
Approximation of Experimental Physical Values with Non-typical Conditions of Error

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1 Introduction

2 Mathematical Background

3 Formulation of the Problem

A function is one of the most known mathematical objects. An important task which has practical applications, is the approximation of a function or relationship based on some information known about the function or relationship in question. This information may either be determinate or statistical. An example of a determinate piece of information about function $f(x)$ is its range (or the possible values this function may have) on a given interval $[\alpha, \beta]$. Example of a statistical information may be the law of distribution of random errors ξ_i in approximate values $\tilde{y}_i = f(x_i) + \xi_i$ of the function, which in turn can describe a certain physical process (change of temperature over time, for example). In practice, a number n of points x_i can be obtained as results of some kind of physical experiment. Where in this case, the approximation of function $f(x)$ only makes sense if the this function is described by a finite number $m < n$ of parameters (coefficients) c_j , where the true values of said parameters will be denoted as \dot{c}_j , $j = 1, 2, \dots, m$.

This Internal Assessment will focus on the estimation of parameters of the function

$$y = f(\dot{c}, x_i), \quad \dot{c} \in \mathbf{R}^m, \quad x \in [\alpha, \beta], \quad \dot{c} = (\dot{c}_1, \dot{c}_2, \dots, \dot{c}_m) \quad (3.0.1)$$

based on its approximate values

$$\tilde{y}_i = f(x_i) + \xi_i, \quad i = 1, 2, \dots, n, \quad (3.0.2)$$

when additionally it is also known, that: 1. vector $\dot{c} = (\dot{c}_1, \dot{c}_2, \dots, \dot{c}_m)$ belongs to a given limited set D , like for example a parallelepiped in \mathbf{R}^m dimensions; 2. ξ is a limited continuous random value; the median of which $Med(\xi)$ is equal to zero.

Judging by references in scientific works that I read while researching for this IA [*], the most popular linear model of a studied relationship is

$$f(\dot{c}, x) = \sum_{j=1}^m \dot{c}_j \phi_j(x), \quad (3.0.3)$$

specifically in polynomial form, when

$$\phi_1(x) \equiv 1; \quad \phi_j(x) = x^{j-1}, \quad j = 1, 2, \dots, m. \quad (3.0.4)$$

In practice, it is often the case when it is not only necessary to estimate the parameters of a function, but identifying the type (structure) of this function is needed as well. In other words, a finite number L of alternative structures is given

$$f_l(c; x), c \in \mathbf{R}^{m(l)}, \quad l = 1, 2, \dots, L, \quad (3.0.5)$$

and it is necessary to identify to which of L structures of function $f_l(c; x)$ belongs the function $f(\dot{c}, x)$, and after that estimate the vector \dot{c} of its parameters. In our school program, the class has encountered one such task, when it was said to find out if we were dealing with a linear or exponential relationship, be it in either physics or math. However, then, this problem was solved using the exact (or near to exact) values of both of the relationships, so it was easy to distinguish them.

There are countless papers dedicated to the approximation of functions based on their approximate values (in practice - experimental data). Usually, in such papers the consensus is to use a certain condition. This condition is to assume that the mathematical expectancy of error is equal to zero [*].

$$E(\xi) = 0 \quad (3.0.6)$$

However, in this IA this condition will not be used. Here instead of the condition of mathematical expectancy of error ξ being equal to zero, I will assume that the median of the same error ξ being equal to zero,

$$Med(\xi) = 0 \quad (3.0.7)$$

specifically when the algorithm of evaluation of the parameters of the function is based on ideas from the *method of least squares*.

I justify my interest to the condition $Med(\xi) = 0$ by the case when the traditional condition $E(\xi) = 0$ is unachievable. This happens when measurements are taken close to one of the natural limits of the physical relationship being measured. An example of such natural limit is the inability of some magnitude, such as weight, to be negative. In this case, the absolute value of the error made, can only be large (with respect to other errors made) in the *same sign*, either positive or negative. Figure 1 shows an example of this graphically.

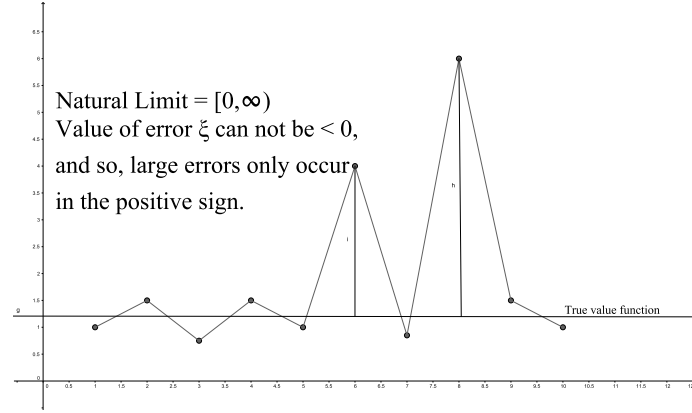


Figure 1: Graphical representation of a case where $E(\xi) = 0$ does not work effectively.

