Covariance Matrix Computation for Parameter Estimation in Nonlinear Models Solved by Iterative Linear Algebra Methods

E. A. Kostina[1]

Minisymposium: Inverse Problems and Optimization

Abstract: For solving constraint parameter estimation and optimal design problems, we need the knowledge of covariance matrix of the parameter estimates and its derivatives. So far numerical methods for parameter estimation and optimal design of experiments in dynamic processes have been based on direct linear algebra methods for computing the covariance matrix and its derivatives. The direct methods are variants of Gaussian elimination and involve an explicit matrix factorization for solving linear systems of equations. They were originally developed for systems of non-linear ODE or DAE where direct linear algebra methods are more effective for forward model problems than iterative methods. On the other hand, for very large scale constrained systems with sparse matrices of special structure, e.g. originating from discretization of partial differential equations, direct linear algebra methods as based on Gauss elimination or orthogonal decompositions are not competitive with iterative linear algebra methods even for forward models. Hence, in case of parameter estimation in PDE models, generalizations of iterative linear algebra methods to the computation of the covariance matrix and its derivatives are crucial for practical applications and this defines the topic of this talk. One of the intriguing results presented in the talk is that solving nonlinear constrained least squares problems by Krylov type methods (conjugate gradient and LSQR) we get as a by-product (practically for free) the covariance matrix and confidence intervals as well as their derivatives.

The talk is besed on joint work with H. G. Bock, O. Kostyukova, I. Schierle and M. Saunders.

[1] Department of Mathematics and Computer Science
University of Marburg
Hans-Meerwein-Straße
35032 Marburg
kostina@mathematik.uni-marburg.de