Using ML and AI to Speed-Up Large-Scale Optimization Problems

Iiro Harjunkoski

Hitachi Energy Research / Aalto University

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Introduction – Focus on Scheduling

Increasing complexity

- Digitalization of industrial production processes
- Maximize synergies through more integrated operations
- Scheduling problems larger → both modeling and solution procedures are cumbersome
- Automatize the decision making

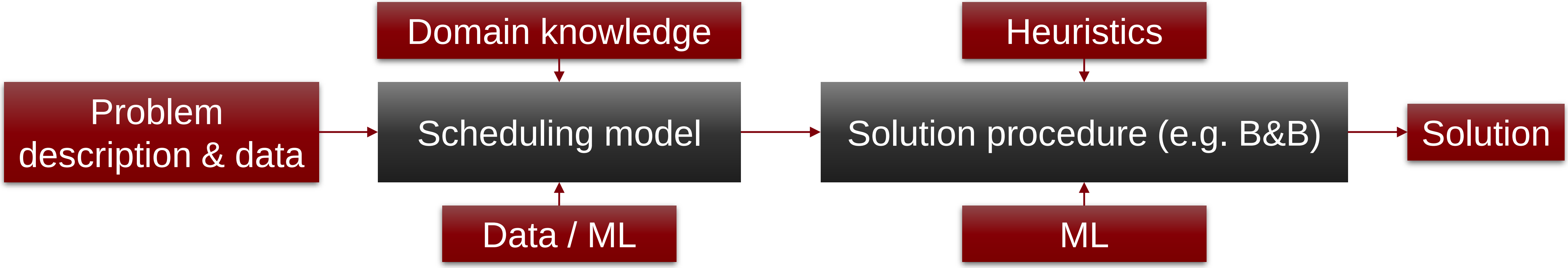
Common approaches to speed up the optimization

- Simplify the problem (i.e., balancing between the solution quality and computing time)
- Apply heuristics to reduce solution space
- Deploy simulation tools to predict complex variable values
- Use decomposition: Divide the problem into smaller subproblems
- + mixture of all of the above

How to Use Machine Learning in the Scheduling Context?

Main steps

- Building the model – often manual effort
  - User / Operator: Apply domain knowledge
  - Automated: Data processing
- Solving the model (mostly 100% automated) but the solution engine can be supported by
  - Manually defined heuristics based on problem understanding
  - Machine Learning (designed by an expert)

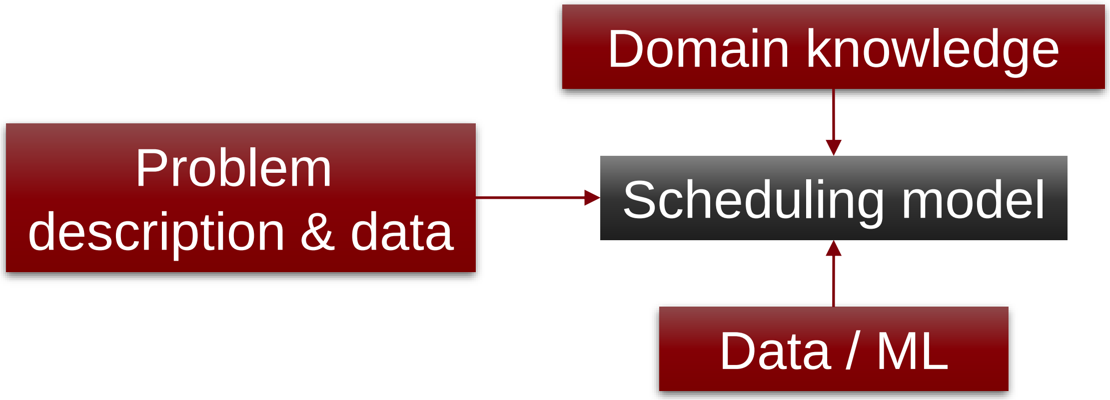


Modeling

Use ML to reduce the sometimes significant and error-prone engineering efforts that can occupy highly-trained personnel on routine tasks

- Can true domain expertise be reliably generated by a system that mainly builds on already existing data?
- If using ML, it is important that the system identifies its own capability limitations / boundaries!

- Modeling of true problems require domain knowledge / problem understanding + data
- Machine Learning can contribute to e.g.
  - Processing large datasets (clustering, forecasting, …)
  - Parameter tuning, surrogate modeling
  - Automatically generated constraints (ALAMO)
  - Creation of cuts

