Advances in Methods for Optimum Experimental Design

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Abstract: Mathematical-physical models are crucial for the simulation and optimization of complex chemical processes. Usually, such models consist of differential equation systems which are nonlinear in states, parameters and controls. Only models which have been validated against experimental data provide reliable descriptions of the processes. Optimum experimental design is used to plan experiments which yield minimal model uncertainty at given experimental effort and under given experimental constraints.

This task leads to intricate non-standard constrained optimal control problems minimizing functionals on the variance covariance matrix of a parameter estimate. Our numerical solution methods are based on the direct approach of optimal control, nonlinear programming methods with structure exploiting linear algebra and a tailored derivative evaluation. Recently a formulation has been found which allows to apply multiple shooting techniques.

As first talk in the minisymposium on experimental design, this talk will introduce the formulation of experimental design problems and give an overview on solution approaches and application scenarios.

Then recent advances in the development and application of experimental design methods will be discussed. Numerical results will be illustrated by examples from chemical engineering.

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