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NUMERICAL DIFFERENTIATION AND INTEGRATION OF NOISY MODEL DATA

1990

1. INTRODUCTION

The modern standard optimization methods of the zero, first and second order are based on computations and comparisons of the values of an objective function, $F(x)$, its first and second derivatives, respectively [1-3]. Thereby $F(x)$ is a priori assumed to be smooth, continuous, convex and twice differentiable function.

However, all the experimental functions are generally measured with some systematical and statistical errors, $E(x)$, i.e., in practice

$$F(x) = T(x) \pm E(x), \qquad (1)$$

where $T(x)$ is the true value of $F(x)$.

Here the results of numerical differentiation are compared with those of integration for a model quadratic objective function

$$F(x) = ax^2 + bx + c \qquad (2)$$

computed with a superimposed randomized error $E(x)$.

2. ERRORS IN NUMERICAL DIFFERENTIATION VERSUS INTEGRATION

The amplifying error effect of numerical differentiation and the dumping error effect of numerical integration with respect to noise inherent in an objective function have been known till now only at a purely qualitative level [4-6].

For example, the noisy experimental data with multipeak spectral structures have been analyzed in [6] to demonstrate the effect of filtering in the course of peak finding and identification stages.

However, presently there are no accepted figure-of-merits (FOM) to evaluate the disastrous action of initial noise component on the values of $F(x)$ and its derivatives except of numerical computational errors obtained from truncated Taylor series.

In turn, this prevents the existing optimization codes to be tested under the conditions close to experimental ones. In addition, the absence of such FOM's retains international standartization in the field of testing optimization procedures.

3. THE COMPUTATIONAL RESULTS ON NUMERICAL DIFFERENTIATION AND INTEGRATION ON NOISY MODEL DATA

The quadratic objective function $F(x)$ (2) has been used as a model one (Fig.1a) with a superimposed random noise component, $E(x)$, specified by uniform distribution function, RNDM(x), within an interval [0,1] (Fig.1b).

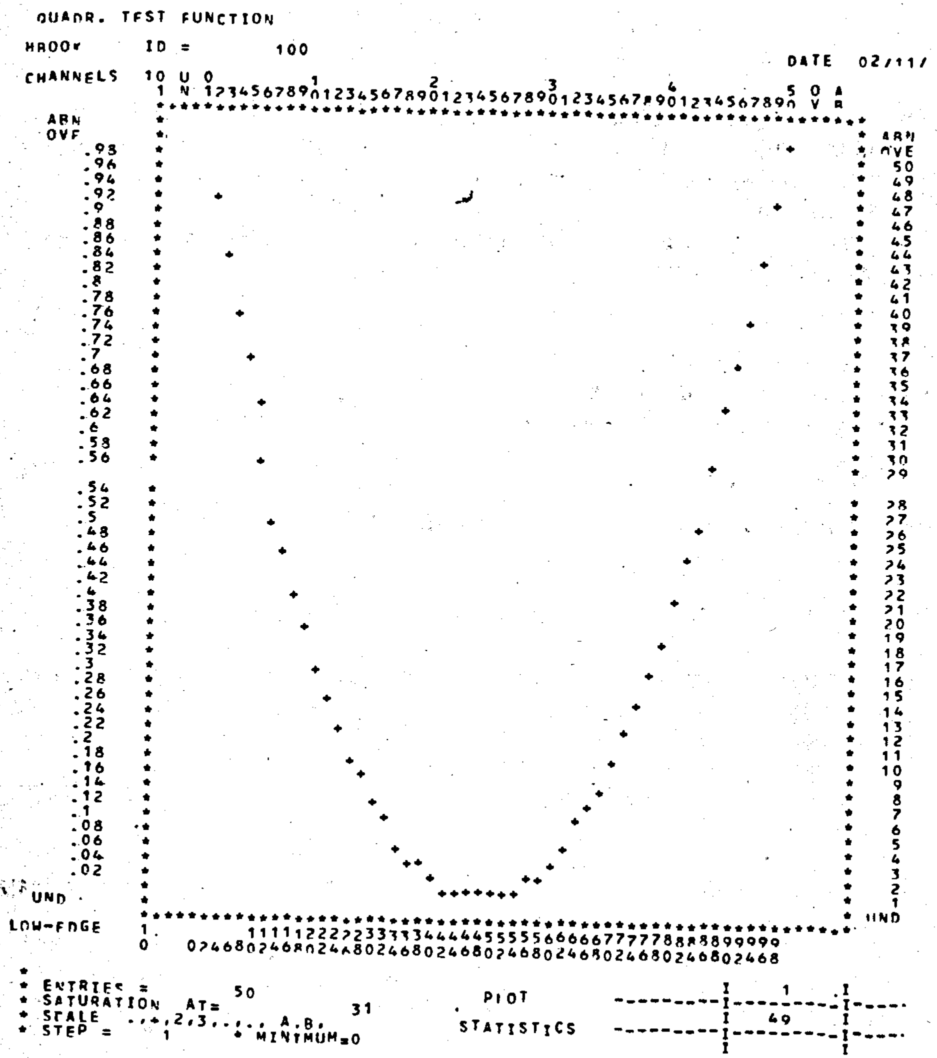
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Fig.1a

