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Examination of Parameters Evaluation Methods in Computational Mechanics

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ABSTRACT

These works present an analysis and comparison of two computational procedures for mathematical models parameters estimation: the approach-in-stages procedure and the ordinary (usual) one. The ordinary procedure is based on a single-step operation to fit the model parameters while the approach-in-stages, a graphical method combining the least squares, permits the evaluation of these parameters (physical characteristics) by a multi-stage-of-identification process. After summarize of the underlying theoretical framework, a presentation of numerical examples as comparison of the two ways of approximation, is set out. Furthermore, results from hyperelastic modeling are compared using each of the two approximation procedures to characterize rubbery materials by the strain energy density function.

Keywords: *Computation, Approximation Methodologies, Approach in Stages, Least-Square, Methods Comparison*

1. INTRODUCTION

To validate a mathematical model of a physical phenomenon, one ought to evaluate the parameters of the model from experimental data. Frequently, the least squares procedure is used. This procedure is based on a single process that allows fitting the parameters of all of the model terms by the use of all of data within the (investigational) domain of interest. Recently, an approach in stages, a graphical method combining the least squares, permits the evaluation of the model parameters (characteristics) by a multi-stage-of-identification process. The present works attempt to evaluate the two ways of approximation. Comparative and critical analyses of the two procedures are set out in functions approximation and in hyperelastic behavior modeling.

2. USUAL METHODOLOGIES

It is the methodology used in scientific numerical calculation nowadays.

2.1. Linear Least Squares

Let us consider a function f(x) defined in the domain V, to be approximated by the function y(x) generated by a combination of basic functions $\varphi_j(x)$ as follows:

$$y(x) = \sum_{j=1}^{N} a_j \varphi_j(x) \qquad for\ x \in V \qquad (1)$$

$$y(x) = <P(x> \{a\} \qquad (2)$$

where the line vector <P(x)>, the base of approximation, is given by:

$$<P(x)> = <\varphi_1(x), \varphi_2(x),... \ \varphi_N(x)> \qquad (3)$$

$\varphi_j(x)$ are basic functions, {a} is the column vector of unknown parameters a_j. The residue function R(x) is defined for $x \in V$ by:

$$R(x) = f(x) - y(x) \qquad (4)$$

The residue is null when y(x) is a solution. The Galerkine integral formulation [1, 2] for least squares method is given by:

$$W(y) = \int_V \delta R(x) R(x) dv \qquad (5)$$

where δR(x), the weighting function, is the first variation of the residue function. W(y) remains null for y(x) solution. From previous relations, one has:

$$W(y) = <\delta a> \left(\int_V \{P(x)\} < P(x) > dv \{a\} - \int_V \{P(x)\} f(x) dv \right) \qquad (6)$$

where the column vector {P(x)} is the vector transpose of the line vector <P(x)>, the line vector <δa> that of {δa}. W(y) must be null for any variation δa_j of parameters. So, one has to resolve:

$$\int_V \{P(x)\} < P(x) > dv \{a\} - \int_V \{P(x)\} f(x) dv = 0 \qquad (7)$$

For a discrete problem given by (x_k, f_k) data points, with k = 1, M; the relation (7) is rewritten as:

$$\sum_{k=1}^{M}\{P(x_k)\} < P(x_k) > \{a\} - \sum_{k=1}^{M}\{P(x_k)\}\ f_k = 0 \qquad (8)$$

In matrix form, the relation (8) becomes:

$$[\ D_G\ ]\ \{a\} = \{F_G\} \qquad (9)$$

where the matrix coefficients are given by:

$$D_{G_{ij}} = \sum_{k=1}^{M} \varphi_i(x_k)\varphi_j(x_k) \qquad (10)$$

$$F_{G_i} = \sum_{k=1}^{M} \varphi_i(x_k) f_k \qquad (11)$$

The solutions of the problem are given (in a linear least squares sense) by:

$$\{a\} = [\ D_G\ ]^{-1}\ \{F_G\} \qquad (12)$$

The parameters a_j (j=1, N) are evaluated in terms of all (x_k, $f(x_k)$) data points, i. e., for k=1, M.

