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ORTHONORMAL POLYNOMIAL APPROXIMATION OF WATER DROP EVAPORATION DATA WITH ERRORS IN TWO VARIABLES

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Ортонормальная полиномиальная аппроксимация данных
испарения капли воды, заданных с ошибками по обеим переменным

Исследование связано с фитированием экспериментальных данных по испарению капли воды, полученных в результате наблюдений на микроуровне. Аппроксимационный алгоритм построения ортонормированных полиномов применяется для данных с ошибками по обеим переменным. Численный метод здесь обобщается с помощью введения полной дисперсии, включающей обе ошибки. Анализируется ортонормальное и «обычное» разложение аппроксимационной функции.

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Orthonormal Polynomial Approximation of Water Drop Evaporation
Data with Errors in Two Variables

The investigation for fitting drop water evaporation data as a result of original microscope observations is presented. Our approximation algorithm with construction of orthonormal polynomials (orthonormal polynomial expansion method, OPEM) is applied to data with uncertainties in both independent and dependent variables. For this purpose our numerical method is developed here to include both errors. We also review its principles and analyze the orthonormal and «usual» expansions of the approximating function.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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1. INTRODUCTION

The evaporation of liquid drops considered as a physical process is of interest from applied point of view in ecology and for various technical applications. The process of forced evaporation of liquid drops placed within an air flow seems to be more interesting for technical purposes [1]. Up to now the wetting properties of liquids are of considerable interest for research. This is not only because of the various applications in industry, but also due to some unsolved topics in the theory of liquid wetting [2–4]. A general study of drop evaporation is contained in [5]. For general formulae to calculate time of evaporation and evaporation mass of a liquid (not necessarily water) drop placed on non-wettable substrate, we refer to [6, 7]. Here we are interested in the application of evaporation process to a precise optical measurement of the water drop's contact angle during the evaporation. Using this information, one can determine the so-called water spectrum which reflects some properties of water [3]. Due to the dependence of energy spectrum (in the special case of natural waters) on chemical compositions, or physical fields, etc., the spectra reflect the joint influence of all such factors. Generally speaking, the influence of the ecosystem as a whole on the natural waters thus presents a potential application to ecology.

2. PHYSICAL DATA

The water spectrum is determined by the method of evaporating drop taken from the probe and placed on a non-wettable substrate [1] (see here Fig. 1). We consider small water drops *2* of mass 1–10 mg, placed on a hydrophobic substrate *3* with a contact angle θ. Here we study the variations of the wetting angle of a sessile drop of water in two cases: before and after treatment in cleaning station. In the course of evaporation of the drop, as the drop's contact angle changes, we measure the frequency of appearance f of these angles within fixed angle intervals. One can summarize that in this way the «state spectrum» with respect to the contact (wetting) angle is obtained of the corresponding system of contact among the substrate, the water drop and the air. For this purpose, one measures by microscopic observations at regular time intervals (here every 2 minutes) the values for several drops (to enable drawing statistical conclusions). In this way one obtains a set of discrete values $f_i, i = 1, \dots, M$, the frequencies of occurrence of θ_i.

It is known that the water spectrum is sensitive to environmental influences such as radiation [2], physical fields [3], and others. Simultaneously with the probe measurement, one determines the spectrum of the deionized water, the so-called «control». The arithmetic difference between the two spectra is called differential spectrum, which is independent of incidental influences on the spectrum of the probe.

