20th International Conference
ENGINEERING MECHANICS 2014
Svratka, Czech Republic, 12 – 15 May 2014

PARAMETER IDENTIFICATION IN INITIAL VALUE PROBLEMS FOR NONLINEAR ORDINARY DIFFERENTIAL EQUATIONS

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Abstract: *Nonlinear initial value problems (IVPs) for ordinary differential equations are considered. As a representative, a cement hydration model is chosen. The model equation depends on a few parameters that are to be identified on the basis of hydration-related measurements at a sequence of time points. This is done through the minimization of a cost function defined as the sum of squared differences between the measured values and the model response at the same time points. To minimize the cost function, a gradient based algorithm is used. The gradient of the cost function can be calculated either by numerical differentiation or via solving auxiliary initial value problems. The minimization algorithm tends to find a local minimum. Therefore, it is run from different starting points to increase the chance of finding the global minimum. Algorithms are coded in the Matlab environment, and Matlab IVP solvers as well as Matlab Optimization Toolbox and Symbolic Math Toolbox are utilized. The latter makes the derivation of the auxiliary IVPs easy and reliable.*

Keywords: Identification of parameters, Initial value problem, Matlab, Sensitivity analysis.

1. Introduction

Identification of parameters is a frequent problem in modeling real-world phenomena. In a common situation, a phenomenon is observed and its features are quantified through measurements. Next, a mathematical model is formulated that, inevitably, depends on parameters that can be general and known (as general physical constants, for instance) or rather special and known only approximately. Parameters can also determine the basic hypothesis of the mathematical model. As an example, take a possible uncertainty in the relationships between quantities involved in the model. These relationships can be described by, for instance, linear, quadratic, or exponential mathematical expressions, and the first goal of modeling is to identify the classes of dependencies that constitute the model.

In this paper, we focus on the identification of parameters in initial value problems for ordinary differential equations. This subject has been widely studied in the literature. An easily accessible introductory material (Munster, 2009) can serve as an appropriate starting point for beginners in the field. A more advanced application is the subject of the paper (Babadzanjanz et al., 2003). Let us note that we will deal with a problem that is not ill-posed and that can be treated in a straightforward way similar to that used in the papers cited above.

We were motivated by the report (Mareš, 2012), where four parameters of a cement hydration model are identified through a neural network approach. The initial value problem is, see (Mareš, 2012),

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t}(t) = B_1\left(\frac{B_2}{\alpha_\infty} + \alpha(t)\right)\left(\alpha_\infty - \alpha(t)\right)\exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right)C, \tag{1}$$

$$\alpha(0) = 0, \tag{2}$$

where α is the time dependent degree of hydration, B_1 and $B_2$are coefficients related to the cement chemical composition, α_∞ is the limit value of the hydration degree, η represents the microdiffusion of free water through formed hydrates, and C is a constant originating from an expression comprising some

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physical constants such as the universal gas constant, for instance. The initial condition $\alpha(0) = 0$ stands for the hydration degree at time $t = 0$ that is assumed to be zero though a positive value less than α_∞ is also possible. The degree of hydration is measured at time points t_i, in this way, values m_i, i = 1, 2, …, n, are produced. To take account of possibly different importance of the measurements, nonnegative weights $w_i$can be considered. In the sequel, the hydration initial value problem will also be referred to as the state equation, especially in the context that is not limited to the hydration equation but includes other initial value problems too.

Constant C is known, but the values of α_∞, B_1,B_2, and η are to be identified through the minimization of the cost function defined as follows

$$f(\alpha_\infty, B_1, B_2, \eta) = \sum_{i=1}^{n} w_i (m_i - \alpha(t_i))^2 \tag{3}$$

The range of these input parameters is given in Table 1 taken from (Mareš, 2012). As a consequence, we arrive at a constrained minimization of f, where, to obtain the value of f for different inputs, the hydration initial value problem (1)-(2) has to be repeatedly solved.

Tab. 1: Lower and upper bounds for input parameters α_∞, B_1, B_2, and η.

Parameter	Minimum	Maximum
α_∞	0.7	1.0
B_1	10^6	10^7
B_2	10^{-6}	10^{-3}
η	-12	-2

2. Methods

Various approaches are possible for solving the constrained global minimization problem described in the end of Section 1. We have chosen an SQP (sequential quadratic programing) method implemented as the optimization procedure `fmincon` in the Matlab Optimization Toolbox, see (Optimization, 2012). This Matlab function is designed to find a minimum of a constrained nonlinear cost function. The algorithm asks for the gradient of the minimized cost function. The gradient can be either calculated automatically by a numerical differentiation of the cost function or delivered by a user-written Matlab function. To use the latter option, it is necessary to derive and solve auxiliary initial value problems that represent the sensitivity of the solution of the state equation to the input parameters. The sensitivity is, in fact, the derivative of the state solution with respect to an input parameter. The background theory for the derivation of these problems is described in (Kurzweil, 1978), Chapter 14, for instance.