2.2. Collocation by Sub-domains

A method that considers subsets of the domain of interest *V* is the collocation method (Dhatt and Touzot, 1984). It entails choosing N subsets V_1, V_2, V_3 ... V_N (equal to the number of parameters to determine) of the domain *V*. The weighting functions are taken equal to unity inside each sub-domain and null elsewhere (let us note that the Collocation by points method considers Dirac impulses as weighting functions). One has for *j=1, N*:

$$W_j(y) = \int_{V_j} R(x)dv = 0 \qquad (13)$$

So,

$$\int_{V_j} < P(x) > dv\,\{a\} - \int_{V_j} f(x)dv = 0 \qquad (14)$$

The discrete form of the relation (14) in matrix form is as follows:

$$[\ D_C\ ]\ \{a\} = \{F_C\} \qquad (15)$$

The matrix coefficients are:

$$D_{C_{ij}} = \sum_{V_i} \varphi_j(x_k) \qquad (16)$$

$$F_{C_i} = \sum_{V_i} f_k \qquad (17)$$

The same remark is observed: the parameters a_j *(j=1, N)* are also evaluated in terms of all (x_k, f_k), x_k being a member of the combination of the sub-domains.

3. APPROACH-IN-STAGES METHOD

The approach-in-stages procedure graphically evaluates model parameters step-by-step, in a continuous multi-stage process [3].

3.1. Procedure

Let us consider, for $x \in V_N$, $\varphi_N(x)$ being the equivalent function of the function *y(x)* given by eq. (1), that is:

$$y(x) \approx a_N\varphi_N(x) \quad \text{for } x \in V_N \qquad (18)$$

Plotting *y(x)* versus $\varphi_N(x)$, that is, $(\varphi_N(x), y(x))$, should give a linear curve for $x \in V_N$. The method consists of plotting the curve $(\varphi_k(x), y(x))$ by varying k to get a linear portion for certain values of *x*, which defines the identification sub-domain. The partial solution $\varphi_k(x)$ is then determined and the weighting coefficient a_k is given by the slope of the relative linear curve. Reiterating the reasoning leads to the following recurrence formula [3]:

$$y_k(x) = y(x) - \sum_{j=0}^{k-1} a_{N-j}\ \varphi_{N-j}(x)\ ;\ k=1, N \qquad (19)$$

$$y_0(x) = y(x).$$

where $y_k(x)$ is the function to be identified in the sub-domain V_k.

This method evaluates the model's parameters by following increasing order of the variable *x*.

3.2. Approach in Stages by Power Functions

In polynomial nonlinear approximation, the basic functions $\varphi_j(x)$ correspond to power functions x^{β_j}, with β_j a real number. The approach in stages method identifies basic power functions $a_j x^{\beta_j}$ generating the function *y(x)* in a decreasing order [4, 5] and the identification sub-domains are ranked in a decreasing values of *x*, see works of Beda and Chevalier [3]. To begin with small stretches, one should instead identify parameters in increasing values of *x*, that is, instead of plotting the curve $(\varphi_j(x), f(x))$ when *f(x)* is proportional to $\varphi_j(x)$, one rather plots the reciprocal function versus reciprocal basic function. Plotting $(1/\varphi_j(x), 1/f(x))$

permits one to inverse the order of determining the parameters: beginning the identification at lower values of x and finishing at greater values. The solution is obtained when the curve is linear, and the slope corresponds to the reciprocal coefficient $1/a_j$. When $\varphi_j(x)$ is inversely proportional to $f(x)$, one has to plot someway $(\varphi_j(x), f(x))$ to have the good order of determining parameters. Thus, the approach in stages is a procedure of continuous approximation by block (subsets of the domain of interest) of a continuous or discontinuous function.

