СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
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ИССЛЕДОВАНИЙ

Дубна

E11-98-3

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ORTHONORMAL POLYNOMIAL EXPANSION METHOD WITH ERRORS IN VARIABLES

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1998

1 Introduction

Sometimes the measurements in physics have errors in both the independent and dependent variables [1]. This case, so important for physicists, is not given in detail in the standard statistics books, used by physicists. The paper describes an improvement of earlier proposed Orthonormal Polynomial Expansion Method in our papers [2, 3, 4, 5] and in work [6]. Here the uncertainties in the dependent y and the independent x variables are introduced. A new total variance is defined and used:

$$\sigma_{\rm tot}^2 = \sigma_y^2 + (\partial y/\partial x)^2 \sigma_x^2. \tag{1}$$

Here the penalty is the requirement that the derivative $(\partial y/\partial x)$ is available.

2 Method

The method is a generalization of the Forsythe three-term reccurence formula [7] for constructing a set of orthogonal polynomials, using least square method. The generalization consists of : fast and accurate telescoping of fitting series in one dimensional case, normalization of a reccurence procedure [1, 2], stable differentiation and integration in one [5] and many-dimensional case [6], Some applications in high energy physics, nuclear physics and other fields are presented in our papers [2, 3, 4, 5].

The main relation for the one-dimensional case generating polynomials $\{P_i^{(m)}(x)\}$ $(m = 0)$, their derivatives $(m > 0)$ and integrals $(m > 0)$ is:

$$P_{i+1}^{(m)} = \gamma_{i+1}\left((x - \alpha_{i+1})P_i^{(m)} - (1 - \delta_{i0})\beta_i P_{i-1}^{(m)} + m P_i^{(m-1)}\right), \tag{2}$$

where the normalizing γ and recurrence coefficients α and β are presented by scalar products of the polynomials in the test data. One can generates the orthogonal polynomials recursively.

The approximating quantity is sought for in the form:

$$Y^{(m)\rm appr}(x) = \sum_{k=0}^{N} a_k P_k^{(m)}(x) = \sum_{k=0}^{N} c_k x^k, \tag{3}$$

where all calculations are carring out for $x\prime$ in [-1,1] approximating interval, but the prime sign is omitted for brevity. Here c_k are coefficients in an ordinary polynomial series, a_k are coefficients in orthonormal series and $P_k^{(0)}$ are orthonormal polynomials over discrete point set with different weights w_i:

$$\sum_{i=1}^{M} w_i P_k^{(0)}(x_i) P_l^{(0)}(x_i) = \delta_{kl}. \tag{4}$$

Here δ_{kl} is a Kronecker symbol. The relation between a_k and c_k is:

$$c_k = \sum_{i=k}^{N} a_k c_k^{(i)}, \quad k = 0, ..., N. \tag{5}$$

The coefficients $c_k^{(i)}$ are evaluated by recurrence relation:

$$c_0^{(0)} = 1/\beta_0$$

$$c_k^{(i+1)} = 1/\beta_{i+1}[(1-\delta_{0k})c_{k-1}^{(i)} - (1-\delta_{i+1,k})\alpha_{i+1}c_k^{(i)}$$
$$-(1-\delta_{ik})(1-\delta_{i+1,k})\beta_i c_k^{(i-1)}],$$

where $i = 1, 2..., N-1$; $\quad k = 0, 1, ..., i$.

The inherited uncertainties in the coefficients Δc_k are given by the Δa_k with:

$$\Delta c_k = \left(\sum_{i=k}^{N} (c_k^{(i)})^2\right)^{1/2} \Delta a_k, \tag{6}$$

Afterwards the a_k and Δa_k, c_k amd Δc_k are evaluated in natural (unput) units using relations:

$$x = (x\prime - x_0)/x_1, x_1 = 2/(x_{max} - x_{min}), x_0 = -(x_{max} + x_{min})/(x_{max} - x_{min})$$

and Δa_k are evaluted, using [8]:

$$\Delta a_k = \left(\sum_{i=1}^{M} P_k^2(x_i) w_i (Y_i - Y_i^{\mathrm{appr}})^2\right)^{1/2}.$$

The main fitures of our OPEM is the absence of matrix inversion and the optimum condition of matrices involved for high-degree fits.

We introduce the test set of $\{x_i, Y_i, \sigma_{x_i}, \sigma_{Y_i}, i = 1, ...M\}$ values of both variables and their standard deviations. In our algorithm the following χ^2 is minimized:

$$\chi^2 = \sum_{i=1}^{M} (Y_i^{\mathrm{appr}} - Y_i)^2 w_i \to \min. \tag{7}$$

We involve in the OPEM the formula for the total variance as follows:

1.Carrying out the y approximation with the weight function $w = 1/\sigma_Y^2$, depending only on errors of y. We evaluate the values of derivative $\{(\partial y/\partial x)_i\}$ in every point by (2) and (3).