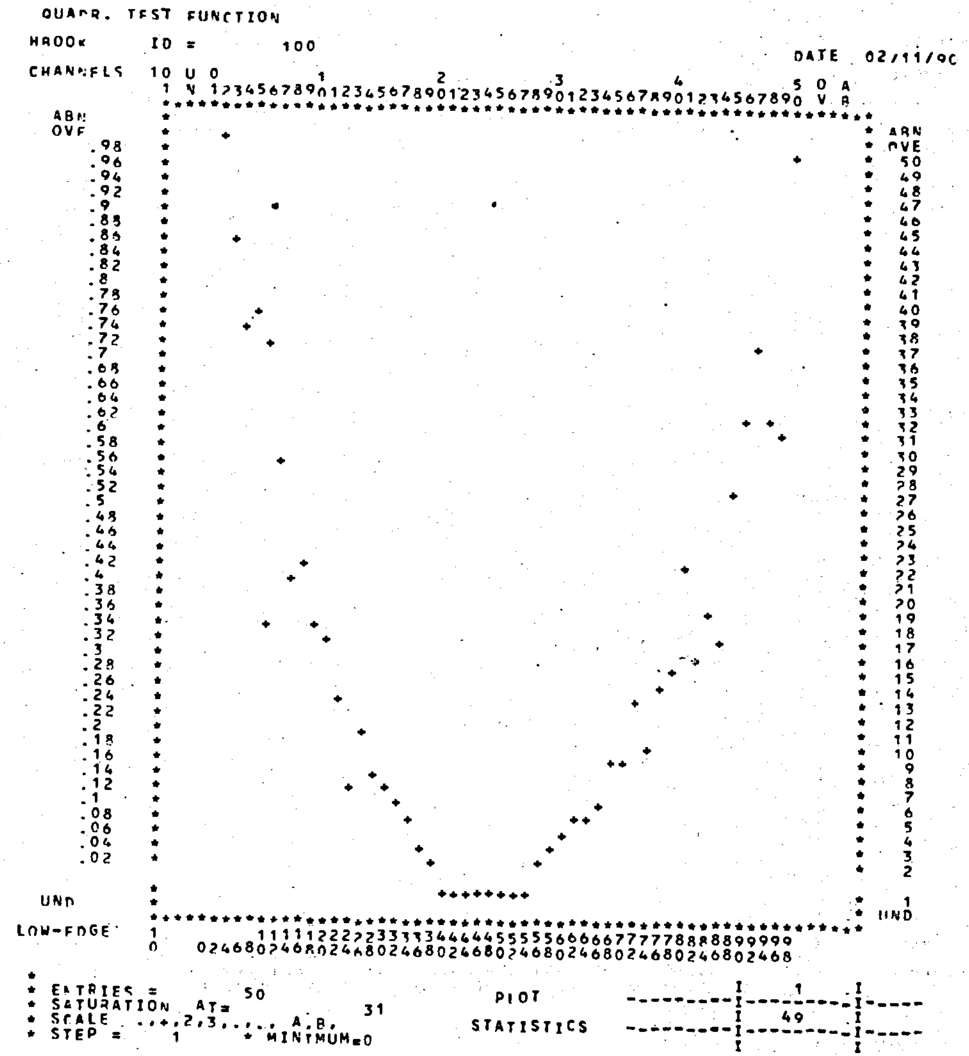
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Fig.1b

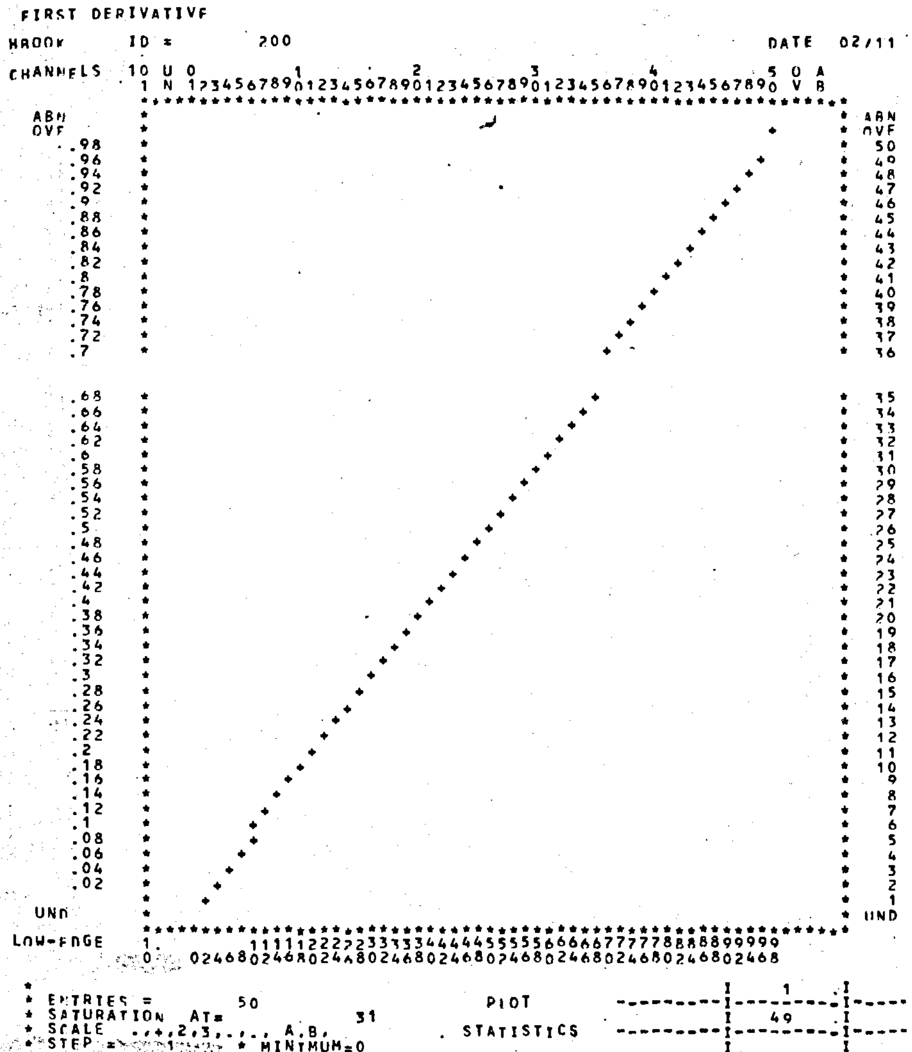
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Fig.2a