4. FINITE DOMAINS LEAST SQUARES

4.1. Approximating a function by block

For a problem with two sub-domains V_1 and V_2 for example, one obtains the following matrix form:

$$[D_{FD}]\{a\} = \{F_{FD}\} \qquad (20)$$

The L first parameters $(a_j, j=1, L)$ to determine in V_1 and the N-L others $(a_j, j= L+1, N)$ in V_2.

$$[D_{FD}] = \begin{vmatrix} D_1 & 0 \\ 0 & D_2 \end{vmatrix} \qquad (21)$$

$$D_{1_{ij}} = \sum_{V_1} \varphi_i(x_k)\varphi_j(x_k) \qquad (22)$$

$$D_{2_{ij}} = \sum_{V_2} \varphi_i(x_k)\varphi_j(x_k) \qquad (23)$$

$$\{F_{FD}\}^T = < \sum_{V_1} \varphi_1(x_k) f_k \ , \ldots\ldots \sum_{V_1} \varphi_L(x_k) f_k \ ,$$
$$\sum_{V_2} \varphi_{L+1}(x_k) f_k \ , \ldots\ldots \sum_{V_2} \varphi_N(x_k) f_k > \qquad (24)$$

Each set of parameters (for each sub-domain) is independently evaluated by finite domains least squares and the function is then a piece-wise function, that is, it is defined by sub-domains. The system is decoupled and corresponds to the Finite Elements method. From relations (17) and (23), one notes that, by the ordinary least squares procedure, the range of calculation domains strongly influences the numerical values of the parameters evaluated.

4.2. Finite Domains Least Squares

To get a function defined by a single expression in the whole domain of interest, one combines the approach in stage with finite domains least squares. In this case, the approximation in the second stage must be in a linear least squares sense and the new function to evaluate is defined as follows:

$$r(x) = f(x) - \sum_{j=1}^{L} a_j \varphi_j(x) \qquad (25)$$

where $a_1\varphi_1(x)$, $a_2\varphi_2(x)$, ... $a_L\varphi_L(x)$ are determined in the first identification sub-domain V_1 by the plot of $(1/\varphi_j(x), 1/f(x))$, that is, by the stages approach method [3]. Thus, the matrix relation is:

$$[D_{FD}]\{a\} = \{F_{SL}\} \qquad (26)$$

where $[D_{FD}]$ is given in relations (21), (22) and (23). $\{F_{SL}\}$ is given by:

$$\{F_{SL}\}^T = < \sum_{V_1} \varphi_1(x_k) f_k \ , \ldots\ldots \sum_{V_1} \varphi_L(x_k) f_k \ ,$$
$$\sum_{V} \varphi_{L+1}(x_k) r_k \ , \ldots\ldots \sum_{V} \varphi_N(x_k) r_k > \qquad (27)$$

With

$$r_k = f_k - \sum_{j=1}^{L} a_j \varphi_j(x_k) \qquad (28)$$

The approach in stages method [3] allows one to first of all determine the partial solutions $a_j x^{\beta_j}$ (real-order power functions), which in their turn allow to provide monomials, that is, integer-order power functions $a_j x^j$ by the linear least squares method [6].

5. RESULTS

5.1. Simulation

Let us consider the following piece-wise function $f(x)$ defined in $V = [0\ 7.5]$ as:

$$\text{for } x \in [0\ 5] \equiv V_1 \quad : f(x) = 4x$$
$$\text{and for } x \in [5\ 7.5] \equiv V_2 \quad : f(x) = \frac{20}{e^5} e^x$$

In Fig. 1, one sees that the curve of the reciprocal function $1/f(x)$ versus reciprocal variable $1/x$ is linear at large values of $1/x$ and the slope is equal to 0.25, which is equal to $1/a_1$. Consequently, one finds that $a_1 = 4$, as the real value of the parameter. One sees also that the linear part of the curve begins at the point where the abscissa $1/x$ equals 0.2 and finishes at $1/x = 200$, that is, from $x = 0.005$ to $x = 5$. The first sub-domain V_1 is then defined by the interval $[0\ 5]$. Defining material behavior by block remains an inadequate description. So, even for a continuous or discontinuous

