APPROXIMATION BY EXPONENTIALS. III.*

THE USE OF THE PRODUCT OF A POLYNOMIAL AND AN EXPONENTIAL FUNCTION

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The author deals with the problem of fitting to experimental data an equation $u = (p_0 + p_1 x + \ldots + p_n x^n) \exp(\omega x)$, where $\omega, p_0, p_1, \ldots, p_n$ are constants, and further a generalized equation $u = q_0 D_0(x) + q_1 D_1(x) + \ldots + q_n D_n(x)$ where $D_i = P_i(x) . \exp(\omega x)$ and $P_i(x)$ is a polynomial of the i-th degree. All D_i are orthogonal functions on the set of numbers x. Special cases are discussed in which these equations are subject to the constraint $u = u_0$ for $x = x_0$.

The character of the above equations makes them well suited for fitting the frequency curves (putting $p_0 = 0$ makes $u = 0$ both for $x = 0$ and $x = \infty$; ω assumed negative) as well as those curves where $u = L =$ const. for $x \to \infty$ (*e.g.* in chemical reaction studies).

General Formulation

Let us have $R > n + 1$ pairs of experimental observations x_i, y_i $i = 0, 1, \ldots R - 1$ obtained *e.g.* on a computer or otherwise.

We search for the unknowns $p_0, p_1, \ldots, p_n, \omega$ of equation

$$u = (p_0 + p_1 x + \ldots + p_n x^n) \exp(\omega x) \qquad (1)$$

such that the sum of the squares of the deviations (SSD)

$$\mathrm{SSD} = \sum_{i=0}^{R-1} (u - y_i)^2 \qquad (2)$$

be a minimum. The problem leads to $n + 2$ equations

$$\frac{\partial \mathrm{SSD}}{\partial p_0} = \frac{\partial \mathrm{SSD}}{\partial p_1} = \ldots = \frac{\partial \mathrm{SSD}}{\partial p_n} = 0\,, \qquad (3)$$

$$\frac{\partial \mathrm{SSD}}{\partial \omega} = 0\,. \qquad (4)$$

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While Eqs (3) are linear in $p_1, p_2, \ldots p_n$, Eq. (4) is a non-linear one. A plausible approach is to pick ω at random, solve the set of Eqs (3) for $p_0, p_1, \ldots p_n$ and calculate SSD which is clearly a function of ω

$$\mathrm{SSD} = \mathrm{SSD}(\omega)\,. \tag{5}$$

The minimum of this function can be found by a number of methods. The one chosen here is based on halving the interval $\langle \omega_1, \omega_2 \rangle$ encompassing the minimum.

The set of normal equations (3) is simplified by introducing

$$[j] = \sum_{i=0}^{R-1} x_i^j \exp(2\omega x_i)\,, \quad [yj] = \sum_{i=0}^{R-1} x_i^j y_i \exp(\omega x_i)\,.$$

Thus we get

$$\begin{aligned} p_0[0] + p_1[1] + \ldots + p_n[n] &= [y0]\,, \\ p_0[1] + p_1[2] + \ldots + p_n[n+1] &= [y1]\,, \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ p_0[n] + p_1[n+1] + \ldots + p_n[n+n] &= [yn]\,. \end{aligned} \tag{6}$$

It is well known that the system has an ill-conditioned matrix. Consequently, the original fitting equation is replaced by

$$u = [q_0 P_0(x) + q_1 P_1(x) + \ldots + q_n P_n(x)] \exp(\omega x)\,, \tag{7}$$

where $P_k(x)$ is a polynomial of the k-th degree in x. All polynomials are assumed to be known, ω has been chosen and the problem is to determine the coefficients $q_0, q_1, \ldots q_n$ so as to make

$$\mathrm{SSD} = \sum_{i=0}^{R-1} (u - y_i)^2 \tag{8}$$

a minimum. This leads now to the conditions

$$\frac{\partial \mathrm{SSD}}{\partial q_0} = \frac{\partial \mathrm{SSD}}{\partial q_1} = \ldots = \frac{\partial \mathrm{SSD}}{\partial q_n} = 0\,. \tag{9}$$

