APPROXIMATION BY EXPONENTIALS. II.*

EXAMINATION OF THE LIMITING CASES OF THE FUNCTION $u = A_1 \exp(\omega_1 x) + A_2 \exp(\omega_2 x)$

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The limiting cases of the function $u = A_1 \exp(\omega_1 x) + A_2 \exp(\omega_2 x)$, or $u = P_1 p_1^x + P_2 p_2^x$, lead for $\omega_2 \to \omega_1$, or $p_2 \to 0$, to relations of the type $u = (A + B_x) p_1^x$, or $u = A p_1^x + B$. The method of approximation by this empirical function is extended to the case of the data with unevenly spaced values of the argument.

The formulas for the sum of squares of deviations based on a sum of two exponentials may be divided into three groups:

Case I. Approximation formula of the general type

$$u_i = M_1 m_1^i + M_2 m_2^i\,, \tag{1}$$

obtained from a more general formula

$$u = P_1 p_1^x + P_2 p_2^x \tag{1a}$$

assuming the uniform spacing of the experimental data. If $x = x_0 + ih$, where h is the increment of the argument, then

$$P_j p_j^x = P_j p_j^{(x_0 + ih)} = P_j p_j^{x_0} (p_j^h)^i = M_j m_j^i$$

for $j = 1, 2$; $i = 0, 1, \ldots R - 1$. R is the number of measured pairs of data. Corresponding formula for the sum of squares, S, is

$$S = [y_i y_i] - M_1 [y_i m_1^i] - M_2 [y_i m^i]\,. \tag{2}$$

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The values of M_1, M_2 are found from equations

$$M_1[m_1^i m_1^i] + M_2[m_1^i m_2^i] = [y_i m_1^i]\,, \qquad (3)$$
$$M_1[m_1^i m_2^i] + M_2[m_2^i m_2^i] = [y_i m_2^i]\,.$$

Case II. Approximation formula

$$u_i = M_1(m_1^i - m_2^i)\,, \qquad (4)$$

which provides that the curve passes through the point $x_0 = 0$, $y_0 = 0$. The value of M_1 is found from equation

$$M_1 = \frac{[y_i m_1^i] - [y_i m_2^i]}{[m_1^i m_1^i] - 2[m_1^i m_2^i] + [m_2^i m_2^i]}, \qquad (5)$$

The sum of squares is

$$S = [y_i y_i] - M_1[(m_1^i - m_2^i)\, y_i]\,. \qquad (6)$$

Case III. Approximation formula

$$u_i = M_1 m_1^i + (1 - M_1)\, m_2^i\,, \qquad (7)$$

which provides that the curve passes through the point $x_0 = 0$, $y_0 = 1$. The value of M_1 is found from equation

$$M_1 = \frac{[(m_1^i - m_2^i)\, y_i] - [(m_1^i - m_2^i)\, m_2^i]}{[m_1^i m_1^i] - 2[m_1^i m_2^i] + [m_2^i m_2^i]}, \qquad (8)$$

the sum of squares

$$S = [y_i y_i] - 2[m_2^i y_i] + [m_2^i m_2^i] - M_1[(m_1^i - m_2^i)(y_i - m_2^i)]\,. \qquad (9)$$

Clearly, for $m_2 = m_1$ Eqs (*3*) are identical and not suitable for evaluation of M_1 and M_2. Eqs (*5*) and (*8*) as well give indefinite expressions for $m_2 = m_1$. It is therefore necessary to examine more closely the case $m_2 \rightarrow m_1$. One possible way is to substitute the relation $m_2 = m_1(1 + x)$, express M_1 and S as functions of m_1 and x and to examine the limits for $x \rightarrow 0$. In case *I*, Eq. (*3*) has the solutions

$$M_1 = \Delta_1/\Delta\,, \quad M_2 = \Delta_2/\Delta\,, \qquad (10)$$

where

$$\Delta = [m_1^i m_1^i][m_2^i m_2^i] - [m_1^i m_2^i]^2\,, \qquad (11)$$

$$\Delta_1 = [y_i m_1^i][m_2^i m_2^i] - [y_i m_2^i][m_1^i m_2^i]\,, \qquad (12)$$

$$\Delta_2 = [y_i m_2^i][m_1^i m_1^i] - [y_i m_1^i][m_1^i m_2^i]\,. \qquad (13)$$