function defined by block (multi-expression), it should be preferable to approximate it by a continuous function defined in the whole domain of interest by a single expression. To overcome this difficulty, one has to approximate at the second identification stage the residue function instead of the real function like in Finite Elements method. The residue function is defined by, for $x \in [0\ 7.5] \equiv V$:

$$R(x) = f(x) - y_1(x) \qquad (29)$$

where $y_1(x) = a_1\varphi_1(x) \equiv a_1 x$. The residue is null in V_1 and is different from the exact function in the second sub-domain V_2. In the second identification sub-domain, the ordinary procedure provides negative valued parameters. To avoid negative-valued solutions, one has to search and locate the unique positive binomial solutions [6]. Table 1 presents parameters values obtained by different methodologies of approximation and Fig. 1(c) illustrates a comparison between exact and estimated curves. From results, the approach in stages (or by finite domains) provides the best values of parameters, particularly that of the first parameter a_1 that remains important for infinitesimal treatment, particularly in materials behavior modeling, Fig. 1(d), (e). It should be noted that by the ordinary procedure the range of the second sub-domain influences very much the estimated value of the parameter a_1, while by the use of the approach in stages it remains independent of the range. The procedure is then a continuum linear procedure by block of a continuous field but is different from the classical Finite Elements [1, 2] procedure for which elementary approximations are independent and initially done, and subsequently, continuity conditions are applied on elementary solutions to render the approximating function continuous.

5.2. Hyperelastic Modeling

In simple tension of rubber, the reduced stress ϕ of the extended Gent-Thomas model for an incompressible material is given by [7]:

$$\phi = 2\left(\frac{K}{\lambda\, I_2} + \sum_{j=1}^{N} C_j\,(I_1 - 3)^{j-1}\right) \qquad (30)$$

I_1, I_2 are invariants of the Cauchy-Green strain tensor, λ the stretch, K, C_j material parameters that must be all positive [8]. Many fitting approaches have been treated to identify the rubber parameters [3, 9-12] for various hyperelastic models, such as the Ogden model [13] , the Beda models [4, 5]), the Yeoh-Fleming model [14] and the extended Gent-Thomas models [7, 15, 16]; and even for constrain models such as that of Flory-Herman and that of Gent-Thomas [17].

5.2.1. Problematic

It is known from the causality principle that the strain energy at small deformation does not depend on large deformation. Thus, to evaluate the parameters of the strain energy function at moderate deformations, preferably one ought not to use large deformation data (that are brought into effect after), the reason why the domains of interest must be restricted in this case at the sole moderate stretches for parameters estimation.

5.2.2. Results

In rubber materials investigation for example, the experimental curve of the rubber behavior sets out two sub-domains in extension: the first is where the experimental curve is concave, that is, moderate deformations; and the second is where it is rather convex, that is, large deformations, Fig. 2. The use of the ordinary procedure to approximate such a function by positive-integer-power-polynomials (Rivlin strain energy function for example) provides systematically negative parameters [3], which are invalid in hyperelastic modeling [8]. On the other hand, the use of all of data (both the falling and the rising parts of the curve) at the same time leads to non optimal solutions for the deduced infinitesimal material characteristics [6]. The approach-in-stages procedure, which highlights the subset of small stretches in the approximation procedure, gives the more appropriate result for the infinitesimal material characteristics in comparison with the ordinary procedure that uses, in a single process, the whole domain of interest for the resolution. For instance, the infinitesimal deformation elastic modulus E (Young's modulus) of the material given by the limiting value of the reduced stress at the vicinity of the unstrained state, is best estimated [6].

6. COMPARATIVE ANALYSIS

Grand merits of the original multi-stage procedure lay on the fact that it could provide solutions under constraint, for instance, the physical values of the parameters estimated in material investigation; It accurately detects the appropriate number and the optimal order of monomials generating the function of approximation. The solutions obtained have a good extrapolation property. The method first of all transforms a nonlinear procedure that provides a multiple sets of optimal solutions to a linear problem that supplies a unique (best) set of solutions. It permits to avoid negative-valued parameters in particular and to control the signs of solutions in general [6]. The abilities of this method allow its use in a vast scientific calculation domain, since the properties previously cited are not possible by the ordinary (usual) procedure. It should also be noted that this method permits an accurate piece-wise identification of function fragments. The multi-stage process of approximation highlights the weigh of basic functions relatively to sub-domains, that is, relatively to states of deformation in hyperelasticity. Consequently, it allows to best reduce the nonlinear behavior laws to linear laws (infinitesimal deformation), Fig. 2(b), see Table 2 for

parameters values. In certain cases, the ordinary methodology remains most appropriate to fit function for data register only, Fig. 2(c), (d); not for physical modeling under parametrical constraint, Tables 3 and 4.