I want to bring attention to the fact, that the argument that this kind of measurement could be withdrawn by human intervention, is invalid for 2 reasons: 1. Any such withdrawal usually leads to loss of information. 2. In cases where the experiment requires high-capacity data collection human intervention may not be possible.

Speaking of the errors, what is meant is not only error that was produced by a faulty measurement, but also any error caused by some factor that was either omitted or unaccounted for in function $f(x)$. Even though both conditions $E(\xi) = 0$ and $Med(\xi) = 0$ are not special cases of each other, it could be argued that from a point of view of solving practical problems, the condition $Med(\xi) = 0$ is the more broad of the two (as in, it is easier to meet). The only requirement for meeting this condition is $P(\xi) > 0$ is 0.5. Hence the condition $Med(\xi) = 0$ allows for some comparatively large random values of error ξ to be on one side of the true function and not on the other, without the approximation to be significantly affected by those large values, unlike the condition $E(\xi) = 0$. With condition $Med(\xi) = 0$ the approximation can account for large peaks in values of ξ .

As mentioned before, I have two aims in this IA. Aim-maximum - to create an algorithm, capable of identifying from a finite number of alternative function structures, to which of those does the relationship in question belong; estimate the parameters of this function accurately; quite securely give an estimate to the accuracy of the calculated approximate values of the function, which belong to the relationship in question. Aim-minimum - to create an algorithm, capable of estimating the parameters of a functional dependence whose structure is known accurately; again, securely give an estimate to the accuracy of the calculated approximate values of the functional dependence.

Its clear that the quality of the solution of this problem is dependant of an array of factors, which include: 1. the ratio between the number n of measurements \tilde{y}_i and the number m of estimated parameters \hat{c}_j . 2. the intensity of error ξ_i 3. the number of L alternatives, and more importantly, the degree of similarity of functions $f_l(c; x)$. This means that to confirm my theoretical reasoning, quite an ambitions computational experiment is required. I will proceed with the necessary calculations using custom software.

4 Algorithm

Approximation of a functional dependence taking this new condition $Med(\xi) = 0$ in mind, has been looked at in mathematics [*]. It is believed that in this case it is necessary to minimize the sum of absolute values of deviations of the modelled dependence $f(c^*, x)$ from the unknown true function $f(\hat{c}, x)$, where c^* is the found optimal value of vector c . This method is referred to as the Least Absolute Deviations (LAD). However, through my research I have found no methods of estimating LAD's accuracy. What value does an optimization method have if there is no way to determining the error it made? In addition, LAD does not presume the existence of priori limitations on the vector \hat{c} . And i must ask the question: What happens if the vector of parameters c^* , providing the minimum of the sum of modulus of errors, does not belong to the set D ?

It is clear, that in every separately taken case (run of an algorithm), the factual accuracy of the model solution (when the true function is known) cannot serve as either a comparative evaluation of two competing algorithms, nor criteria of effectiveness of any given algorithm. It is also clear, that if all, or close to all errors ξ_i have the same sign (the condition $Med(\xi) = 0$, although, the condition $E(\xi) = 0$ as well, allow this, be it with a small probability), then neither method will give any good solutions. And also, with a certain 'layout' of errors ξ_i , a theoretically more sound method might by change give a worse solution than a less sound one. So, when estimating the effectiveness of a method, it is necessary to rely on average results of some number of random solutions. In conjunction with this, the idea lies in the fact that for the quality of constructed approximation $f(c^*, x)$ to $f(\dot{c}, x)$, I take the mathematical expectation

$$E(\rho(c^*, \dot{c})) = \int_D P(c) \rho(c^*, \dot{c}) dc_1 dc_2 \dots dc_m, \quad c = (c_1, c_2, \dots, c_m) \quad (4.0.1)$$

of proximity (distance) $\rho(c^*, \dot{c})$ of function $f(c^*, x)$ from $f(\dot{c}, x)$ where in the role of distance $\rho(c^*, \dot{c})$, one could take on of the functions

$$\rho_1(c^*, c) = \sum_{j=1}^m |c_j^* - c_j| \quad (4.0.2)$$

$$\rho_2(c^*, c) = \sum_{j=1}^m (c_j^* - c_j)^2 \quad (4.0.3)$$

$$\rho_3(c^*, c) = \sqrt{\frac{1}{n} \sum_{i=1}^m (y_i - f(c^*, x_i))^2} \quad (4.0.4)$$

In solving the problem, that I have above labelled as 'aim-minimum', criteria (4.0.1) was considered in a paper by [blak]. Looking ahead, I say that I will suggest a more constructive algorithm than the one occurring in [balk]. I want to note that the problem that I have above labelled as 'aim-maximum' was not looked at in the mentioned paper.

