La Recherche Opérationnelle ou l'art de bien optimiser: un panorama

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• • •

What is Operations Research?

- " OR deals with the development of advanced analytical methods to solve decision or optimization problems",
- OR \sim Combinatorial Optimization \sim Discrete Optimization \sim Continuous Optimization \sim Mathematical Programming \sim Constraint Programming \sim ...
- Main stream: make use of mathematics and computer science to build appropriate models and algorithms.





0/1 KNAPSACK

Input: A finite set U, a size $s(u) \in \mathbb{N}$ and value $v(u) \in \mathbb{N}$ for each $u \in U$. A maximum size $B \in \mathbb{N}$. Goal: Find a subset $U' \subseteq U$ such that $\sum_{u \in U'} s(u) \le B \text{ and } \sum_{u \in U'} v(u) \text{ is maximum.}$

```
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 $\begin{array}{l} \text{Minimize } f(x) \\ \text{subject to} \\ x \in \mathcal{S} \end{array}$

How to solve this kind of problem?
 Exact/optimal algorithms ⇒ optimal solutions.
 Heuristic algorithms ⇒ "good" solutions.

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- Pt2: What is a good model?
- Pt3: Which solution algorithm?

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- 0/1 KNAPSACK: An instance I is a tuple (U, s, v, B),
- The size *n* of *I* is the number of elements, *i.e.* n = |U|,
- What is the smallest time complexity (in the worst case) a computer can achieve to solve the **0/1 KNAPSACK**?

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- Class \mathcal{P} : contains problems solvable in polynomial time of the instance size *n* (easy problems),
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- \mathcal{P} vs \mathcal{NP} ? Assumption: $\mathcal{P} \neq \mathcal{NP}$,

One of the millennium problems of the Clay Mathematics Institute (\$1 million reward)



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- For problems shown to be in \mathcal{NPC} (\mathcal{NP} -hard problems):
 - Option 1: Find an optimal algorithm with the "lowest possible" time complexity (though exponential in n)... or at least, fast enough in practice.
 - Option 2: Find a heuristic algorithm running in polynomial time (so, no guarantee to have the optimal solution).

• Getting a model leading to an effective solution is fundamental!

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- Consider the following scheduling problem,

Single machine total tardiness (SMTT)

Let be *n* tasks to perform on a single processor. Each task *j* is defined by a known processing time p_j and a due date d_j .

For a given schedule s, each task j is given a completion time C_j and a tardiness $T_j = \max(0; C_j - d_j)$. Find a schedule s with minimum $\sum_i T_i$ value.



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- A position based IP formulation (IP_1) ,

$$\begin{array}{ll} \text{Minimize } \sum_{k=1}^{n} T_{[k]} \\ \text{s.t.} \\ & \sum_{k=1}^{k} x_{j,k} = 1 \\ & \sum_{j=1}^{j} x_{j,k} = 1 \\ & T_{[k]} \geq \sum_{\ell=1}^{k} \sum_{j=1}^{n} x_{j,\ell} p_j - \sum_{j=1}^{n} x_{j,k} d_j \\ & \forall k = 1, ..., n \\ & T_{[k]} \geq 0 \\ & \forall k = 1, ..., n \\ & \forall k = 1, ..., n \\ & \forall j, k \end{array}$$

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• For a given instance, provide (*IP*₁) to a commercial solver (e.g. CPLEX, Gurobi, XPress) and press the *Solve* button!

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- For a given instance, provide (*IP*₁) to a commercial solver (e.g. CPLEX, Gurobi, XPress) and press the *Solve* button!
- You should be able to solve instances up to about 50 jobs in size.

Model the problem differently by making use of Lawler's decomposition [2],

[2] Lawler, E.L (1977). A pseudopolynomial algorithm for sequencing jobs to minimize total tardiness, Annals of Discrete Mathematics, 1:331-342.

