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LETTERS TO THE EDITORS

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IMPROVED EVALUATION OF THE PARAMETERS OF LINEARIZABLE RELATIONSHIPS*

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An iterative process is proposed for finding the parameters k_0, k_1 of non-linear regression $y = y(k_0, k_1, x)$, reducible to the form $\tilde{y} = b_0 + b_1 x$ through the transformations $\tilde{y} = \tilde{y}(x, y)$, $\tilde{x} = \tilde{x}(x, y)$, $b_0 = b_0(k_0, k_1)$, $b_1 = b_1(k_0, k_1)$. In each iteration a system of two linear equations $\sum_i c_{i0}[\tilde{y}_i - (b_0 + b_1\tilde{x}_i)] = 0$, $\sum_i c_{i1}[\tilde{y}_i - (b_0 + b_1\tilde{x}_i)] = 0$ is solved, in which the coefficients c_{i0}, c_{i1} figure, determined from the values of k_0, k_1, b_0, b_1 obtained from the preceding iteration: $c_{i0} = \frac{y_i - y(k_0, k_1, x_i)}{\tilde{y}_1 - (b_0 + b_1\tilde{x}_i)} \cdot \frac{\partial y(k_0, k_1, x_i)}{\partial k_0}$, $c_{i1} = \frac{y_i - y(k_0, k_1, x_i)}{\tilde{y}_1 - (b_0 + b_1\tilde{x}_i)} \cdot \frac{\partial y(k_0, k_1, x_i)}{\partial k_1}$. In the first iteration one puts $c_{i0} = 1$, $c_{i1} = \tilde{x}_i$.

The problem of determining the parameters of a bi-parametric empirical curve $y = y(k_0, k_1, x)$, describing the mass of pairs of the experimental data x_i, y_i, $i = 1, \ldots, N$, has been repeatedly discussed in the literature [1–4]. In [1] the author gives in relation to an exponential function a quite fast algorithm for determining the parameters of linearizable functions. However, the proposed algorithm gives a biased evaluation. This paper proposes modification of the algorithm [1], devoid of this shortcoming; to obtain the quickest convergence, sequential use of the methods in [2] and [3] is recommended.

To find the regression parameters k_0 and k_1, one often uses the method of least squares (m.l.s.), i.e. as a criterion of the closeness of the empirical curve to the exponential data one uses the sum $Q = \sum_i [y_i - y(k_0, k_1, x_i)]^2$ [1–4]. Where the random component in the magnitudes y_i has a normal distribution, minimization of Q gives unbiased evaluations for k_0 and k_1. When the regression function y has the form $y = k_0 + k_1 x$, the problem of finding min Q reduces to the solution of a set of two linear equations $\partial Q/\partial k_0 = 0$, $\partial Q/\partial k_1 = 0$ [1]. In the more complex case when the parameters k_0, k_1 enter y in non-linear fashion, for example, $y = k_0 \exp(k_1 x)$, the problem is solved

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either by some method of finding the extreme of the function of many variables [4] or one solves the set of non-linear equations $\partial Q/\partial k_0 = 0$, $\partial Q/\partial k_1 = 0$ by a certain iteration method [3] or (if possible) the initial regression function is converted to linear form $\tilde{y} = b_0 + b_1\tilde{x}$, where $\tilde{y} = \tilde{y}(x, y)$, $\tilde{x} = \tilde{x}(x, y)$, $b_0 = b_0(k_0, k_1)$, $b_1 = b_1(k_0, k_1)$ (in the case of the exponent $\tilde{y} = \ln y$, $\tilde{x} = x$, $b_0 = \ln k_0$, $b_1 = k_1$) and already then one finds the minimum of the expression $Q = \sum_i [y_i - (b_0 - b_i\tilde{x})]^2$ by solving the linear (relative to the unknowns b_0, b_1) set of equations $\partial\tilde{Q}/\partial b_0 = 0$, $\partial\tilde{Q}/\partial b_1 = 0$. However, in the last case the evaluations prove distorted since, instead of the minimum of the function Q, we have the minimum of the function $\tilde{Q}$ [1]. To lessen this distortion it is proposed that the terms in the sum $\tilde{Q}$ be taken with the "weight coefficients" $\sum_i c_i[\tilde{y}_i - (b_0 + b_1\tilde{x})]^2 = 0$, $c_i = \left[1/\left(\frac{\partial\tilde{y}(x, y)}{\partial y}\right)\Big|_{(x_i, y_i)}\right]^2$ (for the exponent $c_i = y_i^2$) [2]. It has also been proposed for a function of the type $y = k_0 \exp(k_1 x)$ that these "weight coefficients" be more clearly defined in several iterations [1]. In particular, "weight coefficients" of the type $c_i = \left(\frac{y_i - y(k_0, k_1, x)}{\tilde{y}_i - (b_0 + b_1\tilde{x})}\right)^2$ have been proposed, in which the parameters k_0, k_1, b_0, b_1 figure, determined from the preceding iteration [1]. In the first iteration all the c_i values were taken as equal to unity [1].