7. CONCLUSIONS

The multi-stage methodology is most adapted for approximation under constraint and to provide appropriate estimated parameters for smaller values of variable. While the ordinary procedure presents best resolution and is most appropriate for other types of approximation, such as fitting a curve without any constraint on the parameter and when the errors at the smaller values of the considered variable are not considered. The approach-in-stages is enough simple to use by a non-specialist in numerical computation.

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Table 1: Simulation Parameters of f(x) evaluated by Different Procedures and various bases of Approximation

Bases of approximation < P >	Estimated parameters a_N on (4, 0.134759)	Relative Error
Multi-stage Process, *Exact base*		
Stage-1 $< x >$	4	0 %
Stage-2 $< e^x >$	0.1066	20.9 %
Multi-stage Process, *Polynomial base*		
Stage-1 $< x >$	4	0 %
Stage-2 $< x^8, x^9 >$	$(2.557\ 10^{-6},\ 2.562\ 10^{-6})$	/
$< x^7, x^8 >$	$(-1.227\ 10^{-4},\ 3.810\ 10^{-5})$	/
$< x^9, x^{10} >$	$(3.527\ 10^{-6},\ -8.5\,0\ 10^{-8})$	/
Ordinary Methodology (Unique stage process)		
Exact base $< x, e^x >$	(1.4258, 0.1251)	(64.36 %, 7.17 %)
Polynomial base $< x, x^8, x^9 >$	$(3.4521, 1.1671\ 10^{-5}, 1.3744\ 10^{-6})$	(13.70 %, /, /)

Table 2: Evaluated Parameters of Yeoh vulcanizate VC from Different Methodologies

Multi-stage Process (two stages)			
$C_1 = 0.203$ MPa	$K = 0.25$ MPa	$C_2 = 1.6\ 10^{-3}$ MPa	$C_3 = 1.7\ 10^{-4}$ MPa
Ordinary Methodology (single stage process)			
$C_1 = 0.1911$ MPa	$K = 0.3099$ MPa	$C_2 = 0.0035$ MPa	$C_3 = 1.0728\ 10^{-4}$ MPa

Table 3: Evaluated Parameters of Treloar Rubber-1 from Different Methods

Multi-stage Process (Two stages)					
C_1	K	C_2	C_3	C_{15}	C_{16}
0.127 MPa	0.3 MPa	$3.066\ 10^{-4}$ MPa	$7.63\ 10^{-5}$ MPa	$2.672\ 10^{-25}$ MPa	$1.48\ 10^{-26}$ MPa
Ordinary Methodology (Unique stage process)					
C_1	K	C_2	C_3	C_4	C_5
0.1424 MPa	0.2552 MPa	-0.0041 MPa	$4.7292\ 10^{-4}$ MPa	$-1.2249\ 10^{-5}$ MPa	$1.198\ 10^{-7}$ MPa

Table 4: Evaluated Parameters of Treloar Rubber-2 from Different Procedures

Multi-stage Process (Two stages)						
$C_1 = 0.16475$ MPa	$K = 0.27$ MPa	$C_6 = 1.917\ 10^{-10}$ MPa	$C_7 = 1.8815\ 10^{-11}$ MPa			
Ordinary Methodology (Unique stage process)						
C_1	K	C_2	C_3	C_4	C_5	C_6
0.1644 MPa	0.2714 MPa	$6.9412\ 10^{-4}$ MPa	$-1.4202\ 10^{-4}$ MPa	$1.049\ 10^{-5}$ MPa	$-3.3817\ 10^{-7}$ MPa	$4.8\ 10^{-9}$ MPa

