ORTHONORMAL POLYNOMIAL APPROXIMATION OF MINERAL WATER DATA WITH ERRORS IN BOTH VARIABLES

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Abstract

In this paper we introduce the data from mineral water probe with errors in both variables. For this case we apply our orthonormal polynomial expansion(OPEM) method to describe the data in the new error corridor. It received the approximating curves and their derivatives including the errors by weighting approach. The numerical method and approximation results are presented and discussed. The special criteria are carried out for orthonormal and evaluated from it usual expansions. The numerical results are shown in tables and figures.

Key words: orthonormal and usual polynomial approximation, weighted approach, contact mineral water angle data

1 Introduction

The water spectra method applies a drop taken from a water probe to measure the water's state spectrum. In the special experiment the drop is placed on a hostaphan folio- Figure 1[1]. During the whole process of evaporation of the drop, one measures at equal time intervals the drop contact angle with the folio. On X-axis one has the values of the contact angles within fixed angular intervals and on Y-axis the frequency of measurements of these angles.

To compare different state spectra one normalizes each spectrum dividing its Y-values by the number of all measurements and thus obtains a probability distribution . One can change the function $\phi(\theta)$ on the independent angle θ to the function of energy variable F(E) using the following Antonov transformation [2]:

$$f(E) = b\phi(\theta)/\sqrt{1 - (1 + bE)^2},$$

where

$$b = I(1 + cos(\theta_0))/\gamma.$$

Here $I = 5.03.1018m^{-2}$ is the density of water molecules in the surface layer, γ is the surface tension, θ_0 - the initial contact angle.

The so obtained graph after measurements by method in [1] is referred to as energy spectrum $F(E)$ of the probe. E is the energy of Hydrogen bond of investigated water.

On Figure 2 the dependent variable contains the values of the water Hydrogen bond energy. Here we present new detailed information about given data and their errors on both variables of water probe.

The method of water spectra is sensitive to treatment by physical fields as γ-ray treatment of water [1, 2] and to environmental changes of the ecosystem on different water probe [3, 4, 5, 6, 7, 8]. In the present paper we approximate another natural water data taken from a water spring in Bulgaria near the village Lenovo.
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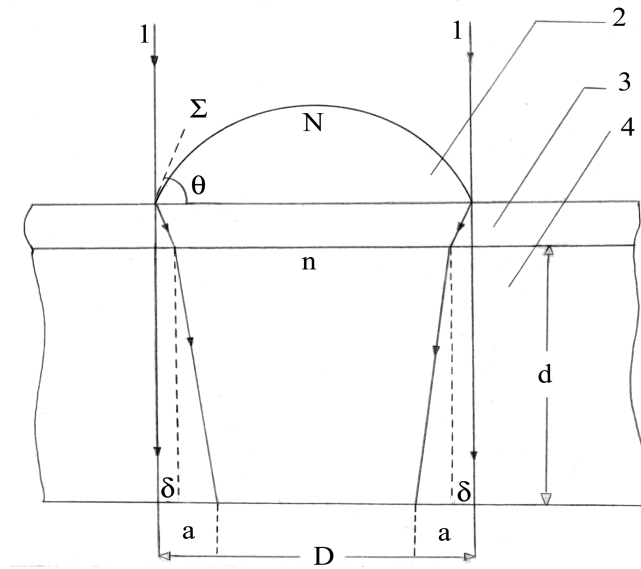[2]Email:todorov_st@yahoo.com
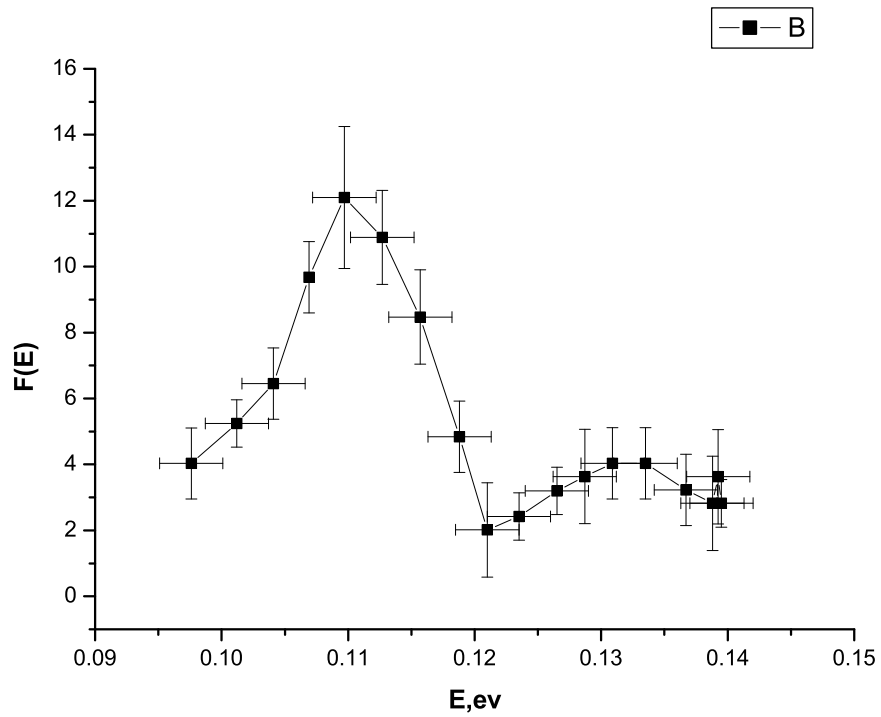
Figure 1: **Experimental setup**

