Parameter Estimation of Viscoelastic Materials: A Test Case with Different Optimization Strategies

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Abstract. In this work, and based on numerical optimization techniques, constitutive parameters for viscoelastic materials are determined using a inverse problem formulation. The optimization methodology is based on experimental results obtained in the frequency domain, for a CFRP-Carbon Fibre Reinforced Polymer, through DMA-Dynamic Mechanical Analysis. The relaxation modulus of viscoelastic materials is given by a summation of decaying exponentiating functions, known as Prony series. Prony series, in time domain, are normally used to determine constitutive parameters for viscoelastic materials. In this paper, using the Fourier transform of the time domain Prony series, a nonlinear constrained least square problem based on Prony series representations of storage and loss modulus, for the considered material, is analyzed. A case study considering the estimation of $2N$ viscoelastic parameters, $N = 1, 2, \cdots 11$, is taken as a benchmark. The nonlinear constrained least square problems are solved using global and local optimization solvers. The computational results as well as the main conclusion are shown.

Keywords: inverse problem, nonlinear optimization, viscoelasticity, constitutive parameters
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INTRODUCTION

Viscoelastic materials are quite more complex to describe than purely elastic materials (see e.g. [1], [2]). In fact, and in opposition to elastic materials, viscoelastic materials are characterized by having strain-rate dependence, loading-history dependence and a energy dissipative behavior due to internal damping mechanisms. Some common phenomena in viscoelastic materials are the creep (strain increases with time for a constant stress), relaxation (stress decreases with time for a constant strain) and, for a cyclic deformation, a phase lag between the applied stress and the obtained strain, is observed. Viscoelastic materials behave as elastic solids and viscous liquids depending on the temperature or time/frequency scale chosen. In fact, the behavior of viscoelastic materials is a combination of the idealized behaviour of purely elastic solids and viscose liquids. These intrinsic material characteristics increase the constitutive modelling complexity due to the associated non-conservative effects (e.g., damping), strain-rate dependence, loading amplitude dependence and type of loading. However, for obtaining accurate results, when viscoelastic materials are considered, these properties must be adequately modeled, especially, when dynamic solicitations are applied to the considered structure (see [2]). The dynamic behavior of viscoelastic materials can be characterized through resonant and non-resonant experimental techniques. Normally, this characterization is made through DMA that characterize the intrinsic evolution of storage (shear) modulus, G', and loss (shear) modulus, G'', with the frequency.

The main goal of this work is to obtain viscoelastic constitutive parameters, specifically for the considered material, directly from frequency domain experimental data, avoiding the used of time-domain experimental data. In fact, time-domain experimental data, is normally obtained considering a static state of deformation, which may not reproduce, exactly, the dynamic response of viscoelastic material when subject to cyclic loadings.

The paper is organized as follows. Next section presents the derivation of the complex modulus equations for a viscoelastic material in frequency domain. In particular, the formulas for the storage modulus and loss modulus are deduced in this section. Then, the nonlinear least square problem to estimate a viscoelastic parameter set is analyzed. Finally, the numerical results are presented and some conclusions are taken.

LINEAR VISCOELASTIC MATERIAL BEHAVIOR

We first briefly review the theoretical background on modeling of linear behavior of viscoelastic materials. The mathematical formulation for this kind of phenomenon may be expressed through a Riemann convolution integral

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(see [3]). In particular, the stress in linear viscoelastic materials is given by the following constitutive equation which is based on the Boltzman's superposition principle

$$\sigma(t) = \int_{-\infty}^{t} G_{rel}(t-\tau)\frac{de}{d\tau}d\tau, \tag{1}$$

where σ is the stress tensor, e is the strain tensor and $G_{rel}(t)$ is the linear relaxation (shear) modulus or, also known as the relaxation kernel. Considering that $\sigma(t) = e(t) = 0$ for $t < 0$, and a discontinuous loading step is applied at $t = 0$, equation (1) is rewritten as

$$\sigma(t) = G_{rel}(t)e(0) + \int_{0}^{t} G_{rel}(t-\tau)\frac{de}{d\tau}d\tau, \tag{2}$$

where e(0) is the limiting value of $e(t)$ when $t \to 0^+$. Applying Laplace transforms to equation (2) and taking $e(0) = 0$, we obtain the following equation in the Laplace domain $\tilde{\sigma}(s) = s\tilde{G}_{rel}(s)\tilde{e}(s)$, where $\tilde{\sigma}$ and $\tilde{e}$ are Laplace transforms stress and strain with variable s, respectively. Assuming s as a pure imaginary variable equal to $j\omega$ we obtain