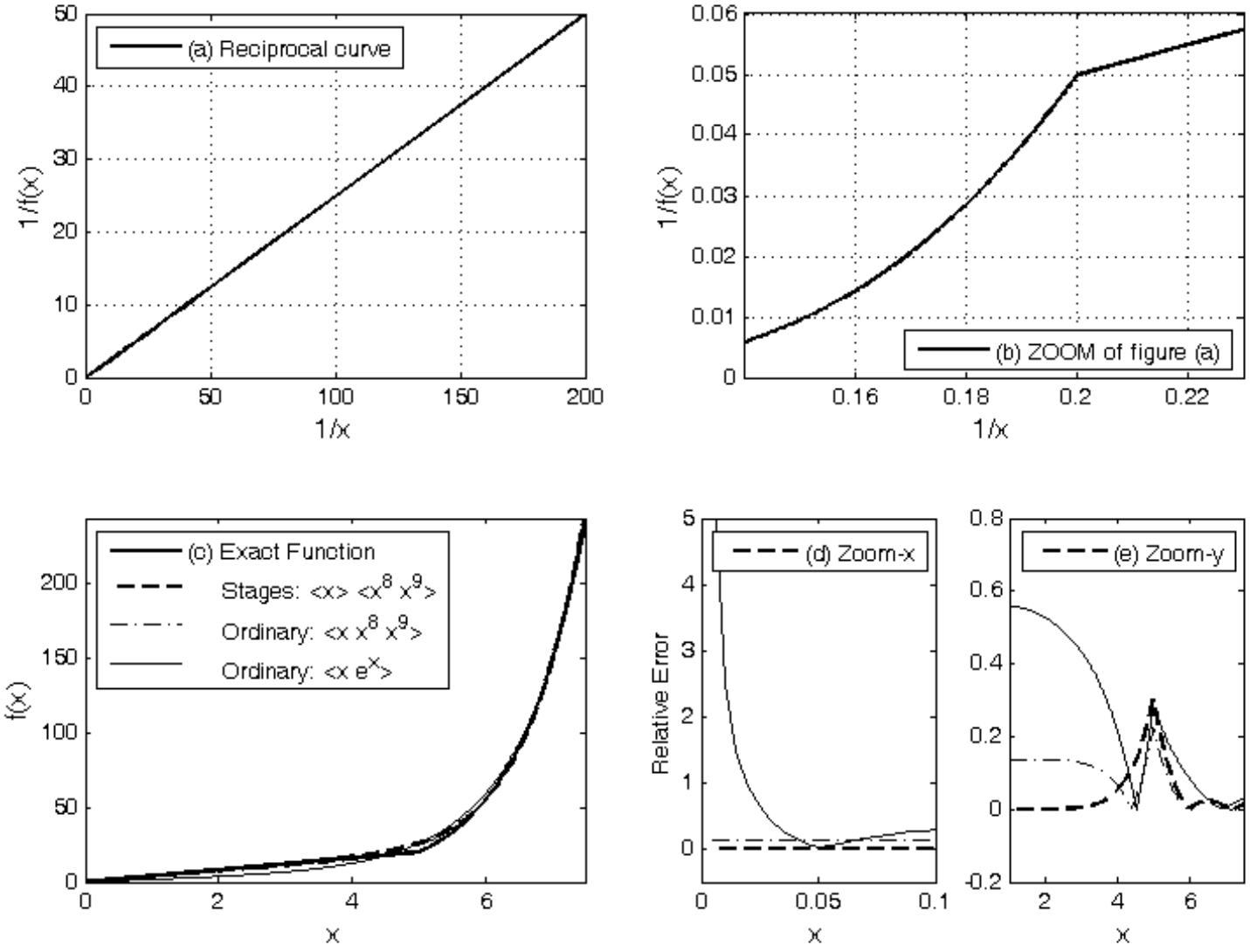

Figure 1: Simulation and Approximation of a Fragmentary Function by Different Procedures