2. Carrying out second y approximation with the total weight function $w_{\mathrm{tot}} = 1/\sigma_{\mathrm{tot}}^2$ using (1) , where the values of derivative are derived at the first step. Here the assumption of Bevington [9] to combine the uncertainties of both quantities and assign them to the dependent variable alone is taken into account. The procedure is iterative.

3 Results, Discussions and Illustrations

To test the algorithm we approximate the quadratic function $y = c_2x^2 + c_1x + c_0$ with errors in x_i and Y_i, given in [10]. Different types of minimizing of $chi-square$ are proposed there: PLOTDATA program fit (standard minimum variance) for the case $\sigma_x = 0$ and Effective Variance Method [11] and full MINUIT [12] program fit, for the case $\sigma_x \neq 0$. The χ^2 in [10] and [11] is found by minimizing the weighted sum of the squared deviations:

$$\chi^2 = \sum_{j=1}^{M} [((x_j - x_j^0)/\sigma_{x_j})^2 + ((Y_j - Y^{appr}(x_j^0))/\sigma_{Y_j})^2]. \tag{8}$$

For each true value x_j^0, there will be a measured x_j Gaussian-distributed about x_j^0 with a standard deviation σ_x, and similarly a measured Y_j Gaussian-distributed about $Y_j^0 = Y(x_j^0)$ with standard deviation σ_{Y_j}. In this case , in addition to the N values of $\{c_k\}$, there are M values of $\{x_j^0\}$, giving a total of $M + N$ unknowns. The total number of experimental points is the M values of x_j plus the M values of Y_j. The number of degres of freedom are $[2M - (M + N)] = (M - N)$. The minimization of the equation (8) has to be performed for the M values of x_j^0 as well for the N values of a_k. An obvious approach is the employment of MINUIT with minimization carried out for all $M + N$ parameters simultaneously.

The above formula can be simplified and it is performed in Effective variance Method [11], without the necessity of including the independent variables as parameters. The method esentially relies on the adequacy of being able to approximate the function $Y(x)$ by a linear function in the neighbourhood of each experimental point (within a range $\sigma x_j, \sigma Y_j$ for each(x_j, Y_j)). The simplified expression is given by eq.(2) in [10], which is analogous to our eq. (7). The minimization in [10] is carried out with MINUIT or iteratively using a standard minimum variance routines. In [13] is shown that such a process does not converges, in general, to the "exact" solution.

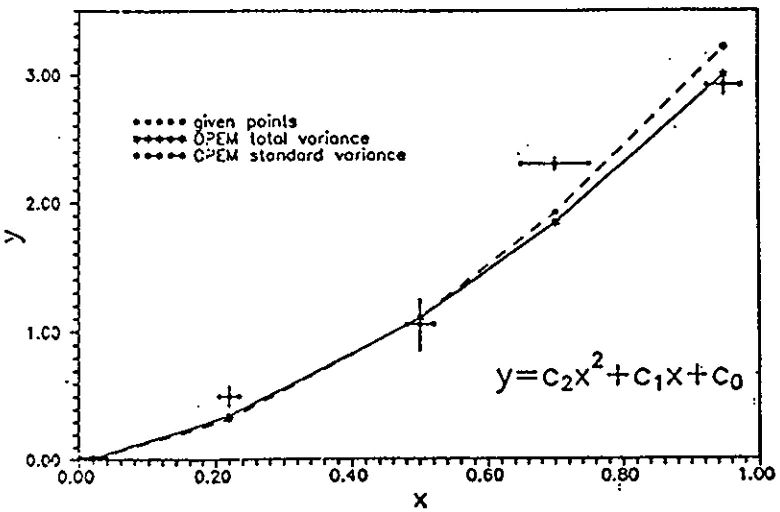

Fig.1

Our results for this simple example are obtained on IBM compatible PC, using FORTRAN 77 codes. The given points, error corridors and two approximated curves by OPEM are given in Fig.1. It is evident that the approximating curve for $\sigma_x \neq 0$ is more suitable to given error corridors. The OPEM results for χ^2 values and the values of coefficients $\{c_k\}$ by eq.(5) and their uncertainties $\{\Delta c_k\}$ (estimated by (6)) are compared in two main cases (respectively in Table 1 and 2) with the methods in [10].

a. Approximation when $\sigma_x = 0$ (Table 1). The result $\chi^2_{\rm OPEM} =$ 14.9418 is equal to calculated by PLOTDATA $\chi^2 = 14.94$ in [10]. The errors in OPEM coefficient c_1 is: 0.305. It is smaller than evaluated corresponding value by PLOTDATA - 0.35.

