Mathematical Algorithmic Optimization

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Areas of Research

The research group MathOpt is embedded in the Faculty of Mathematics at the Otto-von-Guericke-University Magdeburg.

Active research fields include

- direct methods for optimal control,
- mixed-integer optimal control,
- real-time optimization,
- stochastic optimization,
- mixed-integer nonlinear programming.

The main focus of the group is on the application driven development of optimization methods, and their efficient implementation on computers. We believe in the potential of multi-disciplinary cooperation between partners with a profound disciplinary expertise and value the mutual benefit for both sides: novel, innovative approaches and insights in the application field by means of optimization; and a demand/feedback effect that stimulates the development of new methodologies in applied mathematics. Our main application areas are

- automotive engineering,
- chemical engineering,
- economics,
- medicine,
- the psychology of decision making,
- systems biology.

Challenging problems in these areas are treated in interdisciplinary cooperations with scientists from academia and industry.

Members of the group have been involved in industrial projects, e.g., with Daimler, Lufthansa, and BASF. Industrial relevance of our mathematical and computational optimization algorithms is of utmost importance, and we are open for new collaborations. In the following we present some exemplary projects.

Projects

Mixed-integer optimal control

Mixed-integer optimal control problems (MIOCPs) in differential equations have gained increasing interest over the last years. This is probably due to the fact that the underlying processes have a high potential for optimization. Typical examples are the choice of gears in transport or processes in chemical engineering involving on-off valves. However, they combine discrete, nonlinear, and dynamic aspects, and require thus new theory and methods.

Direct methods, in particular all-at-once approaches like the direct multiple shooting method, have become the methods of choice for most practical control problems. In direct methods infinite-dimensional control functions are discretized by basis functions and corresponding finite-dimensional control values that enter into the optimization problem. The drawback of direct methods with binary control functions obviously is that they lead to high-dimensional vectors of binary variables.

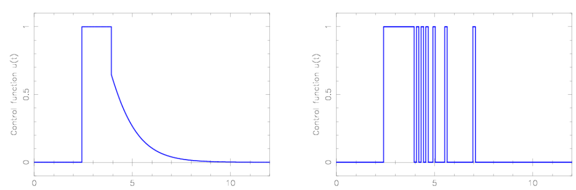

Fig. 1 Control functions, plotted over time. **Left:** Optimal, but relaxed non–integer solution. **Right:** Integer, but suboptimal solution. We develop methods to get integer solutions plus error estimates for the performance loss.

We propose to use an outer convexification with respect to the binary controls. This allows to exploit the advantages of direct methods to efficiently solve non–integer control problems, but provides accurate error estimates on the performance loss of a suboptimal integer solution compared to the optimal one.

Optimal Control in Automotive Engineering

We are interested in the modeling, simulation, and optimization of driving. If energy- or time-optimal driving strategies are to be determined, the gear shifts have an important impact. As stated before, standard approaches to discretize the control problem and to solve a mixed-integer nonlinear program will work only on limited and small time horizons because of the exponentially growing complexity of the problem.

Recent work lead to a tremendous speedup of several orders of magnitude in computational times to obtain optimal solutions, allowing for more complex scenarios. We extended a benchmark mixed-integer optimal control problem to a more complicated case in which a periodic solution on a closed track is considered. Our generic solution approach is based on a convexification and relaxation of the integer control constraint. It may also be used for other objectives, such as energy minimization.

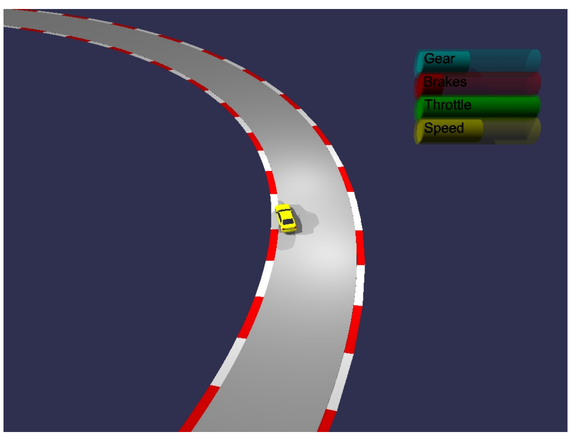

Fig. 2 Visualization of a car driving in a time-optimal way on the virtual racing track. Provably optimal gear shifts are of special interest.

Current work focuses on further speedup, on providing feedback controls (involving gear shifts!) in real-time, and on more detailed mathematical models.

Optimal Control in Chemical Engineering

Many complex processes in chemical engineering involve valves that are either open or closed. Mathematically, valves are binary control functions, hence functions that are either zero or one at any given time. We develop numerical methods for applications such as distillation columns or simulated moving bed processes in which switching by means of valves occurs. Special focus is given on a) start-up procedures of continuous processes or b) periodic operation.

Optimal Control in Systems Biology

Self-organized rhythmic processes are encountered at all levels in cell biology and are a subject of great interest for both biological and mathematical research communities.

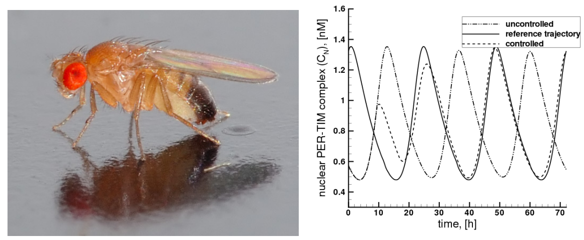

Fig. 3 **Left:** Drosophila melanogaster. Biological rhythms of fruit flies are well understood. **Right:** Simulated phase resetting achieved by an external stimuli that is calculated as the solution of an optimal control problem.

Biological systems are open and kept far from equilibrium by fluxes of matter and energy. For these reasons, the systems are always exposed to external perturbations and the balance between robustness and sensitivity to external stimuli is a crucial issue.

We are interested in particular dynamical properties and structures that occur in the formulation of optimal control problems in the context of

- chemotherapies,
- circadian rhythms,
- signaling pathways.

A special focus is given to integer formulations of possible medical treatments that stem from practical limitations, such as a minimum number of hospital visits.

The Psychology of Human Decision Making

Psychological research that is based on computer-supported tests has been making great progress over the last years, especially in the analysis of human decision making. However, sensitivity information is needed to locally and globally analyze the exact situations and decisions that led to a bad or good overall performance of test persons.

A second important question concerns performance. For many complex scenarios the choices made by humans can only be compared to one another, but not to the optimal solution, as it is unknown. We want to resolve the open scientific question how much and in which situations optimization methods outperform human decisions. Both questions are addressed in an interdisciplinary project.