OPTIMIZATION ALGORITHMS FOR AI AND LEARNING ALGORITHMS FOR OPTIMIZATION PROBLEMS

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ABSTRACT

This PhD course proposes to investigate the interaction of optimisation algorithms and theory with the practice of Artificial Intelligence (mainly Machine Learning models). The first part of the course reviews the different optimisation algorithms proposed in the literature to tune the parameters of Machine Learning models, the theoretical and empirical investigation of how and why such algorithms are successful even on very large scale models and how Bi-Level Optimisation is a (relatively new) tool which can help in solving advanced Machine Learning problems. The second part focuses on the use of Machine Learning and Data Mining tools to help solve Operations Research (i.e., combinatorial optimisation) problems and methods, such as Vehicle Routing, Travelling Salesman, Additive Manufacturing, and more complex decomposition strategies and problems. This part is structured as a review on the effectiveness of different learning models over various aspects of optimization: from the building of good heuristic solutions and the prediction of their quality, to the analysis of problems and structure of their instances to evince important properties. Finally, the third part examines some applications of predictive and prescriptive analytics in the challenging field of healthcare delivery.

Keywords: Non-linear continuous optimisation, Machine Learning, Landscape analysis, Bi-level optimisation, Combinatorial Optimisation, Data Mining.

Aim of the lectures

This PhD course aims at elucidating the deep links between mathematical optimisation and machine learning. The students will be introduced to the following themes and abilities: understand the properties of different kinds of non-linear continuous optimisation algorithms to tune the (hyper-)parameters of machine learning models and how to apply them; understand how to model some advanced machine learning models as bi-level optimisation models; identify situations where machine learning and process mining can be used as a sub-module for combinatorial optimisation problems.

Pre-requisites

Differentiable functions, real multivariate functions, gradient operator, convexity, (simple) basics of Machine Learning; basics of Operations Research, algorithms and complexity.

Plan of the lectures

Non-linear optimisation for the tuning of Machine Learning models (10h)

- Why do we need optimisation for Machine Learning (ML) models?
- First-order methods: principles of Gradient Descent and Stochastic Gradient Descent, convergence analysis.
- Second-order methods: Newton's method, Hessian-free methods, Stochastic Quasi-Newton methods, Gauss-Newton $\Rightarrow$ possible improvements and drawbacks of second-order algorithms for ML optimisation.
- Intermediate methods: Gradient methods with acceleration and momentum.

- Landscape analysis: avoiding bad local minima, geometry of the loss function for Deep Neural Networks.
- Bi-Level Optimisation (BLO): advanced ML model tuning as BLO problems (optimisation of hyper-parameters).

Machine Learning for combinatorial optimisation (10h)

This part will focus on several successful applications of Machine Learning (ML) methods in the context of classical Operations Research (OR) problems.

- *Learning Combinatorial Optimization Algorithms over Graphs* — A greedy procedure, guided by Reinforcement Learning, to solve various graph optimization problems.
- *Learning when to use a decomposition* — Comparison of binary classifiers employed to decide whether a model possesses a structure suited for the application of Dantzig-Wolfe decomposition.
- *What makes a VRP solution good? The generation of problem-specific knowledge for heuristics* — Application of binary classifiers to the Vehicle Routing Problem for the learning of instance and solution structure, in order to distinguish between optimal and non-optimal heuristic solutions.
- *Machine learning meets mathematical optimization to predict the optimal production of offshore wind parks* — Comparison of different Machine Learning approaches in the prediction of the optimal solution value for the offshore wind farm layout problem.
- *A reinforcement learning iterated local search for makespan minimization in additive manufacturing machine scheduling problems* — A meta-heuristic procedure, based upon Iterated Local Search guided by Reinforcement Learning, for the minimization of Makespan in the context of Additive Manufacturing problems.

A paper will be presented in each of the lessons, then a discussion upon obtained results and strengths/weaknesses of each paper will take place. Students are strongly encouraged to take part, actively, to these discussions.

Analytics in Healthcare delivery (4h)

- Introduction to Healthcare and the processes behind the delivery of healthcare services.
- Predictive and Prescriptive analytics in Healthcare: basics of process mining and online optimisation.
- The Emergency Care Pathway: analysis and solutions.

Tentative schedule

The lectures consist of 24 hours divided between the three themes previously described (respectively 10h/10h/4h) and will take place on Friday mornings between 8:30am and 12:30am on the following dates: **17th** and **24th of April**, **8th**, **15th**, **22nd** and **29th of May 2026** in streaming.

Examination

The candidates can choose between different possible forms of exam for this course, to be agreed upon with the teachers.

- Explanation/discussion around a scientific paper of the literature pertinent to the themes of the lectures.
- Implementation and comparison of some of the methods presented during the lectures (e.g., first-order vs second-order method for training a neural network).
- Discussion on how the presented methods could be applied to the students' research lines.
- Other proposal from the student, after agreement with the teachers.