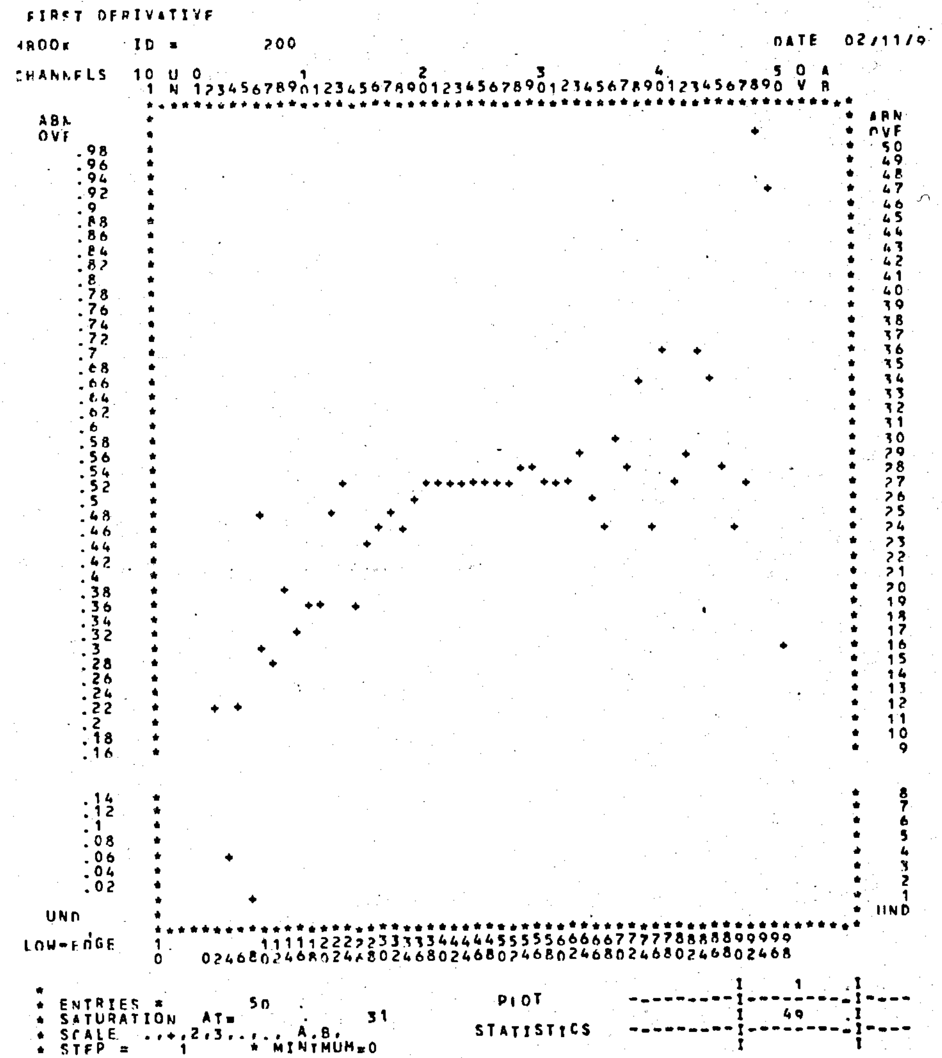
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Fig.2b

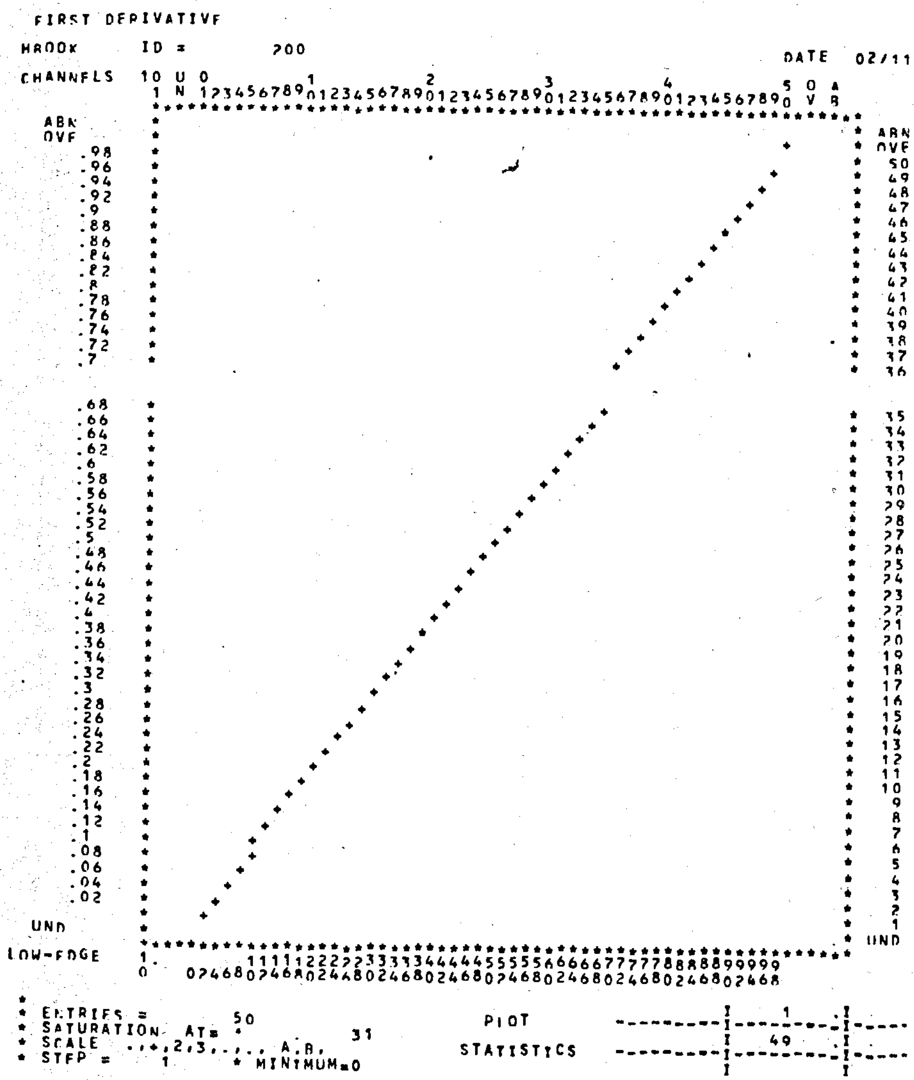
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Fig.3a

