

# Numerical Methods of Optimum Experimental Design Based on a Second-Order Analysis of Parameter Estimates

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**Abstract:** A successful application of model-based simulation and optimization of dynamic processes requires an exact calibration of the underlying mathematical models. Here, fundamental tasks are the estimation of unknown model coefficients by means of real observations and design of optimal experiments.

After an appropriate numerical treatment of the differential systems, the parameters can be estimated as the solution of a finite dimensional nonlinear constrained parameter estimation problem. Due to the fact that the measurements always contain defects, the resulting parameter estimate cannot be seen as an ultimate solution and a sensitivity analysis is required, to quantify the statistical accuracy. The goal of the design of optimal experiments is the identification of those measurement times and experimental conditions, which allow a parameter estimate with a maximized statistical accuracy. Also the design of optimal experiments problem can be formulated as an optimization problem, where the objective function is given by a suitable quality criterion based on the sensitivity analysis of the parameter estimation problem. Usual choice is a function of a covariance matrix.

In this talk we present a new objective function, called the Q-criterion, which is based on a second order sensitivity analysis of parameter estimates. The robustness properties of the new objective function in terms of parameter uncertainties is investigated and compared to a worst-case formulation of the design of optimal experiments problem. It is revealed that the Q-criterion covers the worst-case approach of the design of optimal experiments problem based on the A-criterion. Moreover, the properties of the new objective function are considered in several examples. Here, it becomes evident that the Q-criterion leads to a drastic improve of the Gauss-Newton convergence rate for the underlying parameter estimation problems.

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