GOR Gesellschaft für Operations Research e.V.

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101st Meeting of the GOR Working Group „Real World Optimization“

Mathematical Optimization meets Machine Learning and Artificial Intelligence

Bad Honnef, November, 22 & 23, 2018

Physikzentrum Bad Honnef, Hauptstr 5, 53604 Bad Honnef

Thursday, Nov 22 - 2018: 09:30 – 18:00

All times are still subject to changes

09:30-09:45 **Opening and Welcome** (Jens Schulz)

09:45-10:15 **Marco Lübbecke** (
Introductory talk – AI + ML + Opt = ?

10:15-10:45 **Hergen Schultze** (BASF SE, Ludwigshafen)
Model Based Machine Learning in Quality Management

10:45-11:15 ---------- Coffee Break ----------

11:15-12:00 **Ulf Lorenz** (University of Siegen, Siegen)
Tree Search and Learning - Algorithms and Heuristics in the PSPACE-hard World

12:00-13:30 ---------- Lunch Break ----------

13:00-13:30 **Torben Barth** (Fraport AG, Frankfurt)
Applied analytics at Frankfurt Airport

13:30-14:00 **Kevin Tierney** (Bielefeld University, Bielefeld)
Deep Learning Tree Search for the Container Pre-Marshalling Problem

14:00-14:30 **Renke Kuhlmann** (University of Bremen, Bremen)
Learning to Steer Nonlinear Interior-Point Methods

14:30-15:00 ---------- Coffee Break ----------

15:00-15:30 **Jonas Ostmeyer** (PSI FLS Fuzzy Logik & Neuro Systeme GmbH)
Deep Qualicision: Optimization driven labeling of process

15:30-16:00 **Marius Lindauer (**University Freiburg)
Machine Learning for Automated Algorithm Design

16:00-16:30 **Oliver Bastert** (FICO, München)
Optimizing Machine Learning

---------- Excursion / Walking tour ----------

18:00-22:00 **Conference Dinner**
- Celebrating the 101st meeting of our GOR Working Group -

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Friday, November 23, 2018: 09:00 – 14:30

All times are still subject to changes

07:30-08:45 ---------- Breakfast at hotels ----------

09:00-09:30 **Stefan Helber** (University of Hannover, Hannover)
Modeling and predicting the throughput of stochastic flow lines with limited local buffer capacity via artificial neural networks

09:30-10:00 **Raoul Heese** (Fraunhofer ITWM, Kaiserslautern)
Machine learning-driven screening of operation windows in chemical plants

10:00-10:30 ---------- Coffee Break ----------

10:30-11:15 **Christian Mandl** (TU München, München)
Tba - 45min

----- Taking a Group Photograph for the OR News and Press -------

11:45-12:45 ---------- Lunch Break ----------

12:45-13:15 **Ulrich Reincke** (SAS, Heidelberg)
Autotuning im Machine Learning im Viya- Release von SAS

13:15-13:45 **Jonas Ostmeyer** (PSI FLS Fuzzy Logik & Neuro Systeme GmbH)
Deep Qualicision: Optimization driven labeling of process

13:45-14:15 **Sebastian Hilgert** (DB Analytics, Deutsche Bahn, Frankfurt)
Dispatching in railway operation using simulation and machine learning

14:15-14:30 **Final Discussion – End of the Workshop – Coffee Break**

Location: Physikzentrum Bad Honnef, Hauptstr 5, 53604 Bad Honnef

The Speakers

Torben Barth is part of the analytics group at Fraport and has the role of a senior consultant and data scientist. He is responsible for the development of quantitative solutions at Frankfurt Airport. He obtained his Ph.D. in Operations Research at the Management Engineering department of the Technical University of Denmark (DTU) in 2014. His PhD thesis dealt with the optimization of baggage handling at airports. Since his start at Fraport in 2005 he is involved in the introduction of quantitative decision support solutions for operational and strategic problems.

Raoul Heese obtained his PhD in quantum physics from Ulm University (Germany) in 2016. He has worked as a postdoctoral researcher in Ulm and at the Stanford University (USA). Currently, he is a scientific employee at the Fraunhofer ITWM in Kaiserslautern.

Stefan Helber holds the Chair of Production Management at the Faculty of Economics and Management, Leibniz Universitt Hannover, Germany. He holds a doctoral degree in Business Administration from Ludwig-Maximilians-Universität München. His research interests focus on performance analysis and production planning & scheduling for manufacturing and service systems. His publications address topics such as lot sizing in determinstic and stochastic environments, call center planning, flow line configuration, academic timetabling, project scheduling etc. He is a member of DFG Coordinated Research Center 871 "Regeneration of Complex Capital Goods".

