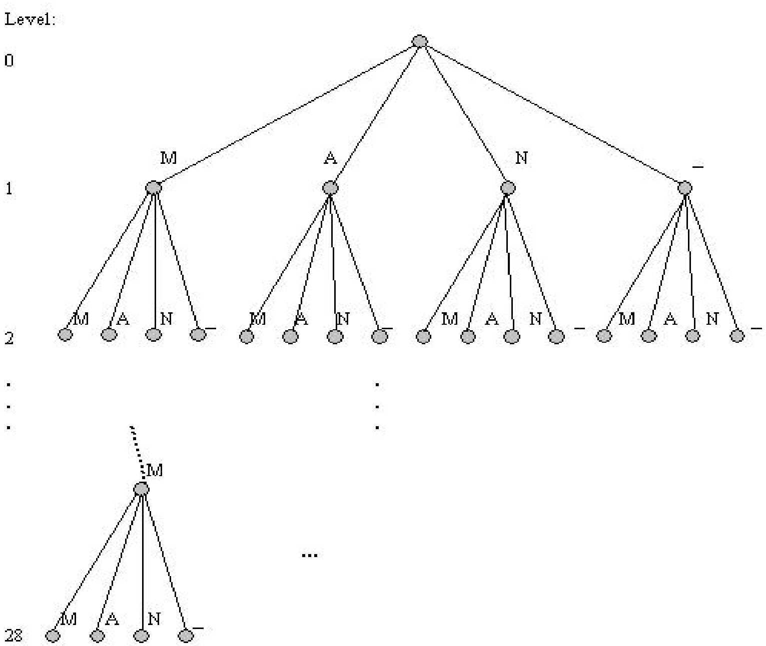
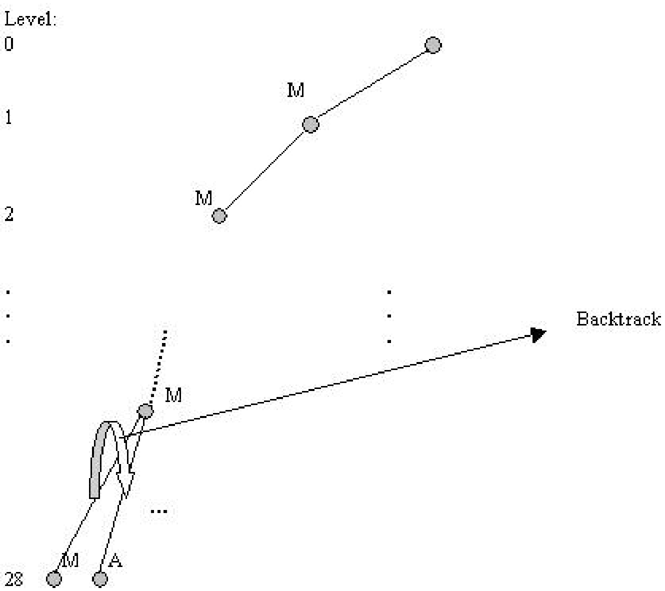
$$F(x)=(x_{17}\vee\bar{x}_{37}\vee x_{73})\wedge(\bar{x}_{11}\vee\overline{x_{12}})\wedge\ldots\wedge(\bar{x}_{2}\vee x_{43}\vee x_{22})$$

Constraint Programming Techniques

- Tree search
- Constraint propagation
- Forward checking
- Lazy clause generation
- Variable ordering heuristics
- …





Modeling and solvers

- Constraint Programming
  - Solvers: OR-Tools, Chuffed, CP Optimizer…
  - The MiniZinc challenge: https://www.minizinc.org/challenge.html
- Mathematical Programming
  - Solvers: Gurobi, CPLEX…
- Answer Set Programming
  - Solvers: Potassco (the Potsdam Answer Set Solving Collection), DLV, …
- SAT
  - Solvers: http://www.satcompetition.org/
- …

The “Zebra Puzzle”

In **five houses**, each with a different **color**, live 5 persons of different **nationalities**, each of whom prefer a different **brand of cigarette**, a different **drink**, and a different **pet**. Given the following facts, the question to answer is:

“Where does the zebra live, and in which house do they drink water?”

- The Englishman lives in the red house.
- The Spaniard owns the dog.
- The Norwegian lives in the first house on the left.
- Kools are smoked in the yellow house.
- …

The “Zebra Puzzle”

- The Norwegian lives next to the blue house.
- The man who smokes Chesterfields lives in the house next to the man with the fox.
- The Winston smoker owns snails.
- The Lucky Strike smoker drinks orange juice.
- The Albanian drinks tea.
- The Japanese smokes Parliaments.
- Kools are smoked in the house next to the house where the horse is kept.
- Coffee is drunk in the green house.
- The Green house is immediately to the right (your right) of the ivory house.
- Milk is drunk in the middle house.

(Stuart Russell and Peter Norvig, Artificial Intelligence: A Modern Approach. 2nd Edition, Prentice Hall, 2003)

CP formulation

- Variables, Domains, Constraints

Possible formulation:

- Variables:
  - Color: Red(C1), Blue (C2), …
  - Nationalities: Englishman (N1), Spaniard (N2), …
  - Drinks: Tea (D1), …
  - Brand of cigarette: Chesterfields (B1), Kools (B2), …
  - Pet: Dog (P1), Fox(P2) …
- Domain of variables:

  {House1, House2, House3, House4, House5}

CP formulation

- Constraints:
  - The Englishman lives in the red house:

    $N1=C1$
  - The Spaniard owns the dog:

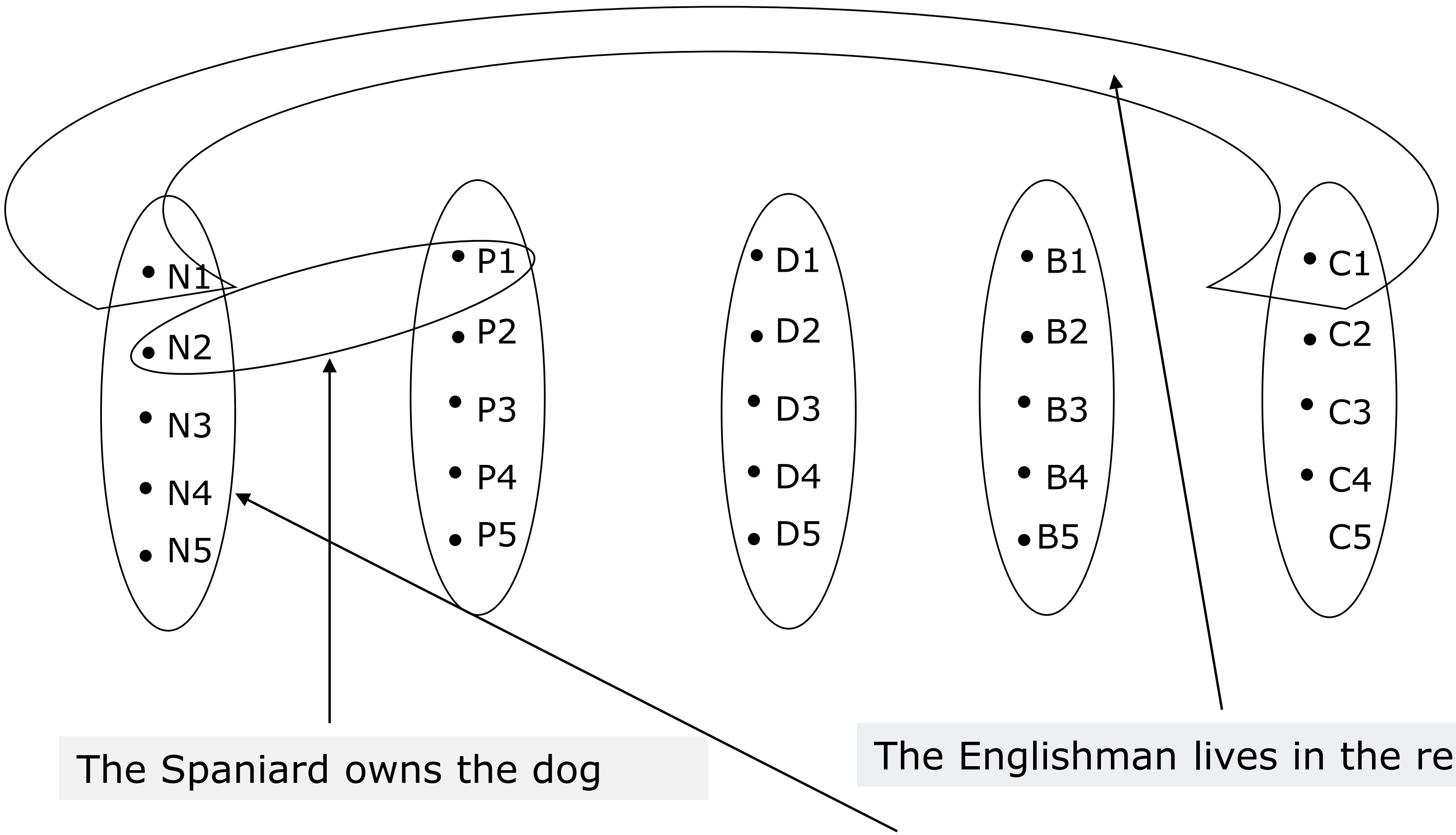
    $N2=P1$

  …
  - The man who smokes Chesterfields lives in the house next to the man with the fox:

    $|B1-P2|=1$

  - $N1 \neq N2$, $N1 \neq N3$, …$N4 \neq N5$
  - …

The "Zebra Puzzle": Hypergraph representation



The Spaniard owns the dog

The Englishman lives in the red house

Two nationalities can not be assigned to the same house

...