The probability density function $P(c)$, $c \in D$ where c is a vector that could be the unknown true vector \dot{c} , that (the function) appears in the m -multi integral (4.0.1), can be constructed on the basis of the formula of the binomial distribution of a random value [*]. In fact, let's say: $c \in D$ is one of the vectors which claims that it is the unknown true vector \dot{c} from function (3.0.3); q_i are the elements of the sequence

$$q_1(c) = \tilde{y}_1 - f(c, x_1), \quad q_2(c) = \tilde{y}_2 - f(c, x_2), \dots, \quad q_n(c) = \tilde{y}_n - f(c, x_n); \quad (4.0.5)$$

where q is a discrete random value, that can assume values

$$r = r(c) = \sum_{i=1}^{n-1} \delta_i(c), \quad (4.0.6)$$

where

$$\delta_i = \delta_i(c) = \begin{cases} 1, & \text{if } q_i(c)q_{i+1}(c) < 0 \\ 0, & \text{if } q_i(c)q_{i+1}(c) \geq 0 \end{cases} \quad (4.0.7)$$

In meaningful terms, the value of r is the number of transitions of sign of the elements of (4.0.5). Where $r \in [0, n-1]$. If it truly happens that $c = \dot{c}$, then the values of q_i would be nothing but the errors ξ_i , and by the condition $Med(\xi) = 0$ the probabilities p_r of events $\eta = r$ could be written as

$$p_r = \frac{\binom{n-1}{r}}{2^{n-1}}, \quad r = 0, 1, \dots, n-1. \quad (4.0.8)$$

Lets move on from discussing the question of the transition of sign with some one vector c , to the analysis of this situation with regards to the whole set D . Say that there exists a partitioning of set D into a family of sub-sets D_1, D_2, \dots, D_n such that the elements (in this case vectors c) of sub-set D_r provide the same number $r-1$ of transitions of sign of elements of (4.0.5). In this way, the priori probability that the unknown true vector $\dot{c} \in D_r$ in given by (4.0.8). However, in any separate case, some of the sub-sets D_r could be empty, meaning that with some vectors of parameters $c \in D$, the number of transitions of sign of (4.0.5) will not equal the given value of r (any one can make sure of this by trying to draw a line which would crossed a given poly-line by guess, in such way that all of the endpoints of this poly-line turned out to be on either side of the guessed line). The priori

probabilities p_r that the unknown true vector \dot{c} is in one of the non-empty sub-sets D_r can be recalculated to the posteriori probabilities p_r^* . Let's define I as the set of the numbers of all the non-empty sub-sets D_r . Then

$$p_r^* = \begin{cases} \frac{p_r}{\sum_{s \in I} p_s}, & r \in I. \\ 0, & r \in \{0, 1, \dots, n-1\} \setminus I \end{cases} \quad (4.0.9)$$

Because in our case the vectors c , are those that could be the true vector \dot{c} , are continuous values, and not discrete ones, then to use formula (4.0.1) we must proceed from estimates p_r^* of the probabilities of event $\dot{c} \in D_r$ to estimates $p_r^*(c), c \in D_r$, of a probability density function. As there is no information which would allow me to somehow rank/sort the 'preference' of vector c in the bounds of each sub-set D_r , it is logical to assume uniform distribution

$$P_r^*(c) = \frac{p_r^*(c)}{\mu(D_r)}, \quad r \in I, \quad (4.0.10)$$

where $\mu(D_r)$ is the measure (analogous to the volume) of sub-set D_r in \mathbf{R}^m dimensions.

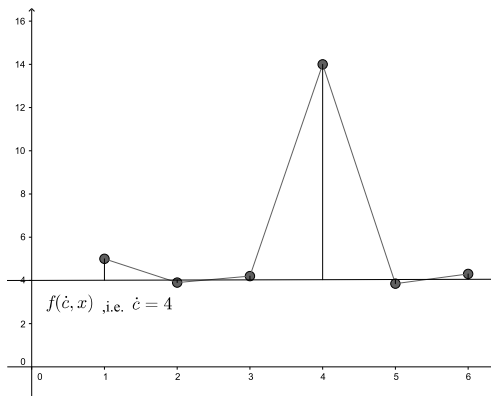
Therefore (4.0.1) becomes

$$E(\rho(c^*, \dot{c})) = \sum_{r \in I} \frac{p_r^*(c)}{\mu(D_r)} \int_{D_r} \rho(c^*, \dot{c}) dc_1 dc_2 \dots dc_m \quad (4.0.11)$$