Sebastian Hilgert studied Logistics at TU Dortmund and Iowa State University and started his profession in the consulting business. He is senior expert for prediction, optimization and simulation at DB Analytics (https://www1.deutschebahn.com/db-analytics-de), leading projects for the different business units of Deutsche Bahn AG in the mobility, logistics and infrastructure sector. He is member of the ASIM (Working group simulation, an expert committee of the German Society for Computer Science (GI)) and the Guideline Committee of the VDI (Association of German Engineers).

Renke Kuhlmann is currently doing his PhD in mathematics at the University of Bremen with a focus on penalty-interior-point algorithms for nonlinear programming. He is one of the main developers of the nonlinear programming solver WORHP to which he contributed with an efficient and robust implementation of an augmented Lagrangian penalty-interior-point algorithm and a post-optimality sensitivity analysis module. His research interests additionally include (mixed-integer) optimal control.

Marius Lindauer is a junior research group lead at the University of Freiburg (Germany) with a focus on Machine Learning for Automated Algorithm Design (ML4AAD) and Automated Machine Learning (AutoML.org). He combines cutting edge techniques from machine learning and optimization to automate the process of hyperparameter optimization, algorithm configuration and algorithm selection.

He received his M.Sc. and Ph.D. in computer science at the University of Potsdam (Germany), where he worked in the Potassco Group. In 2014, he moved to Freiburg as a postdoctoral research fellow. In 2013, he was one of the co-founders of the international research network on COnfiguration and SElection of ALgorithms (COSEAL) and is nowadays a member of its advisory board. In 2016 and 2018, he was a member of the *aad_freiburg* team, which won both editions of the international AutoML competition.

Marco Lübbecke is a full professor and chair of operations research at RWTH Aachen

University, Germany. He received his Ph.D. in applied mathematics from TU Braunschweig in 2001 and held positions as assistant professor for combinatorial optimization and graph algorithms at TU Berlin and as visiting professor for discrete optimization at TU Darmstadt.

Marco's research and teaching interests are in computational integer programming and discrete optimization, covering the entire spectrum from fundamental research and methods development to industry scale applications. A particular focus of his work is on decomposition approaches to exactly solving large-scale real-world optimization problems. This touches on mathematics, computer science, business, and engineering alike and rings with his appreciation for fascinating interdisciplinary challenges.

Jonas Ostmeyer obtained his Diploma (M.Sc. equiv.) in Business Mathematics from TU Dortmund University (Germany) in 2012. As part of his ensuing position as a research assistant at the Chair of Operations Research at Fern Universität in Hagen he worked on his PhD thesis about time flexible lot sizing and scheduling, which is now being reviewed. Furthermore, he used his expertise in mathematical optimization to solve real world problems in several cooperative projects with companies of various industries.

Jonas Ostmeyer works at PSI FLS Fuzzy Logik & Neuro Systeme GmbH, a company of the PSI Software Group. In his position as a Consultant Supply Chain Optimization and Sales he drives the integration of artificial intelligence for business processes optimization into the digitalization strategies of companies across all sectors.

Ulrich Reincke is a Principal Analytics Solution Architect and Data Scientist in the Centre of Excellence at SAS Institute, Heidelberg. Over the last 20 years he has been responsible in different roles for analytical enterprise decision support solutions at SAS. The aim of these solutions is to apply methods of statistics, machine learning, data mining, forecasting and optimization to empower organizations to make better or more profitable fact-based decisions. Prior to SAS Mr. Reincke had positions in the Information Product Department of Deutsche Börse in Frankfurt and in the International Trade Division of The World Bank in Washington DC. His academic background includes degrees in mathematics and economics and international relations.

Hergen Schultze is the head of the research group *Statistics, Machine Learning, and Artificial Intelligence* at BASF SE in Ludwigshafen, Germany. He received his PhD from Georg-August University in Göttingen. His research interest covers non-linear physical systems, machine learning (especially in a lab setting), and optimization of decisions.
www.linkedin.com/in/hergen-schultze

Kevin Tierney joined Bielefeld University as a full professor of Decision and Operation Technologies in April, 2018. He was previously assistant professor at Paderborn University for Operations Research and Decision Support Systems. He earned his PhD from the IT University of Copenhagen, Denmark with a thesis on the topic of "Optimizing Liner Shipping Fleet Repositioning Plans.". He has a Master of Science from Brown University in Computer Science and a Bachelor of Science from Rochester Institute of Technology in Computer Science. He is currently researching applications of machine learning within the field of optimization, as well as optimization problems within the area of maritime transportation.

