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Abstract

The identifiability problem that rises in mixed numerical-experimental problems is one of the most important issues if an experiment has to be designed for the quantification of material parameters. This paper focuses on the relation between various aspects of an experiment and the condition number of the information matrix used in gradient algorithms for the parameter estimation. The initial estimate of the parameter sets permits to indicate whether or not the designed experiment provides the required information. A comparison is made for a tensile specimen and a bend specimen, where different types of measurements are simulated. Various aspects influence the optimal relation between an experiment and a numerical model. The proper analysis of this relationship permits the optimization of the design of an experiment.

1 Introduction

Amongst other methods, the parameters used in numerical models can be properly identified by means of mixed numerical-experimental techniques. Commonly, experimental results and computational simulations are combined in order to minimize an objective function, which should lead to the best agreement between measurements and computations, see Beck and Arnold[1], Draper and Smith[2], Sol and Oomens[3], Meuwissen et al.[4]. This minimization process is often troublesome and convergence may occur to different minima starting from different initial estimates. A troublesome convergence of the estimation process may be due to model errors, measurement errors, an inappropriate objective function or an experiment that does not sufficiently trigger all the material nonlinearities. The latter problem

is related to the question of identifiability and estimability. The lack of identifiability, which is generally due to the existence of multicollinearity, should be investigated in view of the design of the experiment. Several examples are available in literature, especially for linear models, e.g., Hinkelmann and Kempthorne[5], Norton[6], Pukelsheim[7].

In the case of highly nonlinear material behaviour, such an identification analysis becomes particularly difficult. The complete experimental setup, i.e. the geometry of the test specimen, the boundary and loading conditions, the measurement technique and the point(s) of measurement, must be evaluated on beforehand in order to make sure that the proposed experiment provides the required data to identify the parameters accurately. Many experiments are not optimized in the sense that the measurements are not carried out at the right place on the test specimen or the provided data does not allow to identify all parameters independently. A preliminary identification analysis permits to assess whether an experiment provides the requested data. In such an analysis, it is assumed that the computational model is the perfect model for the investigated material. Even in the absence of model errors, an estimation procedure may be troublesome. It is therefore necessary to resolve the identifiability problem completely in this ideal case. Real applications inevitably involve measurements and model errors and the combination of these errors with the presence of multicollinearity may have a baleful influence on the mixed numerical-experimental procedure.

The theory of optimum experimental design[7;8] provides useful answers for many case problems. However, the nonlinear identification of material parameters presents problems which are difficult to cope with. This contribution illustrates that the design of an experiment may have an important influence on the efficiency of mixed numerical-experimental methods. Attention is focused on the efficiency of the experiment, and the influence of measurement errors on the condition of the information matrix. Two problems will be addressed. The first problem is essential in the mixed numerical-experimental optimization procedure. Since measurements of different nature with different dimensions are performed, and since the unknown material parameters also differ in scale and units, it is essential to rephrase the problem in a dimensionless format. On the basis of these dimensionless parameters and measurements a second topic will be treated. For this purpose, an analysis of multicollinearity is carried out, where the influence of the notch depth of a bend specimen, the influence of different types of measurements as well as the location of the measurement points is scrutinized.

2 Optimization of the information matrix used in mixed numerical-experimental methods

An important problem that arises in mixed numerical-experimental methods is the dimensional and scale incompatibility of the material parameters and measured quantities. This section proposes a dimensionless rescaling of the basic estimation problem which is optimized for the condition number of the information matrix.

This step is both important for the iterative parameter estimation procedure and for the identifiability question. This problem has to be treated before the proper analysis of the experiments, since it reflects the procedure experimental information is being dealt with.

2.1 Identifiability of a parameter set

Assume that an experiment is carried out in view of the estimation of a parameter set $\underset{\sim}{\theta}$ of a nonlinear constitutive model for a given material. The measured response from the experiment is stored in a column $\underset{\sim}{m}$, which may contain forces, displacements or other measured quantities. The predicted response of the computational model is given by $\underset{\sim}{h}$, where the computation has been synchronized with the experiment through the use of prescribed forces or displacements.

