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Non-linear optimization of the material constants in Ogden's strain-energy function for incompressible isotropic elastic materials

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0. <u>Abstract</u>

The Levenberg—Marquardt non—linear least squares optimization algorithm is adapted to compute the material constants in Ogden's strain—energy function for incompressible isotropic elastic materials.

In previous papers, three terms have been included in the strain-energy function. In the present paper, four terms are used and it is shown that the optimal values of the eight material constants, which are determined using the Levenberg—Marquardt algorithm, give a much closer fit to experimental data than the strain-energy function with three terms.

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1. Introduction

In a number of publications (see, for example, Ogden (1972), Chadwick *et at* (1977)), elementary methods have been used to determine the material constants μ_i , α_i in the strain-energy function

$$F = \sum_{i=1}^{M} \mu_i P(\lambda(\alpha_i, c)) = \sum_{i=1}^{M} \mu_i \begin{pmatrix} -1 + \alpha_i & -1 + c\alpha_i \\ \lambda & \lambda \end{pmatrix}$$
(0)

for incompressible isotropic elastic materials. In equation (0), F represents the force per unit undeformed area 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

$$\mu_i \boldsymbol{\alpha}_i > 0 \quad \text{for all } i = 1, \dots, M. \tag{1}$$

The parameter c in equation (0) is related to the pure homogeneous deformations 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 (1972).

The set of numerical results for μ_i and α_i (i - 1,2,3) given by Ogden (1972) and the two sets given by Chadwick *et at* (1977) were obtained using *linear* least squares methods to fit curves to the experimental data of Treloar (1944). 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 (1975), James *et al* (1975) and Treloar and Riding (1980) is

contained in Ogden (1981).

Chadwick *et al* (1975) and Ogden (1972) obtained values of μ_i and α_i (i = 1,2,3) by using the fact that, at small strains ($\lambda_{-} \simeq 1$), the computation is dominated by just one term μ_1 p($\lambda_{-}, \alpha_{1-}, c$), with μ_2 p($\lambda_{-}, \alpha_{2,}, c$) and μ_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* (1977) and Ogden (1972) for the data of Treloar (1944) are reproduced for comparison purposes in Table I.

In previous papers, authors using a strain-energy formula of the form (0), have taken M = 3, It was observed by Ogden (1972; p. 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 α_4 - 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 Such techniques obviate the need to calculate the μ_i , α_i (section 2). (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 (1944), the optimal values with M = 3.4 are reported in section 3 and, for M = 4, the curves generated by (0) are plotted in Figures 1, 2, 3. Comparison with the values of Ogden (1972) and Chadwick et al (1977) is presented in Table I and comparison of the accuracy obtained using non-linear optimization methods with the accuracy attained by Ogden (1972) and Chadwick et al (1977) in Table II.

2. <u>A non-linear least squares algorithm</u>

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 (1980) 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 and consequently a large literature of successful applications of the Levenberg-Marquardt algorithm in the L2 norm, and a large amount of associated computer software, has resulted. The Levenberg-Marquardt algorithm in the L₂ norm is available to IBM users as SHARE PROGRAM # 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 (1944) 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 $(\lambda_k - F_K)$ k = 1,...,K with K \geq 2M. Let F_k be the value of F_k yielded by

$$F_{k} = \sum_{i=1}^{M} \mu_{i} \left(\lambda_{k}^{-1+\alpha_{i}} - \lambda k^{-1+\alpha_{i}} \right)$$

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

$$S - S(\mu_1, \alpha_1, \dots, \mu_M \alpha_M) = \sum_{k=1}^{K} E_k^2$$
$$= \sum_{k=1}^{K} \left\{ F_k = \sum_{i=1}^{M} \mu_i \left(\lambda_k^{-1+\alpha_i} - \lambda k^{-1+\alpha_i} \right) \right\}^2$$
(2)

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 <u>x</u> of order 2M defined by

$$\underline{\mathbf{x}} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{2M-1}, \mathbf{x}_{2M}) \mathbf{T} = (\boldsymbol{\mu}_1, \boldsymbol{\alpha}_1, \dots, \boldsymbol{\mu}_M, \boldsymbol{\alpha}_M) \mathbf{T} \quad ,$$

where T denotes transpose.