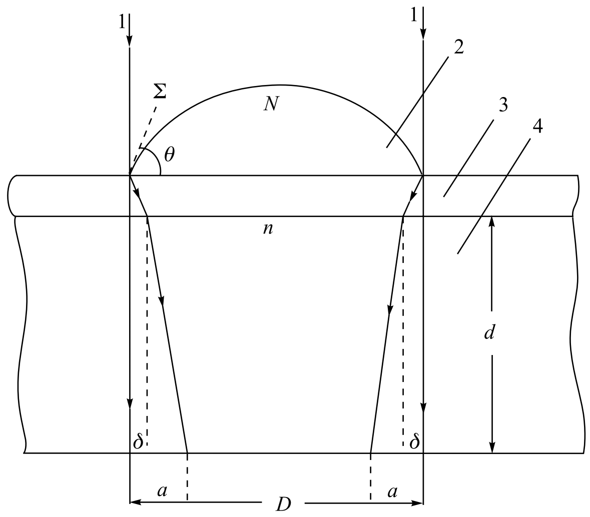

Fig. 1. Experimental setup

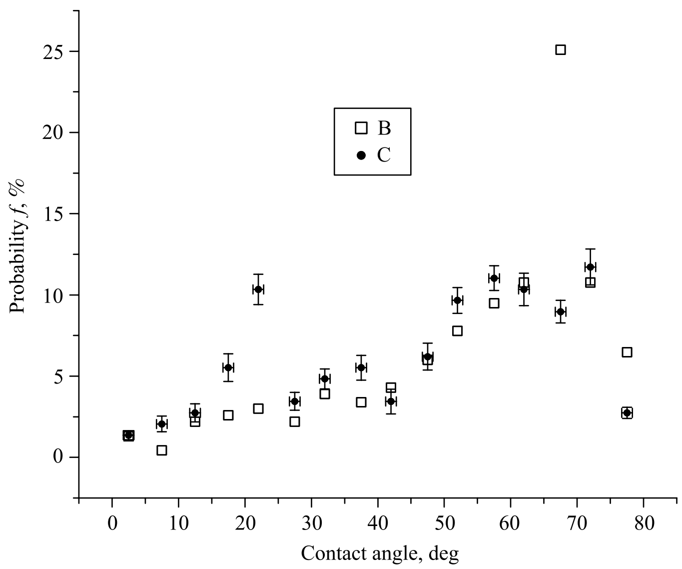

Fig. 2. Experimental data from deionized (B) and non-treated water (C)

Here N and n are the refraction indexes of water and glass correspondingly, d is the thickness of the glass plate, the segment denoted by δ in Fig. 1 can be neglected since $\delta \ll a$, a is a measured width of the dark ring. According to the laws of geometric optics, one can calculate the tangent of contact angle as a function of the above cited parameters as follows:

$$\tan\theta = n/\left(\sqrt{N^2\Delta - n^2} - \Delta^{1/2}\right); \Delta = 1 + d^2/a^2.$$

We present such curves that correspond to the water in Fig. 2 (deionized water control with open squares and non-treated water, probe with full circles).

3. PROBLEM DEFINITION

• To find the best approximation curve of measured water data in Fig. 1, including errors in both variables;

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

• To find the best approximating curve with usual polynomials, evaluated by orthonormal;

• To present the evaluated approximated curves in the evaluated new corridor of errors and in figures and tables.

4. NUMERICAL METHOD — OPEM «TOTAL VARIANCE»

Let the $\{\theta_i, f_i, i = 1, \ldots, M\}$ be arbitrary pairs of monitoring data $\theta = \theta_i$ and $f = f_i$, introduced in Section 2. They are given with experimental errors in both variables — $\sigma(f_i)$ and $\sigma(\theta_i)$. Following the ideas of Bevington (1977) [8] (where his proposal is to combine the errors in both variables and assign them to dependent variable), we consider the total uncertainty (total variance) $S^2(\theta, f)$, associated with (θ, f)(see also [8–10]):

$$S_i^2(\theta, f) = \sigma^2(f_i) + \left(\frac{\partial f_i}{\partial \theta_i}\right)^2 \sigma^2(\theta_i). \tag{1}$$

One defines the errors corridor $C(\theta, f)$, which is the set of all intervals

$$[f(\theta) - S(\theta, f), f(\theta) + S(\theta, f)], \tag{2}$$

associated which each pair (θ, f). The first criterion to be satisfied is that the fitting curve should pass within the errors corridor $C(\theta, f)$. In the cases of errors only in f, (i.e., $\sigma(\theta) = 0$, $\sigma(f) \neq (0)$) the errors corridor $C(\theta, f)$ 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 $f^{\text{appr}}(\theta_i)$ satisfies the expression

$$\chi^2 = \sum_{i=1}^{M} w_i [f^{\text{appr}}(\theta_i) - f(\theta_i)]^2/(M-L) \to \min, \quad w_i = 1/S_i^2 \tag{4}$$

(L — optimal number of polynomials). The preference is given to the first criterion. When it is satisfied, the search of the minimal chi squared stops.

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

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

The polynomials satisfy the following orthogonality relations:

$$\sum_{i=1}^{M} w_i P_k^{(0)}(\theta_i) P_l^{(0)}(\theta_i) = \delta_{k,l} \tag{6}$$

over the discrete point set $\{\theta_i, i = 1, 2, \ldots\}$. Then the orthogonal coefficients are evaluated by the given values f_i, weights and orthogonal polynomials (no matrix inversion):

$$a_i = \sum_{k=1}^{M} f_k w_k P_i^{(m)}(\theta_k). \tag{7}$$

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

$$P_{i+1}^{(m)}(\theta) = \gamma_{i+1}[(\theta - \mu_{i+1})P_i^{(m)}(\theta) - (1-\delta_{i0})\nu_i P_{i-1}^{(m)}(\theta) + mP_i^{(m-1)}(\theta)], \tag{8}$$