Introducing for simplicity

$$D_k(x) = P_k(x) \cdot \exp(\omega x)\,, \tag{10}$$

we get that

$$\frac{\partial \mathrm{SSD}}{\partial q_k} = \sum_{i=0}^{R-1} 2[q_0 D_0(x_i) + \ldots + q_n D_n(x_i) - y_i] \,.\, D_k(x_i)$$

$k = 0, 1, \ldots n$. Introducing again a simplified notation

$$[D_j D_k] = \sum_{i=0}^{R-1} P_j(x_i)\, P_k(x_i) \exp(2\omega x_i)\,,$$

$$[y D_k] = \sum_{i=0}^{R-1} y_i P_k(x_i) \exp(\omega x_i)\,, \qquad (11)$$

we obtain from Eq. (*9*) a set of normal equations in q_k

$$q_0[D_0 D_0] + q_1[D_0 D_1] + \ldots + q_n[D_0 D_n] = [y D_0]\,,$$

$$q_0[D_0 D_1] + q_1[D_1 D_1] + \ldots + q_n[D_1 D_n] = [y D_1]\,,$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (12)$$

$$q_0[D_0 D_n] + q_1[D_1 D_n] + \ldots + q_n[D_n D_n] = [y D_n]\,.$$

Now we require that the polynomials D_k, $k = 0, 1, \ldots n$, be orthogonal on the set of points x_i, $i = 0, 1, \ldots R - 1$, *i.e.* that

$$\sum_{i=0}^{R-1} D_r(x_i)\, D_s(x_i) \begin{cases} = 0 & \text{for} \quad r \neq s\,, \\ \neq 0 & \text{for} \quad r = s\,, \end{cases} \qquad (13)$$

$r, s = 0, 1, \ldots n$.

If it is so the set of normal equations (*11*) simplifies to

$$q_k[D_k D_k] = [y D_k] \qquad (14)$$

$k = 0, 1, \ldots n$, from which q_n can be easily computed.

The requirement of orthogonality can be met *e.g.* by taking

$$D_0(x_i) = 0\,, \quad D_1(x_i) = \exp(\omega x_i) \qquad (15)$$

and all other D_k being defined by the recurrence formula

$$D_{k+1}(x) = (x - A_k)\, D_k(x) - B_k D_{k-1}(x)\,, \qquad (16)$$

$k = 0, 1 \dots n$, where

$$A_k = \frac{\sum_{i=0}^{R-1} x_i D_k^2(x_i)}{\sum_{i=0}^{R-1} D_k^2(x_i)}\,, \quad k = 1, 2, \dots n\,, \tag{17}$$

$$B_k = \frac{\sum_{i=0}^{R-1} x_i D_k(x_i)\, D_{k-1}(x_i)}{\sum_{i=0}^{R-1} D_{k-1}^2(x_i)} = \frac{\sum_{i=0}^{R-1} D_k^2(x_i)}{\sum_{i=0}^{R-1} D_{k-1}^2(x_i)}\,, \quad k = 2, 3, \dots n,\ B_1 = 0\,. \tag{18}$$

We shall give a proof of this statement computing simultaneously the coefficients A_k, B_k. Let us suppose that Eq. (*16*) is valid for $k = 1, 2, \dots, k$ and thus the functions $D_0, D_1, \dots D_k$ are orthogonal in the sense of Eq. (*13*). Multiplying the recurrence formula (*16*) by polynomial $D_j(x_i)$ and summing over all i we get

$$[D_{k+1} D_j] = [x D_k D_j] - A_k[D_k D_j] - B_k[D_{k-1} D_j] \tag{19}$$

(the brackets again indicate summing over i from 0 to $R - 1$).

The following cases are distinguished:

$j < k - 1$: All sums on the right hand side vanish and, accordingly, the left hand side equals zero.

$j = k - 1$: In accord with the assumption we have on the right hand side $[D_k D_{k-1}] = 0$. Taking B_k such that

$$[x D_k D_{k-1}] - B_k[D_{k-1}^2] = 0\,,$$

(compare Eq. (*18*)), then also the left-hand side of Eq. (*19*) vanishes.

