NON-LINEAR OPTIMIZATION OF THE MATERIAL CONSTANTS IN OGDEN'S STRESS-DEFORMATION FUNCTION FOR INCOMPRESSIBLE ISOTROPIC ELASTIC MATERIALS

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Abstract

In previous papers, three terms have been included in Ogden's stress-deformation function for incompressible isotropic elastic materials. The material constants have been calculated by elementary methods and the resulting fits to sets of experimental data have been moderately good.

The purpose of the present paper is to improve upon established correlation between theory and experiment by means of a systematic optimization procedure for calculating material constants. For purposes of illustration the Levenberg-Marquardt non-linear least squares optimization algorithm is adapted to determine the material constants in Ogden's stress-deformation function.

The use of this algorithm for three-term stress-deformation functions improves somewhat on previous results. Calculations are also carried out in respect of a four-term stress-deformation function and further improvement in the fit is achieved over a large range of deformation.

1. Introduction

In a number of publications (see, for example, Ogden [6], Chadwick *et al.* [1]), elementary methods have been used to determine the material constants μ_i , α_i in the stress-deformation function

$$F \equiv \sum_{i=1}^{M} \mu_i p(\lambda, \alpha_i, c) = \sum_{i=1}^{M} \mu_i (\lambda^{-1+\alpha_i} - \lambda^{-1+c\alpha_i})$$
(1)

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for incompressible isotropic elastic materials. In equation (1), F represents the force per unit undeformed area, normal to the principal direction of strain, corresponding to the principal stretch λ . The units of the μ_i are those of F and the α_i are dimensionless (i = 1, ..., M). Considerations of stability and physically realistic response lead to the inequalities

$$\mu_i \alpha_i > 0 \quad \text{for all } i = 1, \dots, M. \tag{2}$$

The parameter c in equation (1) is related to the pure homogeneous deformation of simple tension, pure shear and equibiaxial tension, for which $c = -\frac{1}{2}, -1, -2$ respectively. For further details of the three deformations and the derivation of the corresponding values of c, the reader is referred to Ogden [6].

The set of numerical results for μ_i and α_i (i = 1, 2, 3) given by Ogden [6] were obtained by an *ad hoc* method as were the two sets given by Chadwick *et al.* [1]; all of these values of the constants were derived to fit curves to the experimental data of Treloar [9]. Treloar's data were obtained in three experiments on samples cut from a single sheet of vulcanized natural rubber; his three sets of data are plotted for simple tension, pure shear and equibiaxial tension in Figures 1, 2, 3 respectively. A brief review of other experiments and associated fitted curves by Jones and Treloar [3], James *et al.* [2] and Treloar and Riding [10] is contained in Ogden [7].

Chadwick *et al.* [1] and Ogden [6] obtained values of μ_i and α_i (i = 1, 2, 3) by using the fact that, at small strains $(\lambda \approx 1)$, the computation is dominated by just one term $\mu_1 p(\lambda, \alpha_1, c)$, with $\mu_2 p(\lambda, \alpha_2, c)$ and $\mu_3 p(\lambda, \alpha_3, c)$ increasing in importance as λ increases. The actual values of μ_i , α_i determined by Chadwick *et al.* [1] and Ogden [6] for the data of Treloar [9] are reproduced for comparison purposes in Table 1.

In previous papers, authors using the stress-deformation formula (1), have taken M = 3. It was observed by Ogden [6, page 578], however, that by taking M = 4, a better fit could be obtained for $\lambda > 7.0$. One purpose of this paper is to report numerical results which verify this claim, though it will be seen that Ogden's estimate of $\alpha_4 \approx 10$ is too low for Treloar's data. The other purpose of this paper is to show that superior numerical results for μ_i , α_i (i = 1, 2, ..., M) are obtained using *non-linear* least squares optimization techniques (Section 2). Such techniques obviate the need to calculate the μ_i , α_i (i = 1, 2, ..., M) successively by fitting curves to expanding ranges of data. The optimal values μ_i^* , α_i^* (i = 1, 2, ..., M) are determined as the elements of a vector. For the data of Treloar [9] the optimal values with M = 3, 4 are reported in Section 3 and, for M = 4, the curves generated by (1) are plotted in Figures 1, 2, 3. Comparison with the values of Ogden [6] and Chadwick *et al.* [1] is presented in Table 1 and comparison of the accuracy obtained using non-linear optimization methods with the accuracy attained by Ogden [6] and Chadwick *et al.* [1] in Table 2.

