The need for qualitative reasoning in automated modeling: a case study

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Abstract

This paper demonstrates that qualitative reasoning plays a crucial role for both an efficient and physically correct approach to the automated formulation of an accurate quantitative model which explains a set of observations. The model which "best" reproduces the measured data is selected within a model space whose elements are constructed by exploiting specific knowledge and techniques of the application domain. An automated search, performed at a pure numeric level through system parameter identification methods, may be inefficient because of the computational costs which significantly grow with the dimension of the model space. Even more importantly, a "blind" search over the whole space may yield a model which best fits the observations but does not capture all of the qualitative features of the physical system at study, such as for example discontinuities of the behavior. We approach the selection problem by exploiting a mixture of qualitative and quantitative techniques which require both symbolic and numeric computations. This paper illustrates the suitability of such an approach in the context of a computational environment for the automated formulation of the constitutive law of an actual visco-elastic material.

Introduction

Automated model formulation is one of the major problems in the Qualitative Physics research framework (Addanki, Cremonini, & Penberthy 1991; Capelo, Ironi, & Tentoni 1993; Crawford, Farquhar, & Kuipers 1992; Falkenhaier & Forbus 1991; Ironi & Stefanelli 1994; Iwasaki 1992; Low & Iwasaki 1992; Nayak 1994; Weld 1992). Such an issue involves both the construction of the model space for a given application domain and the selection, within such a space, of the most appropriate model for a given task. The model space may be built either manually or, possibly, automatically in accordance with specific knowledge and techniques of the considered domain, whereas the selection strategy is suggested by the task for which the model is to be used.

This paper deals with the problem of automated model selection, with a focus on the task of finding the most accurate quantitative mathematical model which explains a set of observations.

The accuracy of a model indicates how "closely" the model predictions match the observations. The model accuracy problem has been addressed by some authors (Iwasaki & Levy 1994; Nayak 1994; Weld 1992) in terms of simplification and refinement of models so that the predicted behavior of the resulting model, obtained by a simple search process through a graph of models (Addanki, Cremonini, & Penberthy 1991) does not present discrepancies with the observations. These papers do not consider the resolution of model accuracy, i.e. they do not consider the numeric precision of the model predictions versus the observations.

In accordance with our task, we look for a model which is accurate from both the qualitative and numeric point of view, i.e. a model which captures all and none but the qualitative features of the physical system at study and which best fits the experimental data. Therefore, the problem may be approached in two stages: at first, qualitative techniques may be properly exploited to select within the model space a subset of models which describe the behavior of the physical system at least qualitatively, and then, numerical procedures may be used, in an optimization loop, to identify, within such a set, the model which best refines the quantitative properties of the observed behavior. There are at least two reasons why the optimization loop should not be extended to the whole model space. The most important reason is that the "best" model obtained on the basis of a purely numerical criterion could be not completely consistent, in qualitative terms, with the observations, or, in other words, that it could not capture some important physical features of the modeled system. For example, the presence of discontinuities in the observed data may be not properly represented because, in general, the numerical procedures tend to smooth them. Moreover, the computational costs significantly grow with the number of models which are to be considered.

This paper is mainly about model accuracy: it describes algorithms and problems related to model selection and identification. Our approach is here de-

scribed in the context of a prototype modeling environment for the automated formulation of the constitutive law of an actual visco-elastic material (Capelo, Ironi, & Tentoni 1993; 1995). We consider linear visco-elastic models, i.e. models whose visco-elastic behavior is described by a linear Ordinary Differential Equation (ODE) with constant coefficients. The space of possible linear visco-elastic models is characterized by four classes of ODEs (Capelo, Ironi, & Tentoni 1993). Such a model space has been automatically generated in two steps: at first, following an enumerative procedure and exploiting suitable filters in order to control the combinatorial explosion, complex structures of materials are generated by analogy with mechanical devices where components which reproduce the fundamental elastic and viscous responses are combined either in series or in parallel. Then, the mathematical model of each structure is generated by exploiting suitable connection rules and mathematical models of the basic components, which are expressed through internal state variables. It can be proved that the dimension of the model space is equal to $2n$, if n is the maximum number of components the structures are made up. Of course, n determines the maximum order m of the equations in each class as well.

