

A Higher Order Sensitivity Analysis of Parameter Estimation Problems and its Effect on the Design of Robust Optimal Experiments

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Abstract: The use of computerized simulation to gain knowledge of unknown phenomena and process behaviors is a challenging task in many natural sciences. In order to get a full description of an underlying process, a basic issue is to identify unknown parameters. Basically one estimates these by minimizing the difference between the model response and the measurements. The measurements can be obtained as a result of experiments and always contain defects. Thus the whole system is affected by errors and a sensitivity analysis is necessary. Usually one applies linear confidence regions to determine the statistical accuracy of the solution to parameter estimation problems. But in particular in highly nonlinear cases this may cause problems and linearized regions are not adequate.

To counteract this, we will define a quadratic approximation of confidence regions. The new region is based on a second order representation of the parameter vector depending on the measurement errors. We will see that bounds of the quadratically approximated region can be represented by two Lipschitzians κ and ω , which were introduced by H.G. Bock to formulate a local convergence theorem of the Gauss-Newton method. The Lipschitzian κ is the asymptotic convergence rate and ω is a measure of the curvature of the problem. Furthermore, we will describe how to integrate the new information into robustification of optimum experimental design. It will especially be shown that a robust design of experiments performed by a worst-case design already contains components of the quadratic approximation of confidence region.

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