2.1. Sensitivity equations

The aforementioned initial value problems have the same form, namely

$$\frac{\mathrm{d}v}{\mathrm{d}t}(t) = g(t)v(t) + p(t), \tag{4}$$

where $g(t)$ and $p(t)$ are known functions containing the state solution $\alpha(t)$ the derivative of which we wish to calculate. The equation is equipped with $v(0) = 0$, the initial condition. In detail,

$$g(t) = B_1 \exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right)\left(\alpha_\infty - \frac{B_2}{\alpha_\infty} - 2\alpha(t) + \left(\frac{B_2}{\alpha_\infty} + \alpha(t)\right)(\alpha_\infty - \alpha(t))\eta\alpha_\infty^{-1}\right)C \tag{5}$$

is shared by all the sensitivity equations but p is more input parameter dependent. If the sensitivity (that is, the derivative) to α_∞ is required, then

$$p(t) = B_1 \alpha(t) \exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right) C\alpha_\infty^{-3}$$

$$\times (\alpha_\infty B_2 + \alpha_\infty^3 - \eta\alpha_\infty B_2 + \eta B_2 \alpha(t) - \eta\alpha_\infty^2 \alpha(t) + \eta\alpha^2(t)\alpha_\infty). \tag{6}$$

If B_1 is in the focus of sensitivity analysis, then

$$p(t) = \left(\frac{B_2}{\alpha_\infty} + \alpha(t)\right)\left(\alpha_\infty - \alpha(t)\right) \exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right) C. \tag{7}$$

For B_2, we obtain

$$p(t) = B_1\left(\alpha_\infty - \alpha(t)\right) \exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right) C\alpha_\infty^{-1}. \tag{8}$$

Finally, the differentiation with respect to η results in

$$p(t) = B_1\left(\frac{B_2}{\alpha_\infty} + \alpha(t)\right)\left(\alpha_\infty - \alpha(t)\right)\alpha(t) \exp\left(\frac{\eta}{\alpha_\infty}\alpha(t)\right) C\alpha_\infty^{-1}. \tag{9}$$

To facilitate the process of the derivation of the sensitivity initial value problems, Matlab Symbolic Math Toolbox, see (Symbolic, 2012), was employed. By using this tool, we automatically both derive the sensitivity formulae and obtain the respective Matlab functions that are then called from a sensitivity calculation routine.

The sensitivity of the cost function, represented by the partial derivative of f with respect to $\omega \in \{\alpha_\infty, B_1, B_2, \eta\}$, is as follows

$$\frac{\partial f}{\partial \omega} = 2\sum_{i=1}^{n} w_i(m_i - \alpha(t_i))\alpha'_\omega(t_i), \tag{10}$$

where α'_ω, the derivative of α with respect to ω, is obtained through solving the sensitivity initial value problems (4)-(9), that is, $\alpha'_\omega \equiv v$.

The key point of the calculation is to solve the initial problems. This is done by the ordinary differential equation solver `ode45`, a standard Matlab function. Although its use in the main program as well as in its subroutines is easy and comfortable, it has turned out that the accuracy the gradient calculation is affected by the values of the inner parameters that control the setting of the `ode45`solver. Tuning of these parameters is recommended.

2.2. Results and comments

Outputs of two identification program runs are depicted in Fig. 1. The data were generated from a known state solution, the parameters of which were then “lost” and identified again.

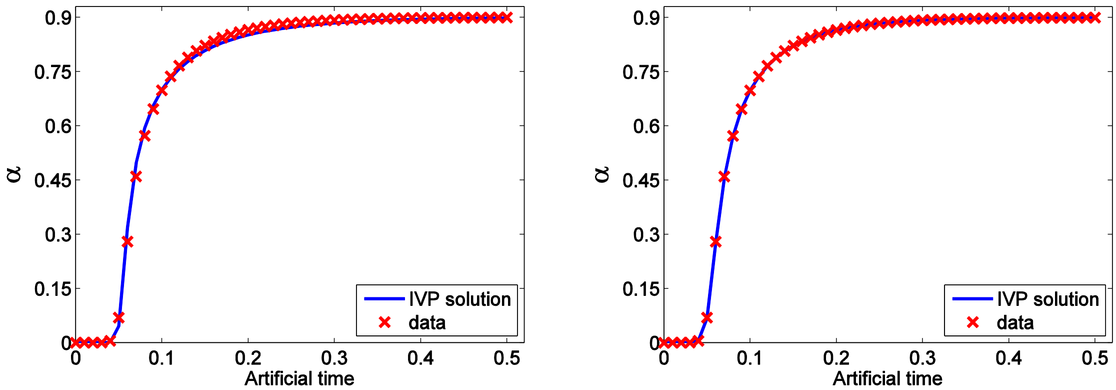

Fig. 1: Measured data and the solution of the hydration problem corresponding to the identified parameters α_∞, B_1, B_2, and η.

In the left graph, one can see that the data points are not exactly matched. The initial cost of 181.932 was reduced to 4.086, which falls short of expectations. The minimization method got stuck at a local minimum. The right graph results from the optimization run starting at a different initial point. The initial cost of 3 408.858 was reduced to 0.0000222.

3. Conclusions

The coupling of a purely numerical software with a computer algebra tool has proved to be effective. It substantially reduces the danger of erroneous derivation of the sensitivity equations and saves coding time. Since the identification problem is a sort of global minimization problem, one has to be careful when using a gradient-based optimization algorithms. A set of different starting points has to be chosen.

Acknowledgements

The authors appreciate the support of the Grant Agency of the Czech Technical University in Prague, grant No. SGS14/003/OHK1/1T/11. The authors also wish to thank Karel Hájek and Ondřej Petlík for their assistance in the project.

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