Rotating workforce scheduling: A constraint model

$$\sum_{k\in 0}^{u_w}(T_{t(j+k)} = O) > 0, \quad j \in TT \tag{1}$$

$$\sum_{k\in 1}^{l_w}(T_{t(j+k)} = O) = 0, \quad j \in TT, T_j = O \wedge T_{t(j+1)} \neq O \tag{2}$$

$$\sum_{k\in 0}^{u_O}(T_{t(j+k)} \neq O) > 0, \quad j \in TT \tag{3}$$

$$\sum_{k\in 1}^{l_O}(T_{t(j+k)} \neq O) = 0, \quad j \in TT, T_j \neq O \wedge T_{t(j+1)} = O \tag{4}$$

$$\sum_{k\in 0}^{u_{sh}}(T_{t(j+k)} \neq sh) > 0, \quad j \in TT, sh \in \mathbf{A} \tag{5}$$

$$\sum_{k\in 1}^{l_{sh}}(T_{t(j+k)} \neq sh) = 0, \quad j \in TT, sh \in \mathbf{A}, T_j \neq sh \wedge T_{t(j+1)} = sh \tag{6}$$

$$T_j = sh_1 \rightarrow T_{t(j+1)} \neq sh_2, \quad j \in TT, (sh_1, sh_2) \in F_2 \tag{7}$$

$$T_j = sh_1 \wedge T_{t(j+1)} = O \rightarrow T_{t(j+2)} \neq sh_2, \quad j \in TT, (sh_1, sh_2) \in F_3 \tag{8}$$

$$\sum_{i\in 1..n}(S_{i,j} = sh) = R_{sh,j}, \quad j \in 1..w, sh \in \mathbf{A} \tag{9}$$

$$\sum_{i\in 1..n}(S_{i,j} = O) = o_j, \quad j \in 1..w \tag{10}$$

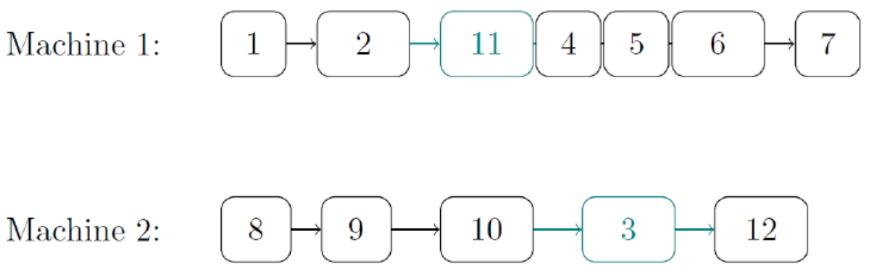
Selected papers: [11, 13]

Alternative model: global constraints for (9) and (10)

$$gcc\_low\_up([S_{i,j} | i \in 1..n], \mathbf{A}, [R_{sh,j} | sh \in \mathbf{A}], [R_{sh,j} | sh \in \mathbf{A}]) \tag{11}$$

$$gcc\_low\_up([S_{i,j} | i \in 1..n], \mathbf{A}^+, [R_{sh,j} | sh \in \mathbf{A}^+], [R_{sh,j} | sh \in \mathbf{A}^+]) \tag{12}$$

Example MIP: Parallel Machine Scheduling



Selected papers: [10]

minimise $Lex(\Sigma_{j \in J}(T_j), C_{max})$, subject to

$$\Sigma_{m \in M}(Y_{j,m}) = 1, \forall j \in J$$

$$\Sigma_{i \in J_0, i \neq j}(X_{i,j,m}) = Y_{j,m}, \forall j \in J, m \in M$$

$$\Sigma_{j \in J_0, i \neq j}(X_{i,j,m}) = Y_{i,m}, \forall i \in J, m \in M$$

$$C_j \geq C_i + s_{i,j,m} + p_{j,m} + V \cdot (X_{i,j,m} - 1), \\ \forall i \in J_0, j \in J, m \in M$$

$$\Sigma_{j \in J}(X_{0,j,m}) \leq 1, \forall m \in M$$

$$\Sigma_{i \in J_0, j \in J, i \neq j}(s_{i,j,m} \cdot X_{i,j,m}) + \\ \Sigma_{i \in J}(p_{i,m} \cdot Y_{i,m} + s_{i,0,m} \cdot X_{i,0,m}) \leq C_{max}, \\ \forall m \in M$$

$$T_j \geq C_j - d_j, \forall j \in J$$

$$T_j \geq 0, \forall j \in J$$

MinZinc

- Constraint modeling language
- Used for modeling constraint satisfaction/optimization problems
  - High-level
  - Solver-independent
    - Model is compiled into FlatZinc that is understood by a wide range of solvers (CP, MIP, …)
- MiniZinc is developed at Monash University
- Free and open-source

Example

Listing 2.1.1: A MiniZinc model aust.mzn for colouring the states and territories in Australia

```
% Colouring Australia using nc colours
int: nc = 3;

var 1..nc: wa;   var 1..nc: nt;  var 1..nc: sa;   var 1..nc: q;
var 1..nc: nsw;  var 1..nc: v;   var 1..nc: t;

constraint wa != nt;
constraint wa != sa;
constraint nt != sa;
constraint nt != q;
constraint sa != q;
constraint sa != nsw;
constraint sa != v;
constraint q != nsw;
constraint nsw != v;
solve satisfy;

output ["wa=\(wa)\t nt=\(nt)\t sa=\(sa)\n",
        "q=\(q)\t nsw=\(nsw)\t v=\(v)\n",
         "t=", show(t),  "\n"];
```

MiniZinc Handbook. Peter J. Stuckey, Kim Marriot, Guido Tack:
https://www.minizinc.org/doc2.2.1/en/MiniZinc%20Handbook.pdf

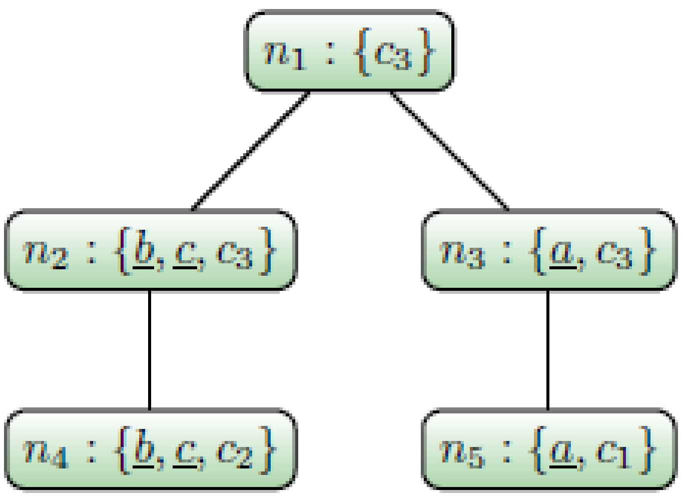
Structural decomposition methods

Structural decomposition methods: Tree decomposition

- Many NP-hard problems are known to become tractable for instances whose treewidth is bounded by some constant *k*

- A promising approach for solving problems using tree decompositions:

Compute a tree decomposition



Compute the solutions by a dynamic programming algorithm

id	c_3	ext.
$n_1 \mid 0$	**S**	$\{(n_2 \mid 0, n_3 \mid 0), (n_2 \mid 2, n_3 \mid 0)\}$
$n_1 \mid 1$	**U**	$\{(n_2 \mid 1, n_3 \mid 0)\}$

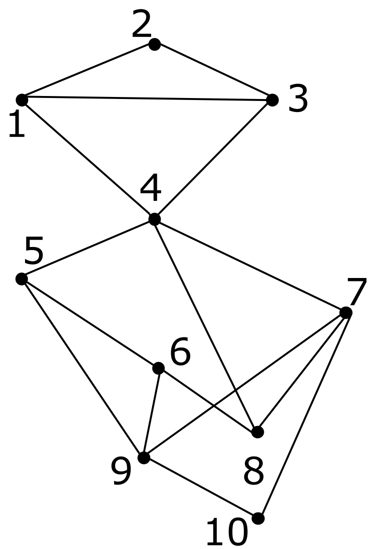
id	$\underline{b}$	$\underline{c}$	c_3	ext.
$n_2 \mid 0$	**F**	**F**	**S**	$\{n_4 \mid 0\}$
$n_2 \mid 1$	**F**	**T**	**U**	$\{n_4 \mid 1\}$
$n_2 \mid 2$	**T**	**T**	**S**	$\{n_4 \mid 3\}$

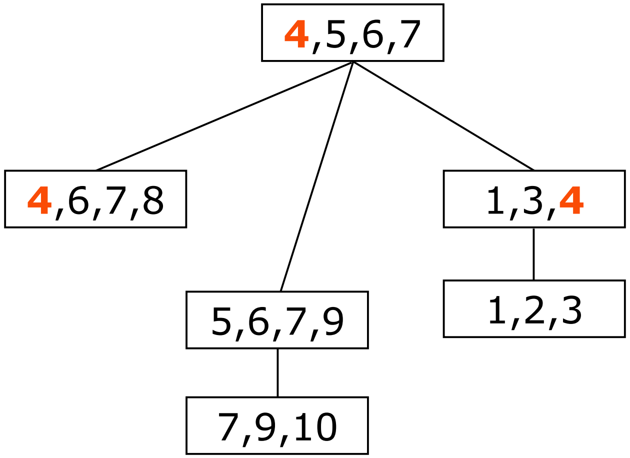
id	$\underline{a}$	c_3	ext.
$n_3 \mid 0$	**F**	**U**	$\{n_5 \mid 0\}$

id	$\underline{b}$	$\underline{c}$	c_2	ext.
$n_4 \mid 0$	**F**	**F**	**S**	-
$n_4 \mid 1$	**F**	**T**	**S**	-
$n_4 \mid 2$	**T**	**F**	**U**	-
$n_4 \mid 3$	**T**	**T**	**S**	-

id	$\underline{a}$	c_1	ext.
$n_5 \mid 0$	**F**	**S**	-
$n_5 \mid 1$	**T**	**U**	-