Mixed numerical-experimental techniques are used to determine the set of parameters $\underset{\sim}{\theta}$ for which the model response $\underset{\sim}{h}(\underset{\sim}{\theta})$ provides the closest fit to the measurements $\underset{\sim}{m}$. Commonly, an objective function is defined to quantify the quality of the fit[1;9]. In the present paper, a quadratic objective function $J(\underset{\sim}{\theta})$ is adopted

$$J(\underset{\sim}{\theta}) = [\underset{\sim}{m} - \underset{\sim}{h}(\underset{\sim}{\theta})]^T \underline{V} [\underset{\sim}{m} - \underset{\sim}{h}(\underset{\sim}{\theta})] \tag{1}$$

The matrix $\underline{V}$ is a positive definite symmetric weighting matrix. The Gauss-Markov estimator is retrieved if the diagonal terms of $\underline{V}$ equal 1 over the variances of the different measurements. If $\underline{V}$ is omitted, a classical least-squares estimator is obtained. The unknown parameters $\underset{\sim}{\theta}$ are determined by minimizing the objective function $J(\underset{\sim}{\theta})$. A classical method to accomplish this minimization is a Gauss-Newton gradient algorithm which leads to an iterative solution of the estimation problem. Details of this algorithm can be found in literature[1]. Other frequently used techniques are given by the method of steepest descent or the Levenberg-Marquardt method.

The iterative update of the parameters $\underset{\sim}{\theta}$ is given by:

$$\delta\underset{\sim}{\theta} = \left[\underline{S}^T \underline{V} \underline{S}\right]^{-1} \left[\underline{S}^T \underline{V} (\underset{\sim}{m} - \underset{\sim}{h})\right] \tag{2}$$

In here, $\underline{S}$ represents the sensitivity matrix which is defined by

$$\underline{S}(\underset{\sim}{\theta}) = \frac{\partial \underset{\sim}{h}(\underset{\sim}{\theta})}{\partial \underset{\sim}{\theta}}. \tag{3}$$

The sensitivity matrix can be computed in a semi-analytical manner[10] or by a finite difference scheme[4].

In analogy to regression problems the matrix $\underline{C}$ given by

$$\underline{C} = \underline{S}^T \underline{V} \underline{S} \tag{4}$$

can be called the information matrix of the nonlinear estimation problem. The condition of this information matrix is a generally accepted indicator for the identifiability of the problem[1].

The entire iterative estimation procedure is started from an initial estimate $\underset{\sim}{\theta}^{(0)}$ of the parameters. The condition of the information matrix will next be analysed in the vicinity of this initial estimate. Evidently, the conclusions from such an analysis do not apply to the whole range of admissible values of the parameters $\underset{\sim}{\theta}$, but an ill-conditioned information matrix at the initial estimate may drive the entire parameter identification to a bad convergence and additional non-unique solutions. The condition of the information matrix has been intensively studied in regression problems[11]. In a linear regression problem, the parameters have to be determined from a set of measurements according to

$$\underset{\sim}{m} = \underline{S}\,\underset{\sim}{\theta} \tag{5}$$

where the sensitivity matrix $\underline{S}$ is a constant matrix. The least squares solution is then given by

$$\underset{\sim}{\theta} = \underline{C}^{-1}\,\underline{S}^T\,\underset{\sim}{m} \tag{6}$$

$$\underline{C} = \underline{S}^T\,\underline{S} \tag{7}$$

which is similar to the linearized equation (2) for the iterative correction $\delta\underset{\sim}{\theta}$ in the case $\underline{V} = \underline{I}$. The condition of the information matrix can be investigated in various ways. The determinant of $\underline{C}$ has to be large, but its value totally depends on the scale of the parameters and measurements. A more efficient method is based on an eigenvalue analysis of the information matrix $\underline{C}$. The ratio of the largest eigenvalue λ_{max} to the smallest eigenvalue λ_{min} is a good measure of multicollinearity, which is called the condition number of $\underline{C}$. The condition number does not change if the entire sensitivity matrix is multiplied by a constant. The larger the value of the condition number, the greater the degree of multicollinearity. It is generally accepted that a condition number less than 100 poses little problem with multicollinearity. Larger values suggest that the linear dependency between the different columns of the sensitivity matrix is too strong, which renders the independent identification of the unknown parameters troublesome. Furthermore, the parameter covariance matrix $\underline{P}$ which is the inverse of the information matrix $\underline{C}$ given by equation (4), is directly affected by the condition of $\underline{C}$. The worser the condition of the information matrix $\underline{C}$, the larger the covariances of the parameters will be.

