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Citation: *AIP Conf. Proc.* **1353**, 23 (2011); doi: 10.1063/1.3589486

View online: <http://dx.doi.org/10.1063/1.3589486>

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A novel criterion for determination of material model parameters

A. Andrade-Campos, R. de-Carvalho and R.A.F. Valente

*Department of Mechanical Engineering, Centre for Mechanical Technology & Automation, GRIDS,
University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal,
Tel: +351.234.370830; Fax: +351.234.370933; e-mail: gilac@ua.pt*

Abstract. Parameter identification problems have emerged due to the increasing demanding of precision in the numerical results obtained by Finite Element Method (FEM) software. High result precision can only be obtained with confident input data and robust numerical techniques. The determination of parameters should always be performed confronting numerical and experimental results leading to the minimum difference between them. However, the success of this task is dependent of the specification of the cost/objective function, defined as the difference between the experimental and the numerical results. Recently, various objective functions have been formulated to assess the errors between the experimental and computed data (Lin et al., 2002; Cao and Lin, 2008; among others). The objective functions should be able to efficiently lead the optimisation process. An ideal objective function should have the following properties: (i) all the experimental data points on the curve and all experimental curves should have equal opportunity to be optimised; and (ii) different units and/or the number of curves in each sub-objective should not affect the overall performance of the fitting. These two criteria should be achieved without manually choosing the weighting factors. However, for some non-analytical specific problems, this is very difficult in practice. Null values of experimental or numerical values also turns the task difficult. In this work, a novel objective function for constitutive model parameter identification is presented. It is a generalization of the work of Cao and Lin and it is suitable for all kinds of constitutive models and mechanical tests, including cyclic tests and Baushinger tests with null values.

Keywords: Parameter identification, Constitutive models, Objective function, Criterion, Optimisation

PACS: 02.70.-c; 02.60.Pn; 02.70.Dh;

INTRODUCTION

Nowadays, the quest for secure input data for simulations and more specifically for finite element method (FEM) codes is increasing due to the increasing demand of the industry on obtaining more reliable numerical results. One of the most important input data for FEM solvers is the material behaviour, mathematically described by the constitutive model equations. Due to the large amount of phenomena required to be described by the FEM codes, the constitutive material models became complex and generally include a large number of parameters to be identified for each specific material. The general methodology for parameter determination of material constitutive models, as an inverse problem, consists in the minimization of a function $\mathcal{L}$ that represents the difference of the experimentally observed material behaviour and the mathematical model chosen to reproduce it,

$$\begin{aligned} \min \quad & f = \mathcal{L}(\mathbf{A}, \mathbf{Z}^c, \mathbf{Z}^e) \\ \text{s.t.} \quad & g(\mathbf{A}, \mathbf{Z}^c, \mathbf{Z}^e) \leq 0 \\ & \mathbf{A}_{\min} \leq \mathbf{A} \leq \mathbf{A}_{\max} \end{aligned} \tag{1}$$

where $\mathbf{A}$ represents the array of parameters that needed to be determined and $\mathbf{Z}$ stands for the set of measured properties, such as the stress, strain, etc. The superscripts c and e stand for computed and experimental values. The function g defines the set of functions used in the constraints of the optimisation process and $\mathbf{A}_{\min}$ and $\mathbf{A}_{\max}$ are the material parameter bounds. The minimisation is achieved with the assistance of optimisation algorithms, whether they are gradient-based, direct search, metaheuristics or artificial intelligence-based algorithms. However, all these algorithms and their efficiency directly depend on the quality of the information given by the objective function or optimisation criterion, defined as $\mathcal{L}$ in equation 1. Working as a guide, the objective function should efficiently find the best fit to the experimental data, always subjected to some specific constraints. In order to obtain reliable information about the difference between the experimental and numerical values the objective function should fulfill some criteria

[1]:

Criterion 1: the errors of the experimental data should not be accounted for during the parameter identification process. This could be achieved by eliminating the experimental data points considered of doubtful quality.

Criterion 2: for each curve, all the experimental point should be taken in account and should have equal opportunity to be optimised.