Tree decomposition of a graph





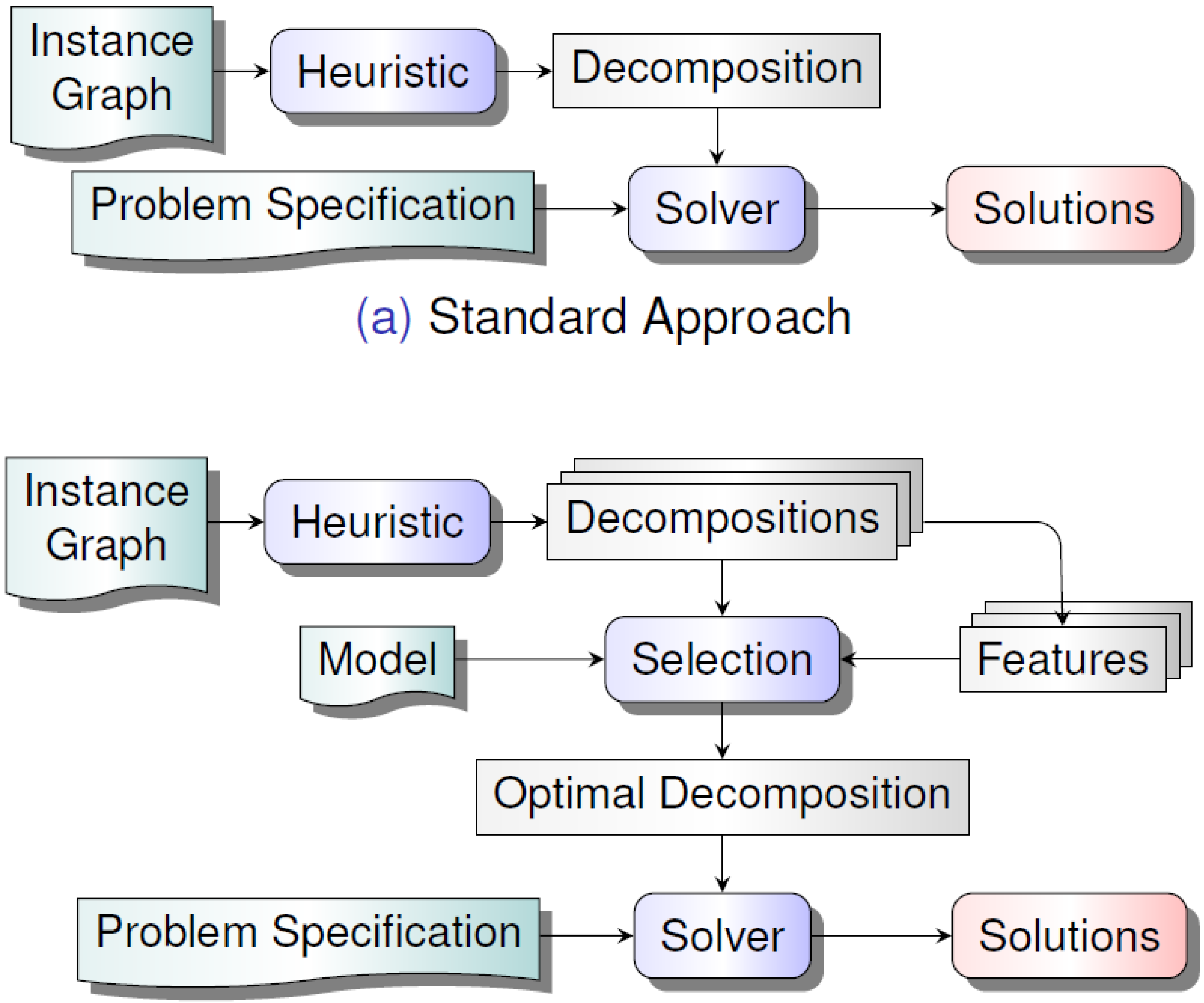
All pairs of connected vertices appear in some node of the tree

Connectedness condition for *vertices*

Width: (*number of vertices in the largest tree node) -1 = 3*

Treewidth: *minimal width over all possible tree decompositions*

Improving the efficiency via machine learning



(a) Standard Approach

(b) Improved Approach

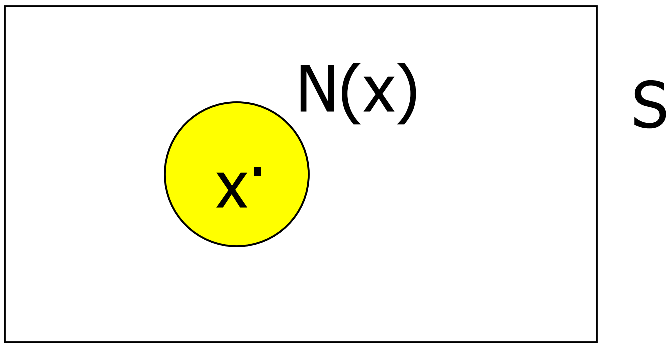
Selected reference [23]

Metaheuristics

Hybrid techniques

Local Search Techniques

- Based on the neighbourhood of the current solution



- The solution is changed iteratively using neighbourhood relations (moves)

- Acceptable or optimal solutions are often reached

Local Search Techniques

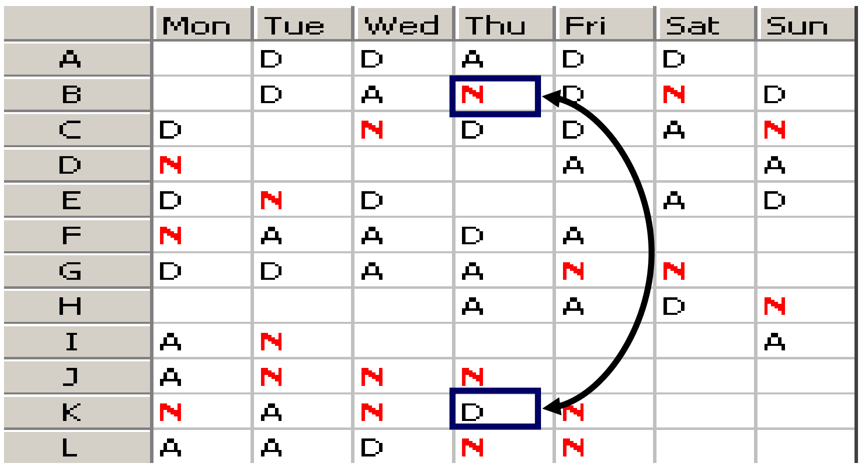
1. Construct the initial solution s
2. Generate neighbourhood N(s) of solution s
3. Select from the neighbourhood the descendant of the current solution
4. Go to step 2

Advanced metaheuristic techniques

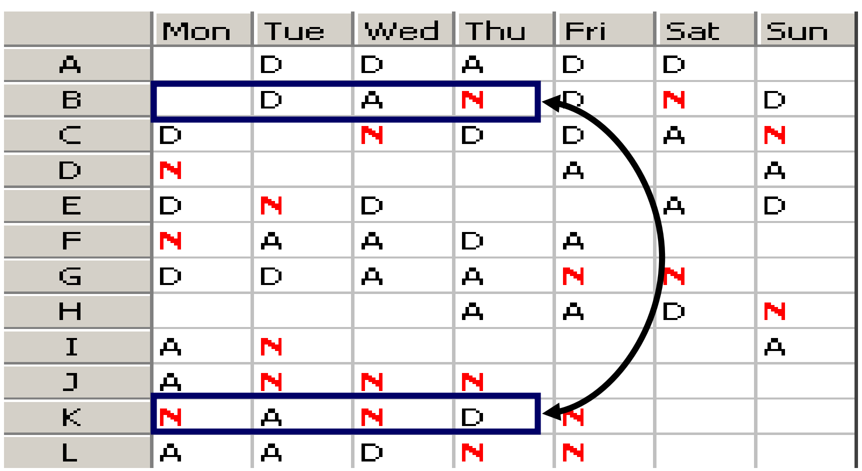
- Simulated Annealing
- Tabu Search
- Iterated Local Search
- …

Metaheuristics include a mechanism to escape local optima

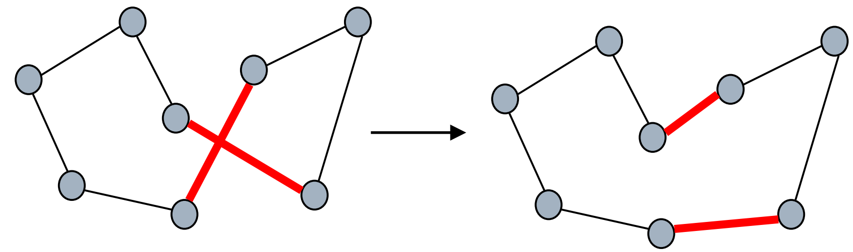
Neighborhoods

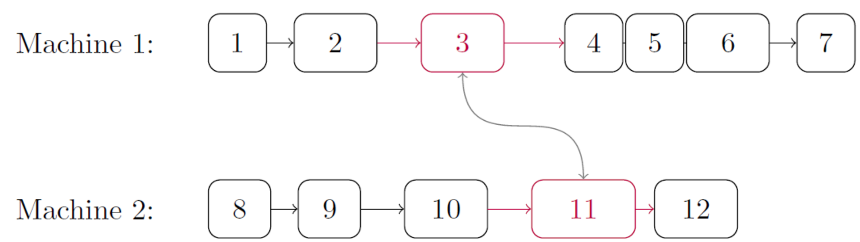


	Mon	Tue	Wed	Thu	Fri	Sat	Sun
A		D	D	A	D	D	
B		D	A	N	D	N	D
C	D		N	D	D	A	N
D	N				A		A
E	D	N	D			A	D
F	N	A	A	D	A		
G	D	D	A	A	N	N	
H				A	A	D	N
I	A	N					A
J	A	N	N	N			
K	N	A	N	D	N		
L	A	A	D	N	N		

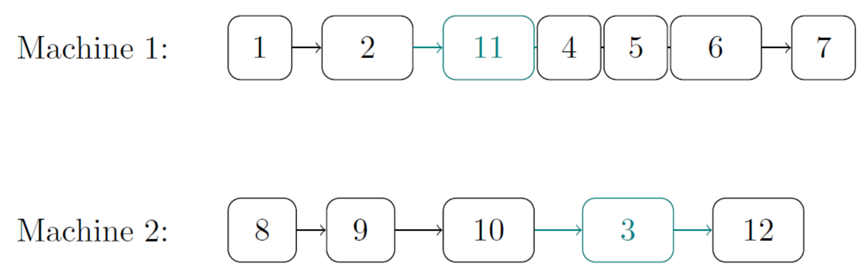


	Mon	Tue	Wed	Thu	Fri	Sat	Sun
A		D	D	A	D	D	
B		D	A	N	D	N	D
C	D		N	D	D	A	N
D	N				A		A
E	D	N	D			A	D
F	N	A	A	D	A		
G	D	D	A	A	N	N	
H				A	A	D	N
I	A	N					A
J	A	N	N	N			
K	N	A	N	D	N		
L	A	A	D	N	N		