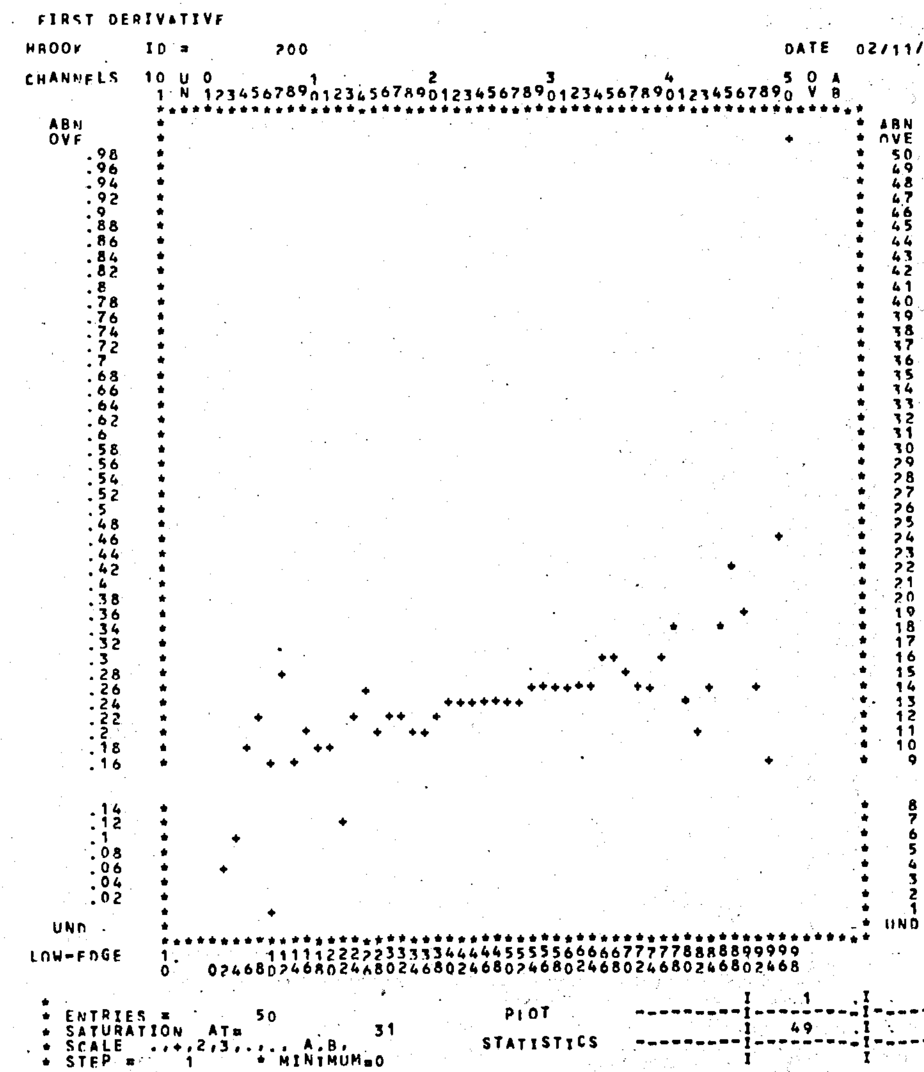
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Fig.3b

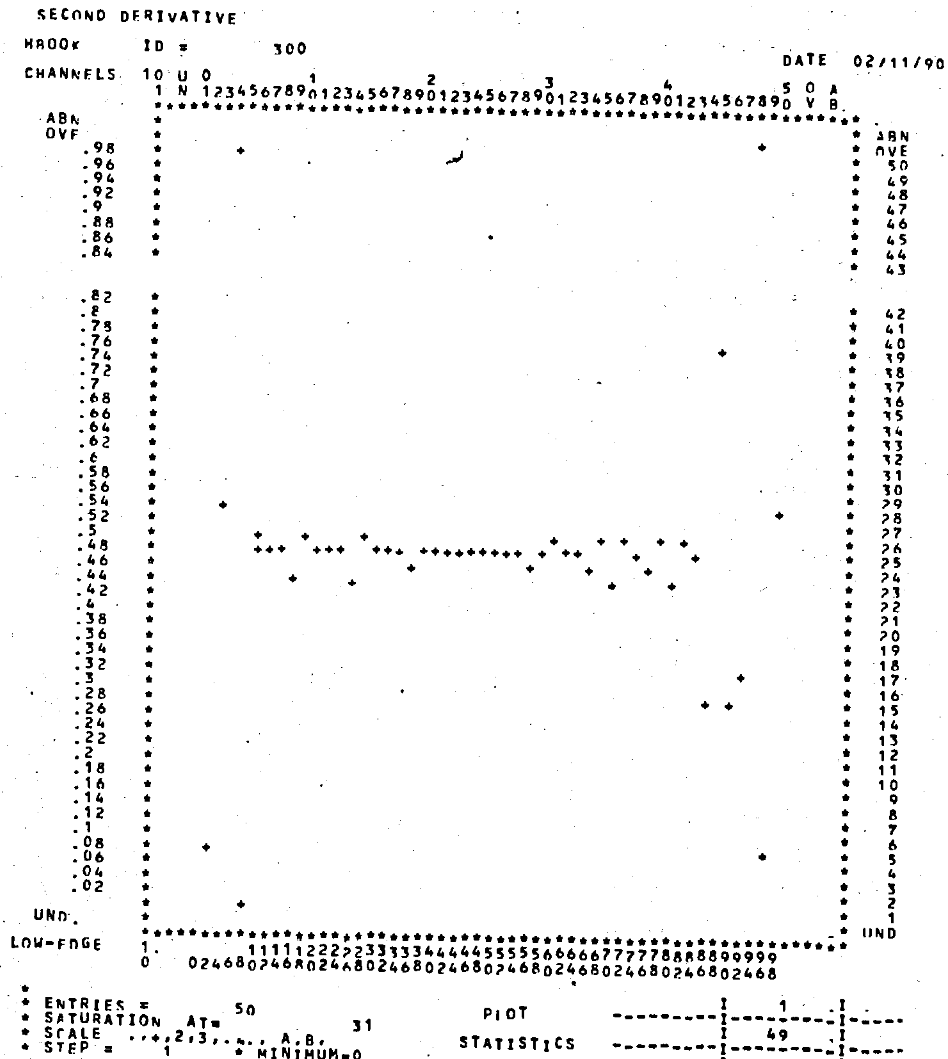
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Fig.4a

