NUMERICAL DIFFERENTIATION OF EXPERIMENTAL DATA USING THE FOURIER TRANSFORM

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The conditions under which the Fourier transform can be used for numerical differentiation of functions that are measured with some error are examined. Methods are given for taking into account boundary conditions on the differentiable function and its derivatives. The effect of the uncertainty of the boundary conditions on the quality of the differentiation is studied in a numerical experiment.

Introduction. The problem of finding the nth order derivative $u(t) = f^{(n)}(t)$ of a function $f(t)$, which is measured with some error in the interval $[t_0, T]$, reduces to solving a Volterra integral equation of the first kind:[1]

$$\int_{t_0}^{t} h(t - \tau)u(\tau)d\tau = \varphi(t), \tag{1}$$

where

$$h(t) = t^{n-1}/(n-1)!, \tag{2}$$

$$\varphi(t) = f(t) - f(t_0) - f^{(1)}(t_0)\frac{(t - t_0)}{1!} - \ldots - f^{(n-1)}(t_0)\frac{(t - t_0)^{n-1}}{(n-1)!}. \tag{3}$$

The regularized algorithms for numerical differentiation are usually constructed for a system of linear algebraic equations, which is the finite-difference analog of Eq. (1) (derivatives of order $(n - 1)$, inclusively, at the point t are set equal to zero, $\varphi(t) = f(t)$ (Refs. 1 and 2)). The most difficult operation is inversion of an $N\times N$ matrix, where $N = (T - t_0)/\Delta t + 1$, and Δt is the spacing of the values of t at which the functions $\varphi(t)$ and $u(t)$ are determined. At the same time, for equations of the convolution type the volume of calculations can be significantly reduced by transferring into the frequency domain.[2–4] This is especially important for problems of large dimension, in particular, when differentiating multidimensional data.[5] In this paper we study the conditions under which the Fourier transform (FT) is applicable in the problem of numerical differentiation, we present methods for taking into account the boundary conditions on the function being differentiated and its derivatives, and in a numerical experiment we perform a comparative analysis of the quality of differentiation performed with the help of the FFT algorithm and by solving a system of linear equations approximating the equation (1).

The conditions under which the Fourier transform is applicable in the problem of numerical differentiation. In order to use the Fourier transform to solve Eq. (1), we extended the functions h, u, and φ in the standard fashion[2]

$$u(t) = \varphi(t) = 0 \quad \text{for } t < t_0 \tag{4}$$

$$h(t) = 0 \quad \text{for } t < 0 \tag{5}$$

This makes it possible to extend the limits of integration in Eq. (1) to infinity. Equation (1) then assumes the following form in the frequency domain:

$$\tilde{h}(\omega)\cdot\tilde{u}(\omega) = \tilde{\varphi}(\omega), \tag{6}$$

where the tilda denotes a Fourier transform, ω is the angular frequency, and the Tikhonov-regularized solution of the starting problem is determined with the help of the inverse Fourier transform from

$$\hat{\tilde{u}}(\omega) = \frac{\tilde{\varphi}(\omega)}{\tilde{h}(\omega)}\cdot\frac{|\tilde{h}(\omega)|^2}{|\tilde{h}(\omega)|^2 + \alpha M(\omega)}, \tag{7}$$

where $M(\omega) \geq 0$ is a prescribed even nonnegative function, and the numerical parameter $\alpha > 0$ (Ref. 1).

One condition for the Fourier transform to be applicable to Eq. (1) under the additional conditions (2)–(5) and hence in order to be able to use Eqs. (6) and (7) is that the functions h, u, and φ must be absolutely integrable. At the same time, the function $h(t)$ defined according to Eqs. (2) and (5) is not absolutely integrable. This difficulty can be overcome by using a method based on the introduction of a "convergence factor."[6] In this method $h(t)$ is premul-

