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METHODS FOR PARAMETER RANKING IN NONLINEAR, MECHANISTIC MODELS

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Abstract: The paper addresses efficient methods for parameter sensitivity analysis and ranking in large, nonlinear, mechanistic models requiring examination of many points in the parameter space. The paper shows how orthogonal decomposition and permutation of the sensitivity derivative is an intuitive and structured method for automatic ranking of the parameters within a candidate set. Provided the model error is Gaussian, and with the problem on a triangularized form, the additional variance associated with each parameter can easily be found. Ranking according to additional variance is therefore another option. The methods are tested on an industrially used simulator model. *Copyright © IFAC 2005*

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1. INTRODUCTION

Analysis of the sensitivity derivative of a model is a necessary step when designing model based parameter estimation algorithms. This paper addresses methods for efficient manual and automated sensitivity analysis for nonlinear models on the general form

$$\hat{y} = g(\theta, u)$$

where $\hat{y} \in \mathbb{R}^{n_y}$ is the model output vector, $\theta \in \mathbb{R}^{n_\theta}$ the parameter vector and $u \in \mathbb{R}^{n_u}$ is a measured input vector which may be present in the model. The sensitivity derivative of the model outputs to the parameter vector is defined as

$$S = W^{\frac{1}{2}} \frac{d\hat{y}(\theta, u)}{d\theta} \in \mathbb{R}^{n_y \times n_\theta}$$

where $W^{\frac{1}{2}}$ is a diagonal weighting matrix. Each column of the sensitivity derivative will express one parameter's sensitivity in all outputs, and can therefore be viewed as the sensitivity direction for the corresponding parameter.

The focus in this paper is on situations when the sensitivity derivative is on numerical form, as opposed to situations when an analytical expression for S can be found. Since the model is nonlinear, global identifiability can generally not be proven. To increase the probability that the model is identifiable over the whole parameter space, the sensitivity derivative must be checked for as many parameter vector values as possible. If the model is also nonlinear in the input vector u, then u will affect the sensitivity derivative, and S needs to be calculated for a wide range of values of u as well. This requires efficient automated sensitivity analysis methods.

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In sensitivity analysis, the following properties of the sensitivity derivative are of interest:

- Many large values in a column are an indication of high sensitivity to the corresponding parameter.
- Large differences in the norms of the columns indicate large differences in sensitivity or poor scaling.
- Degree of linear dependence between columns

Many linear transformations of S or $S\ S$ will reveal these properties. A search into relevant literature databases covering the control engineering domain verify that eigenvector transformation of $S\ S$ is the most commonly used method. Eigenvector transformation can be used for manual parameter ranking through ordering the eigenvalues of $S\ S$ according to size, and inspecting the corresponding eigenvectors to determine which parameters are the most significant contributors to this particular direction. Generally this may not be a trivial task since the eigenvector decomposition produces linear combinations of the original directions of the problem (columns of S).

A large condition number, $\kappa = \sqrt{\frac{\max eig(S'S)}{\min eig(S'S)}}$, indicates either weak individual sensitivity or linear dependence within S. Eigenvalue transformation can therefore be used for automatic ranking of the parameters, by removing (combinations of) columns from S and calculate the condition number of the corresponding sub-matrices of $S\ S$. As an automated method this will give a trial and error method.

An alternative method for automatic ranking proposed in this paper utilizes the original directions of S, and reduces the column space of S into an orthogonal set of vectors in a successive manner. This provides an intuitive and structured way of ranking the parameters and is carried out as follows. From the non-selected set of columns in S, select the column with the highest norm, form a unit vector, and remove this direction (by projection and subtraction) from the non selected set of columns. The procedure is repeated until all columns have been selected. The order of selection is stored in a permutation matrix. This economical QR decomposition with permutation of the sensitivity derivative will give a triangular form of $S\ S$. The same form can be found by LDL decomposition and permutation of $S\ S$. Successive orthogonalization with permutation is described by example in section 3 of this paper.

If the deviation between the actual and simulated output vectors, i.e. the model error $\varepsilon = y \quad \hat{y}(\theta)$, can be assumed to be a stochastic process with Gaussian properties, then $tr(S\ S)^{\ 1}$ gives an estimate of the lower limit of the parameter covariance (Söderström and Stoica 1989). (Berntsen 1977) showed that if $S\ S$ is already on a triangular form, a particularly easy form of the individual variance contribution of each parameter can be found, see section 4. This can be applied to an already ordered set of parameters or used as another method to rank the parameters.

Manual inspection of $S\ S$ can in simple cases give sufficient information to rank the parameters. Manual inspection is however also useful in more complex cases to gain initial insight into important features of the problem, and provide a basis to understand or second-guess the ranking done by automated procedures. A transformation of $S\ S$ which is particularly useful for manual inspection is presented in section 2.

All three methods have been applied to an example 21 6 sensitivity derivative in section 5. Manual inspection has been used initially to reveal the most important properties of the example matrix. Next, the parameters have been ranked through successive orthogonalization and by smallest additional variance. The methods have also been applied to a larger, industrial example, and the results of this analysis have been summarized in section 6. Conclusions are given in section 7.

2. MANUAL INSPECTION OF $S\ S$

In the following a transformation of $S\ S$ giving a particularly useful form for manual inspection, is demonstrated. The following is valid for any sensitivity derivative S with dimension $n_y \quad n_\theta$, $n_y \quad n_\theta$, but for pedagogical reasons, an n_y 3 matrix, $S = \begin{bmatrix} a & b & c \end{bmatrix}$, is used. a, b, c are the column vectors.

Cross multiplication of S gives

$$S\ S = \begin{bmatrix} a^{\ 2} & a, b & a, c \\ b, a & b^{\ 2} & b, c \\ c, a & c, b & c^{\ 2} \end{bmatrix}$$

where , denotes the inner product and the Euclidian norm of a vector. The squared norms on the diagonal give a measure of the total sensitivity of each individual parameter. Large inner products in the off diagonal elements indicate that the two vectors have large elements in the same places (linear dependence), and/or a large norm of the vectors involved. To separate the information about the impact of each individual parameter from the information about linear dependence, the norms $(S(i, i) > 0)$ are extracted and $S\ S$ to written on the form shown in equation (1).

In (1) the first and last matrices contain information about the "strength" of each parameter, as sensitivity vector length. The off diagonal terms of the middle matrix can be recognized from the