In linear regression methods, the problem of multicollinearity is alleviated in two steps. First a change of variables is carried out which transforms the problem into a fully dimensionless regression problem. Secondly, another estimation procedure is used which is less sensitive to multicollinearity. A well-known procedure is ridge regression. The parameter set, initially given by equation (6), is then determined from

$$\underset{\sim}{\theta} = [\underline{C} + \alpha\underline{I}]^{-1}\,\underline{S}^T\,\underset{\sim}{m} \tag{8}$$

where α is a positive coefficient, generally smaller than unity. For nonlinear problems, the Levenberg-Marquardt algorithm is obtained from equation (2) through

the addition of the same term $\alpha \underline{I}$ to the information matrix. The Levenberg-Marquardt algorithm has always been presented as a compromise between the steepest descent method and Gauss-Newton method. The analogy with the linear regression methods confirms that the Levenberg-Marquardt algorithm is indeed less sensitive to multicollinearity. The second step to cope with multicollinearity thus exists for both linear and nonlinear estimation problems. The first step, which is undoubtfully more important is mostly omitted in nonlinear estimation problems. The use of a Markov estimator already neutralizes the influence of the units of the measured response. However, the units and scale of the parameters and the incompatibility of forces, displacements and strains persists. Applying an ad-hoc supplementary weighting to the matrix $\underline{V}$ is often performed, which generally leads to an enhanced information matrix. This implies that it makes little sense to compare the efficiencies of experiments in which different types and numbers of measurements are used, if the sensitivity matrix is not rendered dimensionless in a rigorous manner.

2.2 Dimensionless information matrix

The dimensional incompatibility problem in estimation methods is well-known for linear regression analyses[11], where the regressor plays the role of the sensitivity matrix. Standardized regression coefficients can be computed, which permit a correlation analysis that is totally independent of the choice of scale for the regressor or the regression coefficient. However, this procedure cannot be applied in a trivial manner if regressor variables with different units exist for the same regression coefficient. This is typically the case when different types of measurements are performed in an experimental analysis (e.g., the applied force or the displacement of an LVDT). Another procedure is therefore proposed for nonlinear parameter estimation problems.

The nonlinear relation between the predicted output and the unknown parameter set is therefore linearized in the vicinity of the initial estimate $\underset{\sim}{\theta}^{(0)}$

$$\delta \underset{\sim}{h} = \underline{S}\, \delta \underset{\sim}{\theta} \tag{9}$$

The variation of the output $\delta \underset{\sim}{h}$ and the sensitivity matrix are next divided into blocks according to the different types of measurements that are carried out, i.e., forces, displacements, strains, etc. If two different types are used the following equation ensues

$$\begin{bmatrix} \delta \underset{\sim}{h}_1 \\ \delta \underset{\sim}{h}_2 \end{bmatrix} = \begin{bmatrix} \underline{S}_1 \\ \underline{S}_2 \end{bmatrix} \delta \underset{\sim}{\theta} \tag{10}$$

If the number of blocks equals n_b and the number of parameters n_θ, a reference value can be defined for each output block, i.e., h_i^R $(i = 1 \rightarrow n_b)$, and each parameter, i.e., θ_k^R $(k = 1 \rightarrow n_\theta)$. Each output item is rescaled and made dimensionless by dividing it by its block reference value. The same operation is carried out for the unknown parameters. The dimensionless items are denoted with $\underset{\sim}{h}^\star$ and $\underset{\sim}{\theta}^\star$.