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tiplied by $\exp(-ct)$, where $c > 0$, and the limit $c - 0$ is taken in the final results. Calculating the Fourier transform of the function (2) and premultiplying by $\exp(-ct)$ we obtain, taking into account Eq. (5),

$$\tilde{h}_c(\omega) = \int_0^\infty \frac{t^{n-1}}{(n-1)!} \exp\{-(c + j\omega)t\}dt = \frac{1}{(c + j\omega)^n}, \quad (8)$$

where $j^2 = -1$. As shown in Ref. 6, for $n = 1$ the possibility of using Eq. (8) in the limit $c - 0$ for calculating a convolution of the form (1) using Eq. (6) is guaranteed in the case $\tilde{f}^{(1)}(0) = 0$. It is easy to show that for $n > 1$ the necessary condition for the existence of the limit when using $\tilde{h}_c(\omega)$ instead of $\tilde{h}(\omega)$ in Eq. (6) and letting $c - 0$ is

$$\tilde{f}^{(1)}(0) = \ldots = \tilde{f}^{(n)}(0) = 0 \quad (9)$$

This condition, together with the requirement that the functions $f^{(1)}(t)$, ..., $f^{(n)}(t)$ be absolutely integrable (necessary in order for the Fourier transform to be applicable to them), imposes restrictions on the function $f(t)$ that is being differentiated. These restrictions are that this function and all its derivatives up to order $(n - 1)$ inclusively must vanish in the limit $|t| - \infty$. The transfer function $\tilde{h}(\omega)$ in Eqs. (8) and (7) will then have the form

$$\tilde{h}(\omega) = 1 / (j\omega)^n, \quad \omega \neq 0. \quad (10)$$

For $\omega = 0$, according to Eqs. (9), we set in Eq. (7) $\hat{\tilde{u}}(0) = 0$.

We note that the restrictions on the function $f(t)$ were formulated for infinite limits of integration $t_0 = -\infty$ and $T = \infty$. In real situations the limits of integration are finite, i.e., the condition for absolute integrability is satisfied. In addition, when the FTT algorithm is used to obtain a linear and not a cyclical convolution[7] the number of readings of the function $f(t)$ increases as a result of the addition of the zero values for $t < t_0$, so that the requirement that the function extended in this manner and its derivatives up to order $(n - 1)$ vanish at the ends of the interval is formally satisfied, even if it is not satisfied for the starting function $f(t)$ (defined on the interval $[t_0, T]$). Nonetheless, the possible jumps at the points t_0 and T of the extended function can substantially distort the results of differentiation (see the numerical example 2 given below). For this reason, we shall study a numerical example of the differentiation of such a function under the condition that the requirement indicated above is satisfied at the ends of the interval $[t_0, T]$.

Numerical example 1. For the model function $f(t)$ vie chose the Gaussian curve shown in Fig. 1a. The discrete representation of the function contained 32 values in the interval $[t_0, T]$ and was extended on both sides by $N/2$ zero values. The parameters of the Gaussian curve were chosen so that at the ends of the interval $[t_0, T]$ the values of the function and its derivatives were close to zero. Additive noise $\varepsilon\theta(t_1)$, where θ_1 are random numbers distributed uniformly in the interval $[-1, 1]$, was superposed on $f(t_1)$. Two noise levels were used: $\varepsilon = 0.01$ and $\varepsilon = 0.1$. Thus the perturbed function $f_\varepsilon(t) = f(t) + \varepsilon\theta(t)$ was differentiated by two methods: using the FTT algorithm[7] (to calculate the spectral characteristics appearing in Eq. (7) and the inverse Fourier transform of Eq. (7)) and also by solving a system of $N = 32$ linear equations, approximating Eq. (1), by the method of A.N. Tikhonov.[1] In both cases a zero-order stabilizer was used ($M(\omega) = 1$ in Eq. (7)), and the regularization parameter was determined based on the discrepancy. The results of the calculation of the first three derivatives are presented in Fig. 1. The calculations show that the quality of the differentiation is virtually identical for both algorithms. However the differentiation performed with the help of the FTT is much faster, the gain in speed in this case ($N = 32$) being several factors of 10 (the calculations were performed on a BESM-6 computer). The gain in speed increases rapidly as N increases.[3]