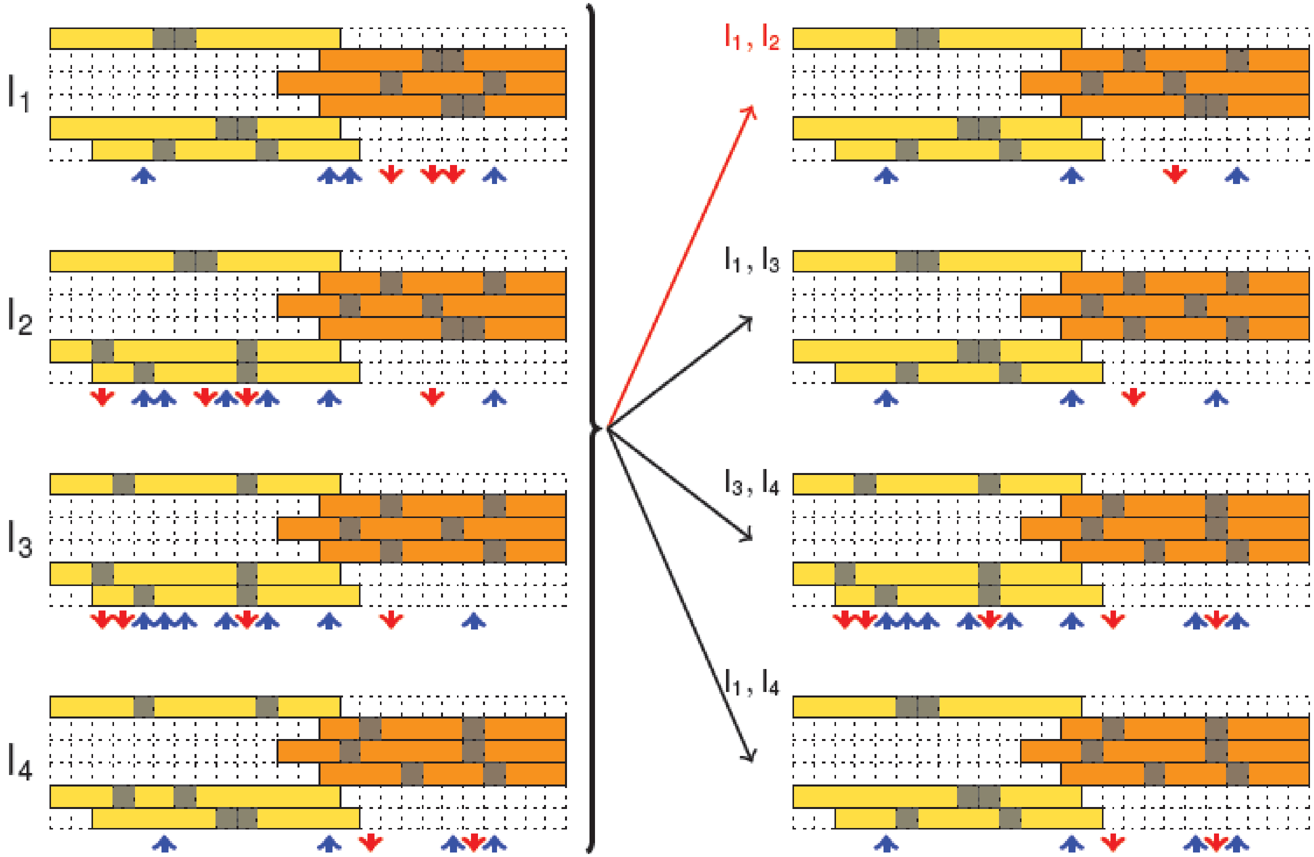
(a) Before Move Application



(b) After Move Application

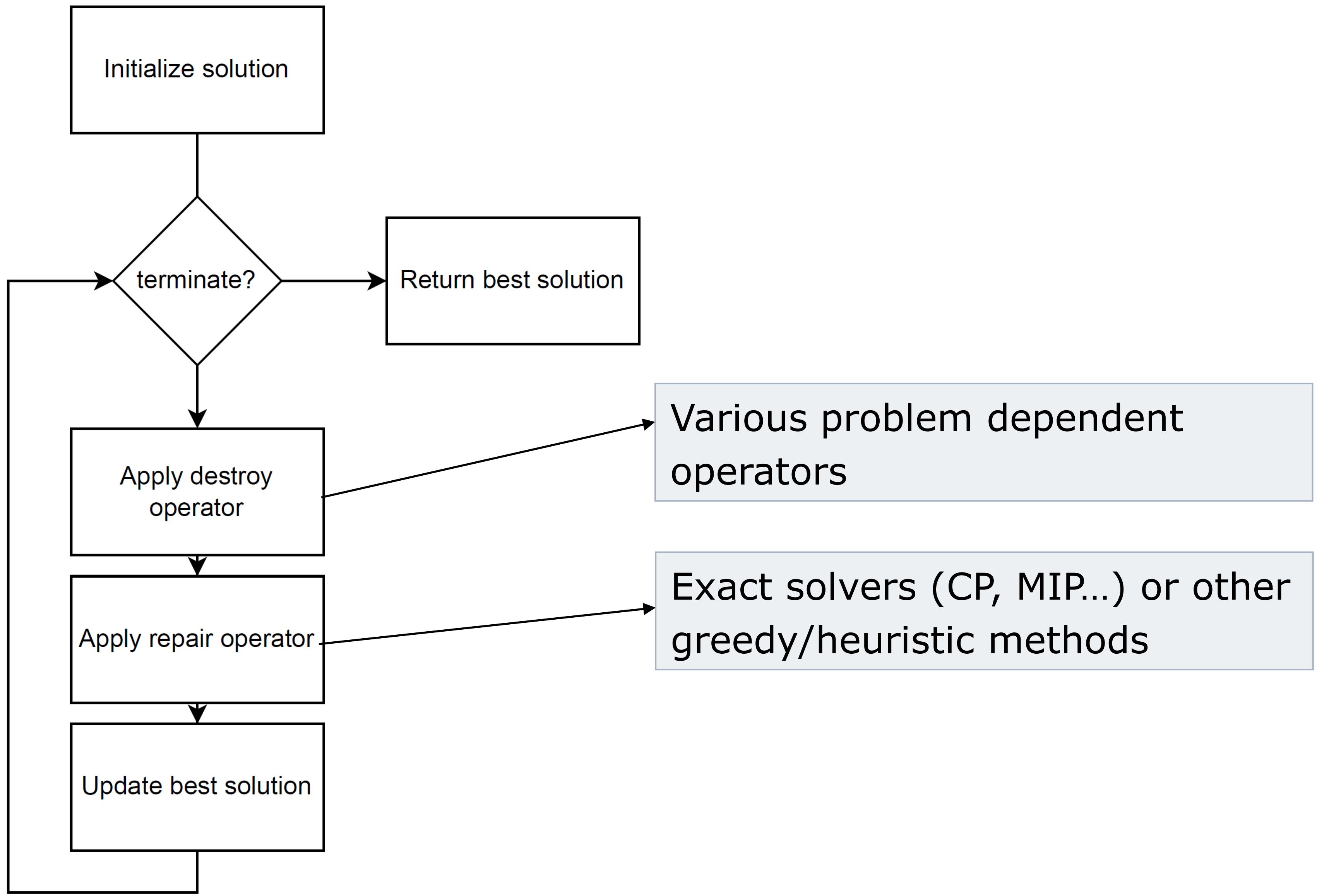
Selected papers: [10,14,3]

Memetic Algorithms: Crossover

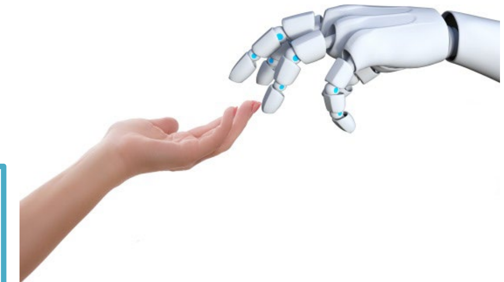


Selected papers: [16]

Large neighborhood search



Hybrid techniques



Methods of Artificial Intelligence (Machine Learning, Heuristics...)

Methods of Logic

Mathematical Optimization

...

$$S_{i,d,t} \leftrightarrow \bigwedge_{x=1}^{sl_t} U_{i,d,x} \bigwedge_{y=sl_t}^{sl_{max}} \neg U_{i,d,y}$$

$$\begin{aligned} minimize\ f = \ & 30 * \sum_{\substack{s \in S \\ k \in K \\ d \in \{1 \ldots 7\}}} C_{skd}^{S1} \\ & + 15 * \sum_{\substack{n \in N \\ s \in S \\ d \in \{1 \ldots 7\}}} (C_{nsd}^{S2a} + C_{nsd}^{S2b}) \\ & + 30 * \sum_{\substack{n \in N \\ d \in \{1 \ldots 7\}}} (C_{nd}^{S2c} + C_{nd}^{S2d}) \end{aligned}$$

Automated algorithm selection

Instance space analysis

Hyper-heuristics

Case Study: Test Laboratory Scheduling

Algorithm Selection - Motivation

Often, several search algorithms are available for solving a particular problem

- **No free lunch theorem**
- ". . . for any algorithm, any elevated performance over one class of problems is offset by performance over another class"
- ". . . any two algorithms are equivalent when their performance is averaged across all possible problems"

Wolpert and Macready, "No free lunch theorems for optimization", 1997
Wolpert and Macready, "Coevolutionary free lunches", 2005

Algorithm Selection - Motivation

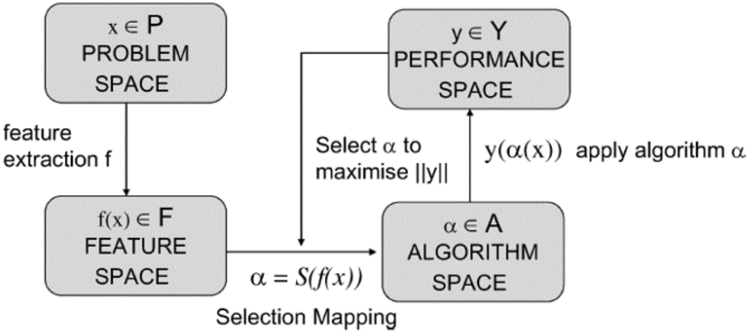
Often, several search algorithms are available for solving a particular problem

- **No free lunch theorem**
- "...for any algorithm, any elevated performance over one class of problems is offset by performance over another class"
- "...any two algorithms are equivalent when their performance is averaged across all possible problems"

⇒ How to select the best algorithm for a specific problem instance?