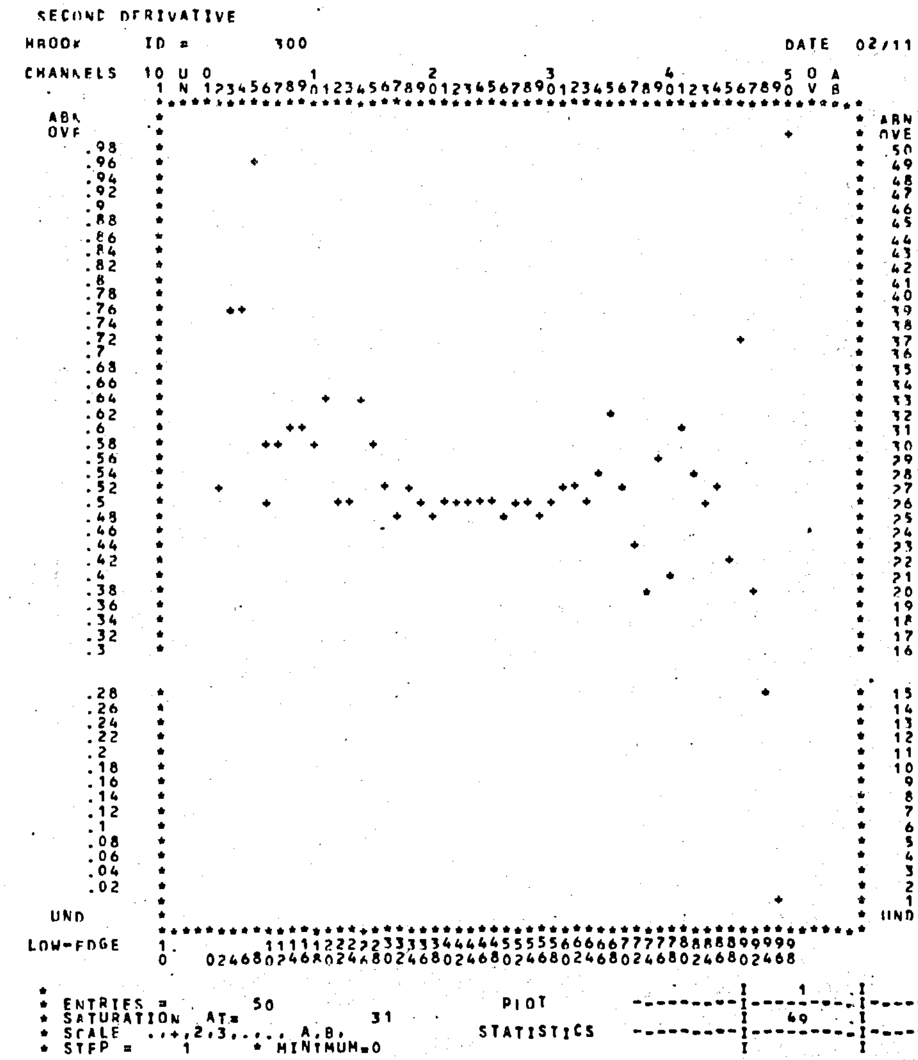
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Fig.4b

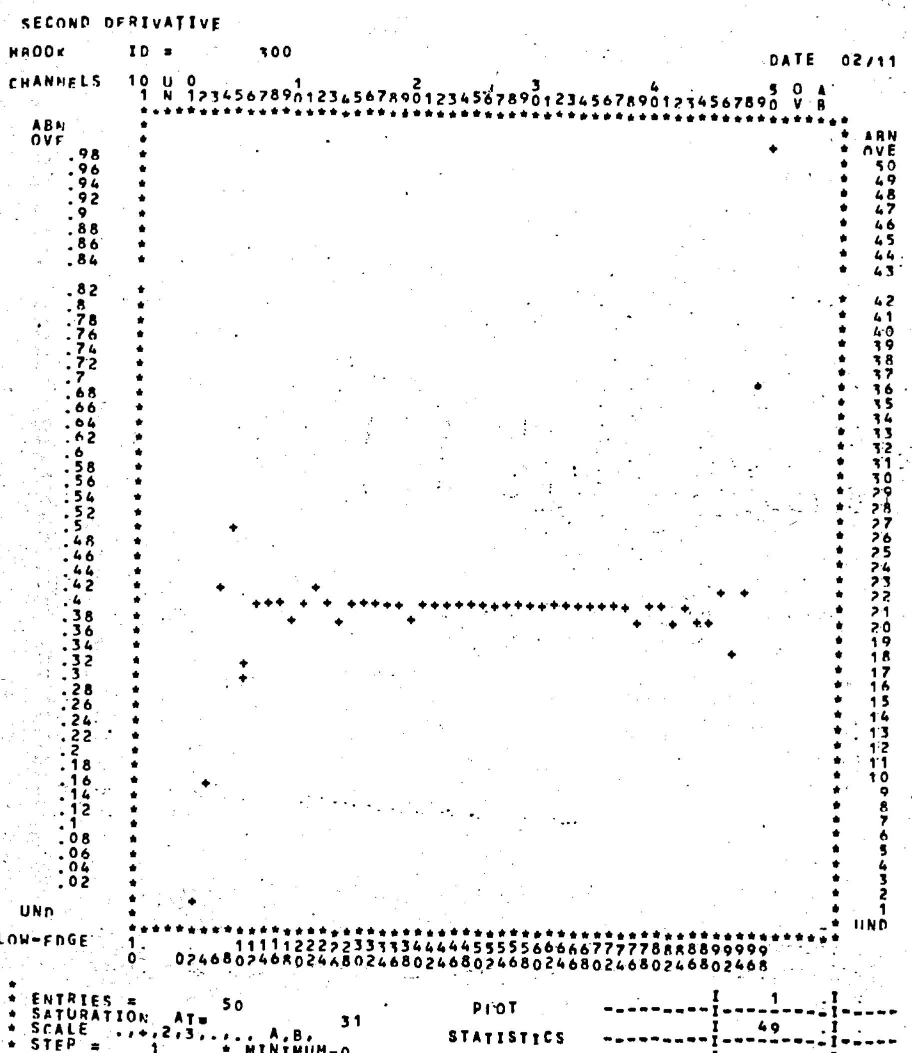
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Fig.5a