Method	μ1	α1	μ2	α2	μ3	α3	μ4	α4
Twizell and Ogden $M = 4, c = -\frac{1}{2}$	6.27	1.23	-0.054	-1.99	0.036	4.44	0.80(-15)	19.49
Twizell and Ogden M = 4, c = -1	6.26	1.21	-0.067	-1.99	0.059	4.43	0.94(15)	19.49
Twizell and Ogden M = 4, c = -2	6.17	1.26	-0.091	-2.01	0.046	4.26	1.00(-14)	19.49
Twizell and Ogden $M = 3, c = -\frac{1}{2}$	2.22	2.26	-0.448	-2.01	0.39(-6)	10.01	_	
Twizell and Ogden M = 3, c = -1	3.31	1.79	-0.689	-1.99	0.20(-5)	9.88	_	_
Twizell and Ogden M = 3, c = -2	5.39	1.46	-0.530	-2.02	0.19(-5)	9.68	_	_
Ogden (1972) all <i>c</i>	6.3	1.3	-0.1	-2.0	0.012	5.0	-	_
Chadwick <i>et al.</i> (1977) equation (5.4) all <i>c</i>	3.0	2.0	-0.81	-1.25	0.37(-4)	7.82	_	-
Chadwick <i>et al.</i> (1977) equation (5.5) all <i>c</i>	3.24	2.0	-0.1	-2.0	0.62(-5)	8.7	_	-

TABLE 1. Numerical values of $\mu_i(kg \ cm^{-2}), \alpha_i \ (i = 1, ..., M; M = 3 \ or 4)$

Whereas the main aim of the present paper is to provide a systematic numerical procedure which ensures a close overall fit to Treloar's data, it is emphasized that this is different from the aims of Ogden [6] and Chadwick *et al.* [1]. In particular Chadwick *et al.* [1] were motivated by the desire to obtain modifications of the neo-Hookean ($\alpha_1 = 2$) and Mooney-Rivlin ($\alpha_1 = 2, \alpha_2 = -2$) strain-energy functions, these being widely accepted as prototype models of the behaviour of rubberlike materials. Also, the above authors did not obtain separate fits to Treloar's [9] simple tension, pure shear and equibiaxial tension data sets, as is done in the present paper, but obtained values of μ_i , α_i (i = 1, 2, 3) appropriate to all three deformations simultaneously.

	S				
	$c=-\tfrac{1}{2}$	c = -1	c = -2		
Twizell and Ogden $M = 4, c = -\frac{1}{2}$	6.30	_	-		
Twizell and Ogden $M = 4, c = -1$	-	0.36	_		
Twizell and Ogden $M = 4, c = -2$	-	-	1.92		
Twizell and Ogden $M = 3, c = -\frac{1}{2}$	12.80	_	_		
Twizell and Ogden M = 3, c = -1	_	0.63	_		
Twizell and Ogden M = 3, c = -2	-	_	2.47		
Ogden (1972)	302.90	1.60	3.91		
Chadwick <i>et al</i> . (1977) equation (5.4)	20.40	2.83	10.32		
Chadwick <i>et al.</i> (1977) equation (5.5)	16.10	1.44	4.42		

TABLE 2. Sums of squares (S)