Wolpert and Macready, "No free lunch theorems for optimization", 1997
Wolpert and Macready, "Coevolutionary free lunches", 2005

Algorithm Selection Problem, Rice (1976)



Rice, "The algorithm selection problem", 1976

Smith-Miles, "Cross-disciplinary perspectives on meta-learning for algorithm selection", 2009

Algorithm Selection Problem, Rice (1976)

Input:

- **Problem space** P that represents the set of instance of a problem class
- **Feature space** F that contains measurable characteristics of the instances generated by a computational feature extraction process applied to P
- Set of considered **algorithms** A for tackling the problem
- **Performance space** Y maps application of an algorithm on an instance to a set of performance metrics

Algorithm Selection Problem: For a given problem instance $x \in P$, with features $f(x) \in F$, find the selection mapping $S(f(x))$ into the algorithm space, such that the selected algorithm $\alpha \in A$ maximizes the performance mapping $y(\alpha(x)) \in Y$.

Back to the Example: Rotating Workforce Scheduling

- Varying demand for different shifts

Shift	Mon	Tue	Wed	Thu	Fri	Sat	Sun
D	1	1	1	1	1	1	1
A	1	1	1	1	1	1	0
N	1	1	1	1	1	1	1

- 4 employees, cyclic schedule
- Regulations constraining shift assignments
- 5-7 days on work, 2-4 days off
- D: 2-5 days, A: 2-4 days, N: 2-3 days
- No D after A or N, no A after N

Back to the Example: Rotating Workforce Scheduling

Problem space P:

- 20 initial real-life instances
- 2000 generated instances

Kletzander et al., "Exact methods for extended rotating workforce scheduling problems", 2019

Musliu, "Heuristic methods for automatic rotating workforce scheduling", 2006

Back to the Example: Rotating Workforce Scheduling

Problem space P:

- 20 initial real-life instances
- 2000 generated instances

Algorithm space A:

- Constraint programming model:
  - MiniZinc modelling language
  - Lazy clause generation solver Chuffed
- Metaheuristic combining methods from:
  - Min-conflict heuristics
  - Tabu search
  - Random walk

Kletzander et al., "Exact methods for extended rotating workforce scheduling problems", 2019

Musliu, "Heuristic methods for automatic rotating workforce scheduling", 2006

Back to the Example: Rotating Workforce Scheduling

Performance space Y:

- Satisfaction problem
- Measure runtime to feasible solution (timeout 1000 seconds)

Back to the Example: Rotating Workforce Scheduling

Performance space Y:

- Satisfaction problem
- Measure runtime to feasible solution (timeout 1000 seconds)

Feature space F: How to get features from instance data?

- n employees
- Length of schedule w
- Set of work shifts $\mathbf{A}$ + day off O, $\mathbf{A}^+ = \mathbf{A} \cup \{O\}$
- Temporal requirement matrix R
- Min and max work block length ℓ_w and u_w
- Min and max block lengths for shifts and days off ℓ_s and u_s ($s \in \mathbf{A}^+$)
- Set of forbidden sequences $\mathbf{F}$

Direct Instance Features

Take instance data to directly use as features:

- Number of employees n
- Number of shifts m
- Minimum and maximum length of work blocks ℓ_w and u_w as well as blocks off shift ℓ_O and u_O.
- Minimum, maximum and average for each of the sets $\{\ell_s \mid s \in \mathbf{A}\}$ and $\{u_s \mid s \in \mathbf{A}\}$.
- Number of forbidden sequences f.

Advanced Instance Features

Compute features from relations, matrices, graphs, ...

- *workFraction*: Percentage of all days spent working
- *shiftFraction*: Distribution of requirements between shifts
- *blockTightness*: $blockTightness = up - low$
- *avgBlockLength*: Lower and upper bound for the average block length
- *shiftBlockTightness*: Freedom in choosing block lengths for individual shift types
- *shiftDayFactor*: Regularity of shifts throughout the week
- *dayFraction*: Workload in relation to the number of employees for individual days
- *dailyChange*: Change in workload between consecutive days

Model Features

Run fast algorithm initializations, heuristics, ...

- MiniZinc to FlatZinc conversion statistics
  - Number of boolean and interger variables
  - Number of boolean and integer constraints
- Initialization in Chuffed:
  - Number of variables, propagators, SAT variables
  - Number of binary, ternary, and long clauses
  - Average length of long clauses

Algorithm Selection

Use any supervised machine learning approach of your choice:

- Bayesian Networks
- Decision Trees
- k-Nearest Neighbor
- Random Forests
- Multilayer Perceptrons
- Support Vector Machines
- Deep Neural Networks

Algorithm Selection and Analysis for RWS

- Method: Random Forests
- Chuffed vs. metaheuristic: accuracy 80%
- Predict timeout: accuracy 93%
- Feasible vs. infeasible: accuracy 98%
- Regression on magnitude of runtime: correlation 0.7 to 0.8

Learning within Algorithms

In this tutorial section: Decision between different algorithms

Other option: Selection / learning within algorithms

- Later in this tutorial: Learning to select algorithm components (hyper-heuristics)
- Example for tree search: Variable / value selection

Learning without Features

Finding adequate features is one of the main challenges in algorithm selection

$\Rightarrow$ What about algorithm selection without features?

- Recent research direction
- Directly use instance data as time series for Recurrent Neural Network (RNN)
- Application to online 1D bin packing

Alissa, Sim, and Hart, "Automated algorithm selection: from feature-based to feature-free approaches", 2023

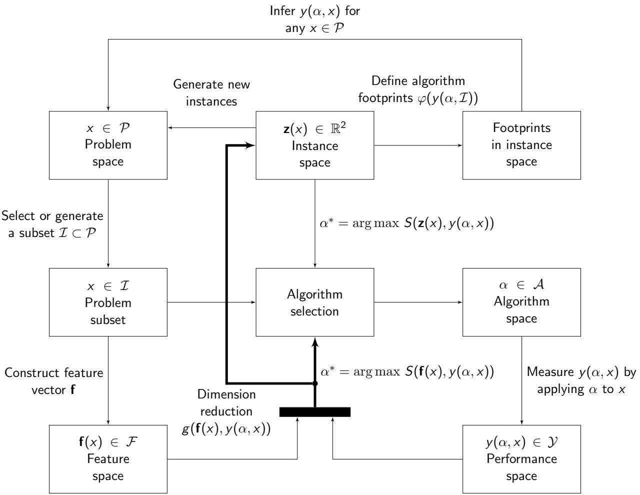
Instance Space Analysis - Motivation

How do we analyze which method works well on which instances?
How do we evaluate a new method for our problem?

- Use benchmark instances
- Better in the average?
- Better in certain cases?
- Do the benchmark instances cover all interesting areas?

$\Rightarrow$ How to check instances and features to make sure that we can properly identify strengths and weaknesses of different algorithms?

Extending Rice's Framework, Smith-Miles et. al. (2014)



Smith-Miles et al., "Towards objective measures of algorithm performance across instance space", 2014

Extending Rice's Framework, Smith-Miles et. al. (2014)

Extensions to Rice's framework:

- Separation of **Problem space** P and available **sub-space of instances** I
- **2-dimensional instance space** for visualization of instance and features distributions
- Selection mapping can either be computed from the feature space or from the instance space
- Performance can be visualized in the instance space and inferred for unseen instances

Instance Space Analysis

Goals:

- Visualize distribution and diversity of instances
- Assess adequacy of features
- Identify regions of strength **footprints** and weaknesses
- Infer where additional instances might be needed

Smith-Miles and Muñoz, "Instance Space Analysis for Algorithm Testing: Methodology and Software Tools", 2023

Instance Space Analysis

Goals:

- Visualize distribution and diversity of instances
- Assess adequacy of features
- Identify regions of strength **footprints** and weaknesses
- Infer where additional instances might be needed

Software Tool: MATILDA

`https://matilda.unimelb.edu.au/matilda/`

`https://github.com/andremun/InstanceSpace`

Smith-Miles and Muñoz, "Instance Space Analysis for Algorithm Testing: Methodology and Software Tools", 2023

Back to the Example: Rotating Workforce Scheduling

Sub-space of instances I:

- 20 initial real-life instances
- 2000 generated instances

Kletzander et al., "Exact methods for extended rotating workforce scheduling problems", 2019

Musliu, "Heuristic methods for automatic rotating workforce scheduling", 2006

Back to the Example: Rotating Workforce Scheduling

Sub-space of instances *I*:

- 20 initial real-life instances
- 2000 generated instances

Algorithm space *A*:

- **2 constraint programming models**:
  - Model 2 extends model 1 by additional constraint to check sequences at the start of each block
- Metaheuristic

Same performance space *Y* (runtime) and feature space *F*

Kletzander et al., "Exact methods for extended rotating workforce scheduling problems", 2019

Musliu, "Heuristic methods for automatic rotating workforce scheduling", 2006

Original Projection

- Bound extreme outliers
- Normalization using Box-Cox and Z transformation
- Remove low diversity features
- Retain features with high correlation to performance
- Clustering

Kletzander, Musliu, and Smith-Miles, "Instance space analysis for a personnel scheduling problem", 2021