Therefore, our problem may be reformulated as follows: given a set of observations obtained in response to standard experiments on an actual material, we have to identify the equation $E_{i,m}$, where m is the order of the equation, and i an index between 1 and 4 which marks the classes of ODEs in the model space. The identification of the equation $E_{i,m}$ requires to determine i, m, and the numeric values of the parametric coefficients in the equation. The value of i is given by the comparison of the qualitative properties of the material, which are abstracted from the data, with the simulated behaviors of the models of ideal materials in the model space (Capelo, Ironi, & Tentoni 1995); whereas m and the values of the coefficients are identified through an optimization loop so that both the goodness of fitting and the significance of the numerical values of parameters are met at best in accordance with the Akaike criterion (Akaike 1974).

This paper is organized as follows: the next section gives a characterization of the model space. Then, the model selection strategy is presented with particular emphasis on the problems related to system parameter identification (Ljung 1987) and on the advantages which may derive from qualitative reasoning.

Model space characterization

Mathematical modeling process of most physical systems follows a reasoning flow whose fundamental inferences are synthesized in Figure 1: first experimental data are collected, then a set of models is chosen, then the "best" model in the set is calculated.

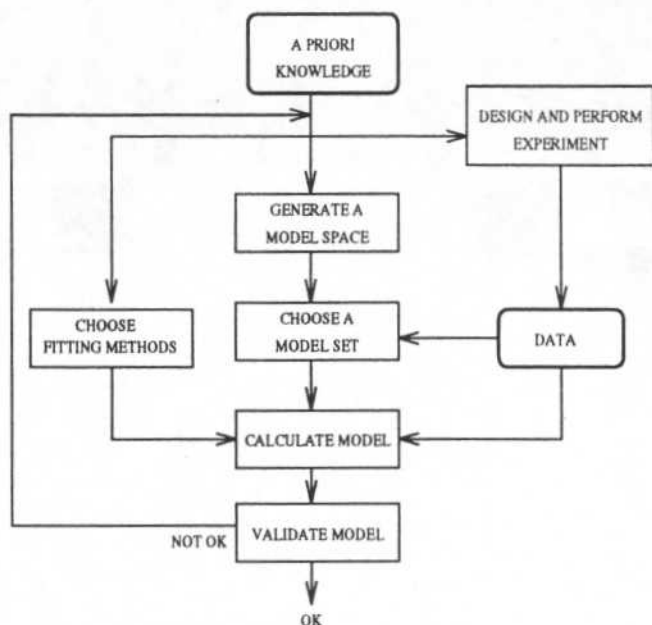The obtained model may be not adequate because:

Figure 1: Basic inferences in the modeling process

1. the numerical procedure failed to find the "best" one according to the fixed criterion;

2. the numerical methods and the fitting criterion were not well chosen;

3. the chosen model set does not give "a good enough" description of the physical system

If the model may not be considered as an adequate one, the failure reason should be looked for in the various steps in the procedure. Let us remark that the data could be not informative enough to provide guidance in selecting good models. The proper a priori knowledge must be exploited in order to address all of the above mentioned problems, among those the proper model set selection is the most crucial one. Therefore, as a first step towards an efficient automated selection of the most accurate model, the characterization of the space of candidate models is essential.

In (Capelo, Ironi, & Tentoni 1993) we gave a characterization of the space of candidate models for visco-elastic materials, automatically generated under the assumption of linear basic models of elasticity and viscosity, respectively $s = Ee$ and $s = \eta\dot{e}$ (s denotes the stress, e the strain, E, η are constants and dot denotes the time derivative), and proved that:

Theorem 1. The set $\mathcal{FE}$ of all the admissible linear models can be partitioned into the following four classes ($\mathcal{FE} = \bigcup_{i=1}^{4} \mathcal{FE}_i$):

$$\mathcal{FE}_1 = \{FE_{1,m} : \qquad \sum_{i=0}^{m} D^i s = \sum_{i=0}^{m} D^i e \ , \ m \geq 0\}$$

$$\mathcal{FE}_2 = \{FE_{2,m} : \qquad \sum_{i=0}^{m} D^i s = \sum_{i=1}^{m+1} D^i e \ , \ m \geq 0\}$$

$$\mathcal{FE}_3 = \{FE_{3,m} : \qquad \sum_{i=0}^{m} D^i s = \sum_{i=0}^{m+1} D^i e \ , \ m \geq 0\}$$

$$\mathcal{FE}_4 = \{FE_{4,m} : \qquad \sum_{i=0}^{m+1} D^i s = \sum_{i=1}^{m+1} D^i e \ , \ m \geq 0\}$$

where D^i denotes the i−th time derivative operator.