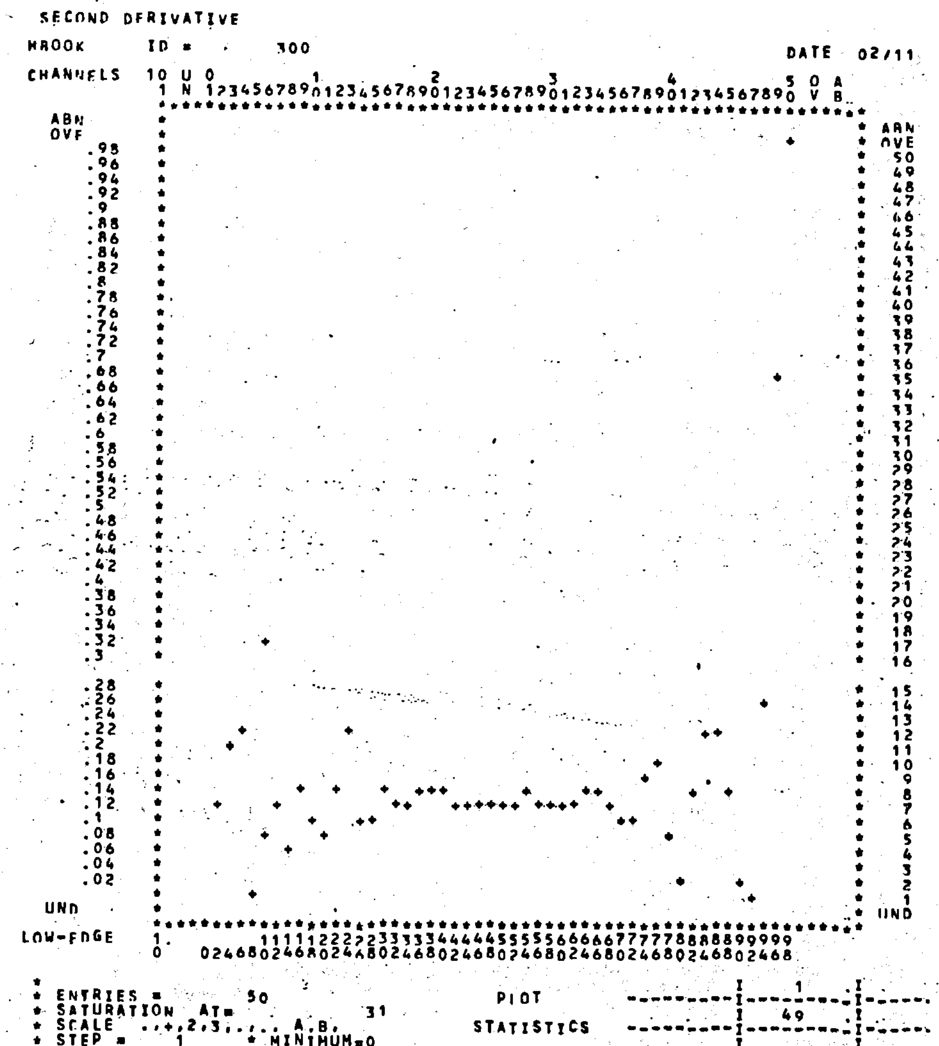
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Fig.5b

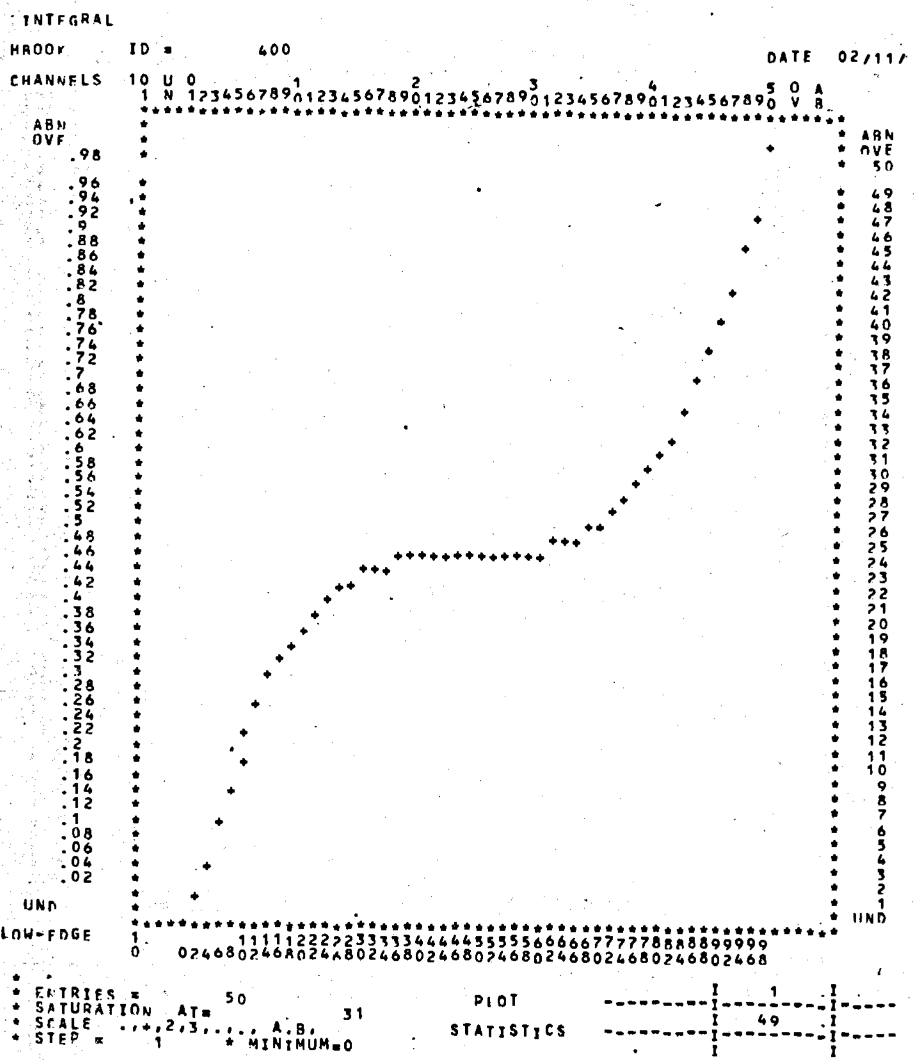
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Fig.6a