Let us show by an example that the iteration procedure proposed in [1] does not converge to the values k_0, k_1, ensuring min Q (it converges to similar but different values).

As an example let us take the function $y = 100\exp(-x)$ with the values $x_i = 1, 2, \ldots, 10$, and with the following set of random additions $\varepsilon_i = 0.2010$; 2.3218; 1.1728; 0.2850; 1.9032: −1.1726; 2.3144; −0.8856; −0.7848; 1.6638; put out by the generator of normally distributed random magnitudes with a dispersion equal to four. The results of the count are reflected in Table 1. The first column of the table indicates the sources of the techniques used to calculate a pair of the corresponding columns of values.

The proposed modification of the method [1] is that the "weight coefficients" are determined as follows. Let us write the equations $\partial Q/\partial k_0 = 0$, $\partial Q/\partial k_1 = 0$ in explicit form:

$$\sum_i (y_i - y(k_0, k_1, x_i))\frac{\partial y(k_0, k_1, x_i)}{\partial k_0} = 0, \quad \sum_i (y_i - y(k_0, k_1, x_i))\frac{\partial y(k_0, k_1, x_i)}{\partial k_1} = 0.$$

Table 1

Iteration No.	[1]		[3]		Modified [1]	
	k_0	k_1	k_0	k_1	k_0	k_1
1	21,58	−0,3198	21,58	−0,3198	21,58	−0,3198
2	66,01	−0,6267	55,41	−0,7368	64,15	−0,6301
3	79,68	−0,7604	86,62	−0,8700	83,68	−0,8024
4	83,31	−0,7942	90,15	−0,8598	88,87	−0,8486
5	84,05	−0,8011	90,02	−0,8591	89,82	−0,8572
6	84,19	−0,8024	90,01	−0,8590	89,98	−0,8587
7	84,21	−0,8027	90,01	−0,8590	90,01	−0,8590
8	84,22	−0,8027	90,01	−0,8590	90,01	−0,8590

Let us premultiply each equation by the magnitude $(\tilde{y}_i-(b_0+b_1\tilde{x}_i))/(\tilde{y}_i(b_0+b_1\tilde{x}_i))$, identically equal to unity (it is assumed that the probability $\tilde{y}_i - b_0 + b_1\tilde{x}_i$ is equal to zero):

$$\sum_i \left[\frac{y_i - y(k_0,k_1,x_i)}{\tilde{y}_i - (b_0 + b_1\tilde{x}_i)} \cdot \frac{\partial y(k_0,k_1,x_i)}{\partial k_0}\right](\tilde{y}_i - (b_0 + b_1\tilde{x}_i)) = 0,$$

$$\sum_i \left[\frac{y_i - y(k_0,k_1,x_i)}{\tilde{y}_i - (b_0 + b_1\tilde{x}_i)} \cdot \frac{\partial y(k_0,k_1,x_i)}{\partial k_1}\right](\tilde{y}_i - (b_0 + b_1\tilde{x}_i)) = 0.$$

The values in square brackets will be considered as "weight coefficients". They depend on k_0, k_1, b_0 and b_1, determined in the preceding iteration. In the first iteration, the "weight coefficients" in the first equation are taken as equal to unity and in the second to $\tilde{x}_i$.

From the method of constructing the iteration procedure, it will be seen that if the iterations converge to certain values of k_0^*, k_1^*, then these values are stationary, (i.e. $\left(\frac{\partial Q(k_0, k_1)}{\partial k_0}\right)\Big|_{(k_0^*, k_1^*)} = 0$, $\left(\frac{\partial Q(k_0, k_1)}{\partial k_1}\right)\Big|_{(k_0^*, k_1^*)} = 0$) for the function Q. The fact that in the above example the method of [3] and the modified [1] converge to the same values also confirms this fact.

From the above example, one may suggest the following recommendation. To obtain the quickest convergence, it is best to determine the initial k_0 and k_1 values by the method of [2], since it gives the best results in one iteration (in the example: 66.79 and -0.6038). Further refinement (if such is required) is achieved by the method of [3], since it has the highest rate of convergence in the vicinity of the extreme.

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