The linearity assumption is actually acceptable, although the constitutive law of a material may be non-linear and may contain non-constant coefficients. In fact, most materials show a linear time dependent behavior in the limit of infinitesimal deformation and even in finite deformation as long as the strain remains below a certain limit, which depends on the material.

The elements in $\mathcal{FE}$ are formal equations, that is ODEs whose non-zero coefficients are given the symbolic unitary value, and describe the mechanical behavior of ideal visco-elastic materials. The models of actual materials are to be looked for in the set $\mathcal{E} = \bigcup_{i=1}^{4} \mathcal{E}_i$, where $\mathcal{E}_i$ is a class of ODEs with the same structure of $\mathcal{FE}_i$ but whose coefficients take value in $\mathbb{R} - \{0\}$. The numeric values of the non-zero coefficients are strictly dependent on the material, and therefore they may be identified only from the experimental data.

Let us remark that for $m = 0$, the equations $FE_{i,m}$ are limit cases and model respectively the elastic structure (H), the viscous one (N), and the simplest composite structures $(H|N, \ H - N$, where $|$ denotes the parallel operator and $-$ the series one; these two structures are known in the literature as Kelvin (K) and Maxwell (M) models). If n is the maximum number of basic components a structure is made up, the number of equations in each class $\mathcal{FE}_1$, $\mathcal{FE}_2$ is equal to $n/2$ if n is even and the integer part of $n/2 + 1$ otherwise; whereas it is equal to the integer part of $n/2$ in the classes $\mathcal{FE}_3$, $\mathcal{FE}_4$. The index m, which implicitly defines the order of the ODE corresponding to a structure made up of n components, is equal to the integer part of $n/2$ or $n/2 - 1$ if n is odd or even, respectively.

The classes of equations are in correspondence one-to-one with suitable classes of analogical structures, which are called reference classes. We proved (Capelo, Ironi, & Tentoni 1995) that the whole enumerated set of analogical structures, with the exception of the limit cases, can be partitioned into four equivalent classes as well since any complex structure is equivalent to a structure in one of the reference classes.

The first stage in the model selection process lies in choosing a proper model set, i.e. the class $\mathcal{FE}_i$ which exhibits the same qualitative behavior of the real material. Therefore, in order to compare the response to the same kind of experiment (either creep or relaxation) of an actual material with those of the ideal ones, we implemented (Capelo, Ironi, & Tentoni 1995) algorithms
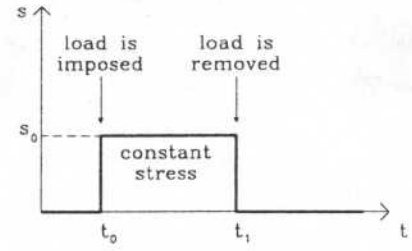

Figure 2: Stress input signal for static creep test: a constant stress state is imposed for a time $\Delta t = t_1 - t_0$.
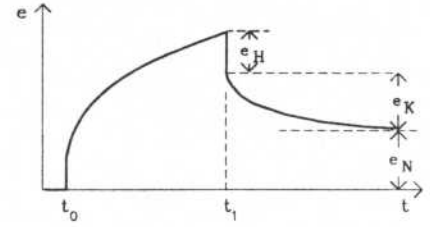

Figure 3: A typical strain response to a stress step excitation

for both the interpretation of the observed responses and the derivation of the profiles of the responses of the ideal materials in terms of the qualitative properties which may characterize the mechanical behavior of an, either ideal or actual, visco-elastic material.

As we have collected experimental data on different visco-elastic materials, such as inks, rubbers, and drugs, obtained by means of static creep experiments only, let us concentrate on such kinds of tests. A static creep experiment consists of applying an external force on the material and observing the caused deformation. However, the analysis of relaxation data, which are obtained by imposing a deformation and measuring the corresponding produced stress, is similarly carried out. As far as the standard form of the applied stress input signal is concerned, it is mathematically modeled by $s(t) = s_0[H(t - t_0) - H(t - t_1)]$, where $s_0 > 0$ is a constant, t_0, t_1 are the significant time-points, and $H(t)$ is the Heaviside function (Figure 2).