Figure 2: **Experimental data from (B) with their errors**

2 Main problem definition

- To find the best approximation curves of measured water data on Fig.2 taking into account

- To extend our original Orthonormal polynomial expansion method (OPEM), according some criteria, to evaluate orthonormal description of given data;

- To find the best approximating curve with usual polynomials, evaluated by orthonormal, according some criteria.

3 Numerical method–OPEM "total variance"

Let the $\{E_i, F_i, i = 1, ...M\}$ are arbitrary pairs of monitoring data $E = E_i$ and $F = F_i$, introduced in section 2. They are given with experimental errors in both variables-$\sigma(F_i)$ and $\sigma(E_i)$. Consider the total uncertainty (total variance) $S^2(E, F)$ [9, 10, 11], associated with (E, F)

$$S_i^2 = \sigma^2(F_i) + (\frac{\partial F_i}{\partial E_i})^2 \sigma^2(E_i), \tag{1}$$

according the ideas of Bevington (1977)[9], where his proposal is to combine the errors in both variables and assign them to dependent variable. One defines the errors corridor $C(E, F)$, which is the set of all intervals

$$[F(E) - S(E, F), F(E) + S(E, F)], \tag{2}$$

.

3.1 orthonormal expansion criteria

The first criterion to be satisfied, is that the fitting curve should pass within the errors corridor $C(E, F)$. In the cases of errors only in F, (i.e. $\sigma(E) = 0, \sigma(F) \neq (0)$) the errors corridor $C(E, F)$ reduces to the known set of intervals

$$[F - \sigma(F), F + \sigma(F)], \tag{3}$$

for any F. The second criterion is, that the fitting curve $F^{appr}(E_i)$ satisfies the expression

$$\chi^2 = \sum_{i=1}^{M} w_i [F^{appr}(E_i) - F(E_i)]^2 / (M - L), w_i = 1/S_i^2. \tag{4}$$

should be minimal (L-number of polynomials). The preference is given to the first criterion. When it is satisfied, the search of the minimal chi- squared stops. Some details of the calculation procedure are given in Forsythe's paper [12] and in our works [13, 14, 15].