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

$$\underline{\mathbf{x}}^{(r+1)} = \underline{\mathbf{x}}^{(r)} - [(\mathbf{p}^{(r)})^{\mathrm{T}} \mathbf{p}^{(r)} = \gamma^{(r)} \mathbf{I}]^{-1} (\mathbf{p}^{(r)})^{\mathrm{T}} \underline{\mathbf{E}}^{(r)}; r = 0, 1, 2, \dots (3)$$

where $\gamma^{(r)}$ (r = 0,1,2,...) is an arbitrary parameter and $\underline{E} = (E_1, E_2,...,E_k)^T$ is the vector of errors (see equation (2)). The matrix I is the identity matrix of order 2M and P is the matrix of first derivatives of order k x 2M whose element p_{k_1} . at the rth iterate is given by

$$P_{ki}^{(r)} = \frac{\partial E_k}{\partial x_i} \Big| \underline{x} = \underline{x}(r) \quad (k = 1, \dots, K ; I = 1, \dots, 2M ; r = 0, 1, 2, \dots).$$

(5)

Thus

$$P_{k,2\ell-1}^{(r)} = -\left\{\lambda_k^{-1+\alpha\binom{r}{\ell}} - \lambda_k^{-1+c\alpha\binom{r}{\ell}}\right\}$$

and

$$P_{k,2\ell}^{(r)} = -\mu_{\ell}^{(r)} \left\{ \lambda_k^{-1+\alpha_{\ell}^{(r)}} - c\lambda_k^{-1+c\alpha_{\ell}^{(r)}} \right\}_{\ell n \lambda_k}$$

for k = 1,...,K; $\ell = 1,...,M$; r = 0,1,2,....

Marquardt (1963) has shown that a sufficiently large $\gamma^{(r)}$ always exists such that

$$\mathbf{S}^{(\mathbf{r}+\mathbf{l})} < \mathbf{S}^{(\mathbf{r})} \tag{4}$$

(unless $\underline{x}^{(r)} = \underline{x}^*$), where $S^{(r)}$ denotes the value of S at the r^{th} 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
$$T(\gamma^{(r)}/u) \leq S^{(r+1)}$$
, let $\gamma^{(r+1)} = \gamma^{(r)}/u$;
(b) if $T(\gamma^{(r)}/u) > S^{(r+1)}$ and $T(\gamma^{(r)}) < S^{(r+1)}$, 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 $T(\gamma^{(r)}u^n)$
 $\leq S^{(r+1)}$. 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 (3) 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.

3. Numerical results

The optimal values of μ_i , α_i . (i = 1,...,M) for M = 3 and M = 4 were determined using the Levenberg-Marquardt algorithm for the data of Treloar (1944) relating to his simple tension experiment (c = -¹/₂). These values are contained in Table I. Also contained in Table I are the set of values of μ_i , α_i (i = 1,2,3) obtained by Ogden (1972) and the two sets obtained by Chadwick *et at* (1977 : pp. 74,75). The minimum sums of squares, defined by equation (2), were also determined for all five sets of values for the simple tension experiment ; the five values of S are contained in Table II.

The two optimal sets of material constants obtained by the non-linear optimization algorithm, and those obtained by Chadwick *et at* (1977) and Ogden (1972), were also used to determine the value of S for the data of Treloar relating to his pure shear (c = -1) and equibiaxial tension (c = -2) experiments. These ten values of S are also contained in Table II.