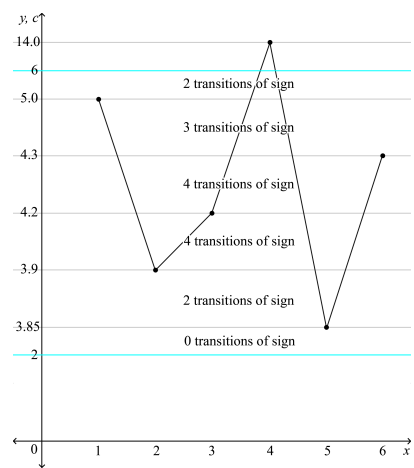
where $\int_{D_r}(\bullet)$ is a laconic (short) notation of a multi integral (in this case a m -multi integral). In the general case, such as this one, the limits of integration of each univariate integral depend on variables, based on which the integration of the external integral relative to the given univariate integral is carried out [*]. (Refer to the example in section 2). This significantly complicates the calculation of these multi integrals. Yet again, looking ahead, I want to note that in the algorithm created, integration is carried out on multidimensional parallelepipeds, when the limits of integration of each integral remain constant.

4.0.1 Illustrative example

For it to be clear, that the following bulky equations lead to success, let's consider an illustrative example, where $m = 1$ (i.e. the vector \dot{c} is a scalar value), $y = f(c; x)$ is a function with one parameter, where \dot{c} is a scalar that has to be found. In this case $n = 6$ and $D = \{c : 2 \leq c \leq 6\}$. In this way, the following graphical representations form.



(a) Graph of proposed example



(b) Illustration of transitions of sign q_i between each \bar{y}_i

Figure 2

Table 1: Table of values for this example

i	x_i	$f(\dot{c}, x_i)$	ξ_i	$\tilde{y}_i = f(\dot{c}, x_i) + \xi_i$
1	1	4	1.0	5.0
2	2	4	-0.1	3.9
3	3	4	0.2	4.2
4	4	4	10	14.0
5	5	4	-0.15	3.85
0	6	4	0.3	4.3

Let the proximity $\rho(c^*, c)$ in (4.0.11), be taken in the form (4.0.3). Then the following simplification takes place.

$$\begin{aligned}
E(\rho(c^*, \dot{c})) &= \sum_{r \in I} \frac{p_r^*}{\mu(D_r)} \int_{D_r} \sum_{j=1}^m (c_j^* - c_j)^2 dc_1 dc_2 \dots dc_m = \\
&\quad \text{expanding } (c_j^* - c_j)^2 \\
&= \sum_{r \in I} \frac{p_r^*}{\mu(D_r)} \sum_{j=1}^m \left[\underbrace{(c_j^*)^2 \int_{D_r} dc_1 dc_2 \dots dc_m}_{=\mu(D_r)} - 2c_j^* \int_{D_r} c_j dc_1 dc_2 \dots dc_m + \int_{D_r} c_j^2 dc_1 dc_2 \dots dc_m \right] = \\
&= \sum_{j=1}^m \left(\sum_{r \in I} \frac{p_r^*}{\mu(D_r)} \left[(c_j^*)^2 \mu(D_r) - 2c_j^* \int_{D_r} c_j dc_1 dc_2 \dots dc_m + \int_{D_r} c_j^2 dc_1 dc_2 \dots dc_m \right] \right) = \\
&= \sum_{j=1}^m \left((c_j^*)^2 \underbrace{\sum_{r \in I} \frac{p_r^*}{\mu(D_r)}}_{\sum_{r \in I} p_r^* = 1} - 2c_j^* \sum_{r \in I} \frac{p_r^*}{\mu(D_r)} \int_{D_r} c_j dc_1 dc_2 \dots dc_m + \sum_{r \in I} \frac{p_r^*}{\mu(D_r)} \int_{D_r} c_j^2 dc_1 dc_2 \dots dc_m \right) \quad (4.0.12)
\end{aligned}$$

And finally:

$$E(\rho(c^*, \dot{c})) = \sum_{j=1}^m \left((c_j^*)^2 - 2c_j^* \sum_{r \in I} p_r^* \frac{\int_{D_r} c_j dc_1 dc_2 \dots dc_m}{\mu(D_r)} + \underbrace{\sum_{r \in I} p_r^* \frac{\int_{D_r} c_j^2 dc_1 dc_2 \dots dc_m}{\mu(D_r)}}_{\text{derivative of this summand on } c_1^*, c_2^*, \dots, c_m^* = 0} \right) \quad (4.0.13)$$

5 Given Examples

6 Conclusion and Reflection

Bibliography