Our procedure gives results for approximating function by two expansions : of orthogonal coefficients $\{a_i\}$ and usual ones $\{c_i\}$ with optimal degree L:

$$F^{appr(m)}(E) = \sum_{i=0}^{L} a_i P_i^{(m)}(E) = \sum_{i=0}^{L} c_i E^i. \tag{5}$$

The orthogonal coefficients are evaluated by the given values F_i, weights and orthogonal polynomials:

$$a_i = \sum_{k=1}^{M} F_k w_k P_i^{(m)}(E_k). \tag{6}$$

Our recurrence relation for generating orthonormal polynomials and their derivatives ($m = 1, 2...$)(or their integrals with m=-1,-2,-3,...) are carried out by:

$$P_{i+1}^{(m)}(E) = \gamma_{i+1}[E - \mu_{i+1})P_i^{(m)}(E) - (1 - \delta_{i0})\nu_i P_{i-1}^{(m)}(E) + mP_i^{(m-1)}E)], \qquad (7)$$

where μ_i and ν_i are recurrence coefficients, and γ_i is a normalizing coefficient, defined by scalar products of given data. One can generate $P_i^m(E)$ recursively. The polynomials satisfy the following orthogonality relations: $\sum_{i=1}^{M} w_i P_k^{(0)}(E_i)P_l^{(0)}(E_i) = \delta_{k,l}$ over the discrete point set $\{E_i, i = 1, 2, \ldots\}$. All the calculations for the sake of uniformity are carried out for E in[-1,1], i.e. after the input interval is transformed to the unit interval. We remark some advantages of OPEM: It uses unchanged the coefficients of the lower-order polynomials; it avoids the procedure of inversion of the coefficient matrix to obtain the solution, the minimal chi-squared stops. All these features shorten the computing time and assure the optimal solution by the criteria(2) and (4).

3.2   the usual expansion criteria

The inherited errors in usual coefficients are given by the inherited errors in orthogonal coefficients:

$$\Delta c_i = (\sum_{k=1}^{L}(c_i^{(k)})^2)^{1/2}\Delta a_i, \qquad (8)$$

$$\Delta a_i = [\sum_{k=1}^{M} P_i^2(E_k)w_k(F_k - F_k^{appr})^2]^{1/2}. \qquad (9)$$

where coefficients $c_i^{(k)}$ are defined by orthonormal expansion of polynomials

$$P_k = \sum_{i=0}^{k} c_i^{(k)}E^i, k = 0, .., L \qquad (10)$$

and explicitly constructed by recurrence relation in [13].

The procedure is iterative because of the evaluation of derivatives on every iteration step and the result of the k^{it}-th consequent iteration is called below the k^{it}-the approximation. We note that in every iteration step the algorithm find the best approximation using given before criteria.

We can add the other criteria for optimal number of polynomials for usual expansion. Having the L_a we continue with finding the optimal L_c the **minimal value** in

$$max(c_i(L), i = 1, L) \qquad (11)$$

in usual coefficients through all steps of iterations $k^{it} = 1, 2, ..9$ or we are asking the **minimal value** of the maximal distance between functions, evaluated by orthonormal and usual expansions

$$max|(F_{a,k}^{appr} - F_{c,k}^{appr})|, k = 1, M \qquad (12)$$

through all iterations. We investigate both criteria, but we prefer the last one.

4   Approximation results

The main important results from approximation between $2 \div 10$ degrees for iterations $1 \div 9$ are