2. A non-linear least squares algorithm

In this section the Levenberg-Marquardt iterative algorithm for calculating the optimal values μ_i^* , α_i^* (i = 1, ..., M) is outlined. The algorithm was published in 1963 by Marquardt and is similar to the method published in 1944 by Levenberg. In these two papers the L_2 norm is used in the minimization process; Shrager and Hill [8] discuss the implementation of the Levenberg-Marquardt algorithm in the L_1 and L_∞ norms. The L_1 norm is particularly beneficial when the experimental data for λ and F contain one or more wild points, and the L_{∞} norm when the errors in the experimental values of F are negligible. The L_2 norm has enjoyed much more use than the other two, as error estimates have long been available in the literature. Consequently a large literature of successful applications of the Levenberg-Marquardt algorithm in the L_2 norm, and a large amount of associated computer software, has resulted. The Levenberg-Marquardt algorithm in the L_2 norm is available to IBM users as Share Problem #1428 and from the NAG (Numerical Algorithms Group) subroutine library where it is implemented in Fortran as E04GAF and in Algol as E04GAA.

The data of Treloar [9] used in this paper contain no wild points and so the outline of the Levenberg-Marquardt algorithm which follows is related to the L_2 norm.

Suppose there are K data pairs (λ_k, F_k) for k = 1, ..., K with $K \ge 2M$. Let \hat{F}_k be the value of F_k yielded by

$$F_k = \sum_{i=1}^M \mu_i \left(\lambda_k^{-1+\alpha_i} - \lambda_k^{-1+c\alpha_i} \right)$$

and let $E_k = F_k - \hat{F}_k$ be the error in F_k . The least squares criterion requires that

$$S = S(\mu_{1}, \alpha_{1}, \dots, \mu_{M}, \alpha_{M}) = \sum_{k=1}^{K} E_{k}^{2}$$
$$= \sum_{k=1}^{K} \left\{ F_{k} - \sum_{i=1}^{M} \mu_{i} (\lambda_{k}^{-1+\alpha_{i}} - \lambda_{k}^{-1+c\alpha_{i}}) \right\}^{2}$$
(3)

be minimized; this minimum of S being reached by obtaining optimal values μ_i^*, α_i^* of the parameters μ_i, α_i (i = 1, ..., M). In order to implement the Levenberg-Marquardt algorithm to minimize S, it is convenient to introduce a vector x of order 2M defined by

$$\mathbf{x} = (x_1, x_2, \dots, x_{2M-1}, x_{2M})^T = (\mu_1, \alpha_1, \dots, \mu_M, \alpha_M)^T,$$

where T denotes transpose.

The Levenberg-Marquardt algorithm calculates iteratively a sequence of points $\mathbf{x}^{(r)}$ (r = 0, 1, 2, ...) with $\mathbf{x}^{(0)}$ some initial point chosen so that the sequence $\{\mathbf{x}^{(r)}\}$ will converge to a point $\mathbf{x}^* = (\mu_1^*, \alpha_1^*, ..., \mu_M^*, \alpha_M^*)^T$ that minimizes S (the superscript r denoting the r th iterate). The algorithm calculates the vector $\mathbf{x}^{(r+1)}$ from the vector $\mathbf{x}^{(r)}$ using the equation

$$\mathbf{x}^{(r+1)} = \mathbf{x}^{(r)} - \left[\left(P^{(r)} \right)^T P^{(r)} + \gamma^{(r)} I \right]^{-1} \left(P^{(r)} \right)^T \mathbf{E}^{(r)}, \quad r = 0, 1, 2, \dots, \quad (4)$$

where $\gamma^{(r)}$ (r = 0, 1, 2, ...) is an arbitrary parameter and $\mathbf{E} = (E_1, E_2, ..., E_k)^T$ is the vector of errors (see equation (3)). The matrix *I* is the identity matrix of order 2*M* and *P* is the matrix of first derivatives of order $K \times 2M$ whose element p_{k_I} at the *r* th iterate is given by

$$p_{ki}^{(r)} = \frac{\partial E_k}{\partial x_i}\Big|_{\mathbf{x}=\mathbf{x}^{(r)}}, \quad (k=1,\ldots,K; i=1,\ldots,2M; r=0,1,2,\ldots).$$