Applied analytics at Frankfurt Airport

Torben Barth
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This talk illustrates the different analytical approaches at Frankfurt Airport. The presentation shows typical examples of applied analytics at Frankfurt Airport. It sheds a light on the analytics and data science part on the one hand and the mathematical optimization approaches on the other hand. The differences and the dependencies of the two fields in the daily work at Frankfurt Airport will be shown. Furthermore, the concept of a smart data lab at Frankfurt Airport will be introduced which is an organizational structure to promote analytical ideas in the company and to find new approaches for important operational and strategic problems.

Machine learning-driven screening of operation windows in chemical plants

Raoul Heese, Michal Walczak, Tobias Seidel, Norbert Asprion, Karl-Heinz Küfer, Michael Bortz
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Process design using chemical flowsheet simulations is by its nature a multi-criterial optimization task with conflicting goals, where certain design parameter space regions may result in non-convergent or unphysical outcomes of the simulation. Pareto sets, which contain all optimal and feasible best compromises, are a well-established approach to handle such scenarios. Recently, powerful decision support tools have been developed to determine and explore Pareto sets in industrial contexts [1]. Still, it remains a challenge to distinguish feasible from infeasible design parameters. We present an adaptive data exploration algorithm as an alternative approach to approximate Pareto sets using concepts from the field of machine learning. With the help of suitably trained surrogate models, we are able to interpolate and extrapolate both the optimization targets of interest as well as the design parameter space feasibility. Such predictions help us to understand the global structure of the flowsheet simulation data space. Our proposed algorithm can be understood as a sequential design of experiments, where each new simulation run is chosen based on a data-driven utility function. A set of intuitively comprehensive control variables allows us to tune the explorative behavior in various ways. By doing so, we can either achieve a more expansive or a more restrictive sampling in parameter space regions of particular interest. Each additional sample improves our surrogate models and their respective predictions, leading to a better comprehension of the data space structure in whole and the operation window in particular.

[1] M. Bortz, J. Burger, N. Asprion, S. Blagov, R. Böttcher, U. Nowak, A. Scheithauer, R. Welke, K.-H. K"'ufer, H. Hasse, Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets, Computers & Chemical Engineering, Volume 60, 2014, Pages 354-363

Modeling and predicting the throughput of stochastic flow lines with limited local buffer capacity via artificial neural networks

Prof. Dr. Stefan Helber
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Flow lines are frequently used to organize the mass production of physical goods in manufacturing. Such a line consists of serially arranged stations that are designed and equipped to perform dedicated tasks. The product units flow through the line to receive a series of operations at those stations. In a deterministic setting, the slowest station is the system's bottleneck and determines its throughput or production rate (measured in product units per time unit). However, in reality processing times are often stochastic, e.g., because of machine failures. In this case, to avoid blocking and starving, costly buffers can be installed between the stations to limit the propagation of failures up- and downstream of the system. In practice, discrete-event simulation is often used to estimate the production rate of a given (planned) flow line configuration. As an alternative, extremely fast approximate analytical methods have been developed to estimate the production rate of stochastic flow lines without using discrete-event simulation. We use such an analytical method to create and evaluate a large number of hypothetical flow lines and then train an artificial neural network to predict the production rate of flow lines which have not yet been analyzed before. We present first results from a systematic study of this new approach for flow line performance evaluation.

Dispatching in railway operation using simulation and machine learning

Sebastian Hilgert
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Simulation is a surrender to the complexity of a system: instead of an exact formulation of the problem, a model is built, rules are implemented and the simulation delivers a projection, how the system will react and develop. Combined with machine learning, it is possible to go even one step further and build models without rules. This talk is about the methodical approach, how dispatching situations in railway operation are solved, using a simulation model in combination with a Monte Carlo Tree Search (MCTS) and the Upper Confidence Bound applied to Trees (UTC).

Learning to Steer Nonlinear Interior-Point Methods

Renke Kuhlmann
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Interior-point or barrier methods handle nonlinear programs by sequentially solving barrier subprograms with a decreasing sequence of barrier parameters. The specific barrier update rule strongly influences the theoretical convergence properties as well as the practical efficiency. While most global and local convergence analyses consider a monotone update that decreases the barrier parameter for every approximately solved subprogram, computational studies showed a superior performance of more adaptive strategies. This talk interprets the barrier update as a reinforcement learning task. A deep Q-learning agent is trained both by imitation and random action selection. Numerical results based on an implementation within the nonlinear programming solver WORHP show that the agent successfully learns to steer the barrier parameter.