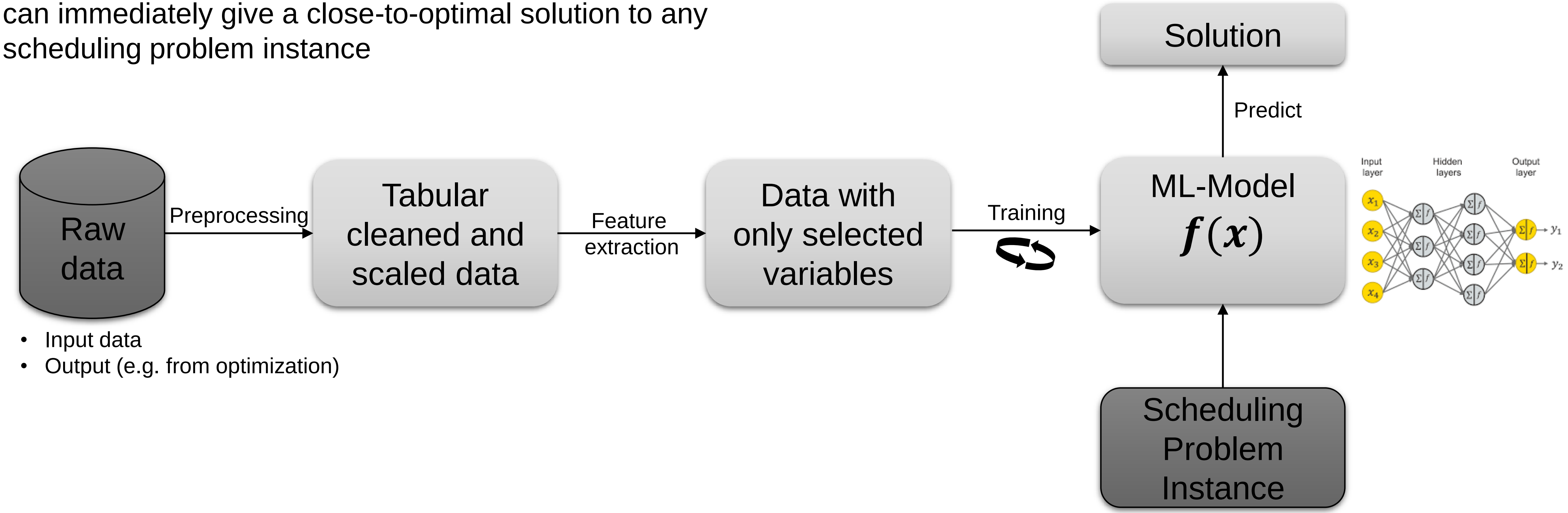


Many contributions in the literature!

Solution

“The Dream”

In an ideal world we can train a prediction model such that it can immediately give a close-to-optimal solution to any scheduling problem instance



- Input data
- Output (e.g. from optimization)

Solution

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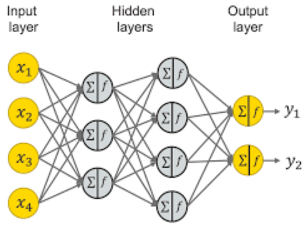
“Reality” – Many avenues, no clear “winner”

Use machine learning to

- Dynamically generate more accurate (up-to-date) scheduling parameters – “forgetting factor”?
- Creating more generic decision-making patterns – solving part of the problem
- Understand and learn to solve a problem (Xavier et al., 2019)
    - ML in B&B search e.g. ECOLE (Provoust et al., 2020)
- IBM CPLEX/Gurobi: Automatically decide upon algorithmic choices in solving QPs, tune parameters during solution
- Use deep reinforcement learning in process scheduling, e.g. OR-GYM (Hubbs et al., 2020b)
- Deploy reinforcement learning to decide on the timing of rescheduling, scheduling algorithms and time budget for the optimization (hyperparameters)



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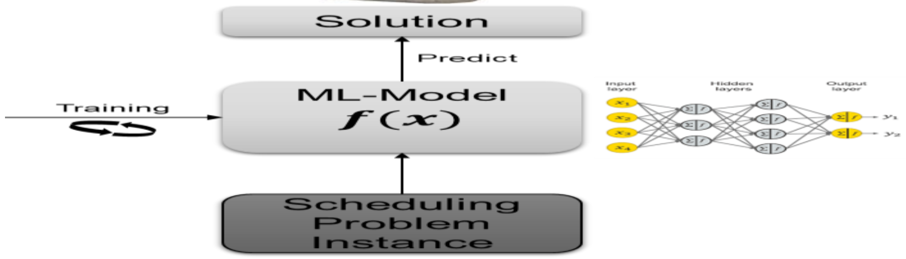
$$\begin{array}{ll} \text{maximize} & \mathbf{c}^{\mathrm{T}}\mathbf{x} \\ \text{subject to} & A\mathbf{x} + \mathbf{s} = \mathbf{b}, \\ & \mathbf{s} \geq \mathbf{0}, \\ & \mathbf{x} \geq \mathbf{0}, \\ \text{and} & \mathbf{x} \in \mathbb{Z}^n, \end{array}$$



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Main Challenges

Automated modeling

Data

Algorithmic complexity

Multiple objectives

Wider deployability

Conclusions / Where are We Today?

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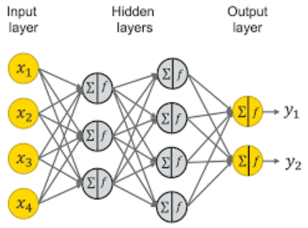
- Combining machine learning to support or complement mixed integer linear programming – already many contributions
  - So far no silver-bullet (will there ever be…)
- Largest benefits (at least “low hanging fruit”) seem to come from effectively combining ML-prediction or clustering & MILP-solution
  - Rather on the modeling than solution level
- Important to have realistic expectations
  - Hype vs. reality
- Needed: Sufficiently large, shared datasets for development
- MILP alone will “hit the wall”
  - Some form of collaborative approaches will become the standard for efficient and successful solution of complex scheduling problems
- Data does not go anywhere… and problems are growing!



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