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Peter Hemker, Stichting Mathematisch Centrum, Amsterdam:

"Nonlinear parameter estimation in initial value problems".

ABSTRACT

A clear recognition of the underlying methodology is a prerequisite for the proper estimation of parameters in scientific models. The notions of consistency and uniqueness can be instrumental in this respect. When experimental data are analysed, in advance a model of the system under investigation has to be known only with a finite number of degrees of freedom. Now a model is called consistent with respect to a set of experimental data if no discrepancy exists between data and model. In general a model will be consistent for parameter values from a subset of the a priori allowed parameter set. A model is unique if all parameters are determined by the data, such that there is no freedom left in the model. It is fundamental that one never can prove a model to be the correct one. However there is the possibility to reject the wrong ones: from a correct operational model (i.e. a model which is consistent and unique) it should be possible to predict future behaviour. Specially, in this light it is clear that not only estimates of the parameters have to be determined, but also estimates of their reliability.

The estimation of a set of parameters is reduced to the solution of a nonlinear least squares problem as follows. Let be given a set of experimental data $\{(t_i, y_i)\}$ – y_i represents the result of a measurement on (some component of) y at time t_i –, and let the model be given by the initial value problem

$$y'(t,p) = f(t,y,p) \,, \qquad y(0,p) = y_0(p) \,. \tag{1}$$

As an estimate of the parameter (vector) p is considered that value of p which minimizes

$$S(p) = \sum (y(t_i,p) - y_i)^2 = \|Y(p)\|^2 \,.$$

The minimization is performed by Marquardt's method.
This method requires values of $\partial y(t,p)/\partial p$, which are obtained by solving the additional set of differential equations

$$y_p'(t,p) = f_p(t,y,p) + f_y(t,y,p) \cdot y_p(t,p), \qquad y_p'(0,p) = \partial y_0(p)/\partial p. \tag{2}$$

The one-way coupling between the nonlinear I.V.P. (1) and this linear set of differential equations (2) is exploited by the use of implicit linear multistep methods (Adams-Moulton or Gear's stiffly stable methods, cf. [1]).

Marquardt's method is realized by means of the singular value decomposition of the Jacobian matrizen $J = \partial y(t_i,p)/\partial p$; [cf. 2,3]. With $J = U \wedge V^T$ the iteration process becomes

$$p^{(n+1)} = p^{(n)} - V(\wedge^2+\lambda)^{-1} \wedge U^T Y(p^{(n)})$$

with some $\lambda = \lambda^{(n)} > 0$.
Initial estimates can be obtained in the usual way (i.e. from steady states or from raw estimates of derivatives) or by combining the parameter estimation process with multiple shooting.

The singular values $\wedge$ and the corresponding columnvectors of V (eigenvectors of J^TJ) yield important information about correlations between the different parameters. These matrices, together with the vector of residuals Y(p), enable us to a certain extend to judge of the consistency, uniqueness and accuracy of the parameters determined.

A program for the determination of parameters in initial value problems is described in [1]. A revised version will become available in [2] and will be described in detail by Van Domselaar [4].

References

[1] P.W. Hemker. Parameter estimation in nonlinear differential equations. Mathematical Centre report MR 134/72.

[2] NUMAL, a library of numerical procedures in ALGOL 60. (P.W. Hemker, W. Hoffmann, P.J. v.d. Houwen and N. Temme eds.) Mathematical Centre, Amsterdam.

[3] J.C.P. Bus, B. v. Domselaar, J. Kok. Nonlinear least squares estimations. Mathematical Centre (to appear).

[4] B. v. Domselaar. Report on nonlinear parameter estimation in differential equations. Mathematical Centre, Amsterdam (to appear).