$j = k$: On the right hand side we have in accord with the assumption $[D_{k-1} D_k] = 0$. Taking A_k such that

$$[x D_k^2] - A_k[D_k^2] = 0\,,$$

compare Eq. (*17*)) the left hand side vanishes.

Thus it has been proven that the polynomial $D_{k+1}(x)$, formulated as shown, is orthogonal to all preceding polynomials. Since, however, D_0, D_1, D_2 are orthogonal, hence all $D_k(x)$ are orthogonal on the given set of points.

The polynomial $D_0(x_i)$ was put equal zero for all i. It is therefore meaningless to take q_0 into consideration in the normal equations (*14*) as well as in the polynomial (7). The polynomial $D_k(x)$ against the original assumption, is of the order $k - 1$ only. Eq. (7) is therefore written anew

$$u = q_1D_1(x) + q_2D_2(x) + \ldots + q_{n+1}D_{n+1}(x) \tag{20}$$

or

$$u = q_1P_1(x) + q_2P_2(x) + \ldots + q_{n+1}P_{n+1}(x)] \exp(\omega x) .$$

The polynomial in the brackets is put in the form of Eq. (*1*). For this purpose we write

$$D_k(x) = D_{k,0} + D_{k,1}x + \ldots + D_{k,k-1} \cdot x^{k-1} . \tag{21}$$

From the definition Eqs (*15*) and (*16*) it follows

$$D_{1,0} = D_{2,1} = \ldots = D_{n+1,n} = 1 , \tag{22}$$

$$D_{k+1,0} = -A_kD_{k,0} - B_kD_{k-1,0} \tag{23}$$

$k = 1, 2, \ldots n$. Finally

$$D_{k+1,k-1} = -A_kD_{k,k-1} + D_{k,k-2} \tag{24}$$

$k = 2, 3, \ldots n$,

$$D_{k+1,i} = -A_kD_{k,i} + D_{k,i-1} - B_kD_{k-1,i} \tag{25}$$

$k = 3, 4, \ldots n;\ i = 1, 2, \ldots n - 2$.

Summing the coefficients of equal powers of x multiplied by the coefficients q_k, one obtains for the sought coefficients p_k of Eq. (*1*)

$$p_i = \sum_{k=1}^{n+1} q_kD_{k,1} \tag{26}$$

$i = 0, 1, \ldots n - 1$. In the sums one has to note that for $i \geqq k$ all $D_{k,i} = 0$.

Choice of the Iteration Method

Thus far we have assumed that the coefficient ω in the exponentials $\exp(\omega x_i)$ is known and obtained thus the coefficients D_k, p_k which have been similarly as SSD a function of ω.

The minimum of this function was searched by successive halving the interval $\langle\omega_1, \omega_2\rangle$ in which it was encompassed. In practice we put $m = \exp \omega$, took a small but otherwise arbitrary m_0 and introduced $m_i = m_0 + ih$, $i = 0, 1, \ldots$; where h

denotes a preselected increment. Gradualy we computed the sums of squared deviations SSD(0), SSD(1), SSD(2) ... For a sufficiently small m_0 SSD at first decreases but ultimately we reach such i when

$$\mathrm{SSD}(i) > \mathrm{SSD}(i-1).$$

This situation is illustrated in Fig. 1*a*. The values SSD(i − 2), SSD(i − 1) and SSD(i) plotted in the figure are there renumbered by indices 0, 2, 4 (see the bottom axis of Fig. 1*a*) and a new SSD(1) is computed with the increment halved. Two cases may occur:

a) SSD(1) ≦ SSD(2). The indices are again changed replacing 1 and 2 by 2 and 4 (Fig. 1*b*).

b) SSD(1) > SSD(2). In this case we have to compute SSD(3) (see Fig. 1*c*) and change the indices by replacing 2 and 0 by 3 and 2. In both cases we return to the original configuration from Fig. 1*a*. with the increment halved. The described halving is repeated until SSD(i − 2), SSD(i − 1) and SSD(i) differ by less than a prescribed accuracy.

