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A Levenberg-Marquardt algorithm for fitting σ-w curves from three-point bend tests for plain and fiber reinforced concretes

Um algoritmo de Levenberg-Marquardt para ajuste de curvas σ-w a partir de ensaios de flexão em três pontos para concretos simples e reforçados com fibras

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Abstract

This technical note describes the implementation of the Levenberg-Marquardt algorithm for the inverse analysis of three-point bend tests on notched specimens of plain and fiber reinforced concretes for determining softening parameters (σ-w curves). Tests indicated that the algorithm is sufficiently efficient and robust.

Keywords: inverse analysis, softening, concrete, Levenberg-Marquardt.

Resumo

Esta nota técnica descreve a implementação de um algoritmo de Levenberg-Marquardt para a análise inversa de dados de ensaios de flexão em três pontos em espécimes de concreto simples ou reforçado com fibras para a determinação de parâmetros de amolecimento (curvas σ-w). Testes indicaram que o algoritmo é suficientemente eficiente e robusto.

Palavras-chave: análise inversa, amolecimento, concreto, Levenberg-Marquardt.

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1. Introduction

A previous article (SOUSA & GETTU, 2006) describes an object oriented programming implementation of a system capable of fitting different types of softening curves to data from three-point-bend tests performed on notched prismatic specimens of plain and fiber reinforced concretes. The approach, implemented in a software named FIT3PB, is based on the minimization of the error function $\vartheta^2(\boldsymbol{a})$, where $\boldsymbol{a}$ is the set of softening parameters. The function $\vartheta^2(\boldsymbol{a})$ is described by the integral of the squared differences along the fitting interval, using a finite differences approach to compute gradient and Hessian of $\vartheta^2(\boldsymbol{a})$. This technical note describes the implementation an alternative based on Levenberg-Marquardt approach to minimize the error function $\vartheta^2(\boldsymbol{a})$ without explicitly computing the Hessian and, thus, reducing the number of calls to the subroutine that evaluates $\vartheta^2(\boldsymbol{a})$, the main drawback of the original implementation.

2. Description of the Computational Implementation

Let it be a load-versus-crack mouth opening displacement (P-CMOD) function

$$P_{num} = f(v, a) \quad (1)$$

where the scalar v is the crack mouth opening displacement (CMOD), $\boldsymbol{a}$ is the vector of softening parameters (e. g. f_t and G_F), and $f(v, \boldsymbol{a})$ is the numerically computed load corresponding to v and the trial softening parameters $\boldsymbol{a}$.
The squared error, in the east squares sense, is

$$\vartheta^2(\boldsymbol{a}) = \int_0^{v_{max}} \left[P_{exp}(v) - f(v, \boldsymbol{a})\right]^2 dv \quad (2)$$

where:
v is the crack mouth opening displacement, usually referred as CMOD
P_{exp} is the experimental value of the applied load corresponding to
a is a set of softening parameters assumed at a step of the fitting process
$f\ (v,a)$ is the value of the applied load, corresponding to a trial set of parameters
The software FIT3PB was implemented according to the following steps:

1. The user introduces the experimental results as a list of P-CMOD pairs, selects a softening model to fit and gives a trial set of softening parameters to start the iterative algorithm;
2. These data are preprocessed to eliminate noise usually present in the beginning of the curve and the P-CMOD pairs are recomputed to create a list with equally spaced abscissas (the same spacing is used for the numerically obtained P-CMOD lists to help in the integration routines);
3. Given the softening model and the current set of parameters, the numerical P-CMOD values – $f(v, \boldsymbol{a})$ – are computed;
4. These values are used to evaluate $\vartheta^2(\boldsymbol{a})$ for the current set of parameters;
5. An optimization routine finds the set of parameters $\boldsymbol{a}$ corresponding to the minimum of $\vartheta^2(\boldsymbol{a})$, using gradient and Hessian of $\vartheta^2(\boldsymbol{a})$ computed with a finite differences scheme;

In this technical note the optimization routine referred in the step 5 is addressed, aiming at improving efficiency and robustness.