The strain response $e(t)$ to a step stress excitation is characterized by either the presence or absence of one or more of the strain properties, which are, namely, an elastic instantaneous deformation, a delayed (still elastic) one, and a viscous irrecoverable deformation (Figure 3). The various combinations of such properties, respectively denoted by e_H, e_K, e_N since they feature the physical properties of the basic structures H, K, N, characterize the prevailing properties of the materials and may be correlated with the modality the basic components are combined. Therefore, the qualitative profiles of the responses to static creep tests of both ideal materials (QB_I) and actual ones (QB_O) are

qualitatively defined in terms of just three logical parameters α_H, α_K, α_N which take on either the value TRUE (T) or FALSE (F) in accordance with the presence or absence of the corresponding strain properties of the considered material.

Algorithms for deriving both QB_I and QB_O are given in (Capelo, Ironi, & Tentoni 1995). More precisely, the qualitative behavior QB_I of each ideal material in the model space is obtained through a simulation algorithm which builds the creep response of the material directly from its structure. For any complex structure C, its equivalent one C_{eq} in the suitable reference class is considered, and $QB_I(C_{eq})$ is generated by exploiting suitable compositional rules. Then, the association of $QB_I(C)$ with the appropriate class of equations is straightforward derived. Let us remind that QB_I =(T,T,F), QB_I =(F,T,T), QB_I =(F,T,F), QB_I =(T,T,T) respectively characterize structures whose correspondent differential models are in the classes $\mathcal{FE}_1$, $\mathcal{FE}_2$, $\mathcal{FE}_3$, $\mathcal{FE}_4$ when $m \geq 1$. The QB_I of the limit structures correspond to the qualitative behavior of the limit equations, i.e. $QB_I(H) = $ (T,F,F), $QB_I(N)$ =(F,F,T), $QB_I(K)$ =(F,T,F), $QB_I(M)$ =(T,F,T). Let us notice that QB_I=(F,T,F) characterizes all of the models in $\mathcal{FE}_3$, and that seven different QB_Is, three of them being limit cases, allow us to classify a material according to its prevailing physical features.

The observed strain properties QB_O are captured through the identification of characteristic shapes in the experimental data plot. First, a qualitative curve description is given in terms of regions which are homogeneous with respect to graphical features such as steepness, convexity and linearity. Then, such features are associated with the proper physical properties: instantaneous elasticity is graphically identified by the curve steepness in t_0 and t_1, whereas delayed elasticity and viscosity are assessed over a time segment where the curve is concave and linear, respectively.

The most plausible candidate model set is given by the class $\mathcal{FE}_i$ whose QB_I perfectly matches QB_O.

Selection of an accurate model

We have seen how the qualitative interpretation of creep experimental data allows us to select a class of plausible models out of $\mathcal{E}$ whose structure is characterized in Theorem 1. We will denote by $\bar{\mathcal{E}}$ such a class, and by $E_m(\mathbf{p})$ (boldface letters indicate vectors) the m-th model in $\bar{\mathcal{E}}$, i.e.

$$\bar{\mathcal{E}} = \{E_m(\mathbf{p}) : \sum_i p_i^{(e)} D^i e = \sum_j p_j^{(s)} D^j s ,$$

$$\mathbf{p} = \begin{bmatrix} \mathbf{p}^{(e)} \\ \mathbf{p}^{(s)} \end{bmatrix} \in \mathbb{R}^{N(m)}, \ \mathbf{p} \neq \mathbf{0} , \ m = 0, .., M\}$$

where: M depends on the maximum number of basic components which are used to generate the model space; the ranges for i and j – and consequently the number $N(m)$ of unknown model parameters $\mathbf{p}$ – depend both on m and on the class, whose structure is constrained by Theorem 1. The integer m indexes the equations in $\bar{\mathcal{E}}$ by increasing differential order and is related to the number of components the model is based on.

After a parametrized set of plausible models has been obtained, the *System Identification* (SI) (Ljung 1987) task is performed, i.e. the problem of selecting the "best" model within the class is addressed.