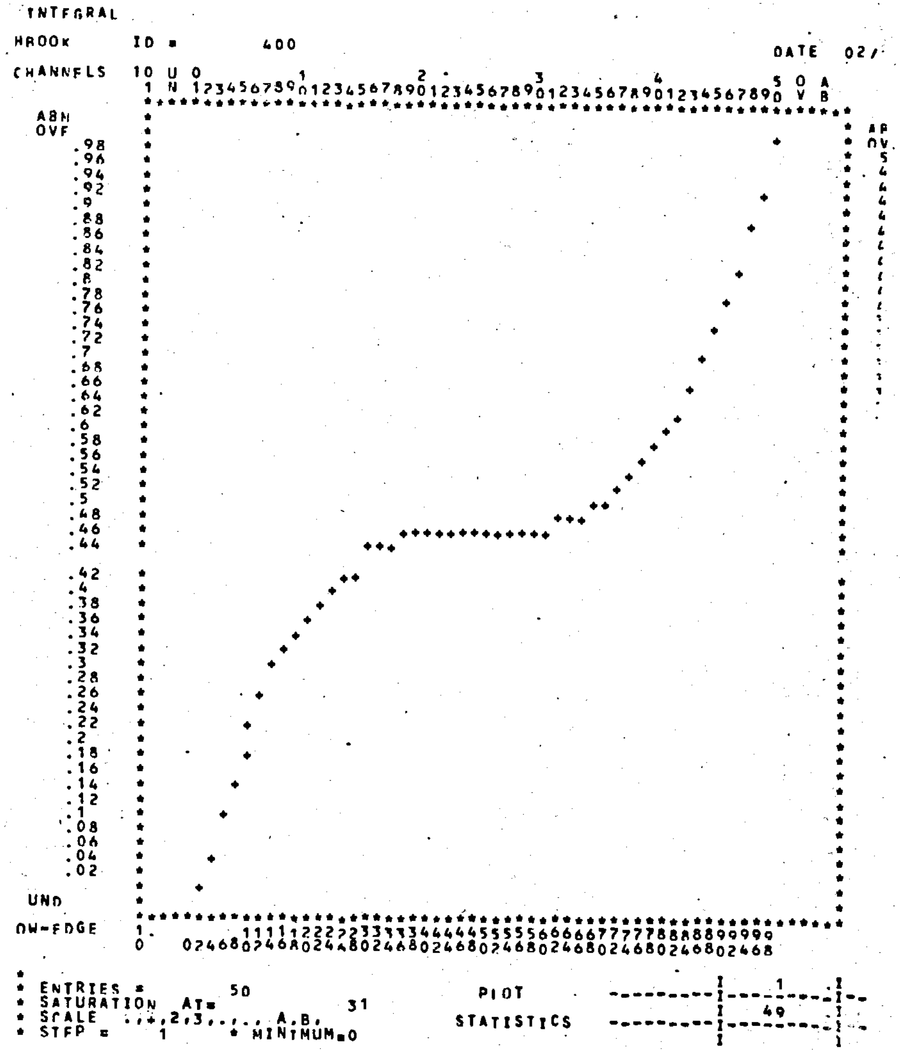
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Fig.6b

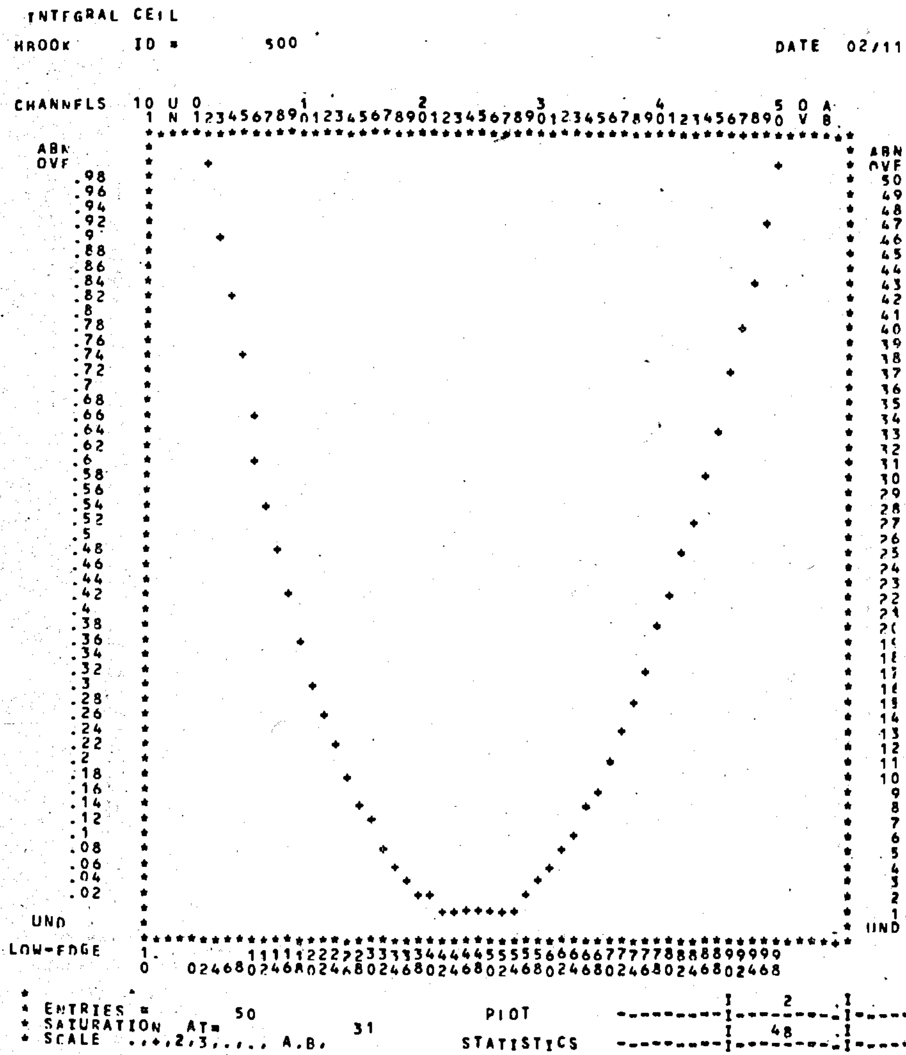
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Fig.7a

