Decision making and uncertainty

5th Summer School of the IMPRS for Advanced Methods in Process and Systems Engineering (IMPRS ProEng)

August 28 - September 1, 2017
in Magdeburg, Germany

IMPRS ProEng
International Max Planck Research School for Advanced Methods in Process and Systems Engineering
Magdeburg

As of August 24, 2017

International Max Planck Research School (IMPRS)
for Advanced Methods in Process and Systems Engineering
Max Planck Institute for Dynamics of Complex Technical Systems
Sandtorstraße 1, 39106 Magdeburg, Germany

http://www.mpi-magdeburg.mpg.de/imprs

Organizational issues

Venue

Max Planck Institute for Dynamics of Complex Technical Systems
Sandtorstraße 1
39106 Magdeburg
Germany

Registration open: 8:30 am – 9:00 am on Monday, August 28, 2017

Contact

Stephanie Geyer
Phone: +49 391 6110-461
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Office: S1.12 (South wing, 1st floor)

Internet access

Eduroam
Please use your eduroam account to access the internet.
https://www.eduroam.org/

MPI-Wifi
In case you are not able to use your eduroam account, please contact Stephanie Geyer for the MPI-Wifi.

UQLab/MATLAB

For the UQLab tutorial on Thursday you need Matlab with statistics toolbox. Please make sure that it is working.

You'll find the installation package for UQLab in our ownCloud. Link and password were sent to you via e-mail.

In case of problems, please contact Stephanie Geyer until Tuesday afternoon.

For participants without their own laptop we'll provide a fully equipped computer for the tutorial (two participants share one computer).

Organizational issues

Lunch

Lunch will be provided at Max Planck Institutes' cafeteria.

For better planning, please choose your preferred lunch until Monday 11:00 am.

There will be a flipchart in front of the seminar room to do that.

Monday, Aug 28, 2017	Clear onion soup with cheese croutons	Baked potatoes filled with cream cheese, cream sauce & salad	Chicken strips (Asian kind) with butter rice
Tuesday, Aug 29, 2017	Celery cream soup	Macaroni with leaf spinach & cheese sauce	Sausage hotpot with curry, French fries & salad
Wednesday, Aug 30, 2017	Vegetable broth with egg drop	Potatoes with mixed vegetables & sauce Hollandaise	Minced meat with mushed potatoes & coleslaw
Thursday, Aug 31, 2017	Broccoli cream soup	Spaghetti with vegetarian Bolognese & cheese	Goulash with beans and ham & potatoes with parsley
Friday, Sep 1, 2017	Chicken broth with egg & vegetable	Boiled eggs in mustard sauce, mushed potatoes & coleslaw	Smoked pork with lemon butter, potatoes with rosemary & salad

Scientific program at a glance

	Morning	Afternoon
Monday, Aug 28, 2017	9:15 – 12:45 **Sebastian Sager** (Otto-von-Guericke University) *"Mathematical Optimization for Clinical Decision Support"*	14:00 – 17:30 **Stratos Pistikopoulos** (Texas A&M) *"Multi-Parametric Model-based Optimization & Control"*
Tuesday, Aug 29, 2017	9:00 – 12:30 **Wolfram Wiesemann** (Imperial College Business School) *"Introduction to Robust Optimization"*	14:00 – 17:30 **Rolf Findeisen** (Otto-von-Guericke University) *"Control and Estimation of Systems under Uncertainty"*
Wednesday, Aug 30, 2017	9:00 – 12:30 **Angela Schoellig** (University of Toronto) *Using Bayesian Models to Make Informed and Safe Decisions Under Uncertainty*	13:30 – 15:00 **Peter M. Flassig** (Rolls-Royce Dtl. Ltd & Co KG) *"Optimization Under Uncertainties: Perspectives From a Jet Engine Manufacturer"*
Thursday, Aug 31, 2017	9:00 – 12:30 **Stefano Marelli** (ETH Zürich) *"Uncertainty quantification and reliability analysis in Engineering"*	14:00 – 16:30 **Stefano Marelli** (ETH Zürich) *"Tutorial: The (Matlab-based) uncertainty quantification software UQLab"*
Friday, Sep 1, 2017	9:00 – 12:30 **Ignacio E. Grossmann** (Carnegie Mellon University) *Title: Recent Theoretical and Computational Advances in the Optimization of Process Systems under Uncertainty*	