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• Dynamic Programming (DP):

 $T[S,0] = \min_{s \le \ell \le e} (T[B_{\ell},0] + T[A_{\ell}, \sum_{j \in B_{\ell} \cup \{j^*\}} p_j] + \max(0; \sum_{j \in B_{\ell} \cup \{j^*\}} p_j - d_{j^*}))$ with j^* the longest task in S, B_{ℓ} (resp. A_{ℓ}) tasks before j^* (resp. after) when sequenced in position ℓ .
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• You should be able to solve instances up to 100 tasks in size.

Intermediate conclusions

Pit stop

- MP and DP are approaches usable for building models,
- MP and DP can be used also to solve your problem,
- The effectiveness of MP solvers is continuously improved: good challengers for the exact solution of decision/optimization problems.

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The GED problem

Let $G = (V, E, \mu, \xi)$ and $G' = (V', E', \mu', \xi')$ be two undirected attributed graphs, with μ (resp. μ') is the set of labels attached to vertices in V (resp. V'), and ξ (resp. ξ') is the set of labels attached to edges in E (resp E').

Let λ be and *edit path*: a minimal set of operations (deletion, insertion, substitution) to transform *G* into *G'*.

Find λ^* with minimal cost $d(\lambda) = \sum_{o \in \lambda} c(o)$.

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 - Variables:

 $\begin{aligned} x_{i,k} &= \begin{cases} 1 & \text{if } i \in V \text{ is matched with } k \in V' \\ 0 & \text{otherwise} \end{cases} \\ y_{ij,k\ell} &= \begin{cases} 1 & \text{if } (i,j) \in E \text{ is matched with } (k,\ell) \in E' \\ 0 & \text{otherwise} \end{cases} \\ |V| \times |V'| \text{ variables } x_{i,k} \text{ and } |E| \times |E'| \text{ variables } y_{ij,k\ell}. \end{aligned}$

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$$\sum_{(k,\ell)\in E'} y_{ij,k\ell} \le x_{i,k} + x_{j,k} \qquad \forall k \in V', \forall (i,j) \in E \quad (C)$$

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$$|V| + |V'| + |V'| \times |E|$$
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• Objective function:

 $\overline{\sum_{i \in V} \sum_{k \in V'} C_{v}(i,k)} x_{i,k} + \sum_{(i,j) \in E} \sum_{(k),\ell \in E'} C_{e}(ij,k\ell) y_{ij,k\ell} + CSTE$

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Same $x_{i,k}$ variables.

 $y_{ij,k\ell} = \begin{cases} 1 & \text{if } (i,j) \in E \text{ is matched with } (k,\ell) \in \tilde{E'} \\ 0 & \text{otherwise} \end{cases}$ with $\tilde{E'} = E' \cup \{(\ell,k)/(k,\ell) \in E'\}$ $|E| \times |E'| \text{ variables } x_{i,k} \text{ and } 2 \times |V| \times |V'| \text{ variables } y_{ij,k\ell}.$

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 $\sum_{(i,j)\in E} \sum_{(k,\ell)\in \tilde{E}'} y_{ij,k\ell} \le d_{i,k} x_{i,k} \qquad \forall i \in V, \forall k \in V' \quad (\mathsf{D})$

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t _{avg} (s)	#Opt	t _{avg} (s)	#Opt
395.33	25	20.26	25

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t _{avg} (s)	#Opt	d _{avg} (%)	t _{avg} (s)	#Opt	d _{avg} (%)
880.74	25	604.11	497.07	365	0.70

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Final conclusions

Conclusion

Thinking about the model is as less as important as thinking about solution algorithms.

Designing models occur when dealing with a problem... but also when designing optimization algorithms.