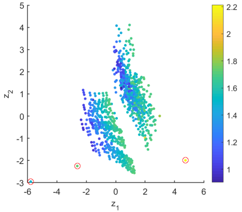
Original Projection

- Bound extreme outliers
- Normalization using Box-Cox and Z transformation
- Remove low diversity features
- Retain features with high correlation to performance
- Clustering

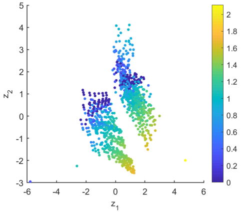
$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} -0.45 & -0.39 \\ 0.45 & 0.40 \\ 0.50 & 0.08 \\ -0.32 & 0.37 \\ 0.23 & -0.63 \end{pmatrix}^{\intercal} \cdot \begin{pmatrix} maxShiftDayFactor' \\ maxDayFraction' \\ employees' \\ minAvgBlockLength' \\ blockTightness' \end{pmatrix}$$

Kletzander, Musliu, and Smith-Miles, "Instance space analysis for a personnel scheduling problem", 2021

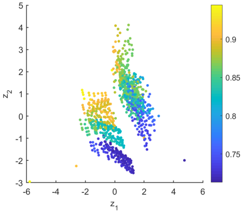
Original Feature Distribution



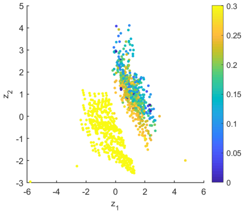
employees



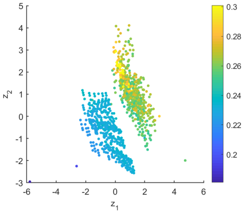
blockTightness



minAvgBlockLength



maxShiftDayFactor



maxDayFraction

Original Feature Distribution

- Good visualization of feature distribution
- Most influential features:
  - Possible block length distributions (*blockTightness*, *minAvgBlockLength*)
  - Instance size (*employees*)
  - Distribution throughout the week (*maxShiftDayFactor*)
  - Daily workload (*maxDayFraction*)
- 2 separated visible clusters
- Several real-life instances are outliers

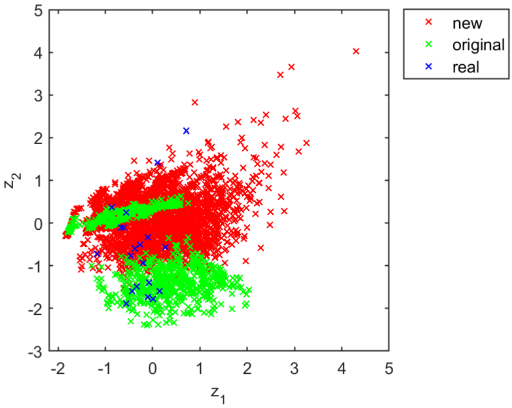
Original Feature Distribution

- Good visualization of feature distribution
- Most influential features:
  - Possible block length distributions (*blockTightness*, *minAvgBlockLength*)
  - Instance size (*employees*)
  - Distribution throughout the week (*maxShiftDayFactor*)
  - Daily workload (*maxDayFraction*)
- 2 separated visible clusters
- Several real-life instances are outliers

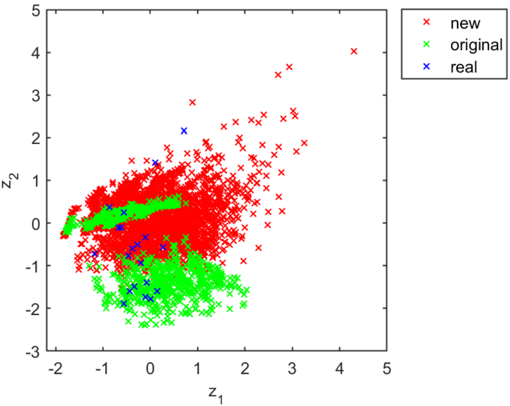
Analysis indicates more instances would be beneficial

- Adapt instance generator
  - Cover gap
  - Include real-life instances
  - Increase number of employees
- Added 3480 new instances

Extended Instances

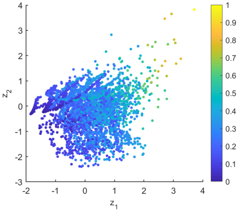


Extended Instances

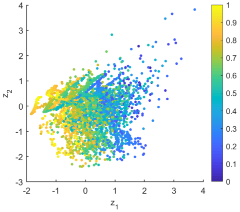


$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} -0.31 & 0.31 \\ 0.02 & -0.57 \\ -0.47 & -0.08 \\ 0.44 & 0.15 \end{pmatrix}^{\mathsf{T}} \cdot \begin{pmatrix} minDayFraction' \\ maxDayFraction' \\ maxAvgBlockLength' \\ minAvgBlockLength' \end{pmatrix}$$

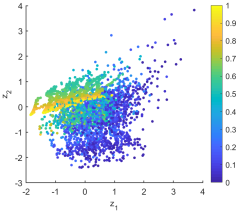
Extended Instance Set - Feature Distribution



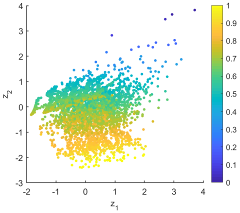
minAvgBlockLength



maxAvgBlockLength



minDayFraction

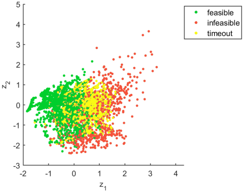


maxDayFraction

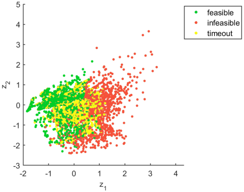
Extended Instance Set - Feature Distribution

- z_1: Axis for *avgBlockLength*
  - Low minimum and high maximum on the left
  - High minimum and low maximum on the right
- z_2: Axis for *dayFraction*
  - Low minimum and high maximum on the bottom
  - High minimum and low maximum on the top
- Gap is closed and real-life instances are well covered

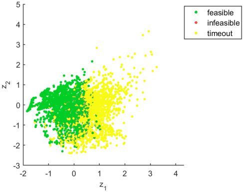
Algorithm Results - Feasibility



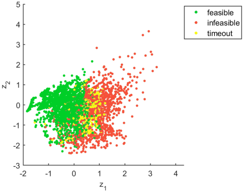
Chuffed model 1



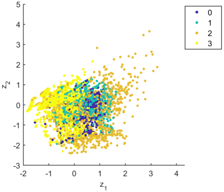
Chuffed model 2



Metaheuristic

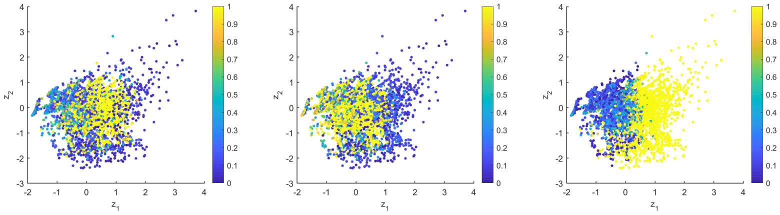


All methods combined



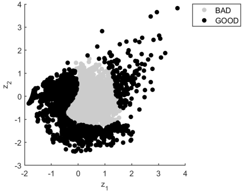
Number of results

Algorithm Results - Runtime

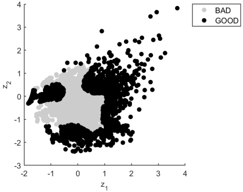


Chuffed model 1 | Chuffed model 2 | Metaheuristic

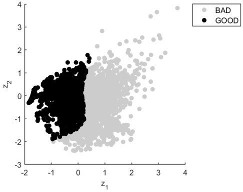
Algorithm Results - Footprints



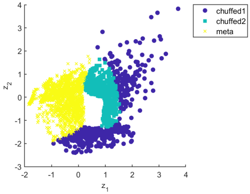
Chuffed model 1



Chuffed model 2



Metaheuristic



SVM portfolio

Algorithm Results

- Clearly visible boundaries between feasibility and infeasibility
  - Due to bounds for number of blocks on z_1-axis
  - Due to high demand fluctuations on z_2-axis
- Instances along this boundary are most difficult

- Strong and weak areas can be generalized to footprints
- Algorithm portfolio can be calculated from instance space
  - Recommended algorithm for each instance
  - Generalization to further areas can be attempted
  - Some areas might not have any well-performing algorithms
    $\rightarrow$ can be reported as hard to solve

$\Rightarrow$ Instance Space Analysis allows deep insights in algorithm behaviour and instance distribution

Automated algorithm selection

Instance space analysis

Hyper-heuristics

- CHeSC
- Reinforcement learning
- Real-world problem domains

Case Study: Test Laboratory Scheduling

Example: CP

- Modern CP solvers internally employ heuristics
- Large Neighborhood Search (LNS):
  Repeatedly apply partial relaxation, then reconstruct

Thomas and Schaus, "Revisiting the Self-adaptive Large Neighborhood Search", 2018

Example: CP

- Modern CP solvers internally employ heuristics
- Large Neighborhood Search (LNS):
  Repeatedly apply partial relaxation, then reconstruct

Relaxation

Random x% of variables are relaxed

Propagation Guided Fix groups of dependent variables

Value Guided Relax variables with same value

Precedency based Assume values are start times, build partial random order

...

Thomas and Schaus, "Revisiting the Self-adaptive Large Neighborhood Search", 2018

Example: CP

- Modern CP solvers internally employ heuristics
- Large Neighborhood Search (LNS):
  Repeatedly apply partial relaxation, then reconstruct

Relaxation

Random $x\%$ of variables are relaxed

Propagation Guided Fix groups of dependent variables

Value Guided Relax variables with same value

Precedency based Assume values are start times, build partial random order

...

Reconstruction

Limited backtracking search

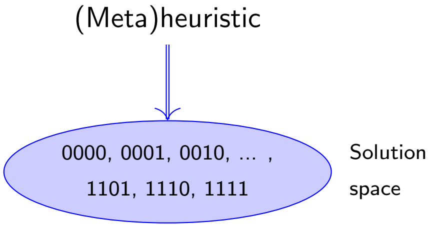
Variable selection:
First Fail, Most Recent Conflict, Weighted Degree

Value selection:
Min/max domain, random, value sticking,...