2.1 Computation of Partial Derivatives

Considering *n* (*n* even) equally spaced segments along the fitting interval (spacing *h*), using the Simpson´s rule for numerical integration, Eqn. 2 can be rewritten as:

$$\vartheta^2(\boldsymbol{a}) = \sum_{i,j=0}^{n} \left\{P_{exp}(v_i) - f(v_i, \boldsymbol{a})\right\} m_{ij} \left\{P_{exp}(v_j) - f(v_j, \boldsymbol{a})\right\} \quad (3)$$

when

$$m_{ij} = \frac{4h}{3}\ for\ i = j\ odd;\ m_{ij} = \frac{2h}{3}\ for\ i = j\ even;$$

$$m_{ij} = \frac{h}{3}\ for\ i = j = 0\ or\ n;\ and\ m_{ij} = 0\ for\ i \neq j$$

The gradient of $\vartheta^2(\boldsymbol{a})$ is given by

$$\frac{\partial \vartheta^2(\boldsymbol{a})}{\partial a_k} = -2 \sum_{i,j=0}^{n} \frac{\partial f(v_i, \boldsymbol{a})}{\partial a_k} m_{ij} \left\{P_{exp}(v_j) - f(v_j, \boldsymbol{a})\right\} \quad (4)$$

The Hessian of $\vartheta^2(\boldsymbol{a})$ is given by

$$\frac{\partial^2 \vartheta^2(\boldsymbol{a})}{\partial a_k \partial a_l} = 2 \sum_{i,j=0}^{n} \left\{ \frac{\partial f(v_i, \boldsymbol{a})}{\partial a_k} m_{ij} \frac{\partial f(v_j, \boldsymbol{a})}{\partial a_l} - \frac{\partial^2 f(v_i, \boldsymbol{a})}{\partial a_k \partial a_l} m_{ij} \left[P_{exp}(v_j) - f(v_j, \boldsymbol{a})\right] \right\} \quad (5)$$

According to PRESS et al. (2007), the second term of the integrand can be neglected (actually the reference does not just neglect, but also gives acceptable reasons for this assumption). The Hessian matrix becomes

$$\frac{\partial^2 \vartheta^2(\boldsymbol{a})}{\partial a_k \partial a_l} = 2\sum_{i,j=0}^{n}\left\{\frac{\partial f(v_i,\boldsymbol{a})}{\partial a_k} m_{ij} \frac{\partial f(v_j,\boldsymbol{a})}{\partial a_l}\right\} \quad (6)$$

This means that a finite differences scheme is no longer necessary to evaluate the Hessian matrix, which can be approximated by the positive definite matrix represented by Eqn.6. Thus, the gradient and the Hessian of the error function $\vartheta^2(\mathrm{a})$ can be computed according to Eqn. 7.

$$\begin{cases} \dfrac{\partial \vartheta^2(\boldsymbol{a})}{\partial a_k} = -2\displaystyle\sum_{i,j=0}^{n}\frac{\partial f(v_i,\boldsymbol{a})}{\partial a_k} m_{ij}\left\{P_{exp}(v_j) - f(v_j,\boldsymbol{a})\right\} \\ \dfrac{\partial^2 \vartheta^2(\boldsymbol{a})}{\partial a_k \partial a_l} = 2\displaystyle\sum_{i,j=0}^{n}\left\{\frac{\partial f(v_i,\boldsymbol{a})}{\partial a_k} m_{ij} \frac{\partial f(v_j,\boldsymbol{a})}{\partial a_l}\right\} \end{cases} \quad (7)$$

The functions $P_{exp}(v_i)$ and $f(v_i,\boldsymbol{a})$ are described in terms of polygonal functions, using the same abscissas. In order to compute the derivatives $\frac{\partial f(v_i,\boldsymbol{a})}{\partial a_k}$, the finite differences scheme consists of giving increments da_k to the parameter a_k, maintaining the others, a_r, approximating the partial derivative by

$$\frac{\partial f(v_i,\boldsymbol{a})}{\partial a_k} \cong \frac{f(v_i,a_r,a_k+\delta a_k) - f(v_i,a_r,a_k)}{\delta a_k} \quad (8)$$

This generates the derivative of each ordinate of the P-CMOD curve with respect to the softening parameters. These values are used to perform the integrations using the Simpson´s rule in the same manner described in Eqn. 3.