In order to identify the ODE which refines the quantitative properties of the given material, both the order of the equation and the numeric values of its parametric coefficients must be determined. It is clear that if m, and consequently $N(m)$, is increased, the goodness of fitting improves, though not indefinitely because of both the numerical errors and the noise on experimental data. However, the significance of the numeric values of the model parameters may not improve as well. As a matter of fact, a higher order model may better fit the data while its coefficients lose significance, and their physical interpretation may consequently fail. Moreover, the information about the number of retardation times (Ferry 1970; Whorlow 1980), which is a feature of the material strictly related to the order of the equation, can be lost if our focus is only on the goodness of fitting. Let us remind that the retardation times are parameters associated with the state changes which subsequently occur in the material. For example, in polymeric materials they can be associated with the break of either the hydrogen or Van der Waals bonds which does not occur at simultaneous times. From the modeling point of view, the retardation times are specified in the arguments of exponential functions whose sum defines the solution of the ODE model.

The SI task is performed through an optimization loop aimed at determining an index $m^* \in \{0, .., M\}$ and a vector $\mathbf{p}^* \in \mathbb{R}^{N(m^*)}$ so that both the goodness of fitting and the parameter significance issues are met at best. Figure 4 illustrates how this goal is achieved. For each m, the tentative model $E_m(\mathbf{p})$ goes through a *parameter identification* process (detailed in Figure 5) and the values $\mathbf{p}^*$ of its coefficients are computed in such a way that $E_m(\mathbf{p}^*)$ best fits the data. Then, the adopted SI optimality criterion is checked for a minimum with respect to m: the resulting quantitative model $E_{m^*}(\mathbf{p}^*)$ succeeds in balancing goodness of fitting and parameter significance.

For the hierarchical structure of our search model set, the problem of determining a model whose order is optimal with respect to both the goodness of fitting and the number of parameters finds a strict analogy with the theory of time series (Choi 1992) where several optimality criteria have been proposed. Among those, we considered the Akaike Information Criterion (Akaike 1974), which can be formulated as follows:
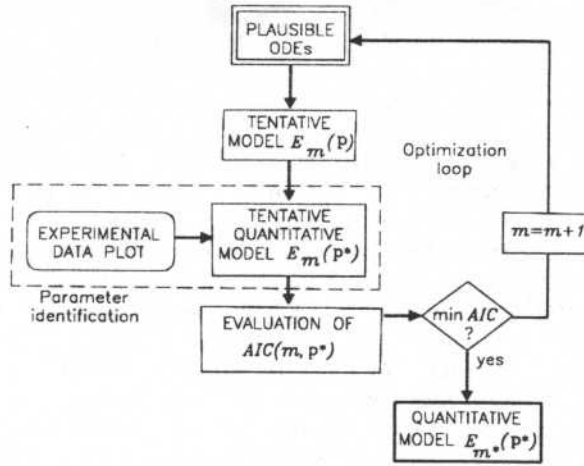
Figure 4: System identification task: the quantitative model is obtained through an optimization loop

Figure 5: Parameter identification process: given $E_m(\mathbf{p})$ and the experimental data, optimal values $\mathbf{p}^*$ are computed.

Akaike Criterion: The model which best fits the experimental data and preserves parameter significance corresponds to the minimum of the function:

$$AIC(m) = 2N(m) - 2\log[\text{maximized likelihood}].$$

Since the experimental errors can be assumed to be independent and normally distributed, the maximum likelihood method corresponds to the least squares method and $AIC(m)$ may be rewritten as follows:

$$AIC(m) = 2N(m) + N_{\text{exp}}\log S^2(m, \mathbf{p}^*) ,$$

where N_{exp} is the number of experimental points and $S^2(m, \mathbf{p}^*)$ the sum of squares of residuals performed by the best fitting model $E_m(\mathbf{p}^*)$. More precisely, for the current m the optimal $\mathbf{p}^*$ is the result of a parameter identification process (see Figure 5) which provides a numerical solution to the following minimization problem:

Find $\mathbf{p}^*$ such that

$$S^2(m, \mathbf{p}^*) = \min_{\mathbf{p} \in \mathbb{R}^{N(m)}} S^2(m, \mathbf{p}) , \qquad (\mathcal{P}1)$$

where

$$S^2(m, \mathbf{p}) = \sum_{i=1}^{N_{\text{exp}}} [e(\mathbf{p}, \bar{t}_i) - e_i]^2, \ \{(\bar{t}_i, e_i)\}_{i=1,..,N_{\text{exp}}} \text{ are}$$

the experimental points ($\bar{t}_1 \equiv t_0$) and, if $\mathbf{De}$ is the vector of the time derivatives of e and $\mathbf{e}^0$ suitable initial conditions, $\{e(\mathbf{p}, \bar{t}_i)\}_{i=1,..,N_{\text{exp}}}$ is the numerical solution of the initial value problem:

