Numerical Methods and Software for Nonlinear Optimum Experimental Design Problems

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Abstract: We use nonlinear differential algebraic equation systems (DAE) to model dynamic processes, e. g. from chemical reaction kinetics or chemical engineering. To obtain realistic process simulations the models have to be validated by estimating the unknown values of the model parameters from experimental data.

The statistical quality of the estimate depends on the experimental setup and the experimental processing and can be described by the variance-covariance matrix. Minimizing a suited function on it leads to complex non-standard optimal control problems. Special challenges are the intricate objective function which depends implicitly on derivatives of the parameter estimation problem, state constraints, and the integrality of a part of the variables. We present numerical approaches to treat these difficulties, including the direct approach for optimal control, methods of sequential quadratic programming, and a tailored computation of the required first and second derivatives. We exploit the problem structures given by multi-experiment formulations.

As a consequence of the nonlinearity of the models, the variance-covariance matrix depends on the values of the model parameters. We employ a worst-case formulation to achieve robustness of the experimental design with respect to parameter uncertainty.

Numerical results of the application of our methods — implemented in the software packages VPLAN — to processes from chemical industry show a high potential for saving experimental expenses. Selected examples are presented in the talk.

References:

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