The sensitivity matrix $\underline{S}$ is transformed accordingly

$$\underline{S}^{\star} = \begin{bmatrix} \underline{S}_1^{\star} \\ \cdots \\ \underline{S}_{n_b}^{\star} \end{bmatrix} = \begin{bmatrix} \frac{\partial \underset{\sim}{h}_1}{\partial \theta_1} \frac{\theta_1^R}{h_1^R} & \cdots & \frac{\partial \underset{\sim}{h}_1}{\partial \theta_{n_\theta}} \frac{\theta_{n_\theta}^R}{h_1^R} \\ \cdots & \frac{\partial \underset{\sim}{h}_i}{\partial \theta_k} \frac{\theta_k^R}{h_i^R} & \cdots \\ \frac{\partial \underset{\sim}{h}_{n_b}}{\partial \theta_1} \frac{\theta_1^R}{h_{n_b}^R} & \cdots & \frac{\partial \underset{\sim}{h}_{n_b}}{\partial \theta_{n_\theta}} \frac{\theta_{n_\theta}^R}{h_{n_b}^R} \end{bmatrix} \tag{11}$$

The entire minimization of the objective function can thus be rephrased in this dimensionless format. The reference values of the block output items h_i^R and the parameters θ_k^R are now determined by minimizing the condition number of the information matrix $\underline{C}^{\star} = (\underline{S}^{\star})^T \underline{S}^{\star}$. This minimization is carried out in the absence of the matrix $\underline{V}$. The influence of measurement noise will be added afterwards. The minimization of the condition number can be carried out in a straightforward manner by a direct search method, e.g., the Nelder-Mead simplex search. This procedure takes little computational effort. An optimal condition number is obtained which rescales the sensitivities in an appropriate manner. Changing units or scales of the parameters, forces or displacements does not affect this optimum nor the dimensionless matrices. The reference values can be maintained in the iterative procedure for the minimization of J, but they will be less optimal if the parameter set tends away from the initial estimate. Nevertheless, this procedure provides a versatile approach to transform the parameter identification into a dimensionless and unscaled procedure. On the basis of these optimized condition numbers, experiments can be compared. The influence of the variances of the Markov estimator in the matrix $\underline{V}$ can be added by transforming the variances of each output item into its corresponding dimensionless form. The influence of the measurement accuracy on the condition number can then be assessed by changing the variances of the measured output items.

3 Analysis of experiments

A tensile test and a bending test will next be examined. In this analysis, it is implicitly assumed that no model errors exist. The identification analysis must predict a well-conditioned information matrix, since the addition of model errors to a weak conditioned information matrix easily leads to an unestimable parameter set. As an example, a gradient-enhanced damage model is used to describe the nonlinear material behaviour upon failure.

3.1 Material model

The material is described with an isotropic strain-based gradient-enhanced damage formulation, in which an intrinsic length scale exists [12;13]. It is a classical isotropic continuum damage constitutive relation, in which the damage D depends on a nonlocal equivalent strain $\bar{\varepsilon}_{eq}$. This nonlocal characteristic is computed from the

field of local equivalent strains ε_{eq} in the vicinity of the material point via a partial differential equation of the Helmholtz type:

$$\bar{\varepsilon}_{eq} - c\nabla^2\bar{\varepsilon}_{eq} = \varepsilon_{eq} \tag{12}$$

The parameter c is a material parameter with the dimensions of length squared. The local equivalent strain adopted here is based on the positive principal strain components[14]

$$\varepsilon_{eq}(\boldsymbol{\varepsilon}) = \sqrt{\sum_{j=1,2,3} \left(\varepsilon_j^+\right)^2} \tag{13}$$

The damage evolution law that governs the failure response is given by

$$D = 1 - \frac{\kappa_i}{\kappa} e^{-\beta(\kappa-\kappa_i)} . \tag{14}$$

In here, κ represents a deformation history parameter, which equals the ultimate nonlocal equivalent strain $\bar{\varepsilon}_{eq}$ that the material has experienced in its loading history. Furthermore, κ_i and β are material parameters, which govern the initiation and the evolution of damage respectively. More computational details can be found in literature[12].

Assuming that the classical elastic parameters (Young's modulus E and Poisson's ratio ν) have been determined in the elastic region, the estimation procedure has to deal with 3 remaining unknown parameters, i.e., c, κ_i and β. The elastic parameters for the simulated material equal $E = 100000\ MPa$ and $\nu = 0.3$. The current set of remaining parameters for which the identification analysis is performed equals $c = 5\ mm^2$, $\kappa_i = 0.001$ and $\beta = 100$.