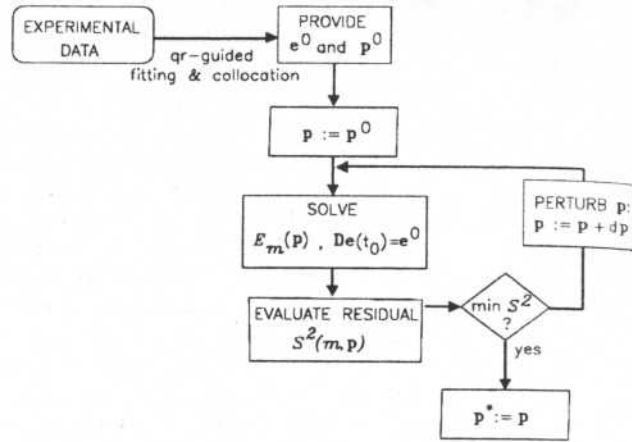$$E_m(\mathbf{p}) , \quad \mathbf{De}(t_0) = \mathbf{e}^0 . \qquad (\mathcal{P}2)$$

Since parameter identification problems are often ill-posed, some attention must be paid to the choice of the numerical schemes.

As regards the choice of the solver for $(\mathcal{P}2)$, we have adopted a numeric differentiation scheme proposed by Klopfenstein-Reiher (Klopfenstein 1971), which has proved especially effective as a stiff ODE solver and performs quite well also on non-stiff ODEs. As a matter of fact, traditional methods, such as explicit Adams or Runge-Kutta (Gear 1971), are inadequate since the ODEs which are solved during the process may be stiff according to the extent of instantaneous elasticity featured by the modeled materials.

In order to obtain a good numerical performance from both the ODE solver and the minimization algorithms, equations have been scaled. To tackle the non-linear least squares optimization problem $(\mathcal{P}1)$, we have adopted the Levenberg-Marquardt (Moré 1977) method, which is efficient and robust. The main problem with optimization algorithms is that a "good" guess $\mathbf{p}^0$ of the solution must be provided in order to ensure convergence to the true solution rather than to a local minimum. This is generally a difficult task, since $\mathbf{p}^0$ may not have an explicit physical meaning.

Moreover, $\mathbf{e}^0$ must be given to completely define problem $(\mathcal{P}1)$. A common way of dealing with unknown initial conditions is to treat all or some of them as parameters to be identified. The obvious drawback of this approach is the increased computational complexity, i.e. higher costs and an augmented risk of numerical instability due to the greater number of parameters involved.

In the light of the above considerations, the following strategy, which exploits both the a priori knowledge

and the experimental data, has been implemented in order to automatically provide a good guess of both $\mathbf{p}^0$ and $\mathbf{e}^0$ so that the convergence to the global minimum may be successfully achieved by the identification procedure.

If $QB_O = (\alpha_H, \alpha_K, \alpha_N)$ is the qualitative abstraction of the creep data, and $\chi(\alpha) = 1$ (or 0) if $\alpha =$T (or F respectively), the experimental curve can be suitably fitted by a function whose shape is suggested by QB_O, as well as by the linearity assumption:

$$y(t; QB_O, \mathbf{c}, \boldsymbol{\lambda}) = \chi(\alpha_K) \cdot \sum_{i=1}^{r} c_i(1 - \exp(-\lambda_i t)) +$$
$$+ \chi(\alpha_N) \cdot c_{r+1} t + \chi(\alpha_H) \cdot c_{r+2}$$

where $\mathbf{c}, \boldsymbol{\lambda}$ are "fine tuning" positive parameters, and the number r of exponential components is related to the current value of m. If $y(t)$ is the function characterized by values of $\mathbf{c}, \boldsymbol{\lambda}$ which minimize the distance between $y(t_i)$ and e_i $(i = 1, .., N_{\exp})$, then $\mathbf{e}^0 := \mathbf{D}y(t_0)$. Finally, the initial estimate $\mathbf{p}^0$ is obtained by collocating the ODE on the experimental grid, i.e. $\mathbf{p}^0$ is the least squares solution of the following linear system:

$$\sum_i p_i^{(e)} D^i y(t_k) = \sum_j p_j^{(s)} D^j s(t_k) \ , \ (k = 1, .., N_{\exp}).$$

An example

In order to show how numerical accuracy by itself does not guarantee that the qualitative physical features of the material are correctly represented by the resulting quantitative model, we consider the following example.