2.2 Algorithm for Error Minimization

The Levenberg-Marquardt algorithm for minimization of the function $\vartheta^2(\boldsymbol{a})$ consists in disturbing the approximated Hessian matrix by multiplying the diagonal elements by a factor $(1+\lambda)$, where λ is modified at each iteration step according to the following algorithm:

1. Start with a trial set of parameters ($\boldsymbol{a}^s$), where the superscript s refers to the current iteration
2. Compute $\vartheta^2(\boldsymbol{a}^s)$;
3. Pick a small value of λ, e.g. λ=0.001;
4. Compute gradient vector $\boldsymbol{g}^s$ and the Hessian matrix $\boldsymbol{H}^s$ according to Eqn. 7;
5. Compute the modified Hessian ($\boldsymbol{H}^{*s}$) matrix by multiplying the diagonal elements of the Hessian matrix ($\boldsymbol{H}^s$) by $(1+\lambda)$;
6. Compute ($\boldsymbol{d}^s$), the vector with the increments by solving the linear system ($\boldsymbol{H}^{*s}.\boldsymbol{d}^s = -\boldsymbol{g}^s$);
7. If $\|\boldsymbol{d}^s\|$ is small enough, break;
8. Evaluate $\vartheta^2(\boldsymbol{a}^{s+1})$ at $\boldsymbol{a}^{s+1} = \boldsymbol{a}^s + \boldsymbol{d}^s$;
9. If $\vartheta^2(\boldsymbol{a}^{s+1}) \geq \vartheta^2(\boldsymbol{a}^s)$, multiply λ by 10 and return to step 4 with $\boldsymbol{a}^s$;
10. If $\vartheta^2(\boldsymbol{a}^{s+1}) < \vartheta^2(\boldsymbol{a}^s)$, divide λ by 10, and return to step 5 with $\boldsymbol{a}^{s+1}$ instead of $\boldsymbol{a}^s$.

The iterative process stops when the condition in step 7 is satisfied or a maximum number of iterations is reached.

3. Application tests

The described algorithm has been implemented in the system FIT3PB, and tested for plain and fiber reinforced concretes. Running a series of test data from notched beam specimens tested in a three-point-bend setup by FERNANDES (2010) for plain concrete, and by BARRAGÁN (2002) for fiber reinforced concrete, the obtained parameters matched the previous ones computed with the former implementation of FIT3PB. Figure 1 present the experimental load-CMOD curves, with the corresponding fitted curves displayed in the details, resulting from the inverse analysis on data from two different plain concrete specimens. Two softening models were used: an exponential model (HORDIJK, 1991) and a bilinear model. Similar results are presented in Figure 2 showing the inverse analysis results of a trilinear model fitted to data from a fiber reinforced concrete specimen.

4. Conclusions

The implementation of a Levenberg-Marquardt algorithm for the least square fitting of a softening curve from three-point-bend specimens has been described. The intention is to improve efficiency and robustness of an inverse analysis system to deal with more complex problems related to fitting of a time dependent model to a group of specimens tested at different loading rates. The implemented algorithm uses a finite difference scheme only for determining the gradient of the error function $\vartheta^2(\boldsymbol{a})$, approximating the Hessian matrix through a dyadic product of such gradient by itself, as described in Eqn. 7.
Although exhaustive tests have not been developed, the implemented Levenberg-Marquardt algorithm has shown improved performance, both in terms of efficiency and robustness.