The sets of optimal values of μ_i , α_i (i = 1,...,M) determined for both M = 3 and M = 4 by the Levenberg-Marquardt algorithm are seen to satisfy the inequality (1). In addition each optimum value α_i^* for M = 3 is seen to satisfy the condition

$$\alpha_i \leq -1 \text{ or } \alpha_i \geq 2$$
 (5)

(Chadwick *et al* (1977; p.63). This is not so for M = 4; he re the optimal value of α_1 ($\alpha_1^* = 1.23$) violates (5). In their paper Chadwick *et at* reject Ogden's (1972) value of $\alpha_1 - 1.3$ because it, too, violates (5); it is noted that for M = 4 the Levenberg-Marquardt algorithm yields optimal values μ_i^* and α_i^* which are very close to those of Ogden (1972). Other grounds for accepting values of α_i

between 1 and 2 have been summarized by Ogden (1981).

For Treloar's simple tension data, the minimum value of S obtained by the Levenberg-Marquardt algorithm with M = 3 is smaller than the three values of S yielded by the values of μ_i , α_i (i = 1,2,3) of Chadwick *et al* †(1977) and Ogden (1972). For pure shear and equibiaxial tension, however, the minimum value of S with M = 3 is superior only to that of Chadwick *et at* (i) (1977 ; p.74).

It is seen that the computed minimum values of S relating to Treloar's equibiaxial tension data are very large, indicating that while the optimal values of μ_i , α_i (i = 1,...,M; M = 3 or 4) computed in the present paper fit the simple tension and pure shear data closely. The same observation may be made of the values of μ_i , α_i . (i = 1,2,3) given in Ogden (1972) and Chadwick *et al* (1977). Figures 1,2,3 contain the curves of best and worst fit for simple tension, pure shear and equibiaxial tension, respectively, as well as the data points of Treloar (1944). It is seen that using four terms in (0) gives a very close fit for large strains for all three experiments.

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 (0) to experimental data ; the wide availability of relevant software enforces this point. It has further been verified that the use of four terms in the strain energy function produces a much closer fit than the use of three terms. This was suggested in 1972 by Ogden (1972) but his estimated value of α_4 , for Treloar's data has been seen to be too low by a factor of about 2, though it is almost equal to α_3^* for the case M = 3. Not one of the five sets of μ_i , α_i (i = 1,...,M; M = 3 or 4) contained in Table I yields a close fit to the data of Treloar (1944) simultaneously for each of the simple tension, pure shear or equibiaxial tension data sets.

	μ_1	α ₁	μ_2	α ₂	μ3	α ₃	μ_4	α_4
Twizell and Ogden (i)	6.27	1.23	-0.054	-1.99	0.036	4.44	0,8(-15)	19.49
Twizell and Ogden (ii)	2.22	2.26	-0.45	-2.01	3.88(-7)	10.01	-	-
Ogden (1972)	6.3	1 ,3	-0.1	-2.0	0.012	5.0	-	-
Chadwick <i>et al</i> (i) eqn. (5.4)	3-0	2.0	-0, 1	-2.0	3.7(-5)	7.82	-	-
Chadwick <i>et al</i> (ii) eqn. (5.5)	3.24	2.0	-0. 1	-2.0	6.2(-6)	8.7	-	-

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Table I : Numerical values of μ_i , α_i (i = 1, ..., M; M = 3 or 4)

Table II : Sums of squares (S).

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Method	S				
	Simple tension	Pure shear	Eqtubiaxial tension		
Twizell and Ogden (i)	6.3	1.40	3.77		
Twizell and Ogden (ii)	12.8	2.20	9.81		
Ogden (1972)	302.9	1.60	3.91		
Chadvi ck et al (i)	20.4	2.83	10.32		
Chadwick <i>et at</i> (ii)	16. 1	1.44	4.42		



Figure 1: Best- and worst-fitting curves for Treloar's simple tension data.



Figure 2: Best- and worst-fitting curves for Treloar's pure shear data.



Figure 3: Best- and worst-fitting curves for Treloar's equibiaxial tension data.

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