3.2 Tensile test

A tensile test has been examined in which different simulated measurements have been performed. The damaging specimen is shown in Figure 1. The specimen has a length of 100 mm, a width that varies from 20 mm to 18 mm and a thickness of 1 mm. The mechanical response of the specimen for the current parameter set

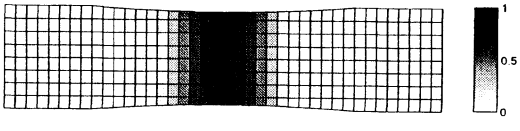

Figure 1: Damaging tensile specimen.

does not present snap-back. Four cases have been examined. The first case uses the applied force F and the measurement of an axially placed LVDT or strain gage Δd at the center of the specimen with a gage length of 10 mm. In the second

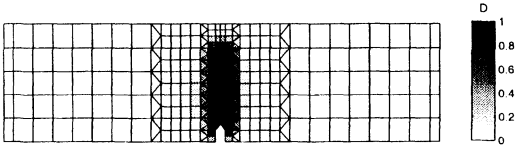

Figure 2: Damaging bend specimen.

case, the gage length of the LVDT is reduced to 5 mm. The third case uses the applied force and the nodal displacements $\underset{\sim}{u}$, while the fourth case is constructed from the force and nodal strains $\underset{\sim}{\varepsilon}$. The references values for the rescaling to a dimensionless format of the measured output items and the parameters differ from case to case, but typical values are $c^R = 9\ mm^2$, $\kappa_i^R = 4.10^{-4}$, $\beta^R = 100$, $F^R = 300\ N$ and $u^R = 0.17\ mm$. The condition numbers for the different cases are: 1683 (LVDT 10 mm), 143 (LVDT 5 mm), 122 ($F, \underset{\sim}{u}$) and 84 ($F, \underset{\sim}{\varepsilon}$). This first example shows that only the last case provides a condition number less than 100. Clearly, the amount and quality of the information increases depending on the number and types of measurements.

3.3 Bending test

The second simulated experiment is a classical three-point bending test, for which the specimen is shown in Figure 2. The specimen is $220mm$ long, $50mm$ high and 20 mm thick. The notch has a width of 5 mm with variables depths, ranging from 2.5 mm to 22.5 mm. Three cases are examined, where each case uses the applied load F. The first case adds the crack-opening displacement at the notch (COD). The second case uses the entire nodal displacement field $\underset{\sim}{u}$ in the beam, while the third case adds all nodal strain components $\underset{\sim}{\varepsilon}$. The results of the minimization of the condition number is given in Table 1. Clearly, the best condition number is

	Notch depths					
Case	2.5 mm	5 mm	7.5 mm	10 mm	12.5 mm	22.5 mm
$F - COD$	556	676	455	349	292	240
$F - \underset{\sim}{u}$	54	66	57	74	104	115
$F - \underset{\sim}{\varepsilon}$	18	34	26	40	70	62

Table 1: Condition numbers for different cases and notch depths

achieved by considering F and $\underset{\sim}{\varepsilon}$. Furthermore, it is noticed that the condition of an experiment with a COD-measurement improves if the notch depth increases, while this has the opposite effect for the two other cases. A small notch gives an experiment which provides a maximum of information if displacement fields or strain fields are measured at the surface of the specimen.

The influence of the standard deviation s of the measurements is analyzed by varying s for one of the output blocks (each case has two output blocks). It should

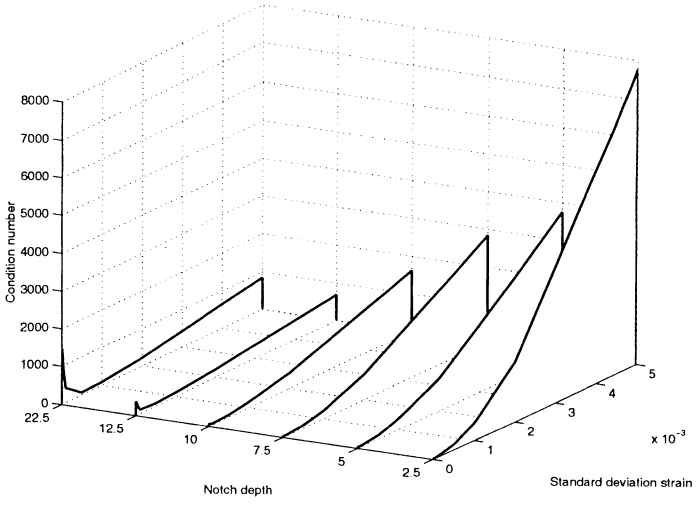

Figure 3: Influence of the standard deviation on the condition number.