By arrangement of these expressions we get $\Delta = x^2 A_1 + x^3 A_{2+} \ldots$, $\Delta_1 = xB_1 + x^2 B_{2+} \ldots$, $\Delta_2 = xC_1 + x^2 C_{2+} \ldots$, where A_j, B_j, C_j, $j = 1,2$ are independent of x, and $C_1 = -B_1$. As a consequence, for $x \to 0$ both coefficients M_1, M_2 approach infinity with opposite signs. In contrast, the limit for the sum of squares is finite.

Cases II *and* III give both the same results: The value of M_1 goes to infinity for vanishing x. However, the formulas for S give a finite value. From the above results it further follows that in the neighbourhood of $m_2 \to m_1$ the approximation formulas (*1*), (*4*) and (*7*) in the given form lose their significance. Also the numerical computations for m_2 close to m_1 carry great errors since the expression $M_1 m_1^i + M_2 m_2^i$ represents the difference of two almost same quantities because $M_1 \approx -M_2$. Thus in the computation as many as 4, 5 or even more orders of accuracy are lost. A substitute for these formulas, which does not lose its meaning for $m_2 \to m_1$ and gives accurate results, is found similarly: Substituting $m_2 = m_1(1 + x) = m(1 + x)$ and in all expansions retaining only the terms with x. For the general Case *I* the substitutive formula is

$$u_i = (N_1 + iN_2)\, m^i \,, \qquad (14)$$

or generally for $x = x_0 + ih$

$$u = (R_1 + xR_2)\, p^x \,. \qquad (15)$$

In special cases $y_0 = 0$ and $y_0 = 1$ we get for $i = 0$

$$u_i = iN_2 m^i \quad \text{and} \quad u_i = (1 + iN_2)\, m^i \,. \qquad (16, 17)$$

The other extreme, when m_2 vanishes poses no numerical difficulties in contrast to the previous one. It should be noted that the approximation formulas (*1*), (*4*) and (*7*) do not transform into a single exponential, since $\lim m_2^i = 0$, for $m_2 = 0$ and $i > 0$, but $\lim m_2^i = 1$, for $i = 0$. Thus in the limit $m_2 = 0$ the formulas (*1*), (*4*) and (*7*) take the following form

$$u_0 = M_1 + M_2 \,, \quad u_i = M_1 m_1^i \quad \text{for} \quad i > 0 \,, \qquad (1a)$$

$$u_0 = 0 \,, \quad u_i = M_1 m_1^i \quad \text{for} \quad i > 0 \,, \qquad (4a)$$

$$u_0 = 1 \,, \quad u_i = M_1 m_1^i \quad \text{for} \quad i > 0 \,. \qquad (7a)$$

One of the supposition here and in the earlier paper[1] was the assumption of an equal spacing of R pairs of experimental data (y_i, x_i), $i = 0, 1 \ldots R - 1$, *i.e.* $x_i = x_0 + ih$, where h is the increment of the argument. Let us assume now that the distribution of the values of x_i along the x axis is arbitrary. We shall perform the calculation under these more general conditions for one special case of the approximation formula of the following type

$$u = P_1 \exp(\omega_1 x) + P_2 \exp(\omega_2 x), \tag{18}$$

which can be modified by introducing $m_j = \exp(\omega_j)$, $j = 1, 2$, to give

$$u = P_1 m_1^x + P_2 m_2^x . \tag{19}$$

Let m_1 and m_2 be known (*e.g.* by an arbitrary estimate). The coefficients P_1 and P_2 are calculated from the equations

$$P_1[11] + P_2[12] = [y1], \quad P_1[12] + P_2[22] = [y2] \tag{20}$$

following from the conditions

$$\partial S/\partial \omega_1 = \partial S/\partial \omega_2 = 0 \tag{21}$$

of the minimum sum of square deviations

$$S = \sum_{i=0}^{R-1} (u_i - y_i)^2 . \tag{22}$$

For brevity we introduced in Eqs (*20*) the following notation

$$[jk] = \sum_{i=0}^{R-1} m_j^{x_i} m_k^{x_i}, \quad [yj] = \sum_{i=0}^{R-1} y_i m_j^{x_i}, \tag{23}$$