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 $P_i^m(\theta)$ recursively. Some details of the calculation procedure are given in Forsythe paper [11] and in our papers [12–14]. The inherited errors in usual coefficients are given by the inherited errors in orthogonal coefficients:

$$\Delta c_i = \left(\sum_{k=i}^{L} (c_i^{(k)})^2 \right)^{1/2} \Delta a_i, \tag{9}$$

$$\Delta a_i = \left[\sum_{k=1}^{M} P_i^2(\theta_k) w_k (f_k - f_k^{\text{appr}})^2 \right]^{1/2}, \tag{10}$$

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

$$P_k = \sum_{i=0}^{k} c_i^{(k)} \theta^i, \quad k = 0, \ldots, L \tag{11}$$

and explicitly constructed by recurrence relation in [12–14]. The comparison among MINUIT, effective variance method and OPEM «total variance» for parabola is also given there (for χ^2 and $(\Delta c/c)$). The results are comparable.

All the calculations for the sake of uniformity are carried out for θ in $[-1, 1]$, i.e., after the input interval is transformed to the unit interval. We remark some *advantages* of OPEM: It uses the unchanged coefficients of the lower-order polynomials; it avoids the procedure of inversion of the coefficient matrix to obtain the solution. All these features shorten the computing time and assure the *optimal solution* (by the criteria (2) and (4)). The procedure is iterative because of the evaluation of derivatives on every iteration step, and the result of the $k^{\rm it}$th consequent iteration is called below the $k^{\rm it}$th approximation.

• First iteration step: $(k^{\rm it} = 1)$ Approximation with

$$\{f_i, \theta_i, w_i = 1/\sigma^2(f_i), i = 1, \ldots, M\}.$$

Evaluation of the optimal approximating curve $f^{{\rm ap}1,L}$ $(df^{{\rm ap}1,L}/d\theta)$.

• Second iteration step: $(k^{\rm it} = 2)$ Approximation with

$$\{f_i, \theta_i, w_i = 1/S_i^2, i = 1, \ldots, M\}.$$

Evaluation of the optimal approximating curve $f^{{\rm ap}2,L}$ $(df^{{\rm ap}2,L}/d\theta)$, etc.

The extended algorithm presented here is called *OPEM «total variance»*.

5. APPROXIMATION RESULTS

Figures 3 and 4 present the obtained optimal OPEM approximation. Figure 3 shows the given data (C) and approximating values (D) by OPEM «total variance». Figure 4 contains the given and approximating curves and two types of evaluated data — lower border E and higher border F, presenting the new corridor, related to (2). It is well seen that the given f as curve (C) values and calculated by OPEM approximating values $f_a^{{\rm appr},13}$ as (D) are between the error corridor $C(\theta, f)$.

Table 1 presents the given and approximating values by OPEM with usual and orthonormal coefficients at calculated optimal degree L of $M = 16$ given values of contact angle θ, f, σ_θ and σ_f, and approximating values with orthonormal coefficients $f_a^{{\rm appr},13}$, differences $\Delta(f, f_a^{{\rm ap},13}) = (f - f_a^{{\rm appr},13})$, total variance $S(13)$ (Eq. (1)) and approximating values with usual coefficients $f_c^{{\rm appr},10}$ and

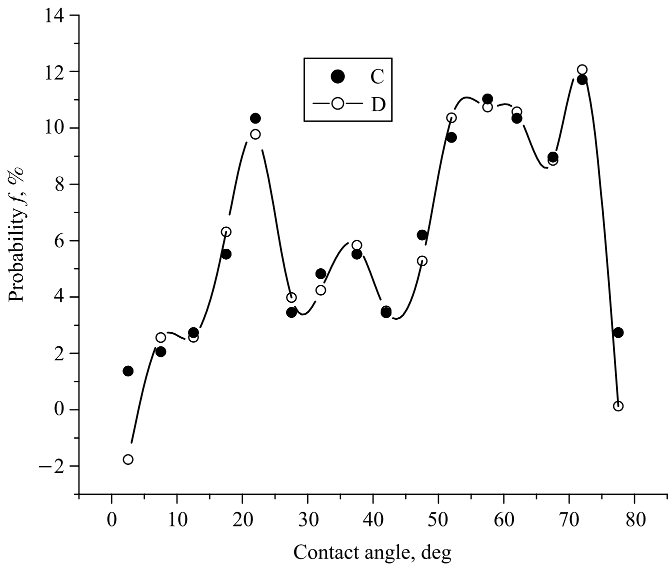

Fig. 3. OPEM approximation by 13th degree orthonormal polynomials (D) of non-treated water data (C)