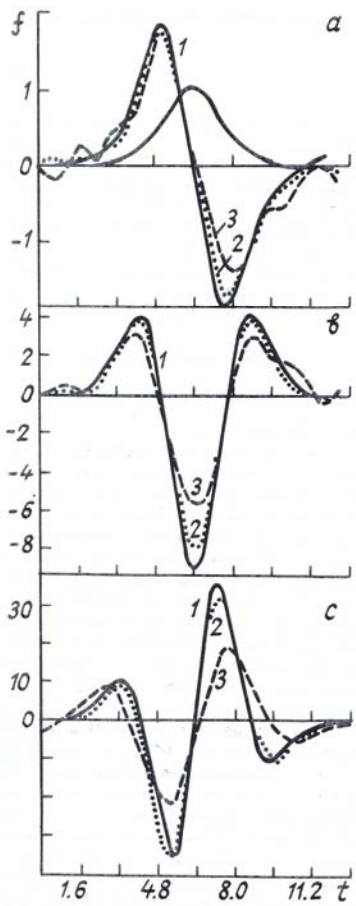

FIG. 1. Numerical differentiation of the model function f(t) with the help of the Fourier transform: 1) exact value; 2, 3) the values of the first (a), second (b), and third (c) derivatives calculated with 1% and 10% noise.

Taking into account the boundary conditions (differentiation of arbitrary functions). Let $f(t)$ be an arbitrary differentiable function, not necessarily equal to zero (like its derivatives up to order $(n - 1)$) at the boundaries of the interval $(t_0, T]$. We shall construct the function $f_p(t) = f(t) - p(t)$, satisfying the necessary boundary conditions,

$$f_p(t_0) = f_p(T) = 0; \quad \dots;$$

$$f_p^{(n-1)}(t_0) = f_p^{(n-1)}(T) = 0 \tag{11}$$

In order $f_p(t)$ satisfies the $2n$ equations (11) we shall seek $p(t)$ in the form of a polynomial of degree $(2n - 1)$:

$$p(t) = \sum_{k=0}^{2n-1} a_k \frac{(t - t_0)^k}{k!} \tag{12}$$

with $2n$ coefficients a_k, determined from the equations following from Eq. (11):

$$p(t_0) = f(t_0), \quad p(t) = f(T); \quad \dots ;$$

$$p^{(n-1)}(t_0) = f^{(n-1)}(t_0), \quad p^{(n-1)}(T) = f^{(n-1)}(T). \tag{13}$$

The derivative $f^{(n)}(t)$ sought is found (after numerical differentiation of the function $f_p(t)$) from the formula:

$$f^{(n)}(t) = f_p^{(n)}(t) + \sum_{k=0}^{n-1} a_{n+k} \frac{(t - t_0)^k}{k!} \tag{14}$$

The boundary values of the derivative $f^{(1)}(t_0)$ and $f^{(n)}(T)$ sought (if they exist) can be taken into account similarly; in so doing, the polynomial (12) will be of degree $(2n + 1)$. If information about the boundary values of the derivatives of one or another order is not available, it is natural to set them equal to zero (see Refs. 1 and 2). The effect of such assumptions will be studied below in a numerical experiment.

Numerical example 2. For the model function we chose the parabola $f(t) = at^2 + bt + c$, shown in Fig. 2a, on which noise was superposed (analogously to the example 1, $\varepsilon = 0.01 f_{max}$), and the first and second derivatives of this function were calculated using the Fourier transform. The regularization parameter α was determined based on the discrepancy. In calculating the first derivative the variants in which the boundary values of the derivative sought are unknown (in this case they were set equal to 0 — Fig. 2b) and when $f^{(1)}(t_0)$ and $f^{(1)}(T)$ are known (Fig. 2c) were studied. The coefficients in the cubic polynomial $p(t)$ had the following form:

$$a_0 = f(t_0); \quad a_1 = \frac{1}{\Delta t}\left[f^{(1)}(T) - f^{(1)}(t_0)\right] - 2a_2\Delta t;$$

$$a_2 = \frac{3}{2\Delta t^2}\left[f^{(1)}(T) + f^{(1)}(t_0)\right] - \frac{3}{\Delta t^3}\left[f(T) - f(t_0)\right];$$