Table 1: **OPEM approximations results for every step approximation**

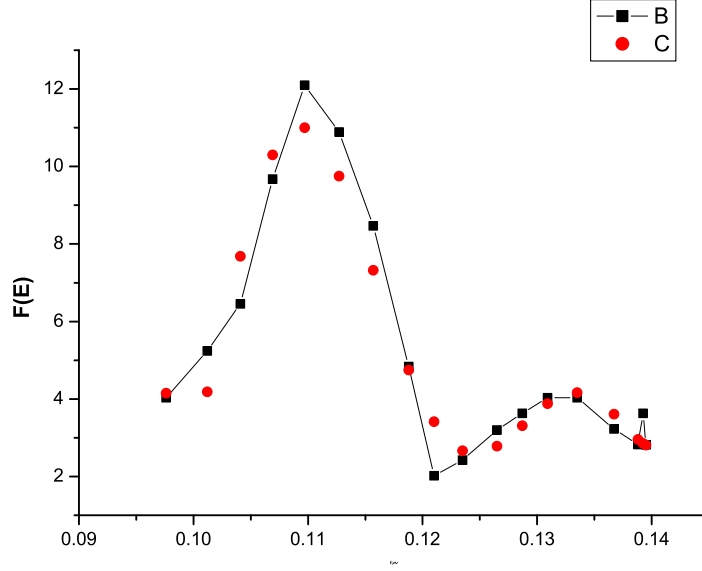| k^{it}	1	2	3	4	5	6	7	8	9
$L(2 \div 10)$	7	6	6	6	6	5	6	5	6
$\chi^2 * 10^{-1}$	5.61	4.23	3.99	3.79	3.77	6.81	3.75	6.65	3.63
$max|(F_a - F_c)|$	14.96	3.48	6.75	4.8	4.63	7.53	4.91	0.081	9.33

Figure 3: **OPEM approximation by 6-th degree orthonormal polynomials (C)(2-nd iteration) of experimental water data(B)**

$max|(F_a - F_c)|$. We see from the Table 1, that from iteration number $2 \div 5$ with optimal number $L_a = 6$ the results are good for both expansions and for usual expansion the 8-th iteration with optimal number $L_c = 8$ they are also good.

Note: It is very interesting to present on figures the three curves - given(B), approximated by orthogonal polynomials(C) and received from it by usual polynomials(D) at different iteration steps.

Below the figures 3,4,5,6 present the different approximations results with 2-nd, 3-rd and 4-th iterations.

The Table 2 presents the given and approximating values by OPEM with usual and orthonormal coefficients by calculated optimal degree $5-th$ in $8-th$ iteration of $M = 18$ given values of following characteristics: energy E , distribution F , σ_E and σ_F, and from $5-th$ column - the approximating values with orthonormal coefficients $F_a^{appr,5}$, approximating values with usual coefficients $F_c^{appr,5}$, differences $\Delta(F_a, F_c) = (F_a^{appr,5} - F_c^{appr,5})$, total variance $S(5)$ (equation (1). The Table 2 shows good coincidence between two descriptions. For comparison we can see the previous results for OPEM applications in [13, 14, 15, 16, 17].
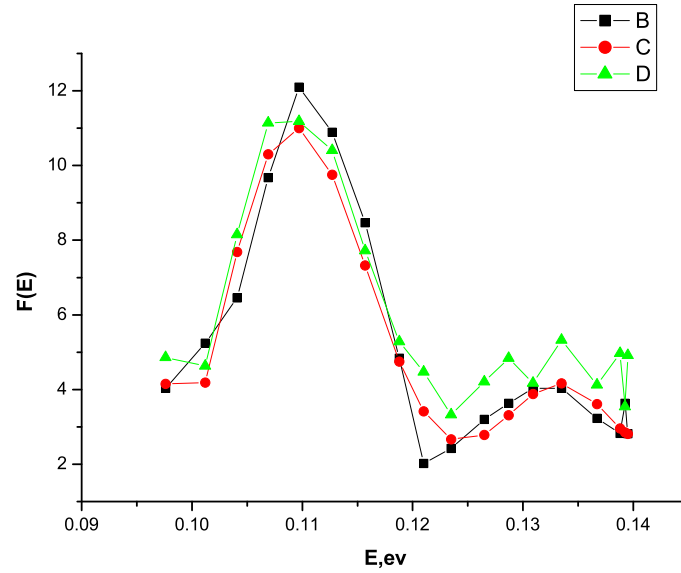
Figure 4: **OPEM approximation by 6-th degree(iteration-2-nd) orthonormal polynomials (C) and received usual expansion(D) of experimental water data(B)**
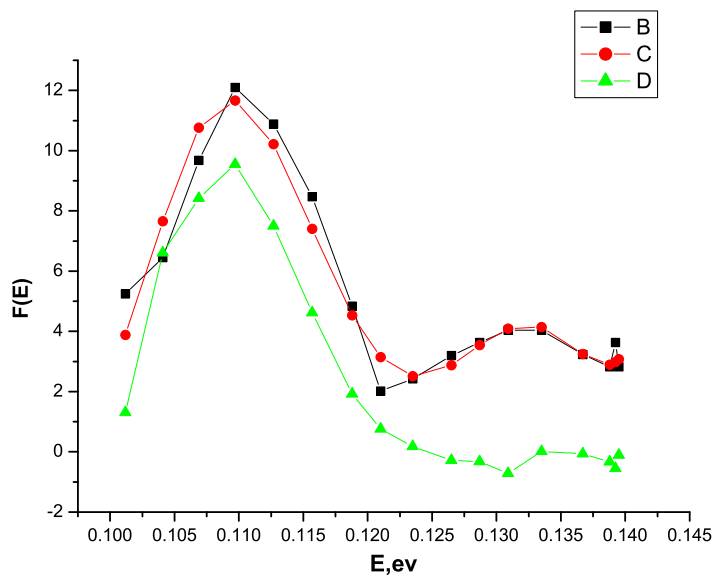