Thomas and Schaus, "Revisiting the Self-adaptive Large Neighborhood Search", 2018

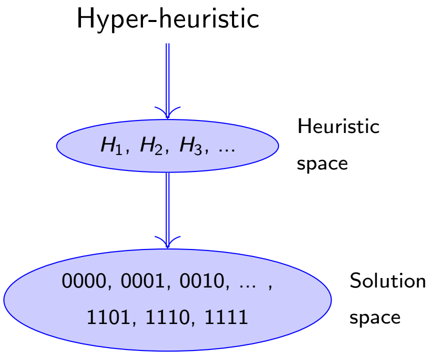
(Meta)heuristic approach

- Operates on set of (possible) solutions
- Implementation defines sample order

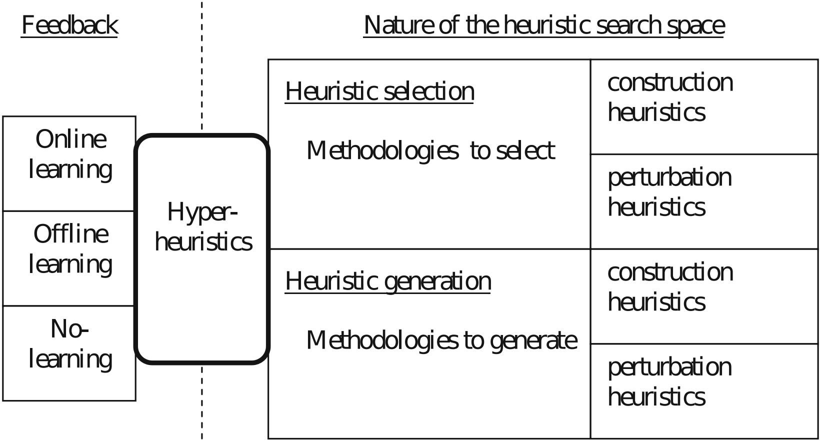


Hyper-heuristic approach

- Operates on set of (low-level) heuristics
  - Complete algorithms
  - Algorithmic components
- Indirectly explore solution space via low-level heuristics

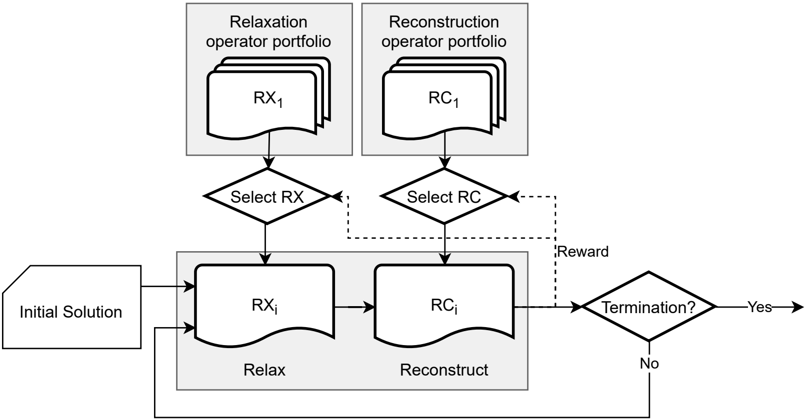


Classification



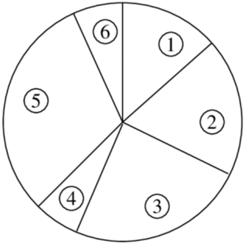
Source: Burke et al., "A Classification of Hyper-Heuristic Approaches: Revisited", 2019

Example: CP - Adaptive Large Neighborhood Search



Example: CP - Operator selection

- Assign weight to each operator
- Select relaxation and reconstruction operator based on current weight (Roulette Wheel Selection)



Laborie and Godard, "Self-adapting large neighborhood search: Application to single-mode scheduling problems", 2007

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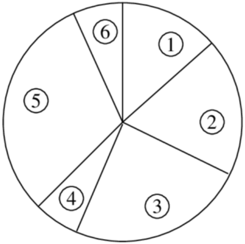
Example: CP - Operator selection



- Assign weight to each operator
- Select relaxation and reconstruction operator based on current weight (Roulette Wheel Selection)

- Update weights according to result:

$$weight_{t+1}(o) = (1 - \alpha) * weight_t(o) + \alpha * \frac{\Delta c}{\Delta t}$$

Laborie and Godard, "Self-adapting large neighborhood search: Application to single-mode scheduling problems", 2007

Thomas and Schaus, "Revisiting the Self-adaptive Large Neighborhood Search", 2018

Example: CP - Results

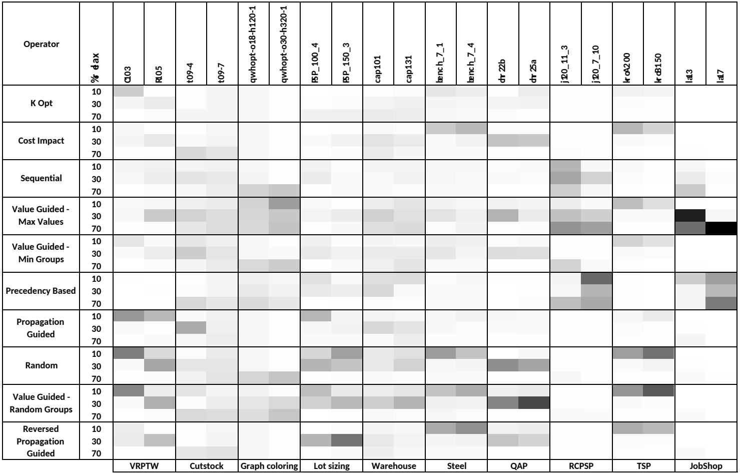


Fig. 1. Heat map of the relaxation operators selection for the Eval window approach

Thomas and Schaus, "Revisiting the Self-adaptive Large Neighborhood Search", 2018

Cross-Domain Heuristic Search Challenge

- Proposed in 2011[1]
- 6 problem domains:
  - Max-SAT, Bin Packing, Personnel Scheduling, Flow Shop, TSP, VRP

[1] Ochoa et al., "HyFlex: A Benchmark Framework for Cross-Domain Heuristic Search", 2012

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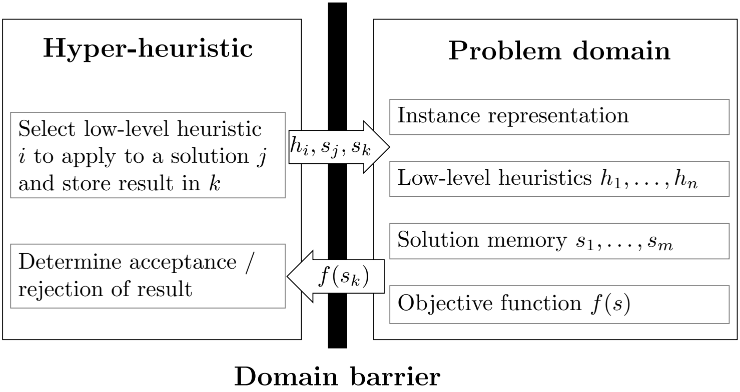
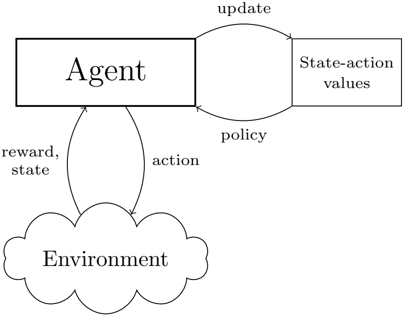
HyFlex

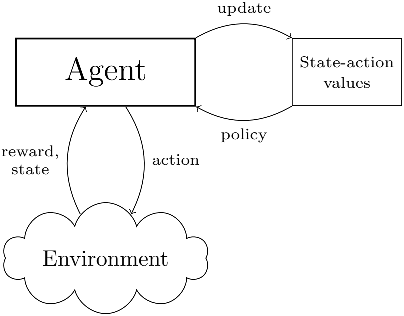

Hyper-heuristic
Select low-level heuristic i to apply to a solution j and store result in k
Determine acceptance / rejection of result
h_i, s_j, s_k
$f(s_k)$
Problem domain
Instance representation
Low-level heuristics $h_1, \ldots, h_n$
Solution memory $s_1, \ldots, s_m$
Objective function $f(s)$
Domain barrier

Reinforcement learning



Selected references [21, 22]

Reinforcement learning

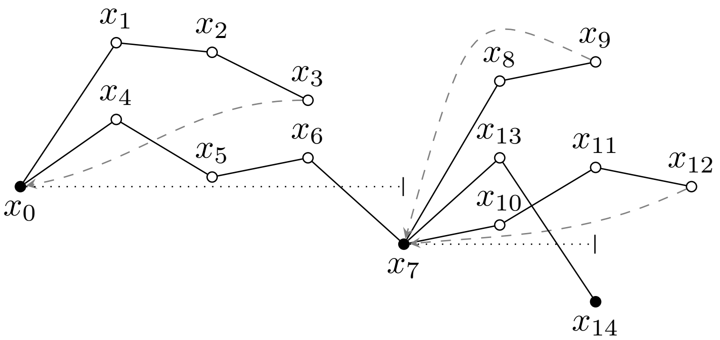


- Natural fit
  - Actions: low-level heuristics
  - Reward: Function of objective value
- Different options for remaining components:
  - State representation
  - Decision policy
  - Update rule

Selected references [21, 22]

RL - Solution chains

- Periodically reset solution, if no improvement found
- Balance long, expensive chains with short chains of limited reach
  - Best results following Luby's sequence



Chuang and Smith, "A study of agnostic hyper-heuristics based on sampling solution chains", 2017

RL - State representation

- Issue: Most interesting information is hidden
- Intuition: Extract information from search history and trajectory of objective value

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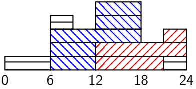
- Issue: Most interesting information is hidden
- Intuition: Extract information from search history and trajectory of objective value

- Last heuristic
- Last heuristic type
- Last change sign
- Last change magnitude
- Chain progress
- Steps since last improvement magnitude
- Steps magnitude and time
- Objective relative to initial or best
- Relative number of improving / 0-cost heuristics
- Measures of recent heuristics
- ...