Hydra 2.0: Advances in Per-Instances Algorithm Configuration

Marius Lindauer
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In the last decade, research on algorithm configuration has shown that many algorithms are sensitive to their parameter configurations. To achieve peak performance, these parameters have to be adjusted accordingly. This applies to many fields in AI, such as algorithms for satisfiability solving, AI planning, mixed integer programming or machine learning. However, the parameter configuration has not only be optimized once, but it can be selected on a per-instance base. Therefore, the field of per-instance algorithm configuration (PIAC) combines algorithm configuration to find well-performing parameter configurations, and algorithm selection to select a configuration for a given instance. In my talk, I will present the PIAC approach Hydra and its recent improvements applied to both combinatorial problems (such as Boolean satisfiability problems) and automated machine learning.

ML + AI + Opt = ?

Marco Lübbecke
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Machine learning (ML), artificial intelligence (AI), and mathematical optimization (MO) are long standing and well established research fields. From a research perspective, there are some natural directions where ML/AI and MO may benefit from each other (and we sketch a few). From an applications perspective, there is the natural ordering of ML/AI ("predictive") first, MO ("prescriptive") second, but other cases are conceivable. In this talk, I will discuss some research, applications, and perspectives that I personally find challenging, interesting, exciting, or boring. In particular, a recent surge of interest ("hype" is not exaggerated) pushed ML and AI into companies/startups and newspapers. Not so much MO. I briefly discuss implications for "our" field (which I still think is MO).

Deep Qualicision: Optimization driven labeling of process data position paper

Dipl.-Wirt.-Math. Jonas Ostmeyer
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In this talk artificial intelligence (AI), and especially machine learning, in an industrial sense is on focus. Using artificial intelligence to optimize business processes is part and parcel of digitalization strategies for many companies. However, applying AI methods from AI applications such as character or speech recognition to make, for example, decisions for production process optimization does not directly lead to the desired results due to the lack of stably labeled data.

To solve this problem the concept of qualitative labeling has been introduced. The approach that combines key performance indicator (KPI) driven optimization with goal conflict-based clustering is the core component of a machine learning method that has already proven its value in an industrial environment under the name Deep Qualicision.

Autotuning in Machine Learning in Viya-Release of SAS

Ulrich Reincke
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The Viya release from SAS (cloud-capable, in-memory, parallelized, multi-API) provides a new hardware architecture for autotuning of machine learning algorithms. Autotuning means training a universe of model parameterizations and data partitions in automatic test series. The efficiency of these test series is driven by genetic algorithms and design of experiments, leading to improvements in ROC, lift, or misclassification rates. The result translates directly into reduced error rates, increased campaign response rates and increased customer value. The presentation provides an example of Gradient Boosting, and a final profit calculation on the basis of a concrete example. Finally we will discuss one of the most common mistakes in predictive modeling: the often neglected operationalization of the model score code, which leaves many theoretically profitable machine learning applications of innovative data science departments in the study or experimental stage.

Optimization Challenges in AI Systems for Materials Research

Dr. Hergen Schultze
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An Artificial Intelligence (AI) system is able to perceive its environment, to process the perceived, to independently solve problems, to make decisions, to act and to learn from the consequences of these decisions and actions. In BASF research we are discovering and developing new materials with tailored application properties based on the molecular ingredients and the process conditions the materials are synthesized, formulated, and applied. To create such systems and to include AI into the materials research workflow we collaborate with lab automation engineers. In the real world, learning from data and making decisions about experiments is especially hard as data is expensive, still erroneous and decisions have direct real world consequences. In our talk we share our vision, highlight the challenges, and focus on how to compute decisions in such an environment. Machine learning models such as Gradient Boosted Trees or Gaussian Processes lead to mixed-integer or Bayesian optimization problems. We report about work we are doing in close collaboration with Prof. Misener at Imperial College or Dr. Bortz at Fraunhofer ITWM.

Deep Learning Assisted Heuristic Tree Search for Container Pre-Marshalling

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The container pre-marshalling problem (CPMP) is concerned with the re-ordering of containers in container terminals during off-peak times so that containers can be quickly retrieved when the port is busy. The problem has received significant attention in the literature and is addressed by a large number of exact and heuristic methods. Existing methods for the CPMP heavily rely on problem-specific components (e.g., proven lower bounds) that need to be developed by domain experts with knowledge of optimization techniques and a deep understanding of the problem at hand. With the goal to automate the cost and time-intensive design of heuristics for the CPMP we propose a new method called Deep Learning Heuristic Tree Search (DLTS). It uses deep neural networks to learn solution strategies and lower bounds customized to the CPMP solely through analyzing existing (near-) optimal solutions to CPMP instances. The networks are then integrated into a tree search procedure to decide which branch to choose next and to prune the search tree. DLTS produces the highest quality heuristic solutions to the CPMP to date with gaps to optimality below 2% on real-world sized instances.