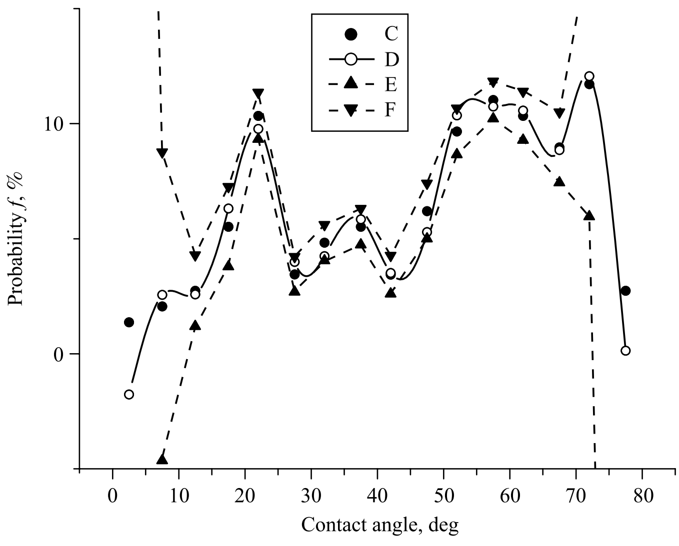

Fig. 4. Given data (C) and OPEM approximation values by 13th degree orthonormal polynomials (D), the lower border (E) and the higher border (F) of error corridor

Table 1. OPEM approximation of contact water angle data

No.	θ	f	$\sigma(\theta)$	$\sigma(f)$	$f_a^{\mathrm{appr},13}$	$\Delta(f, f_a^{\mathrm{ap},13})$	$S(13)$	$f_a^{\mathrm{appr},10}$	$f_c^{\mathrm{appr},10}$
1	2.5	1.37	0.8	0.28	–1.76	–3.135	3.32	1.516	1.516
2	7.5	2.06	0.8	0.48	2.56	0.502	0.77	2.027	2.027
3	12.5	2.74	0.8	0.55	2.57	0.165	0.85	2.644	2.644
4	17.5	5.52	0.8	0.85	6.31	–0.795	0.94	6.766	6.766
5	22.0	10.34	0.8	0.93	9.77	0.564	0.95	7.303	7.302
6	27.5	3.45	0.8	0.53	3.98	–0.535	0.63	5.153	5.149
7	32.0	4.83	0.8	0.62	4.24	0.583	0.62	4.046	4.037
8	37.5	5.52	0.8	0.76	5.83	–0.319	0.77	4.293	4.275
9	42.0	3.44	0.8	0.76	3.50	– 0.067	0.77	4.960	4.940
10	47.5	6.20	0.8	0.83	5.28	–0.914	0.88	6.313	6.293
11	52.0	9.66	0.8	0.80	10.3	–0.697	0.92	8.491	8.425
12	57.5	11.03	0.8	0.76	10.70	0.288	0.79	11.256	11.150
13	62.0	10.34	0.8	1.00	10.50	–0.232	1.09	11.001	11.932
14	67.5	8.97	0.8	0.70	8.84	–0.121	0.70	8.677	8.776
15	72.0	11.72	0.8	1.10	12.06	–0.346	1.62	12.334	12.309
16	77.5	2.74	0.8	0.34	0.13	2.608	8.86	0.791	1.963

Table 2. OPEM approximations results for every step approximation

k^{it}	1	2	3	4	5	6
L (9–15)	13	13	13	13	13	13
χ^2	1.29489	0.99864	0.99891	0.99941	0.99914	0.99914
L (9–12)	10	10	11	11	11	11
χ^2	2.36404	2.22976	2.22488	2.17006	2.16189	2.15843

orthogonal coefficients $f_a^{\mathrm{appr},10}$. For comparison one can see the previous results for OPEM applications in [13, 15, 16].

For numerical experiments with new presented data (with errors in both variables) the best results for χ^2 are summarized in Table 2. The k^{it}th iterations are from 1 to 6. The optimal results for χ^2 with the polynomial degree L are shown at corresponding iterations for two cases: L between 9 and 15 and L between 9 and 12. The second case is for obtaining usual coefficients by special criterion with the minimum of inherited errors ($\Delta c/c$).

6. CONCLUSIONS

• We have developed a new version of OPEM algorithm and Fortran 77 package to include errors in both variables according to (2) and (4), defining new «total variance» and taking into account the respective inherited errors (9) and (10) in coefficients.

• The results show that the orthonormal and usual expansions values are close to given ones in the whole interval.

• The approximating curves are chosen at the 2nd approximation step by optimal degree L to satisfy the proposed criteria (2) and (4).

• Our approximating results with optimal degrees of OPEM orthonormal polynomials for contact (wetting) angle found by orthogonal and usual coefficients show good *accuracy and stability*, as demonstrated in the figures and Tables 1 and 2. We obtained suitable descriptions of the angle variations useful for further investigations and comparison with control curve.

• The presented extended algorithm and package *OPEM «total variance»* with its accuracy, stability and speed can be used in the high-energy data analysis (as shown in our previous papers with earlier versions — for calibration problems [17]).

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