Criterion 3: when using multiple curves, all experimental curves should also have equal opportunity to be optimised, independently of the number of points of each curve.

Criterion 4: if sub-objectives are required, the objective function should be able to deal with the inclusion of these sub-objectives and their account should be done giving equal opportunity to the sub-objective to be optimised.

Criterion 5: different units or scales should not affect the overall performance of the process.

Criterion 6: continuity must be achieved allowing to progressively evaluate the quality of the fitting. Therefore, integer and discrete functions should be avoided in the formulation of the objective function.

Criterion 7: the process should not be dependent of the user. Therefore, the weighting coefficients, useful for achieving some of the above criteria, should be found automatically.

The above criteria are difficult to satisfy in an automatic manner. Generally, these are accomplished manually choosing the weighting coefficients and based on the user empirical experience.

Due to the large success of least square optimization algorithms in previous decades, the curve fitting objective functions are commonly formulated based on the sum of squares of the difference between computed and experimental data (such as stress σ) at the same abscissa value (usually the time t or strain ϵ in material constitutive models). This conventional objective function can be formulated considering an absolute and a relative weight, W^{abs} and W^{rel} respectively, in the following form

$$f = \sum_{j=1}^M \mathcal{L}_j(\mathbf{A}, \mathbf{Z}^c, \mathbf{Z}^e) = \frac{1}{M} \sum_{j=1}^M \frac{1}{N_j} \sum_{i=1}^{N_j} \left[\frac{\mathbf{Z}_i^c - \mathbf{Z}_i^e}{W_j^{\text{abs}} + W_j^{\text{rel}} \mathbf{Z}_i^e} \right]^2 \Rightarrow f = \frac{1}{M} \sum_{j=1}^M \frac{1}{N_j} \sum_{i=1}^{N_j} r_{ij}^2 \text{ with } r_{ij} = \frac{\sigma_i^c - \sigma_i^e}{W_j^{\text{abs}} + W_j^{\text{rel}} \sigma_i^e}. \quad (2)$$

Although the selection of the weighting coefficients is not intuitive, the use of equation 2 has led to good results in previous works [4, 5, 6].

Recently, the mentioned criteria were satisfied by Lin *et al.* [1, 2, 3] with the introduction of new objective functions formulations and automatic weighting factors. Similar to the true strain definition, the concept of true (logarithm) error definition was also used in order to increase the function sensitivity to the parameters. The concept of correspondent computed value was introduced as well. For a pair of experimental and equivalent computed curves, the same fraction is used to choose the corresponding data for the i th experimental data point of the j th curve. This tries to ensure that all the experimental and computed data are involved in the optimisation and the predicted data will be pushed towards the corresponding experimental data. The objective function formulation suggested by Lin and coworkers [1, 2] is

$$f = \frac{1}{M} \sum_{j=1}^M \left\{ \frac{1}{N_j} \sum_{i=1}^{N_j} r_{ij}^2 \right\} \quad \text{with} \quad r_{ij}^2 = \omega_{1ij} \left[\ln \frac{\epsilon^c \left(\epsilon_{N_{ij}}^c \epsilon_{ij}^e / \epsilon_{N_{ij}}^e \right)}{\epsilon_{ij}^e} \right]^2 + \omega_{2ij} \left[\ln \frac{\sigma^c \left(\epsilon_{N_{ij}}^c \epsilon_{ij}^e / \epsilon_{N_{ij}}^e \right)}{\sigma_{ij}^e} \right]^2. \quad (3)$$

The weighting factor for the i th experimental data point of the j th curve developed by Cao and Lin [1] is expressed as $\omega_{ij} = \theta \cdot \epsilon_{ij}^e / \sum_{j=1}^M \sum_{i=1}^{N_j} \epsilon_{ij}^e$, where $\theta = \sum_{j=1}^M N_j$ is a scaling factor proportional to the number of total data points. It is important to note that $\omega_{11} + \omega_{21} + \dots + \omega_{N_j M} = \theta$. As illustrated in figure 1, the use of the Lin's correspondent computed value avoids that curves with small size would show small objective function value. Although curve 2 seems to better model the experimental behaviour of the material, curve 3 presents a smaller objective function if the sum of squares objective function is used. The sum of errors using the objective function proposed by Cao and Lin can numerically demonstrate the fact that curve 2 fits best to the experimental data. However, the new objective function formulation was only applied using experimental data obtained with monotonous tests and unified elasto-viscoplastic constitutive equations. Therefore, no zero or negative values of the measured variables (such as stress and strain), either experimental or computed, were taken in account. It is important to note that equation 3 has no real value if $\epsilon^e = 0$ or $\sigma^e = 0$, leading to $r_{ij} \rightarrow \infty$.