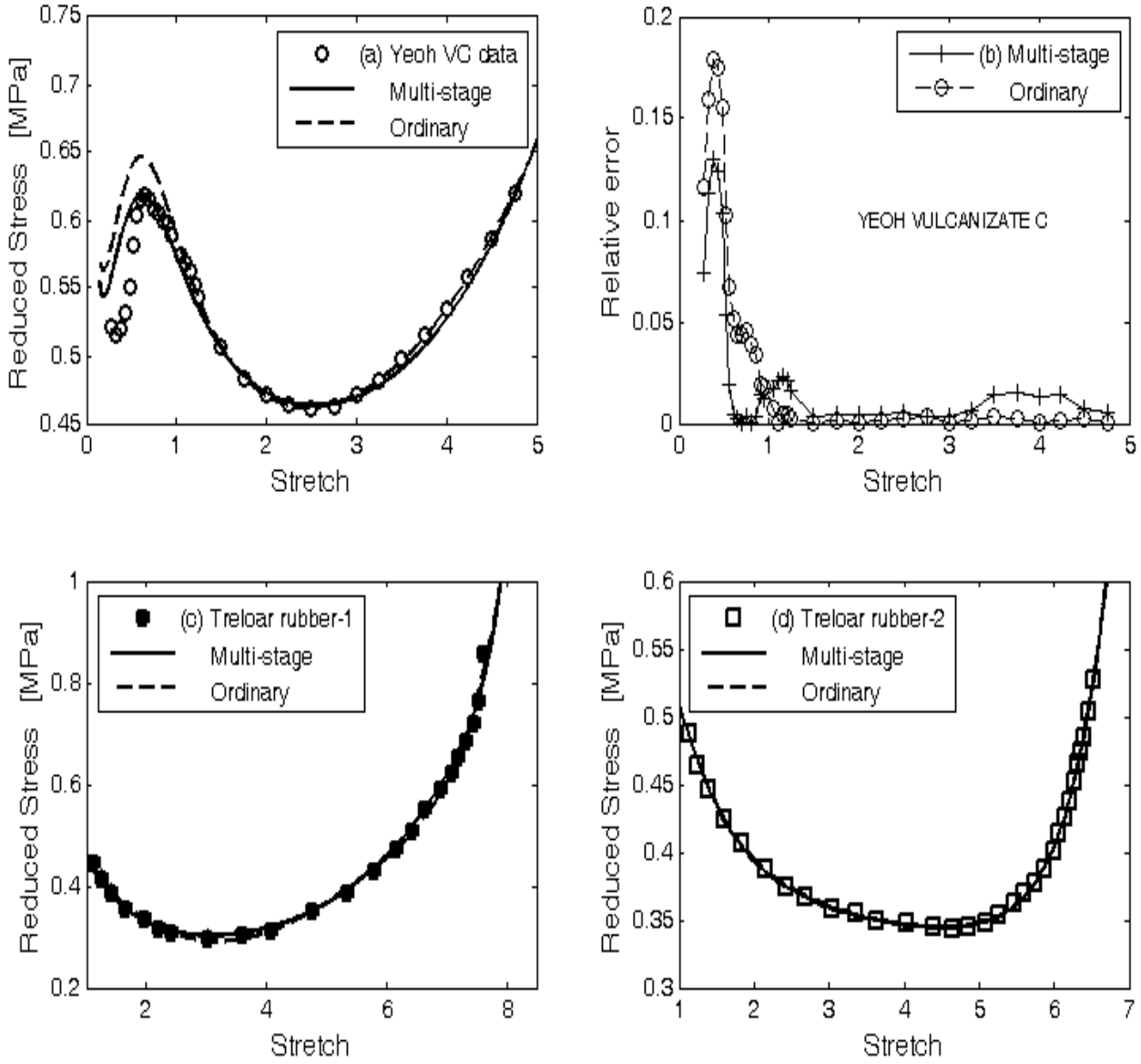

Figure 2: Comparison of Experimental Data with Predictions of the Estimated (from the two different procedures) Reduced Stresses