Thus

$$p_{k,2l-1}^{(r)} = -\left\{\lambda_k^{-1+\alpha_k^{(r)}} - \lambda_k^{-1+c\alpha_k^{(r)}}\right\},\,$$

and

$$p_{k,2l}^{(r)} = -\mu_l^{(r)} \left\{ \lambda^{-1+\alpha_k^{(r)}} - c\lambda_k^{-1+c\alpha_k^{(r)}} \right\} \ln \lambda_k$$

for k = 1, ..., K; l = 1, ..., M; r = 0, 1, 2, ...

Marquardt [5] has shown that a sufficiently large $\gamma^{(r)}$ always exists such that

$$S^{(r+1)} < S^{(r)} \tag{5}$$

(unless $\mathbf{x}^{(r)} = \mathbf{x}^*$), where $S^{(r)}$ denotes the value of S at the rth iteration (r = 0, 1, 2, ...). It is clear therefore that the method converges from poor starting values $\mu_i^{(0)}$, $\alpha_i^{(0)}$ (i = 1, ..., M) and convergence proceeds as follows:

(i) arbitrarily choose $\gamma^{(0)}$ and a parameter u > 1; say $\gamma^{(0)} = 0.01$ and u = 10;

(ii) let $T(\gamma^{(r)})$, $T(\gamma^{(r)}/u)$ be the values of $S^{(r)}$ when $\gamma^{(r)}$ and $\gamma^{(r)}/u$, respectively, are used in equation (3);

(iii) calculate $S^{(r+1)}$, $T(\gamma^{(r)})$ and $T(\gamma^{(r)}/u)$;

(iv) then

(a) if $T(\gamma^{(r)}/u) \le S^{(r+1)}$, let $\gamma^{(r+1)} = \gamma^{(r)}/u$;

(b) if $T(\gamma^{(r)}/u) > S^{(r+1)}$ and $T(\gamma^{(r)}) \le S^{(r+1)}$, let $\gamma^{(r+1)} = \gamma^{(r)}$;

(c) if $T(\gamma^{(r)}/u) > S^{(r+1)}$ and $T(\gamma^{(r)}) > S^{(r+1)}$, increase $\gamma^{(r)}$ by successive multiplication by u until the positive integer n is reached such that $T(\gamma^{(r)}u^n) \le S^{(r+1)}$. Let $\gamma^{(r+1)} = \gamma^{(r)}/u^n$;

(v) test for convergence of all the material constants μ_i , α_i (i = 1, ..., M) to the required accuracy. If the accuracy criterion is met the iterations cease, otherwise r is incremented by unity and control returns to (ii).

The convergence tests described in steps (iv) and (v) of the strategy do lead to increased computer time and storage in comparison with less sophisticated methods. With $\gamma^{(r)} \equiv 0$, for instance, the Levenberg-Marquardt algorithm (4) becomes the Gauss-Newton algorithm which, for some problems, may well converge faster, from good initial values, than the Levenberg-Marquardt algorithm. From poor initial values, however, the Gauss-Newton method may diverge while the Levenberg-Marquardt algorithm will converge. It is this factor which highlights the superior reliability of the Levenberg-Marquardt algorithm, and which makes it especially valuable for fitting a curve of the form (1) to experimental data.

3. Numerical results

The optimal values of μ_i , α_i (i = 1, 2, 3, 4) were computed using the Levenberg-Marquardt algorithm for the laboratory data of Treloar [9] relating to his simple tension, pure shear and equibiaxial tension experiments for which

[6]

 $c = -\frac{1}{2}$, -1, -2 respectively. These optimal values for M = 4 are contained in Table 1. With the exception of α_4 , corresponding material constants vary slightly between experiments. Ideally, this variation would not happen and a possible explanation for its occurrence is the presence of errors in experimental observations. The minimum sums of squares, defined by equation (3), were then computed for the three sets of material constants with their corresponding sets of experimental data; these three values of S are contained in Table 2.