FIGURE 1. Experimental and computed curves. Example for objective function comparison [1].

NOVEL CRITERION

Consider a curve defined analytically as $y = f(x)$, as showed in figure 2a. Numerically, the curve can be defined by a set of points. Therefore, the information of the analytical description $f(x)$ of the curve is not available. In these cases, the equation of the length of a curve can be approximated by the following expression

$$l = \int_a^b \sqrt{1 + \left(\frac{dy}{dx}\right)^2} = \int_a^b \sqrt{dx^2 + dy^2} \approx \sum_{i=1}^N \sqrt{dx^2 + dy^2} = \sum_{i=1}^N \sqrt{(x_{i+1} - x_i)^2 + (y_{i+1} - y_i)^2}. \quad (4)$$

If x and y have different units and magnitude, the length (or dimension) of the larger variable will *monopolize* the length distance. Therefore, it is convenient to normalize these distances. The concept of calculation of the correspondent computed-experimental point is called *weighted length*, in opposition to the *weighted distance* proposed in [1]. This concept takes into account negative values and curve length equidistant values. Therefore, the weighted lengths of each experimental and computed data points are, respectively,

$$l_{ij}^e = \sum_{k=1}^i \sqrt{\left(\frac{\epsilon_{k+1,j}^e - \epsilon_{k,j}^e}{\epsilon_{\max}^e}\right)^2 + \left(\frac{\sigma_{k+1,j}^e - \sigma_{k,j}^e}{\sigma_{\max}^e}\right)^2} \quad \text{and} \quad l_{ij}^c = \sum_{k=1}^i \sqrt{\left(\frac{\epsilon_{k+1,j}^c - \epsilon_{k,j}^c}{\epsilon_{\max}^c}\right)^2 + \left(\frac{\sigma_{k+1,j}^c - \sigma_{k,j}^c}{\sigma_{\max}^c}\right)^2} \quad (5)$$

where $\epsilon_{\max}$ and $\sigma_{\max}$ are the maximum absolute values. The correspondent computed value is given by the equivalent length, $l_{ij}^{\text{eq}} = l_{ij}^e \left(\frac{l_{N,j}^c}{l_{N,j}^e}\right)$, that is responsible by the absolute curve scaling.

Overall Multi-objective function

Considering the least square structure and the true error definition, the objective function suggested for each i data point in the j^{th} curve is given for a stress-strain mechanical model

$$r_{ij}^2 = \left\{ \sqrt{\omega_{ij}^\sigma} \ln \left[1 + \left| \frac{\sigma^c(l_{ij}^{\text{eq}}) - \sigma_{ij}^e}{\sigma_{ij}^e} \right| \right] \right\}^2 + \left\{ \sqrt{\omega_{ij}^\epsilon} \ln \left[1 + \left| \frac{\epsilon^c(l_{ij}^{\text{eq}}) - \epsilon_{ij}^e}{\epsilon_{ij}^e} \right| \right] \right\}^2. \quad (6)$$

The use of the module or absolute function prevents a non proportional error when the experimental value and the computed value present different signs. Figure 2b illustrates this function for the experimental-computed ratio proportion. Although the logarithm function is well prepared for large values when $(\epsilon^e, \sigma^e) \rightarrow 0$, zero divisions should be avoided. Therefore, the denominators of equation 6 should respect the following rule

$$\text{if } |\sigma^e| < \frac{\sigma_{\max}}{N^2} \quad \text{then} \quad \sigma_{\text{denominator}}^e = \min \left(1, \frac{\sigma_{\max}}{N^2} \right). \quad (7)$$

The global objective function follow the same structure as equation 3, $f = \frac{1}{M} \sum_{j=1}^M \left\{ \frac{1}{N_j} \sum_{i=1}^{N_j} r_{ij}^2 \right\}$, that allows giving the same opportunity to all curves to be optimised. In order to different units and different magnitude do not interfere with the equality criterion for each data point, weighting coefficients should be used.