Figure 5: **OPEM approximation by 6-th degree(the 3-rd iteration)-the orthonormal polynomials (C) and received usual expansion(D) of experimental water data(B)**
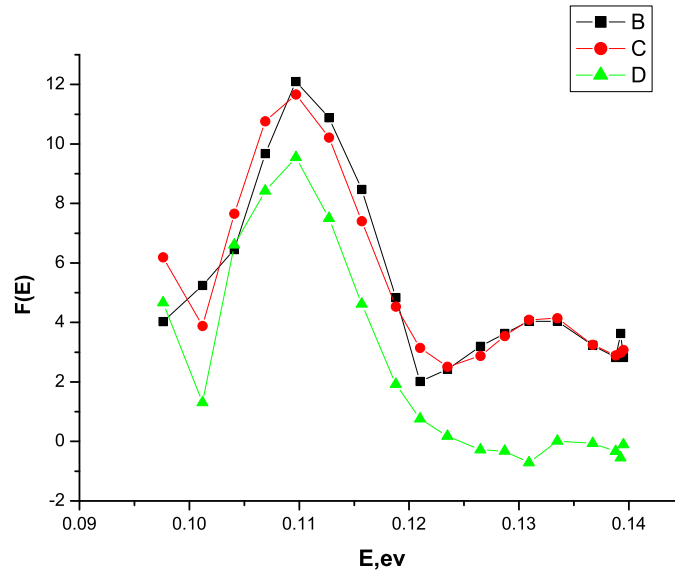
Figure 6: **OPEM approximation by 6-th degree(the 4-th iteration) orthonormal polynomials (C) and received usual expansion(D) of experimental water data(B)**
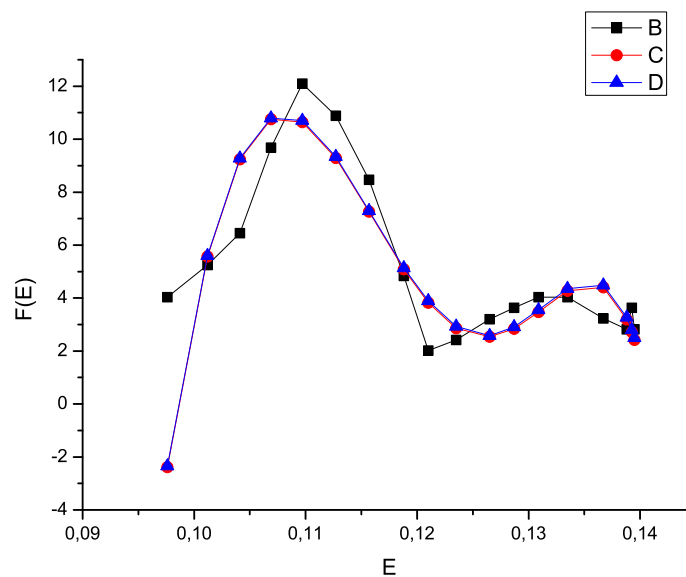

