# Numerical Solution of Large-Scale Optimal Control Problems in Robust Optimum Experimental Design

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**Abstract:** Estimating model parameters from experimental data is crucial to reliably simulate dynamic processes. In practical applications, however, it often appears that the experiments performed to obtain necessary measurements are expensive, but nevertheless do not guarantee sufficient identifiability. The optimization of one or more dynamic experiments in order to maximize the accuracy of the results of a parameter estimation subject to cost and other technical inequality constraints leads to very complex non-standard optimal control problems: find control variables $\xi$ that minimize a function $\varphi$ of a covariance matrix

$$\min_{\xi} \quad \varphi(C(x,p,\xi))$$

such that state variables $x$, parameters $p$ and control variables $\xi$ satisfy DAE model, control constraints

$$c_1(\xi) \geq 0 \quad \text{or} \quad = 0$$

and state constraints

$$c_2(x,p,\xi) \geq 0.$$

One of the difficulties is that the objective function is a function of a covariance matrix and therefore already depends on a generalized inverse of the Jacobian of the underlying parameter estimation problem. Another difficulty is that the optimization results depend strongly on the assumed values of parameters which are only known to lie in a - possibly large - confidence region. Hence, robust optimal experiments are required that solve worst-case (min-max) optimization problems

$$\min_{\xi\in\Omega} \max_{\|\Sigma(p-p_0)\|\leq\gamma} \varphi(C(x,p,\xi)).$$

We suggest new efficient solution methods for such problems. Numerical results for real-life applications from chemistry and chemical engineering will be presented.

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