At first, we illustrate the result obtained when the SI task is performed on a subset of plausible models, preliminarily selected within the whole model space by matching the qualitative observed behavior against the ideal ones. Then, for the same experimental data, we show the result obtained when the SI task is performed blindly on the whole model space. In this example, the dimension of the model space is equal to 20.

Let us consider a set of data related to a rubber-like material; the creep experiment was carried out at $50°C$ over a time range of 141 s, keeping the stress at a constant value of 200 Pa.

The experimental curve and the computer outcome of its qualitative interpretation are illustrated in Figure 6. The system correctly identifies the qualitative physical properties featured by the given material, i.e. delayed elasticity and viscosity, and assesses its qualitative behavior at $QB_O = $ (F,T,T).

Consequently, the plausible model class

$$\mathcal{FE}_2 = \{\sum_{i=1}^{m+1} D^i e = \sum_{j=0}^{m} D^j s , \ m \geq 1\}$$

is identified within the model space as the subset of models which are consistent with the observations.
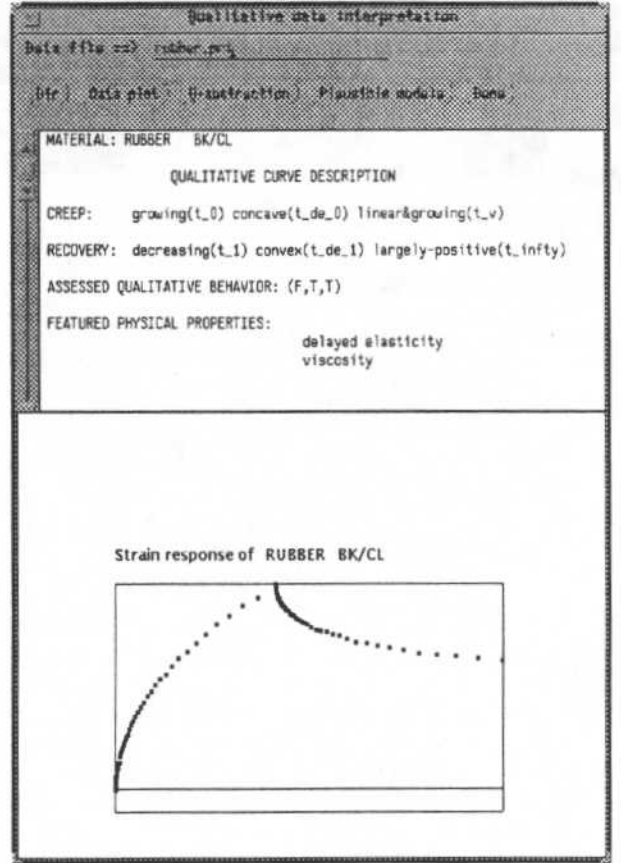

Figure 6: Qualitative interpretation of the creep experimental response of a rubber-like material

Then, the SI optimization loop is performed on the parametrized set of models

$$\mathcal{E}_2 = \{E_m(\mathbf{p}) : \sum_{i=1}^{m+1} p_i^{(e)} D^i e = \sum_{j=0}^{m} p_j^{(s)} D^j s ,$$
$$\mathbf{p} = \begin{bmatrix} \mathbf{p}^{(e)} \\ \mathbf{p}^{(s)} \end{bmatrix} \in \mathbb{R}^{N(m)}, \mathbf{p} \neq \mathbf{0} , \ m \geq 1\}$$

which embodies $\mathcal{FE}_2$, in order to find the optimal numerical values of m and $\mathbf{p}$ which identify the quantitative model of the material.