Figure 7: **OPEM approximation by 5-th degree(the 8-th iteration) orthonormal polynomials (C) and received usual expansion(D) of experimental water data(B)**

Table 2: OPEM approximation of contact water energy data

$No.$	$E[ev]$	$F(E)$	σ_E	σ_F	$F_a^{appr,5}$	$F_c^{appr,5}$	$\Delta(F_a, F_c)$	S
1	0.1395	2.820	0.025	0.72	2.421	2.503	8.169-02	2.2072
2	0.1392	3.627	0.025	1.43	2.721	2.799	7.796-02	2.9469
3	0.1388	2.822	0.025	1.43	3.192	3.266	7.420-02	2.2173
4	0.1367	3.227	0.025	1.08	4.408	4.484	7.614-02	1.8114
5	0.1335	4.035	0.025	1.08	4.272	4.353	8.125-02	1.3297
6	0.1309	4.035	0.025	1.08	3.467	3.549	8.161-02	1.3126
7	0.1287	3.632	0.025	1.43	2.840	2.905	6.474-02	2.6050
8	0.1265	3.200	0.025	0.72	2.534	2.583	4.910-02	0.9395
9	0.1235	2.422	0.025	0.72	2.861	2.932	7.089-02	0.5500
10	0.1210	2.017	0.025	1.43	3.821	3.889	6.886-02	3.4402
11	0.1188	4.840	0.025	1.08	5.091	5.137	4.575-02	5.1487
12	0.1157	8.470	0.025	1.43	7.259	7.291	3.272-02	8.2753
13	0.1127	10.887	0.025	1.43	9.290	9.334	4.365-02	5.3774
14	0.1097	12.095	0.025	2.15	10.647	10.700	5.320-02	4.6238
15	0.1069	9.677	0.025	1.08	10.750	10.793	4.292-02	6.4789
16	0.1041	6.452	0.025	1.08	9.243	9.276	3.293-02	15.8508
17	0.1012	5.242	0.025	0.72	5.569	5.601	3.178-02	6.0766
18	0.0975	4.030	0.025	1.08	-2.384	-2.347	3.714-02	86.5354

5   Conclusions

- We have developed new version of OPEM algorithm and Fortran 77 package to include errors in both variables according (2) and (4), defined new "'total variance"' and taking into account the respective inherited errors (8) and(9) in coefficients.

- The approximating curves are chosen at $2 - nd, 3 - rd, 4 - th$ approximation step by optimal degree $L_a = 6$ and at 8-th iteration step by optimal degree $L_c = 5$ to satisfy the proposed criteria (2),(4) and (11), (12). The results show that the orthonormal and usual expansions values are close to given ones in the whole interval.

- Our approximating results with optimal degrees of orthonormal polynomials for contact (wetting) angle found by orthogonal and usual coefficients show good **accuracy and stability**, demonstrated from Figures and Tables 1,2. We received suitable descriptions of the energy variations useful for further investigations.

- The presented extended algorithm and package OPEM "total variance" with its accuracy, stability and speed can be used in other cases of data analysis (as it it shown in our previous papers with earlier versions - for calibration problems in high energy physics [18]).

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