Fitting Equation Subject to Constraints

If the fitted equation is required to satisfy additional constraints, *e.g.* passing through given points, the derivation procedure is somewhat modified. This will be shown on a particular case when the fitted equation is required to pass through $x = 0$, $y = y_0$.

In the calculation of the coefficients we start from

$$u = q_1 D_1(x) + q_2 D_2(x) + \ldots + q_{n+1} D_{n+1}(x), \tag{27}$$

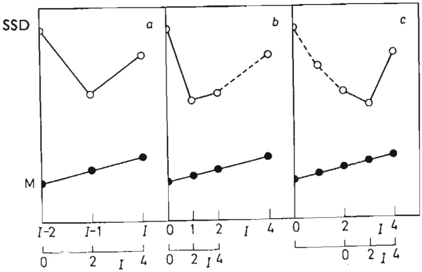

FIG. 1
The Iteration Method

TABLE I

A Comparison of the Fitted (u) and Observed (y) Values

x	y	u for $n = 3$	u for $n = 4$	u for $n = 5$
0	1·00	1·000	1·0000	1·0000
1	1·40	1·364	1·4003	1·4002
2	1·50	1·556	1·4977	1·4979
3	1·46	1·468	1·4674	1·4673
4	1·27	1·224	1·2631	1·2629
5	0·98	0·939	1·9687	1·9687
6	0·66	0·680	1·6789	1·6789
7	0·43	0·471	0·4436	0·4438
8	0·30	0·316	0·2746	0·2748

TABLE II

Results of p_k, ω and SSD

SSD	$n = 3$ $1{\cdot}060 \,.\, 10^{-2}$	$n = 4$ $1{\cdot}418 \,.\, 10^{-3}$	$n = 5$ $1{\cdot}417 \,.\, 10^{-3}$
p_0	1·000 00	1·000 00	1·000 00
p_1	0·874 19	2·039 97	2·286 58
p_2	0·720 31	−0·259 91	−0·700 87
p_3	−0·074 37	0·560 31	0·809 48
p_4	—	0·022 24	−0·052 84
p_5	—	—	−0·004 71
ω	−0·642 872	−0·869 550	−0·870 481

containing orthogonal polynomials. The coefficients $q_1, q_2, \ldots q_{n+1}$ are not independent now: Stipulating $y = y_0$ for $x = 0$ we have necessarily

$$y_0 = q_1 D_1(0) + q_2 D_2(0) + \ldots + q_{n+1} D_{n+1}(0)\,, \tag{28}$$

q_1 for instance may be regarded to be a function of the remaining n coefficients $q_2, \ldots q_{n+1}$.

The sum of square deviations

$$\mathrm{SSD} = \sum_{i=0}^{R-1} [q_1 D_1(x_i) + \ldots + q_{n+1} D_{n+1}(x_i) - y_i]^2$$

is now a function of n coefficients $q_2, q_3, \ldots q_{n+1}$ and ω. Let us assume again ω to be known. Then

$$\frac{\partial \mathrm{SSD}}{\partial q_k} = 2 \sum_{i=0}^{R-1} (q_1 D_1 + q_2 D_2 + \ldots + q_{n+1} D_{n1}) . [D_k - D_1 D_k(0)]$$

(the argument x_i of the polynomials D_k is omitted) $k = 2, 3, \ldots n + 1$. Putting the right-hand side equal zero one obtains after some arrangements

$$\begin{aligned}
-q_1[D_1D_1]\, D_2(0) \quad &+ q_2[D_2D_2] &&= [yD_2] - [yD_1]\, D_2(0) \\
-q_1[D_1D_1]\, D_3(0) \quad &+ q_3[D_3D_3] &&= [yD_3] - [yD_1]\, D_3(0) \\
&\ldots\ldots\ldots\ldots\ldots\ldots \\
-q_1[D_1D_1]\, D_{n+1}(0) &+ q_{n+1}[D_{n+1}D_{n+1}] &&= [yD_{n+1}] - [yD_1]\, D_{n+1}(0) \,.
\end{aligned} \qquad (29)$$