FIGURE 2. (a) The length of a curve. (b) Analysis of the mathematical structure of the proposed objective function.

Weighting coefficients

It is of utmost importance that the weighting coefficients are chosen automatically without any manual or empirical influence. In this work, the weighting coefficients suggested by Cao and Lin [1] will be extended to the possibility of using negative values curves. Hence, the weighting coefficient for the strain is defined as

$$\omega_{ij}^{\varepsilon} = \theta \cdot \frac{|\varepsilon_{ij}^e|}{\sum_{j=1}^M N_j \sum_{i=1}^{N_j} |\varepsilon_{ij}^e|}. \quad (8)$$

A similar expression is used for the stress component. The use of absolute values allows to maintain the fact that, for $\theta = \sum_{j=1}^M N_j$, $\omega_{11} + \omega_{21} + \dots + \omega_{N_j M} = \theta$. The weighting coefficients balance the experimental data points in order to reduce the weight of the denominator. Large experimental points, as denominators, diminish and scale the absolute difference between the computed and the experimental data point. Figure 3 shows the strain and stress weighting coefficients for the experimental data of the example illustrated in figure 1. Additionally, the weighting coefficients for two linear experimental curves are showed in the same figure.

FIGURE 3. Weighting coefficients for the example of figure 1 and for two linear experimental curves.

In the first subfigure, it can be seen that both the stress and strain weighting factors are proportional to the magnitude of the stress and strain values, respectively. This property gives to all experimental data point equal opportunity to be optimised, diminishing the influence of the magnitude of the experimental value (used as denominator).

From the figure with the two linear experimental curves, in which one of them has negative values, it is possible to see that negative values do not affect the value of the weight, being the weight always positive. Furthermore, the slope of the weight curve has the same magnitude whereas the data points are positive or negative. Note that both curves present the same sum of weights (equal to the number of points).

NUMERICAL ANALYSIS

Hyperelastic Yeoh model

Hyperelastic models are generally defined through a strain energy or strain potential function. In this case, the strain potential function Ψ only depends on the first invariant and is given as $\Psi_{\text{Yeoh}} = \sum_{i=1}^3 c_i (I_1 - 3)^i$ with $I_1 = \lambda^2 + \frac{2}{\lambda}$ for

TABLE 1. Results obtained with the classical square error and the proposed objective function.

	Initial values (c_i)	Boundaries [$c_{\min}, c_{\max}$]	Final value	Iterations	Parameters
Classical Square error	0.004	[-10,10]	5.8×10^{-6}	39	0.0112
	0.02				0.0189
	0.01				1.30×10^{-15}
New OF	0.004	[-10,10]	0.01643	38	0.0111
	0.02				0.0193
	0.01				5.628×10^{-14}

the particular case of uniaxial tensile in incompressible materials. $\lambda = \lambda_1$ is the principal uniaxial stretch. In agreement with Holzapfel and Martins *et al.* [7], for an isotropic incompressible material ($J = 1$), the Cauchy stress can be written as a function of the strain invariants, $\sigma = 2 \left(\lambda^2 - \frac{1}{\lambda} \right) \left(\frac{\partial \Psi}{\partial I_1} + \frac{1}{\lambda} \frac{\partial \Psi}{\partial I_2} \right)$, leading to the following expression for the Cauchy stress of the Yeoh model:

$$\sigma_{\text{Yeoh}} = 2 \left(\lambda^2 - \frac{1}{\lambda} \right) \left[c_1 + 2c_2(I_1 - 3) + 3c_2(I_1 - 3)^2 \right]. \quad (9)$$