Monday | August 28, 2017

8:30	Welcome and Registration
9:00	**Opening of the Summer School** Andreas Seidel-Morgenstern Max Planck Institute for Dynamics of Complex Technical Systems
9:15	**Mathematical Optimization for Clinical Decision Support** Sebastian Sager Otto-von-Guericke University
10:45	*Coffee break*
11:15	**Mathematical Optimization for Clinical Decision Support** Sebastian Sager Otto-von-Guericke University
12:45	*Lunch*
14:00	**Multi-Parametric Model-based Optimization & Control** Stratos Pistikopoulos Texas A&M
15:30	*Coffee break*
16:00	**Multi-Parametric Model-based Optimization & Control** Stratos Pistikopoulos Texas A&M

Social Event

18:00	**Get-Together Barbecue** organized by the IMPRS PhD Students Meeting point: cafeteria area at the Max Planck Institute

Monday | August 28, 2017

Prof. Dr.-Ing. Andreas Seidel-Morgenstern
Spokesperson oft he IMPRS ProEng
Max Planck Institute for Dynamics of Complex Technical Systems

Prof. Dr. Sebastian Sager
Otto-von-Guericke University

Mathematical Optimization for Clinical Decision Support

We give an introduction into parameter estimation, experimental design, and online optimization methods for dynamic systems. We discuss what particular challenges arise in clinical practice, using the example of Acute Myeloid Leukemia. We focus on decision making under uncertainty for treatment schedules.

Prof. Stratos Pistikopoulos
Texas A&M

Multi-Parametric Model-based Optimization & Control

Model based multi-parametric programming provides a complete map of solutions of an optimization problem as a function of, unknown but bounded, parameters in the model, in a computationally efficient manner, without exhaustively enumerating the entire parameter space. In a Model-based Predictive Control (MPC) framework, multi-parametric programming can be used to obtain the governing control laws – the optimal control variables as an explicit function of the state variables. The main advantage of this approach is that it reduces repetitive on-line control and optimization to simple function evaluations, which can be implemented on simple computational hardware, such as a microchip, thereby opening avenues for many applications in chemical, energy, automotive, and biomedical equipment, devices and systems.

In this presentation, we will first provide a historical progress report of the key developments in multi-parametric programming and control. We will then describe PAROC, a prototype software system which allows for the representation, modelling and solution of integrated design, operation and advanced control problems. Its main features include: (i) a high-fidelity dynamic model representation, also involving global sensitivity analysis, parameter estimation and mixed integer dynamic optimization capabilities; (ii) a suite/toolbox of model approximation methods; (iii) a host of multi-parametric programming solvers (POP – parametric Optimization] for mixed continuous/integer problems; (iv) a state-space modelling representation capability for scheduling and control problems; and (v) an advanced control toolkit for multi-parametric/explicit MPC and moving horizon reactive scheduling problems. Algorithms that enable the integration capabilities of the systems for design, scheduling and control are presented along with applications in sustainable energy systems, process intensification, smart manufacturing and personalized healthcare engineering.

Tuesday | August 29, 2017

9:00	**Introduction to Robust Optimization** Wolfram Wiesemann Imperial College Business School
10:30	*Coffee break*
11:00	**Introduction to Robust Optimization** Wolfram Wiesemann Imperial College Business School
12:30	*Lunch*
14:00	**Control and Estimation of Systems under Uncertainty** Rolf Findeisen Otto-von-Guericke University
15:30	*Coffee break*
16:00	**Control and Estimation of Systems under Uncertainty** Rolf Findeisen Otto-von-Guericke University

Social Event

19:30	**Guided City Tour** through Magdeburg Meeting point: Monastery "Unserer Lieben Frauen" Regierungsstraße 4 in 39104 Magdeburg

Tuesday | August 29, 2017

Prof. Dr. Wolfram Wiesemann
Imperial College Business School

Introduction to Robust Optimization

Traditionally, uncertainty-affected decision problems are solved by modelling the uncertain problem data as random variables and subsequently discretising the outcomes of these random variables. Although this is a very natural approach, it has several shortcomings: it requires the exact specification of the underlying stochastic process (which is rarely available in practice), and it results in a curse of dimensionality for dynamic (multi-stage) problems, which implies that the computation times grow exponentially with problem size. In this lecture, we review the rapidly growing literature on robust and distributionally robust optimization, which aims to alleviate the aforementioned shortcomings. A robust optimization problem specifies an uncertainty set that contains all possible values for the uncertain problem parameters, and it seeks the best decision in view of the worst parameter realization. A distributionally robust optimization problem, on the other hand, specifies an ambiguity set that contains all possible probability distributions that could govern the uncertain problem parameters, and it seeks the best decision in view of the worst probability distribution. Topics covered include the reformulation and solution of static and dynamic (distributionally) robust optimization problems as well as discrete robust optimization.