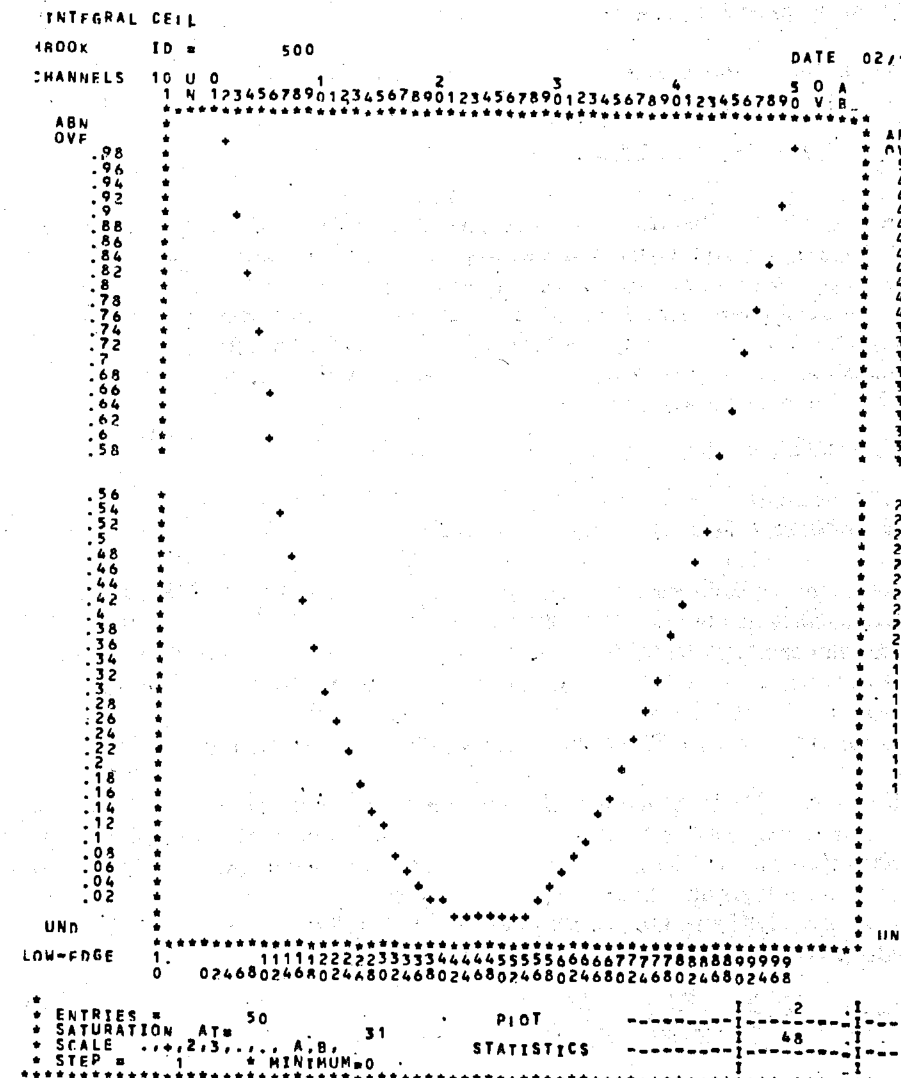
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Fig.7b

All the ordinate values have been normalized within [0,1] as follows

$$y_{norm} = \frac{(y - y_{min})}{(y_{max} - y_{min})}. \quad (3)$$

3.1 Model Data with $E(x) = 0$

The smooth unimodal function (2) has been numerically differentiated by means of the central difference formula

$$F'(x) = \frac{F(x + \Delta x) - F(x - \Delta x)}{2\Delta x} \quad (4)$$

to result in Fig.2a. The differentiation subroutine DGT3 (IBM SSP library) based on the Lagrangian interpolation polynomial of degree 2 relevant to the 3 successive points [7] produces the results presented in Fig.3a.

The appropriate numerical second derivatives can be seen in Figs.4a and 5a.

Integration by means of subroutine RGAUSS (LIBCERN library) is illustrated by total Riemann integral values, RI, (fig.6a) and cell Riemann integral values, CI (Fig.7a). These latter are defined as

$$CI(x_i) = RI(x_i) - RI(x_{i-1}). \quad (5)$$

3.2 Model Data with $E(x) = T(x) * RNDM(x)$

The computational results for these data are presented in Figs.1b-7b. The average error level corresponds there to 50%.

The total crackdown of differentiation procedures and the excellent stability of integration one are clearly seen from the parallel graphic patterns presented.

3.3 A Figure-of-Merit (FOM1) to Evaluate Different Transforms

Many experimental data are known to be measured with the lower error values, $E(x)$, corresponding to 1-10% of $T(x)$ [8]. This requires an algebraic FOM to be used for quantitative estimates of the distortions produced by such transforms as differentiation, integration, smoothing, filtering, etc.

Let us consider some metrics, say, based on Manhattan l_1-norm, $|| * ||_1$. Then the initial $F(x)$ data from Figs.1a and 1b can be evaluated by

$$FOM1(F) = \frac{1}{n} \sum_{i=1}^{n} \frac{|F_i(x_b) - F_i(x_a)|}{|F(x_b) - F(x_a)|_{max}}, \quad (6)$$

where n is the number of points. This FOM corresponds to an average absolute deviation normalized within [0,1].

All other pair graphical patterns can be propossed in an analogous manner to result in FOM1(F'), FOM1(F"), etc.

Then a propagation factor, e.g., EPF(F'), for a first derivative transform will be equal to

$$EPF(F') = \frac{FOM1(F')}{FOM1(F)}. \quad (7)$$

Analogous estimates, FOM2, can be made with Euclidean l_2-norm, i.e., $|| * ||_2$.

4. CONCLUSION

The presented results on error propagation effects in numerical differentiation and integration of model noisy functions clearly show the powerful stabilizing action of integration as compared to differentiation.

These conclusions support the previous computational evidence gained in investigating the integration weighing method of global optimization [9,10].

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