For each m, optimal values $\mathbf{p}^*$ of the coefficients are determined, and AIC is evaluated for each tentative quantitative model $E_m(\mathbf{p}^*)$. The AIC values together with the relative errors of the computed model solutions with respect to the experimental data ($\sqrt{S^2(m, \mathbf{p}^*) / e_i^2}$) are reported in the second column of Table 1. The minimum value of AIC (-1304.2) is taken at $m = 4$. Therefore, the most accurate model the system eventually associates with the given material is a fifth-order ODE; for this model, the calculated

Table 1: AIC values (and relative errors) corresponding to every tentative model identified in $\cup_i \mathcal{E}_i$

	$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_3$	$\mathcal{E}_4$
$m = 1$	-938.4 (9.347 e-02)	-1024.0 (5.617 e-02)	-1134.2 (2.881 e-02)	-1068.4 (4.311 e-02)
$m = 2$	-1168.9 (2.344 e-02)	-1230.0 (1.631 e-02)	-1281.5 (1.184 e-02)	-1249.9 (1.446 e-02)
$m = 3$	-1290.1 (1.125 e-02)	-1297.7 (1.076 e-02)	-1304.1 (1.023 e-02)	-1300.6 (1.057 e-02)
$m = 4$	-1305.5 (1.015 e-02)	**-1304.2** (1.022 e-02)	-1302.7 (1.020 e-02)	-1305.3 (1.016 e-02)
$m = 5$	-1304.6 (1.008 e-02)	-1303.3 (1.016 e-02)	-1303.1 (1.005 e-02)	-1303.6 (1.014 e-02)

values of $\mathbf{p}^{(e)}$ are: 9.248 Pa · s, 1.068e+03 Pa · s^2, 1.466e+04 Pa · s^3, 2.768e+04 Pa · s^4, 4.966e+03 Pa · s^5. Figure 7 shows the strain response, computed according to this model, versus the experimental data.

We have also performed a blind search over the whole model space $\mathcal{FE}$, in spite of the higher computational effort (20 models were identified rather than the 5 models in $\mathcal{E}_2$). Table 1 shows the AIC values corresponding to all the tentative quantitative models identified in $\cup_i \mathcal{E}_i$. In this case, the minimum value of AIC is taken at $m = 4$, but within $\mathcal{E}_1$, which is characterized by $QB_I = (T,T,F)$. This means that the given material would be eventually associated with a fourth-order ODE model which is numerically accurate, i.e. optimal with respect to goodness of fitting and order, but is not qualitatively consistent with the observations as it does not correctly capture the qualitative strain properties $QB_O = (F,T,T)$ featured by the material. The application of the Akaike criterion to the whole search space may fail as the criterion alone does guarantee numerical but not physical accuracy. The implemented selection procedure emulates the expert skills at limiting the candidate search space to equations which are suggested by her expertise in interpreting the observations.

Conclusion

This paper discusses, through a case study, the importance of qualitative reasoning techniques for a correct approach to automated modeling even if the goal is the formulation of an accurate quantitative model: numerical accuracy by itself may be meaningless as it does not guarantee that the physical features are properly
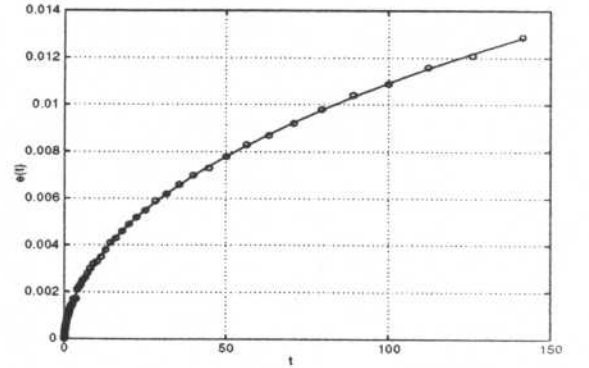

Figure 7: Measured (o) vs computed (–) strain, according to the most accurate model identified by the system

represented. The search model set is properly chosen within the model space for the domain when it satisfies a qualitative accuracy criterion, i.e. any of its elements qualitatively represents the physical properties captured by the observations. Besides the evident advantage which derives from this first selection, the computational costs are significantly reduced because of the reduced dimension of the search space. Moreover, the restriction of the search space to all and none but the qualitative meaningful models allows us to better delimit the a priori knowledge which could be conveniently exploited in the next steps of the automated modeling process. More precisely, as we have shown in our specific case, such knowledge may suggest a proper choice of either the initial conditions needed for solving the initial value problem or a good initial guess for the model parameters. In the context of a system whose goal is to automate all steps in the modeling process, the issue to suitably perform such choices is crucial with respect to numerical costs (running time, numerical instability).

Acknowledgement

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