where $j, k = 1, 2$. Substituting now m_1 and m_2 by $m_1(1 + r_1)$ and $m_2(1 + r_2)$, and taking m_j as constants and r_j as variables, we can express both coefficients P_j, $j = 1, 2$, and the sum of square deviations (Eq. (*22*)) as functions of r_1 and r_2. Providing that r_1 and r_2 are sufficiently small we can neglect higher powers of r_j in the expansion of $(1 + r_j)$ and write

$$(1 + r_j)^{x_i} = 1 + \binom{x_i}{1} r_j + \binom{x_i}{2} r_j^2 + \binom{x_i}{3} r_j^3 , \tag{24}$$

for $j = 1, 2$; $i = 0, 1, \ldots R - 1$.

Introducing the polynomials

$$L_0 = Q^{x_0} + Q^{x_1} + \ldots + Q^{x_N} ,$$

$$L_1 = \binom{x_0}{1} Q^{x_0} + \binom{x_1}{1} Q^{x_1} + \ldots + \binom{x_N}{1} Q^{x_N} ,$$

$$L_2 = \binom{x_0}{1}^2 Q^{x_0} + \binom{x_1}{1}^2 Q^{x_1} + \ldots + \binom{x_N}{1}^2 Q^{x_N},$$

$$L_3 = \binom{x_0}{2} Q^{x_0} + \binom{x_1}{2} Q^{x_1} + \ldots + \binom{x_N}{2} Q^{x_N}, \tag{25}$$

$$L_4 = \binom{x_0}{1}\binom{x_0}{2} Q^{x_0} + \binom{x_1}{1}\binom{x_1}{2} Q^{x_1} + \ldots + \binom{x_N}{1}\binom{x_N}{2} Q^{x_N},$$

$$L_5 = \binom{x_0}{3} Q^{x_0} + \binom{x_1}{3} Q^{x_1} + \ldots + \binom{x_N}{3} Q^{x_N}, \quad N = R - 1,$$

in which $Q = m_j m_k$, $j, k = 1, 2$, we can easily express $[jk]$ as a polynomial of the 3rd degree in r_1 and r_3. Thus approximately

$$[jk] = L_0 + L_1(r_j + r_k) + L_2 r_j r_k + L_3(r_j^2 + r_k^2) + + L_4(r_j^2 r_k + r_j r_k^2) + L_5(r_j^3 + r_k^3). \tag{26}$$

Similarly for $j = 1, 2$

$$[yj] = \sum_{i=0}^{N} y_i m_j^{x_i}(1 + r_j)_j^{x_i} = y_0 m_j^{x_0} + y_1 m_j^{x_1} + \ldots + y_n m_j^{x_N} + \tag{27}$$

$$+ r_j \left[\binom{x_0}{1} y_0 m_j^{x_0} + \binom{x_1}{1} y_1 m_j^{x_1} + \ldots + \binom{x_N}{1} y_N m_j^{x_N}\right] +$$

$$+ r_j^2 \left[\binom{x_0}{2} y_0 m_j^{x_0} + \ldots + \binom{x_N}{2} y_N m_j^{x_N}\right] +$$

$$+ r_j^3 \left[\binom{x_0}{3} y_0 m_j^{x_0} + \ldots + \binom{x_N}{3} y_N m_j^{x_N}\right].$$

Thus the problem formally becomes that treated earlier since all sums $[jk]$ and $[yj]$ were expressed as polynomials in r_1 and r_2. The sum of square deviations can also be found by the earlier described method as a polynomial having for instance the following form

$$S = S_0 + S_1 r_1 + S_2 r_2 + \ldots + S_8 r_1^3 + S_9 r_2^3. \tag{28}$$

To this polynomial we then apply the iteration procedure described earlier[1] for finding the corrections r_1 and r_2.

REFERENCES

1. Slavíček E.: This Journal *35*, 2885 (1970).

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