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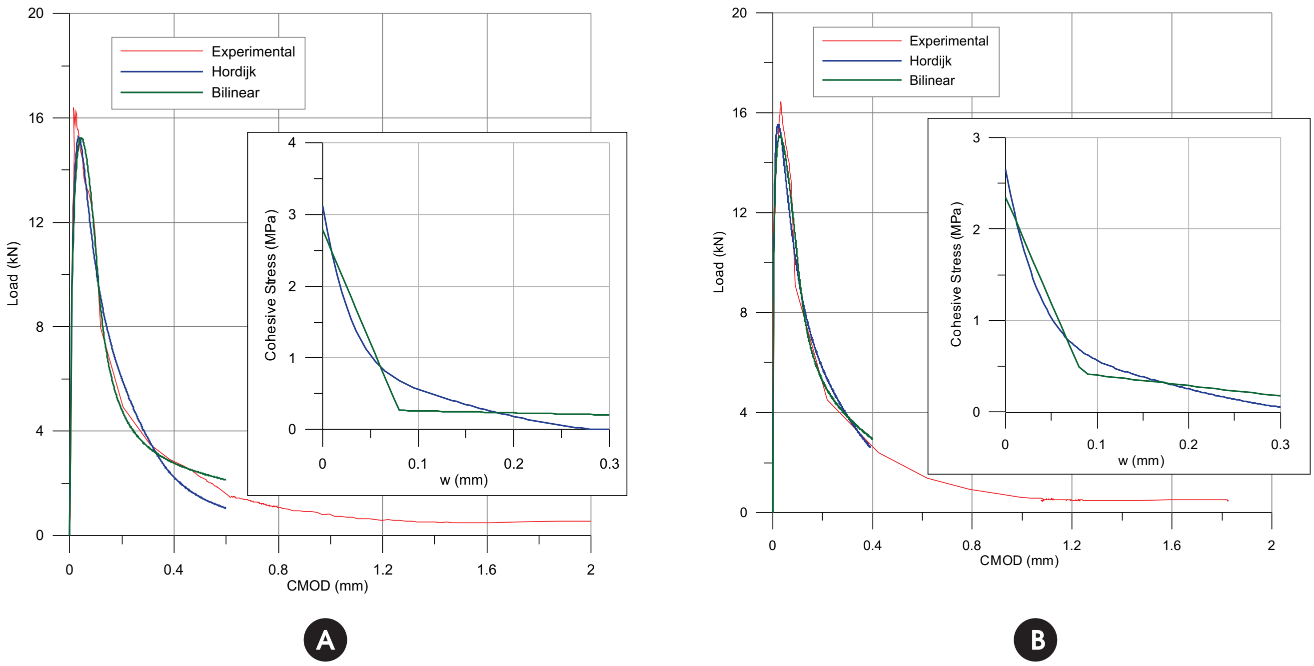
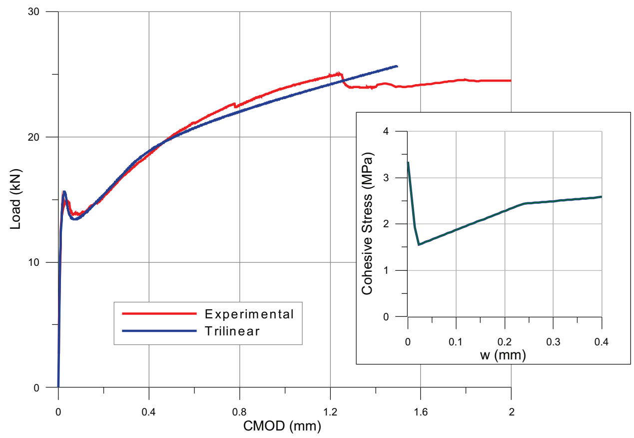
Figure 1 – Application of the implemented algorithm to three-point-bend data from tests on notched specimens of plain concrete



Paulo, Brazil), and Dr. Bryan E. Barragán (Universitat Politècnica de Catalunya, Spain).

Figure 2 – Application of the implemented algorithm to three-point-bend data from tests on notched specimens of fiber-reinforced concrete



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