Numerical Methods for Nonlinear Experimental Design

Stefan Körkel and Ekaterina Kostina

Interdisciplinary Center for Scientific Computing, University of Heidelberg
Im Neuenheimer Feld 368, D-69120 Heidelberg, Germany
stefan@koerkel.de*
ekaterina.kostina@iwr.uni-heidelberg.de

Summary. Nonlinear experimental design leads to a challenging class of optimization problems which occur in the procedure of the validation of process models. This paper discusses the formulation of such problems for a general class of underlying process models, presents numerical methods for the solution and shows their successful application to industrial processes.

Key words: experimental design, parameter estimation, variance-covariance matrix, multiple experiments, nonlinear constrained optimization

1 Introduction

To obtain reliable simulations of dynamic processes, e.g. in physics, chemistry, biology, or engineering, good models of the processes are required. A promising approach is to use models based on laws of nature. Usually the model equations contain quantities whose values are known only very roughly, we call them parameters. They may appear in a highly nonlinear way. To determine their values, experiments are carried out and the resulting data is analyzed by the method of nonlinear parameter estimation. The statistical reliability of the estimates can be described by confidence regions and the variance-covariance matrix. Data from numerous and costly experiments are required to obtain reliable parameter estimates.

Our aim is to design experiments whose data yield parameter estimates with maximal statistical reliability. For this purpose, we minimize functionals on the variance-covariance matrix subject to given constraints on operability and costs. The dynamic process model appears as constraint of this nonlinear optimization problem.

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We formulate the class of nonlinear optimum experimental design problems for a general class of process models. We present suited numerical methods for the solution of these intricate problems and apply them to practical processes from industry. Computational results show that enormous savings of experimental costs are possible by the application of our methods.

1.1 Structure of this Paper

This paper opens with a short overview on previous work. Then we present the general problem statement for the class of parameter estimation and experimental design problems we consider. We discuss the numerical difficulties these problems contain and give numerical strategies to solve them. We give a short description of our software package VPLAN where these strategies are implemented. And finally we present numerical results from industry application problems treated by our methods.

1.2 Overview on Previous Work

Experimental design for linear models is well established and discussed e.g. in the text books of Fedorov [11], Atkinson and Donev [1] or Pukelsheim [22]. But for many processes a description which is valid over a higher range requires nonlinear models. Nonlinear experimental design for examples with small nonlinear equation systems has been investigated e.g. by Haines [14], Rudolph and Herrendörfer [25] and Doví, Reverberi and Acevedo-Duarte [10]. Reilly, Bajramovic, Blau, Branson and Sauerhoff [24], Qureshi, Ng and Goodwin [23] and Oinas, Turunen and Haario [21] treat very small special dynamic processes which allow an analytic solution of the differential equations. Lohmann, Bock and Schlöder [19] present a numerical method for experimental design for ordinary differential equations which leads to a simplified formulation, because only the sampling design is optimized. Baltes, Schneider, Sturm and Reuss [9] use a simple search method for the optimization of a nonlinear experimental design problem for a special process. Until our work, a method which allows the efficient numerical solution of a general class of optimum experimental design problems for nonlinear dynamic process models is missing.


2.1 Process Model

The processes we want to treat in this paper are dynamic or stationary, homogeneous or inhomogeneous deterministic systems. We describe their states