Table 1

	Standard variance		OPEM Standard variance	
	χ^2		χ^2	
	14.942		14.9418	
	value	error	value	error
c_2	-0.06625	0.3926	-0.06624	0.59103
c_1	3.32210	0.3518	3.27946	0.30597
c_0	-0.08240	0.0520	0.54921	0.34543

b. Approximation when $\sigma_x \neq 0$ (Table 2). The approximation by OPEM is different in nature in comparison with appropriate methods.The convergence was obtained quickly (2 iterations). The result $\chi^2_{\rm OPEM}$ is 5.93, which is close to $\chi^2 = 4.17$ in [10] (best aproximation by full MINUIT) , 4.28 by Effective Variance Method and 4.34 by their Iterative Fit (5 iterations).

Table 2

	Effect.var.		MINUIT		OPEM tot. var.	
	χ^2		χ^2		χ^2	
	4.2814		4.1754		5.93	
	value	error	value	error	value	error
c_2	1.1390	0.6663	1.1667	0.6666	0.5398	1.0026
c_1	2.0929	0.6228	2.0614	0.6272	3.0061	0.3954
c_0	-0.0244	0.0726	-0.0223	0.0723	0.1551	0.7995

The value of error in OPEM coefficients $c_1 = 0.395$ is smaller than $c_1 = 0.6272$ by MINUIT and $c_1 = 0.6228$ by Effective Variance Method respectively.

For completeness the results by Effective Variance Method (using MINUIT) and full MINUIT are given. The OPEM errors in coefficients are close to MINUIT fit errors. The results for their iterative fit is not given in the tables. We have to note that the OPEM second and third iteration gives $\chi^2 = 5.93$ and the coefficients have the same values as presented respectively.

4 Conclusions

The main result is that OPEM with a total variance is a more accurate algorithm than OPEM with a standard variance - about three times better (Fig.1 and Tables) because of good derivative accuracy. It gives also good results (for linear approximation) in comparison with other popular methods. and it slightly differs from full MINUIT fit and Effective Variance Method (Table 2). The comparative numerical results for the type and accuracy of OPEM and other approximations determine the perspectives of our new approach. It can be included in nonlinear rational approximation to achieve better conditioned set of normal equations, as it is proposed in [14].

This simple and fast algorithm holds very well for many physical applications, espessialy for calibration procedures. With many data points the appropriate methods leads to a very large number of parameters. For real data applications with many- point approximating intervals and for high-degree polynomials the OPEM total variance will be carried out in a following paper.

5 Acknowledgements

The author would like to express her thanks to Prof. G. Ososkov and Prof. I. Duff for useful discussions.

The paper is supported partially by National Fund for Scientific Research (Bulgaria) under contract No. 507/95.

References

[1] R. Powel, W.Hall, and J. Hust, Proceed. in of the Fifth Symposium on Temperature, Washington, DC, 21-24 1971(Instr. Society of America, Pittsburg, PA, 1972), vol. 4, Pt.2, p.1423.

[2] V. Gadjokov and N. Bogdanova, Dubna, JINR commun., P11–12860 (1979); P11–80781 (1980); P11-80122 (1980).

[3] N. Bogdanova and V. Gadjokov , *Comput. Phys. Commun* **24** (1981) 225.

[4] N. Bogdanova, *J. Comput.and Applied Mathematics*,**14** (1986) 345.

[5] N. Bogdanova and T. Kupenova, *Comput. Physics Commun.*,**73** (1992) 170.

[6] V. Gadjokov and J. Jordanova, *Comput. Phys. Commun.* **31** (1984) 53.

[7] G. Forsythe, *J. Soc.Ind. Appl.Mathem.* **5** (1957) 74.

[8] D. J. Hudson, *Lectures on Elementary Statistics and Probaility* (CERN, Geneva,1964).

[9] P.R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill,1969).

[10] G. Jones, Preprint TRI–PP–92–31, A (1992).

[11] J. Orear, *Am.J.Phys.* **50** (1982) 912.

[12] F. James and L.M. Roos, MINUIT CERN Report, D506 MINUIT(1989)

[13] M. Lybanon, *Am. J. Phys* **52** (1984) 276.

[14] G. Vandersteen, Y. Rolain and J. Schoukens, R. Pintlelon, *IEEE Transactions on Instrumentation and Measurement,* **45**, *2, April, 1996.*

Received by Publishing Department
on January 19, 1998.