Introduction

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Introduction

- Depending on the complexity of the problem: Exact or Heuristic algorithms,
- The toolbox of OR (non exhaustive),

Exact algorithms		Heuristic algorithms		
Family	Name	Family	Name	
Branching algorithms	Branch-and-Bound	Constructive algorithms	Priority based	
	Branch-and-cut		Greedy	
	Branch-and-price		Ant CO	
	Branch-and-cut-and-price	Branching algorithms	Beam Search	
Mathematical Programming	LP		Recovering BS	
	MILP		Branch-and-Greed	
	QP		Limited Discrepancy Se	
	SDP	Neighborhood based algorithms	Simulated Annealing	
Dynamic Programming	Forward DP		Tabu	
	Backward DP		Multistart	
	DP across the subsets		VNS	
Constraint Programming		1	GRASP	
Dedicated Approaches			Genetic Algorithms	
			Bees Algorithms	
		Matheuristics	VPLS	
			Local Branching	

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• We will see some of the most interesting approaches (to my opinion),

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Golden rules

- Never design an exponential-time exact or heuristic algorithm for a problem in class *P*,
- If your problem is in class *P*, find the right polynomial-time exact algorithm (dedicated),
- If your problem is in class NPC, don't search for a polynomial-time exact algorithm: optimality ⇒ exponentiality. Do heuristics?

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 Commercial solvers (CPLEX, Gurobi, XPress) of MILP are now very competitive,

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- First design a good MILP model of your problem,
- Solve it thanks to a commercial solver,
- Try to design a more effective exact algorithm, <u>NB:</u> "more effective" means capable of solving to optimality instances of largest size.

Exact solution of the SMTT problem

• Based on Lawler's decomposition, we have designed an exact branching algorithm [5],



[5] Shang, L., T'kindt, V., Della Croce, F. (2018). The Memorization Paradigm: Branch and Memorize algorithms for the efficient solution of sequencing problems.

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- For the SMTT problem, the bouding mechanism was useless due to the presence of a *memorization mechanism*,
- In Branch-and-X algorithms, we can also add *cuts*:

If $(C_1(r) > d_{[r+1]})$ then there is no optimal solution in which task 1 is scheduled in position r,

with $C_1(r)$ the completion time of task 1 in the EDD schedule when task 1 is moved to position r.

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• We improve these results by adding a *memorization mechanism*: remember the exploration you have done so far, to avoid exploring useless subproblems in the future.













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Pit stop

We have seen so far different exact approaches for $\mathcal{NP}\text{-hard}$ optimization problems:

- Mathematical Programming (MILP),
- Dynamic Programming (DP),
- Branch-and-X algorithms.

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- For \mathcal{NP} -hard problems, we are faced with combinatorics \Rightarrow CPU times may become quickly non acceptable,
- Heuristic approaches may become the only option,
- A heuristic algorithm = polynomial running time but no warranty of computing the optimal solution,
- The challenge: (i) find heuristics as close as possible to the optimal solution, (ii) acceptable running time.

• Many heuristics have been designed for that problem (see e.g. [4]),

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[6] Bougleux, S., Brun, L., Carletti, V., Foggia, P., Gauzere, B., Vento, M. (2017). Graph edit distance as a quadratic assignment problem, Pattern Recognition Letters, 87:38-46.
[7] Brun, L. (2017). Graph edit distance: Basics and History, Workshop on Graph-based Representations in Pattern Recognition (GbR 17), Capri (Italy).

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- Two efficient ones:
 - IPFP ([6]): *neighborhood based algorithm* which improves an initial solution by a local search phase in continuous space (QAP),

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 - GNCCP ([6]): *neighborhood based algorithm* intensively using IPFP on reformulations of the QAP.

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- Many heuristics have been designed for that problem (see e.g. [4]),
- Two efficient ones:
 - IPFP ([6]): *neighborhood based algorithm* which improves an initial solution by a local search phase in continuous space (QAP),
 - GNCCP ([6]): *neighborhood based algorithm* intensively using IPFP on reformulations of the QAP.
- Other heuristics exist (some based on branching approaches) but are less efficient than IPFP or GNCCP ([4, 6, 7]),

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- Mathematical Programming strongly exploits the powerfulness of branching algorithms and polyhedral properties,
- We will see a *neighborhood based heuristic* based on Mathematical Programming: *Matheuristics*.