Prof. Dr.-Ing. Rolf Findeisen
Otto-von-Guericke University

Control and Estimation of Systems under Uncertainty

The operation and monitoring of processes is often a challenging task due to the presence of uncertainties, disturbances, and wide variability of operational conditions. Furthermore, models used for design, monitoring and control are only an approximation of reality. We give an introduction and overview on different uncertainty descriptions. Furthermore, we outline how uncertainty and robustness can be considered in optimisation based control and estimation, with a special focus on predictive control. The introduction will be complemented by an introduction to predictive control and optimisation based estimation, setting the stage for robust formulations.

Wednesday | August 30, 2017	
9:00	**Using Bayesian Models to Make Informed and Safe Decisions Under Uncertainty** Angela Schoellig University of Toronto
10:30	*Coffee break*
11:00	**Using Bayesian Models to Make Informed and Safe Decisions Under Uncertainty** Angela Schoellig University of Toronto
12:30	*Lunch*
13:30	**Optimization Under Uncertainties: Perspectives From a Jet Engine Manufacturer** Peter M. Flassig Rolls-Royce Dtl. Ltd & Co KG
15:00	*Coffee break*

Social Event	
15:30	*Departure for excursion*
16:00	**Guided Canoe Tour** on the Elbe river Meeting point: Biber Kanutouristik, Schweizer Haus
19:30	**Conference Dinner** Restaurant „Die Kirche“ Alt Prester 86 in 39114 Magdeburg, phone: +49 391 53 53 352

Wednesday | August 30, 2017

Prof. Dr. Angela Schoellig
University of Toronto

Using Bayesian Models to Make Informed and Safe Decisions Under Uncertainty

Traditionally, planning, control and decision making algorithms have been designed based on a-priori knowledge about the system and its environment (including models of the system dynamics and characterizations of the environment). This approach has enabled successful system operation in predictable situations, where our models are a good approximation of the real system behavior. However, if detailed models are not available, control systems are typically designed to be conservative against the unknown, which may cause drastic performance losses. To achieve safe and efficient system behavior in the presence of uncertainties and unknown disturbances, we aim to enable systems to acquire knowledge during operation and adapt their behavior accordingly. The ultimate goal is to enable high-performance control with safety guarantees for uncertain systems leveraging data collected during operation.

Our work is motivated by applications in the field of robotics such as self-flying and self-driving vehicles. In contrast to their early industrial counterparts, these robots are envisioned to operate in increasingly complex and uncertain environments, alongside humans, and over long periods of time.

In this lecture, we will introduce Gaussian Processes (GPs) as a tool to model uncertainties and gradually learn unknown effects from data. We show how GPs can be combined with robust, nonlinear and predictive control approaches to achieve safe, high-performance system behavior. Examples include automatic, safe controller tuning for aerial vehicles and experience-based speed improvement for self-driving vehicles. The lecture will include two tutorial sections on GPs and safe Bayesian optimization.

Dr. Peter M. Flassig
Rolls-Royce Dtl. Ltd & Co KG

Optimization Under Uncertainties: Perspectives From a Jet Engine Manufacturer

Variations in the performance of engine parts could cause significant effort to be spend on concessions or re-design tasks. It is, therefore, of importance to consider uncertainties and variability to understand the implications of a varying, non-deterministic design and to consistently maintain high level of conformance to the design specifications, i.e. to obtain a robust and a reliable design.

As we know, one important step for aleatory uncertainty quantification is to analyze and quantify the variability of input data for a physical system such as an aero engine. For geometric variations as a result of manufacturing inaccuracies compressor or turbine aerofoils for example are scanned by optical measurement systems. Afterwards it is possible to reduced and map the obtained datasets to parameters of interests. Now, for non-intrusive uncertainty propagation in a probabilistic framework and for optimization under uncertainties the resulting sets of data need to be discussed and quantified from a statistical point of view. In particular this means to define (i) a valid pdf/cfd for each uncertain input parameter and (ii) a positive, semi-definite correlation matrix for example.

With regard to modelling of input uncertainties the talk will focus on general but, in particular, special aspects as well. Additionally, examples of robust design optimization applications for turbomachinery design problems will be presented.

Thursday | August 31, 2017	
9:00	**Uncertainty quantification and reliability analysis in Engineering** Stefano Marelli ETH Zürich
10:30	*Coffee break*
11:00	**Uncertainty quantification and reliability analysis in Engineering** Stefano Marelli ETH Zürich
12:30	*Lunch*
14:00	**Tutorial: The (Matlab-based) uncertainty quantification software UQLab** Stefano Marelli ETH Zürich
15:00	*Coffee break*
15:30	**Tutorial: The (Matlab-based) uncertainty quantification software UQLab** Stefano Marelli ETH Zürich

Thursday | August 31, 2017

Dr. Stefano Marelli & Prof. Dr. Bruno Sudret
ETH Zürich

Uncertainty quantification and reliability analysis in Engineering

Uncertainty quantification (UQ) has gained momentum in the last decades as a staple topic in engineering sciences, especially in the design and optimization of complex structures and systems. Modelling such structures is nowadays possible with an unprecedented degree of fidelity, but the associated computational costs is often large, even when advanced highperformancs-computing facilities are taken into account. Even more so, time and cost constraints of industrial projects allow the engineers to run at most a few hundred to a thousand simulations, thus excluding the adoption of standard Monte Carlo techniques.