TABLE III

Functional and Fitted Values of the Maxwell Distribution

i	x	y	u for $n = 3$	u for $n = 4$	u for $n = 5$
0	0	0	0	0	0
0	0·2	0·240 188	0·213	0·2410	0·240 180
2	0·4	0·670 293	0·750	0·6645	0·670 405
3	0·6	0·827 696	0·770	0·8474	0·826 829
4	0·8	0·635 244	0·568	0·6089	0·638 898
5	1·0	0·337 072	0·358	0·3307	0·329 689
6	1·2	0·129 663	0·202	0·1524	0·132 496
7	1·4	0·037 086	0·108	0·0631	0·045 230

TABLE IV

Sums of Squared Deviations and Parameters of $u = (p_0 + p_1 i + \ldots + p_n i^n) \exp(\omega i)$

n	SSD	ω	p_0	p_1	p_2	p_3	p_4	p_5
3	$2{\cdot}562 . 10^{-2}$	−0·956150	0	− 1·44353	1·99900	− 0·10690	—	—
4	$2{\cdot}353 . 10^{-3}$	−1·397274	0	5·32564	−8·76149	4·41307	0·03285	—
5	$1{\cdot}430 . 10^{-4}$	−1·811065	0	−40·6270	81·0937	−50·7369	11·7375	−0·0074

(as before brackets indicate summation from $i = 0$ to $R - 1$). From these equations $q_2, q_3, \dots q_{n+1}$ can be simply calculated as functions of q_1 and substituted in Eq. (*28*) with the result

$$q_k = a_k + b_k q_1 . \tag{30}$$

where

$$\begin{aligned} a_k &= ([yD_k] - [yD_1]\, D_k(0))/[D_k D_k] , \\ b_k &= [D_1 D_1]\, D_k(0)/[D_k D_k] , \\ k &= 2, 3, \dots n + 1 . \end{aligned} \tag{31}$$

Substituting in Eq. (*28*) there results for q_1

$$y_0 = q_1 + q_1 \sum_{k=2}^{n+1} b_k D_k(0) + \sum_{k=2}^{n+1} a_k D_k(0) . \tag{32}$$

Substituting in Eqs (*30*) we find successively coefficients q_k, $k = 2, 3, \dots n + 1$.

Note that in the original fitting equation

$$u = (p_0 + p_1 x + \dots + p_n x^n) \exp(\omega x)$$

the constraint $u = y_0$ for $x = 0$ necessitates simply $p_0 = y_0$ so that

$$u = (y_0 + p_1 x + p_2 x^2 + \dots + p_n x^n) \exp(\omega x) . \tag{33}$$

Examples

1) A curve given by points carrying "experimental" error, obtained from an arbitrarily drawn curve on a graph paper by rounding off the ordinate to two most significant digits, was approximated by

$$u = P_n(x) \exp(\omega x) ,$$

for $n = 3, 4, 5$. The curve $u = u(x)$ was required to pass through the point (0,1).

Table I summarizes the observed values of y_i for equidistant argument $x = 0, 1, \dots 8$ and further the values of u_i for $n = 3, 4, 5$. Table II gives the coefficients p_k of the polynomial, ω, and SSD. It is noted that due to considerable "experimental" error SSD is not diminished any more on changing from $n = 4$ to $n = 5$.

2) The same equation was fitted to the Maxwell velocity distribution in an ideal gas given by

$$y = (4A/\sqrt{\pi})\, x^2 \exp(-Ax^2) , \tag{34}$$

where x is molecular velocity, A parameter (taken $A = 3$).

In this case the function in Eq. (*34*) was computed precisely to 6 digits for $x = 0$ through 1·4 and the increment equal 0·2. The "experimental" error is thus negligible. Now we require $u = 0$ for $x = 0$.

Table III indicates the functional values of the Maxwell distribution tabulated as a function of x. In addition we have introduced a running index i. The fitted values for $n = 3, 4, 5$ are in the following columns of the table. Finally, Table IV shows SSD, the coefficients of the polynomials and ω. In case of the precise data SSD decreases with increasing n uniformly by an order of magnitude or more.

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