The two sets of material constants obtained by Ogden [6] and Chadwick *et al.* [1] all with M = 3, are contained in Table 1 and the resulting values of S are contained in Table 2. The values of S obtained in the present paper for M = 4 using the non-linear least squares algorithm, are seen to be smaller, leading to a better overall fit to each of the three sets of experimental data.

Sets of optimal values of μ_i , α_i (i = 1, 2, 3) were also computed using the Levenberg-Marquardt algorithm for the same laboratory data of Treloar [9]. These optimal values for M = 3 are also contained in Table 1 and the corresponding values of S are contained in Table 2. The three values of S obtained using the material constants determined for M = 3 are again seen to be smaller than those obtained by Chadwick *et al.* [1] and Ogden [6]. They are not, however, as small as those obtained with M = 4.

It is seen that for M = 3 the values of μ_1 , α_1 , μ_2 , μ_3 for different tests $(c = -\frac{1}{2}, -1, -2)$ differ considerably, but for M = 4 the maximum difference between tests is very small. This justifies the introduction of the fourth term, although there is no obvious physical basis for it. The differences in values of the material constants for M = 4 are small enough not to be detectable within bounds of experimental error, and the set of values

$$\mu_1 = 6.23, \ \mu_2 = -0.071, \ \mu_3 = 0.047, \ \mu_4 = 0.91 \times 10^{-15} (kg \, cm^{-2}) \\ \alpha_1 = 1.23, \ \alpha_2 = -1.99, \ \alpha_3 = 4.38, \ \alpha_4 = 19.49$$
(6)

may be taken to cover all three tests.

In Figures 1, 2, 3 the curves for simple tension, pure shear and equibiaxial tension are plotted for M = 4 and compared with the data points of Treloar [9]. Also included for comparison are the corresponding curves generated by the material constants of Ogden [6] and Chadwick *et al.* [1, page 74]. The figures confirm that the use of four terms in the stress-deformation function (1) gives a very close fit overall for all three experiments. The comparison with Ogden's results should be qualified with the fact that he omitted one of Treloar's simple tension data points in calculating his material constants (two from his Figure 1).

The sets of optimal values of μ_i , α_i (i = 1, ..., M) computed for both M = 3 and M = 4 by the Levenberg-Marquardt algorithm clearly satisfy the inequalities



(2). However, of the optimal values α_1^* for M = 3 only that corresponding to $c = -\frac{1}{2}$ satisfies the condition

$$\alpha_i \leq -1 \quad \text{or} \quad \alpha_i \geq 2,$$
 (7)



(Chadwick *et al.* [1, page 63]). These conditions are sufficient to guarantee the existence of a unique solution to the problem of a shape-preserving deformation of a circular cylinder rotating about its axis. In their paper, Chadwick *et al.* [1] reject Ogden's value of $\alpha_1 = 1.3$ in [6] because it, too, violates (7); it is noted that for all three values of c with M = 4, the Levenberg-Marquardt algorithm yields optimal values μ_1^* and α_1^* which are very close to those of Ogden [6]. The values of α_1^* computed using the non-linear least squares method with M = 3 and c = -1, -2 also violate (7), yet the corresponding values of S are smaller than those

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obtained by either Chadwick *et al.* [1] or Ogden [6]. Grounds for accepting values of α_i , which violate (7) are discussed in Ogden [7]. Indeed such values of α_i are necessary, for example, for bifurcation from a spherical configuration of an inflated, initially spherical shell.

4. Summary

The numerical results reported in the present paper verify that the use of non-linear least squares optimization methods is justified when fitting curves of the form (1) to the experimental data; the wide availability of relevant computer software enforces this point.

It has further been verified that the use of four terms in Ogden's stress-deformation function produces a closer overall fit than the use of three terms, as might be expected. Moreover, the values of the μ_i , α_i (i = 1, ..., M) for different tests are much closer for M = 4 than M = 3, and provide a single set of material constants for all the three tests within the bounds of experimental error.

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