Advanced uncertainty quantification methods focus therefore on non-intrusive (i.e. that don't require the availability of the modelling tools source codes) and parsimonious (i.e. using as few model runs as possible) techniques that are capable of dealing with problems with many input variables.

Lecture 1: Sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis

In the first lecture a general framework for UQ in engineering applications is introduced. Polynomial chaos expansions (PCE) and recent advances in sparse representations are presented to compute at low cost the PDF and moments of quantities of interest (QoI). Global sensitivity analysis (Sobol' indices), which aims at reducing the complexity of a computational model by determining which input parameters drive the uncertainty of the QoI is then introduced. It is shown how sparse PCEs allow for an efficient estimation of Sobol' sensitivity indices.

Lecture 2: Reliability analysis for engineering systems

One of the important questions addressed by engineers is to evaluate the probability that a system of interest fails to fulfill some performance criterion due to uncertainties in its manufacturing properties or operating conditions. Computing such a probability of failure is also known as rare event simulation, since it is expected to be extremely small, say 10-6 - 10-3. In this lecture classical methods referred to as structural reliability methods are first introduced. Recent developments based on the use of Gaussian process modelling (a.k.a. Kriging) in conjunction with active learning algorithms in the context of rare-event simulation are then presented.

Tutorial: UQLab

In this tutorial the (Matlab-based) uncertainty quantification software UQLab (www.uqlab.com) will be used to allow the students to get familiar with the different methods presented in the two lectures. Accordingly, the tutorial will be split into two parts, focusing on the use of PCE for sensitivity analysis and on the use of advanced reliability methods.

Friday | September 1, 2017	
9:00	**Recent Theoretical and Computational Advances in the Optimization of Process Systems under Uncertainty** Ignacio E. Grossmann Carnegie Mellon University
10:30	*Coffee break*
11:00	**Recent Theoretical and Computational Advances in the Optimization of Process Systems under Uncertainty** Ignacio E. Grossmann Carnegie Mellon University
12:30	**Conclusion of the 5th IMPRS Summer School** Andreas Seidel-Morgenstern Max Planck Institute for Dynamics of Complex Technical Systems

Friday | September 1, 2017

Prof. Ignacio E. Grossmann
Carnegie Mellon University

Recent Theoretical and Computational Advances in the Optimization of Process Systems under Uncertainty

Optimization under uncertainty has been an active and challenging area of research for many years. However, its application in Process Synthesis has faced a number of important barriers that have prevented its effective application. Barriers include availability of information on the uncertainty of the data (ad-hoc or historical), determination of the nature of the uncertainties (exogenous vs. endogenous), selection of an appropriate strategy for hedging against uncertainty (robust optimization vs. stochastic programming), handling of nonlinearities (most work addresses linear problems), large computational expense (orders of magnitude larger than deterministic models), and difficulty in the interpretation of the results by non-expert users.

In this lecture, we describe recent advances that address some of these barriers. We first describe the basic concepts of robust optimization, including the robust counterpart, showing its connections with semi-infinite programming. We also we explore the relationship between flexibility analysis and robust optimization for linear systems. A historical perspective is given, which shows that some of the fundamental concepts in robust optimization have already been developed in the area of flexibility analysis in the 1980s. We next consider two-stage and multi-stage stochastic programming in the case of exogenous parameter, for which we describe acceleration techniques for Benders decomposition, hybrid sub-gradient/cutting plane methods for Lagrangean decomposition, and sampling techniques. We then address the generalization to the case of both exogenous and endogenous parameters, which gives rise to conditional scenario trees for which theoretical properties are described to reduce the problem size. To avoid ad-hoc approaches for setting up the data for these problems, we describe approaches for handling of historical data for generating scenario trees. Finally, we illustrate the application of each of these formulations in demand-side management optimization, planning of process networks, chemical supply chains under disruptions, planning of oil and gas fields, and optimization of process networks, all of them under some type of uncertainty.

Social program

Monday: Barbecue at Max Planck Institute, 6:00 pm

Tuesday: Guided City Tour through Magdeburg from Kloster Unserer Lieben Frauen, 7:30 pm

Wednesday: Canoe Tour on the Elbe river, 4:00 pm
Conference Dinner Restaurant „Die Kirche“, 7:30 pm