$$G^*(j\omega) = \frac{\tilde{\sigma}(j\omega)}{\tilde{e}(j\omega)} = j\omega\tilde{G}_{rel}(j\omega) = j\omega\int_{0}^{\infty} G_{rel}(\tau')\exp(-j\omega\tau')d\tau', \qquad s = j\omega, \tag{3}$$

where ω is the circular frequency and $j = \sqrt{-1}$. The complex shear modulus $G^*(j\omega)$ expressed above is the so-called *complex modulus* expressed in the form

$$G^*(j\omega) = G'(\omega) + jG''(\omega), \tag{4}$$

where $G'(\omega)$ and $G''(\omega)$ are the *storage (shear) modulus* and *loss (shear) modulus*, respectively. If the relaxation functions in (1) are expressed as a discrete set of exponential decays,

$$G_{rel}(t) = G_\infty + \sum_{k=1}^{N} g_k \exp(-t/\tau_k), \tag{5}$$

then, from (3), equation (4) reads

$$G^*(j\omega) = G_\infty + \sum_{k=1}^{N} \frac{g_k\tau_k j\omega}{1+\tau_k j\omega}, \tag{6}$$

where N is the relaxation modes defined by their Prony coefficients g_k and their relaxation times τ_k, $k = 1,2,...,N$, and G_∞ is the long term (shear) modulus. Thus, from equation (6), we obtain the Prony series representations of storage and loss (shear) modulus as functions of frequency

$$G'(\omega) = \Re\{G^*\} = G_\infty + \sum_{k=1}^{N} g_k \frac{(\omega\tau_k)^2}{1+(\omega\tau_k)^2}, \tag{7}$$

$$G''(\omega) = \Im\{G^*\} = \sum_{k=1}^{N} g_k \frac{\omega\tau_k}{1+(\omega\tau_k)^2}. \tag{8}$$

OPTIMIZATION PROBLEM

To estimate the parameters $g \equiv (g_1,...,g_N)$ and $\tau \equiv (\tau_1,...,\tau_N)$ of the relaxation problem (5) we use a nonlinear least squares fit based on the average square of deviation between the predicted values $G'(\omega_i)$, $G''(\omega_i)$ calculated from equations (7) and (8), and the measured G'_i, G''_i data at M frequencies ω_i [4]:

$$\min_{g,\tau\in R^N} F(g,\tau) \equiv \sum_{i=1}^{M} \left(\left(\frac{G'(\omega_i)}{G'_i} - 1 \right)^2 + \left(\frac{G''(\omega_i)}{G''_i} - 1 \right)^2 \right). \tag{9}$$

In our numerical experiments, the coefficients g and relaxation times τ will be considered all positive and the constraints based on the ascending ordering of the relaxation times is also imposed:

$$\tau_i < \tau_{i+1} \text{ for } i = 1,2,\cdots N-1.$$

NUMERICAL EXPERIMENTS AND CONCLUSIONS

It is known that when a local optimization technique is applied to minimize the error (9) it is sensible to the starting parameter set $\{g_1^0,...,g_N^0,\tau_1^0,...,\tau_N^0\}$, since the problem may have many local minima. In [5], to overcome this drawback and to force the convergence to the global optimal set, it is suggested that the starting parameter set should be close to the global optimal set. However, this strategy is only possible if the range of the admissible parameters is known and has a small size. However, in our case we have not any information about the starting parameter set and their ranges. Two nonlinear solvers, that are available online on the NEOS servers for optimization at `http://neos.mcs.anl.gov/neos/solvers`, were selected to solve the optimization problem (9): the Ipopt and the Couenne. Ipopt is a local optimizer solver to solve large scale nonlinear optimization problems which implements an interior point barrier method based on a filter line search strategy [6]. On the other hand, Couenne is a global optimization solver that solves nonconvex mixed integer nonlinear optimization problems using a reformulation based on a branch-and-bound algorithm. The choice of N is an important issue for the success of the nonlinear optimization techniques. In the experiment, we test the effect of different numbers of relaxation modes N on the F residual value. In Table 1, we report the the residual value F and the CPU time (in sec.) for estimation of 2 until 22 viscoelastic parameters, which imply to solve eleven nonlinear constrained least squares problems for $N = 1,2,...,11$. First, we conduct the numerical experiments with the two solvers for which the starting parameter set is not provided. By default the solvers use the null vector for starting parameter set. In this case, only the Ipopt was able to obtain an optimal solution for each nonlinear least square problem ($N = 1,2,\cdots,11$). These results are reported in Table 1 in colunms 1-2. Couenne was always unable to run, aborting due to error. In order to find the best parameter set, additional experiments were carried out to show the effect of starting parameter set on the performance of the optimization solvers. We run the Ipopt and the Couenne solvers using for the starting parameter set (for $N = 1,2,\cdots,11$) the optimal set obtained by Ipopt in the previous experiments. These results are reported in Table 1 in columns 3-6.