be noticed that the condition number is only influenced by the relative variation of the dimensionless standard deviations of the output blocks. If a Markov information matrix is used with a constant standard deviation s_F of 5 N for the load and a variable $s_\mathcal{E}$ for the strains, Figure 3 ensues. This Figure shows that small standard deviations $s_\mathcal{E}$ for the strains give best results. In this case, the contribution of the load F to the information matrix is small. Higher values for $s_\mathcal{E}$ result in an information matrix that solely depends on the force F, which leads to a significant increase of the condition number.

4 Conclusions

A procedure has been proposed that allows to transform the optimization process in mixed numerical-experimental methods for the identification of nonlinear material behaviour into a dimensionless format. A dimensionless sensitivity matrix is obtained which has been optimized through a minimization of the condition number of the information matrix. The condition number of the dimensionless information matrix can be used to compare the efficiency of different experiments in which different simulated measurements are made at different locations of the specimen.

An illustration has been given for a classical tensile test and a bending test, making use of a gradient-enhanced damage model. The examples elucidate the importance of the experimental design, i.e., the geometry of the specimen, the type of measurement as well as the number, the location and density of the measurement points. The use of an experiment with an optimally conditioned information matrix (in the vicinity of the initial estimate of a parameter set of a computational model)

is a prerequisite for the actual parameter identification with a mixed numerical-experimental method, where measurement errors and model errors inevitably exist.

References

1. J. V. Beck and K. J. Arnold. *Parameter Estimation in Engineering and Science*. John Wiley & Sons, 1977.
2. N. R. Draper and H. Smith. *Applied Regression Analysis*. John Wiley & Sons, 1981.
3. H. Sol and C.W.J. Oomens, editors. *Material Identification Using Mixed Numerical Experimental Methods*. Proceedings of the Euromech 357 Colloquium, Kluwer Academic Publishers, 1997.
4. M. H. H. Meuwissen, C. W. J. Oomens, F. P. T. Baaijens, R. Petterson, and J. D. Janssen. Determination of the elasto-plastic properties of aluminium using a mixed numerical-experimental method. *Materials Processing Technology*, 75:204–211, 1998.
5. K. Hinkelmann and O. Kempthorne. *Design and analysis of experiments*. Wiley Series in probability and mathematical statistics. John Wiley & Sons, 1994.
6. J. P. Norton. *An Introduction to Identification*. Academic Press, 1986.
7. F. Pukelsheim. *Optimal design of experiments*. Wiley Series in probability and mathematical statistics. John Wiley & Sons, 1993.
8. A. C. Atkinson and A. N. Donev. *Optimum Experimental Designs*. Oxford Statistical Science Series. Clarendon Press, 1992.
9. P. Eykoff. *System identification. Parameter and State Estimation*. John Wiley & Sons, 1974.
10. J. C. Gelin and O. Ghouati. An inverse solution procedure for material parameters in large plastic deformations. *Communications in Numerical Methods in Engineering*, 12:161–173, 1996.
11. D. C. Montgomery and G. C. Runger. *Applied Statistics and Probability for Engineers*. John Wiley & Sons, 1994.
12. R. H. J. Peerlings, R. de Borst, W. A. M. Brekelmans, and J. H. P. de Vree. Gradient-enhanced damage for quasi-brittle materials. *International Journal for Numerical Methods in Engineering*, 39:3391–3403, 1996.
13. M. G. D. Geers, R. de Borst, W. A. M. Brekelmans, and R. H. J. Peerlings. Strain-based transient-gradient damage model for failure analyses. *Computer Methods in Applied Mechanics and Engineering*, 160(1-2):133–154, 1998.
14. J. Mazars and G. Pijaudier-Cabot. Continuum damage theory - application to concrete. *Journal of Engineering Mechanics*, 115(2):345–365, 1989.