A Matheuristic for the GED problem

• We design a Local Branching heuristic (LocBra, [8,9])

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$$x_{i,k} = \left\{ egin{array}{cc} 1 & ext{if } i \in V ext{ is matched with } k \in V' \ 0 & ext{otherwise} \end{array}
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• Neighborhood definition
$$\mathcal{N}(x, x^{\ell})$$
,
 $\mathcal{N}(x, x^{\ell}) = \{x/\Delta(x, x^{\ell}) \le \pi\}$,
with $\Delta(x, x^{\ell}) = \sum_{(i,k) \in S^{\ell}} (1 - x_{i,k}) + \sum_{(i,k) \notin S^{\ell}} x_{i,k}$,
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• Let us denote by $(IP2)_{\pi}^{I}(x^{\ell})$ the model (IP2) with the constraint $x \in \mathcal{N}(x, x^{\ell})$ added,





• Global functionning of the LocBra Matheuristic,



V. T'Kindt









• Diversification,

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- Identify the variables x_{i,k} which modification from the current solution x^l implies a high modification of the objective function,

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- Compute costs c_{i,k}: cost of matching vertices i ∈ V and k ∈ V', Compute costs θ_{i,k}: cost of matching edges from i with edges from k (assignment problem),



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- Let S_{div} be the set of variables $x_{i,k}$ with high σ_i values,
- To get a new solution from x^{ℓ} solve $(IP2)^{D}_{\beta}(x^{\ell})$:
 - Model (*IP*2),
 - Add constraint: $\Delta'(x, x^{\ell}) = \left(\sum_{(i,k)\in S^{\ell}\cap S_{div}}(1-x_{i,k}) + \sum_{(i,k)\in S_{div}\setminus S^{\ell}\cap S_{div}}x_{i,k}\right) \geq \beta$

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Results on PROTEIN database,

Size	IPFP		GNCCP		LocBra	
	Avg Dev (%)	Avg time (s)	Avg Dev (%)	Avg time (s)	Avg Dev (%)	Avg time (s)
20x20	1.05	0.09	0.22	2.05	0.06	6.54
30x30	0.98	0.27	0.20	7.21	0.08	8.68
40×40	1.14	0.59	1.68	23.17	0.39	8.82

For graphs of size 20×20 and 30×30 , we have the optimal solution. For 40×40 we have 63% of optimal solutions.

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• A comparison with ground-truth on CMUHOUSE-NA shows that LocBra strongly outperforms the other heuristics (at most 5% of wrong matchings against more than 20% for the others).

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- Very efficient and quite simple to use (black-box solver for the MIP),
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Beyond OR

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- Let us consider the **Traveling Salesman Problem** (TSP), Input: A connected graph G = (V, E) with V the set of vertices (cities) and \overline{E} the set of edges (routes). Each edge $(i,j) \in E$ is defined by a weight $d_{i,j}$ (distance). We note n = |V|. Coal: Find a permutation S of vertices such that

<u>Goal</u>: Find a permutation S of vertices such that

$$\left(\sum_{k=1}^{n} d_{S[k],S[k+1]} + d_{S[n],S[1]}\right)$$
 is minimum


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- Based on a Branch-and-Cut algorithm exploiting mathematical programming,

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- Time complexity in $O(n^{2.2})$: instance with 13509 cities \approx 12h.

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- Learn how to produce good solutions directly from the TSP instance,

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- Complexity of the predictor: $O(n^2)$... almost the same than LKH heuristic.

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- The right question should be more why using ML,

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- My believe (also expressed somehow in [15]): *ML* and *OR* should no longer be used separately to solve optimization problems.

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- This would make faster the intensification phase ⇒ enable to consider larger neighborhoods ⇒ improve the overall LocBra heuristic.

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- Room for ML to learn if a solution will be dominant or not.

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Thank you for your attention.