TABLE 1. Results obtained by Ipopt and Couenne.

	IPOPT		IPOPT		Couenne	
N-Terms Prony	fval	CPU time $[s]$	fval	CPU time $[s]$	fval	CPU time $[s]$
1	159.856	0.525919	159.944	0.014997	92.1993	384.29
2	160.682	1.54576‡	160.635	1.38279‡	71.1104	1368.75
3	52.9325	0.896862	71.1106	0.088985	52.9325	4263.29
4	105.521	0.738887	33.0931	1.08483	71.1104	11003.29
5	39.1189	1.2898	83.1709	0.335948	20.7001	14730.76
6	43.1837	1.50977	51.3734	0.730888	11.2055	19701.70
7	33.7657	1.43578	32.3742	0.924858	6.12476	26637.09
8	29.4201	1.24381	36.407	0.883864	†	†
9	40.7317	1.91671	37.8198	0.85087	†	†
10	72.8779	2.67359	38.2514	1.19082	1.13206	301.85
11	71.3711	2.09068	74.163	0.230964	†	†

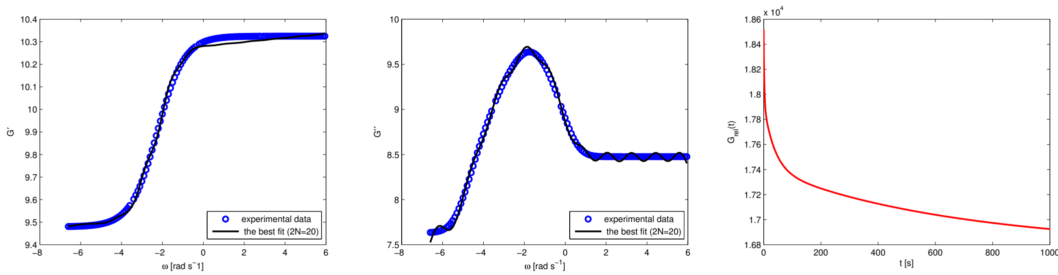
run terminates due to: '†' reach the limit time; '‡'maximum number of iterations

As it was expected, given an initial point close to the local minimum, the results obtained by Ipopt are quite similar to the previous ones since it is a local solver. However, the global Couenne solver was now able to reach the global optimal solution for eight least squares problems ($N = 1,2,3,4,5,6,7,10$). As we can see from Table 1, with too few relaxation modes, the residual value of the objective function is large. In the case of the Couenne solver, the residual value decays rapidly with the number of relaxation modes. The best optimal parameter set was found by Couenne when 20 relaxation modes are used.

TABLE 2. Optimal parameter set.

k	$g_k\,[MPa]$	$\tau_k\,[s]$	k	$g_k\,[MPa]$	$\tau_k\,[s]$
1	565.347	1.96801	6	175.683	17451.3
2	477.644	26.1378	7	368.208	57409.8
3	120.139	312.502	8	0.0047848	1693730
4	360.665	313.019	9	0.00669185	3170850
5	431.935	3488.9	10	8625.22	7115360

In Figure 1(a) and 1(b) are plotted the experimentally measured values of storage and loss moduli vs curve-fit equations of storage modulus (7) and loss modulus (8) using best optimal parameter set estimate (tabulated in Table 2). It is also shown in Figure 1(c) the corresponding relaxation function in the time domain.



(a) Storage modulus (b) Loss modulus (c) Relaxation function

FIGURE 1. The best fit obtained for the storage and loss modulus.

As conclusions, we could determine viscoelastic parameters capable to reproduce efficiently the Storage and Loss modulus data and, consequently, infer the decay of relaxation modulus in the time domain. Using as strategy the local Ipopt solver to obtain an estimate for the initial parameter set from the null vector was important. From the local optimal set as starting parameter set, global optimizer Couenne was able to get the global optimal parameter set. For future work, the anisotropic behavior of the material will be considered, in order to study the dependence of viscoelastic response on the material orientation and loading direction. Also, other non-conventional relaxation models, in the time or frequency domain, will be deduced and tested to improve the fitting accuracy to experimental data.

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