Problem-independent hyper-heuristics on new domains

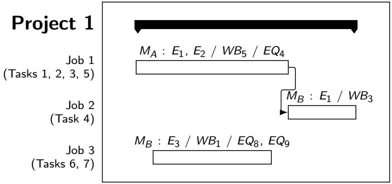
Empl.	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	D	D	D	D	N	N	-
2	-	-	A	A	A	A	N
3	N	N	-	-	D	D	D
4	A	A	N	N	-	-	-

Rotating Workforce Schedule

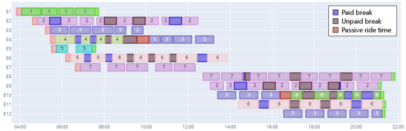


Start	End	E.
6:00	18:00	3
12:00	24:00	2
21:00	9:00	1

Minimum Shift Design



Test Laboratory Scheduling



Bus Driver Scheduling

Automated algorithm selection

Instance space analysis

Hyper-heuristics

Case Study: Test Laboratory Scheduling

Test Laboratory Scheduling Problem (TLSP)

Input

- Scheduling period
- Resources
- Projects and Tasks

Test Laboratory Scheduling Problem (TLSP)

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Solution

- *Grouping* of tasks into jobs

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- *Grouping* of tasks into jobs
- *Assignment* of
  - Execution mode,
  - Starting timeslot, and
  - Resources

  to each job

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- Scheduling period
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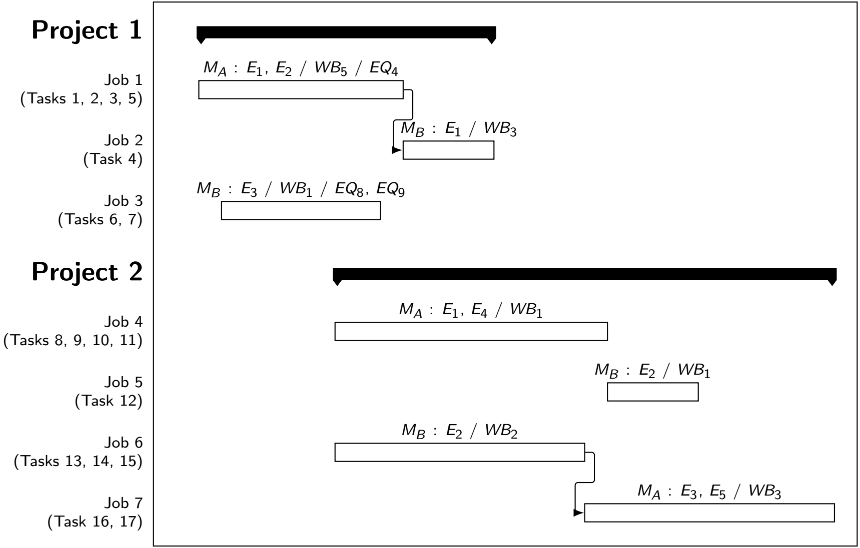
  to each job

Subject to

- Constraints: Grouping restrictions, time windows, precedences, resource availability, ...
- Objectives: Number of jobs, project completion time, preferred resources, ...

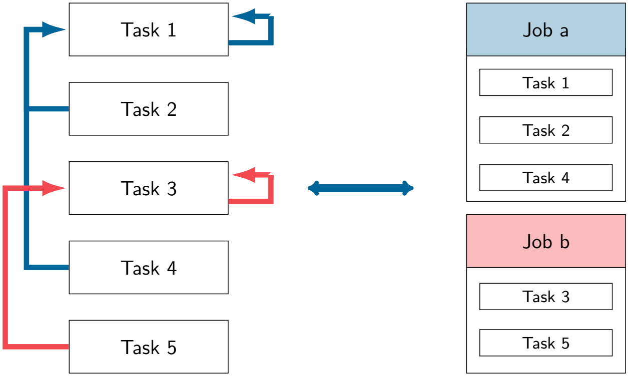
Example schedule



Constraint Programming

Major challenge: Representing grouping

Solution: Representative task for each job



Constraint Programming: Example Constraints

- Resource availability:

$$\text{assigned}[\text{repr}[t], r] = 1 \implies r \in \text{available}_t^{\mathcal{R}}$$

$$\forall t \in \text{Tasks}, r \in \mathcal{R}$$

- Resource requirements:

$$\sum_{r \in \mathcal{R}} \text{assigned}[t, r] = \begin{cases} \max_{t' \in \text{Tasks}:\text{repr}[t']=t} \text{demand}_{t'}^{\mathcal{R}} & \text{if repr}[t] = t \\ 0 & \text{otherwise} \end{cases}$$

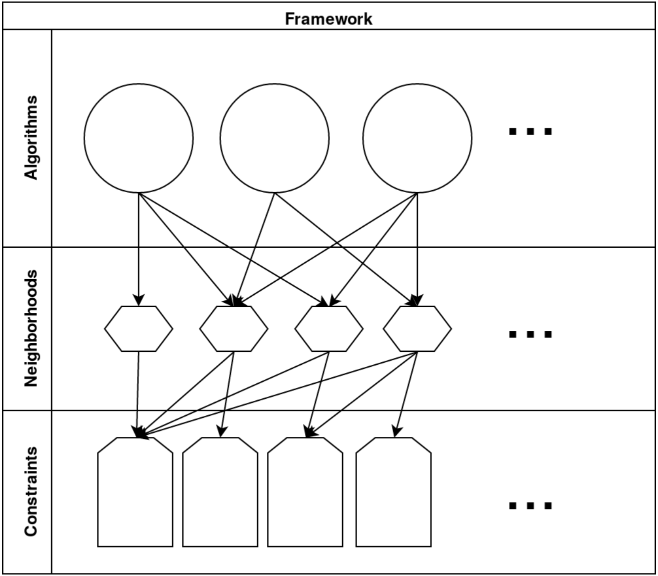
$$\forall t \in \text{Tasks}$$

Very Large Neighborhood Search

Repeatedly generate and solve simplified CP instances:

- Only k projects can be scheduled, the rest of the schedule is fixed
- Initially, $k = 1$, increases when stuck
- Tabu list
- Some scheduling-only steps, with fixed grouping

Meta-heuristics



Meta-heuristics - Neighborhoods

Scheduling neighborhoods

- Timeslot change
- Mode change
- Single resource change
- JobOpt
  - Change all assignments of single job

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Scheduling neighborhoods

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Regrouping neighborhoods

- Transfer task between jobs
- Merge jobs
- Split jobs
  - Move subset of tasks to new job
  - Variant: Linear split

Meta-heuristics - Algorithms

MinConflict Random job, best move in neighborhood for job

- Linear split required
- Hybridization with Random Walk (MC+RW)

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Simulated Annealing Random move in neighborhood, accept using metropolis criterion

- Adapt cooling scheme to reach minimum temperature at time limit

Meta-heuristics - Algorithms

MinConflict Random job, best move in neighborhood for job

- Linear split required
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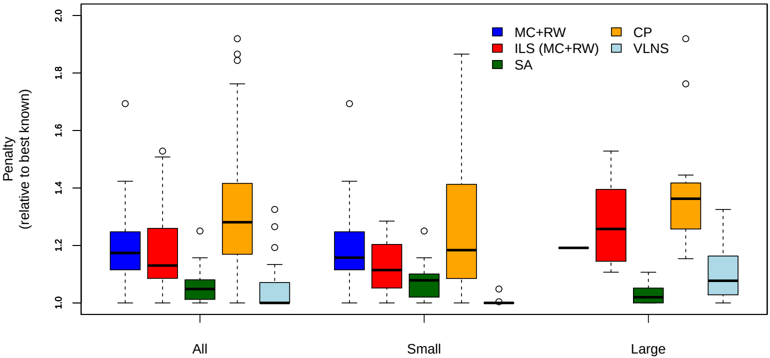
Simulated Annealing Random move in neighborhood, accept using metropolis criterion

- Adapt cooling scheme to reach minimum temperature at time limit

Iterated Local Search Iterate cycles of search and perturbation

- SA or MC+RW used as internal search heuristics
- No improvement for SA

Experimental results



Hyper-heuristics: Low-level-heuristic portfolio

Mutation

- Random move: Mode, time, resources, grouping
- Randomize jobs
- Random walk

Hyper-heuristics: Low-level-heuristic portfolio

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Ruin and recreate

- Delete and reschedule
- Delete and regroup

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Crossover

- Random projects
- Single point XO
- Two point XO

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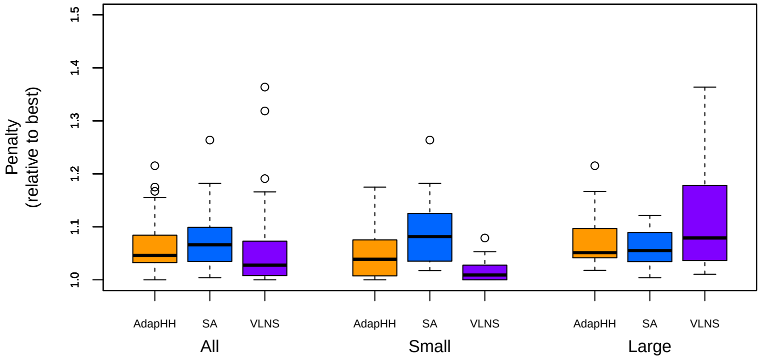
Local search

- HillClimbing
  - mode & time, resources, JobOpt, grouping
- MinConflict
  - mode & time, resources, JobOpt, grouping
- Stochastic hill climbing
  - all neighborhoods
  - high, medium, low T
- Single project CP
- Job-wise greedy

Hyper-heuristics: Experimental results



Conclusions

- Many optimization problems in industry are still solved manually
- AI and optimization offer tremendous potential for further improving solutions in these domains
- Success stories:
  - Test lab scheduling
  - Workforce scheduling
  - Machine scheduling
  - Oven scheduling
  - Sudoku
  - Educational timetabling, Sport timetabling
  - …
- No free lunch
  - Combination of AI and optimization techniques is crucial

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