In order the model can represent realistic values, $\sigma \geq 0 \forall \lambda \geq 1$. Knowing that $\left(\lambda^2 - \frac{1}{\lambda} \right) \geq 0 \forall \lambda \geq 1$, then $c_1 + 2c_2(I_1 - 3) + 3c_2(I_1 - 3)^2 \geq 0$ with $I_1 - 3 \geq 0 \forall \lambda \geq 1$. The polynomial of equation cannot have positive zeros. Therefore, the parameter identification process has the following expression as constraint: $\frac{-2c_2 \pm \sqrt{4c_2^2 - 12c_3c_1}}{c_3} \leq 0$. Figure 4a presents the experimental data obtained from a uniaxial test of a biological muscular tissue [7] that is used in this example. The classical square error objective function will be used in comparison with the proposed objective function (new OF) to identify the three parameters used in the Yeoh model: c_1 , c_2 and c_3 . Table 1 lists the initial and final parameters obtained in the optimisation process. Note that a Newton least square optimisation method was used together with finite differences to calculate the function gradient.

FIGURE 4. (a) Experimental and numerical curves. (b) Evolution of the objective functions. (c) Sensivity of the objective function with the material parameter c_2 .

The Yeoh model curves obtained with the initial and final parameters can also be seen in the figure 4. It can be seen that the final result obtained with both objective functions is similar. Therefore, even for simple and monotonous tests, the new OF can lead to analogous final results with a convergence rate similar to the classical square error (see figure 4b). Figure 4 shows the variation of the objective functions with the material parameter c_2 . From this figure it can be concluded that the proposed objective function has a smoother variation, leading to an easier function to be minimized.

Elasto-viscoplastic model with kinematic and isotropic hardening

The experimental data from a E220BH steel [8] is composed by monotonous tensile and shear tests, and three Bauschinger tests. The constitutive model identified is an elasto-viscoplastic model that takes into account the kinematic and the isotropic work-hardening of the material. The yield function considered can be given as

$$f(\sigma, \mathbf{X}, R) = \bar{\sigma} - R = \sqrt{\frac{3}{2}(\sigma^d - \mathbf{X}) : (\sigma^d - \mathbf{X})} - R \quad (10)$$

where σ^d is the deviatoric part of σ and $\bar{\sigma}$ is the equivalent stress. $\mathbf{X}$ and R represent the back-stress tensor and the isotropic work-hardening, respectively defined as

$$\mathbf{X} = C \frac{1}{\sigma_0} (\sigma - \mathbf{X}) \dot{\varepsilon}^p - \gamma \mathbf{X} \dot{\varepsilon}^p \quad \text{and} \quad R = K(\bar{\varepsilon}^p + \varepsilon_0)^n \quad \text{with} \quad \varepsilon_0 = \left(\frac{\sigma_0}{K} \right)^{1/n}. \quad (11)$$

As represented by the previous equation, the work-hardening combines isotropic and kinematic contributions. K is a material parameter, n the hardening coefficient and σ_0 is the initial yield stress. The non-linear evolution law of the kinematic work-hardening is based in the additive combination of a purely kinematic term (linear Ziegler hardening law) and a relaxation term (the recall term). C and γ are material parameters that must be determined. C is the initial kinematic hardening module and γ define the rate at which the kinematic hardening module decreases with the increasing of the plastic deformation. Note that the equivalent plastic strain rate $\dot{\varepsilon}^p$ can be defined from the plastic work conservation principle, *i.e.*, $\dot{\varepsilon}^p = \frac{(\sigma^d - \mathbf{X}) : \dot{\varepsilon}^p}{\bar{\sigma}}$. Figure 5a shows the experimental and computed curves modeled with the parameters determined using a Levenberg-Marquardt optimisation method. The convergence curve can be seen in figure 5b.

FIGURE 5. (a) Experimental and computed curves for the elasto-viscoplastic constitutive model. (b) Evolution of the objective function.

FINAL REMARKS

In this work, a new optimisation criterion for parameter identification of constitutive models was proposed. This objective function is a generalization of the objective function proposed in [1] and is prepared for negative and zero values of the curves. The objective function was analysed with the aid of an hyperelastic and an elasto-viscoplastic model.

ACKNOWLEDGMENTS

The authors acknowledge the financial support given by the FCT project PTDC/EME/PME/68975/2006.

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