$$\Delta t = T - t_0.$$

In calculating the second derivative the coefficients of the polynomial $p(t)$ of degree[5] have the following form:

$$a_0 = f(t_0); \quad a_1 = f^{(1)}(t_0); \quad a_2 = f^{(2)}(t_0);$$

$$a_3 = \frac{1}{\Delta t}\left[f^{(2)}(T) - f^{(2)}(t_0) - \frac{a_4\Delta t^2}{2!} - \frac{a_5\Delta t^3}{3!}\right];$$

$$a_4 = \frac{12}{\Delta t^3}\left\{\frac{\Delta t}{2}\left[f^{(2)}(T) + f^{(2)}(t_0)\right] - \left[f^{(1)}(T) - f^{(1)}(t_0)\right] - \frac{a_5\Delta t^4}{4!}\right\};$$

$$a_5 = \frac{720}{\Delta t^5}\left\{f(T) - f(t_0) - \frac{\Delta t}{2} \times \left[f^{(1)}(T) + f^{(1)}(t_0)\right] + \frac{\Delta t^2}{12}\left[f^{(2)}(T) + f^{(2)}(t_0)\right]\right\}.$$

The following variants of the boundary conditions were studied:

a) $f^{(1)}(t_0) = f^{(1)}(T) = 0$, and $f^{(2)}(T)$ are known (Fig. 3a).

b) $f^{(2)}(t_0) = f^{(2)}(T) = 0$, $f^{(1)}(t_0)$ and are known(Fig. 3b); and,

c) the boundary values $f^{(1)}$ and $f^{(2)}$ are known (Fig. 3c).

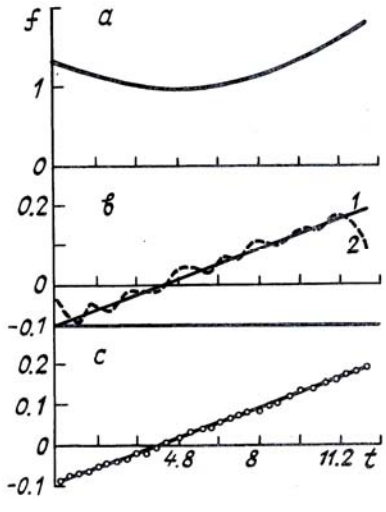

FIG. 2. Effect of the boundary conditions on the calculation of the first derivative: a) differentiable function, 1) exact value of its derivative, 2) results of numerical differentiation with unknown (b) and known (c) boundary conditions (the noise is equal to 1% of the maximum, value of $f(t)$).

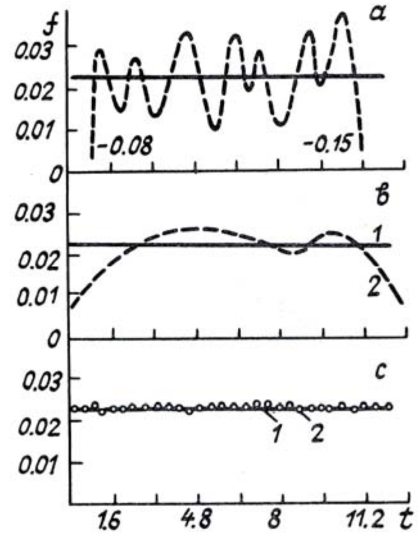

FIG. 3. Effect of the boundary conditions on the calculation of the second derivative (the model function f(t) is the same as in Fig. 2). 1) Exact value of the derivative, 2) derivative calculated with 1% noise for variants a, b, and c of the boundary conditions.

In the case when there is no information about the boundary values of $f^{(1)}$ and $f^{(2)}$ they are set equal to zero. The results obtained were found to be close to the variant a) and are not presented here.

Analysis of the results shows that, first, the solutions obtained with known boundary conditions (Figs. 2c and 3c) are in good agreement with the exact values of the derivatives (the error in the reconstructions falls within the error range in prescribing the differentiable function). Second, the lack of information about the boundary values of the derivative sought degrades the results near the boundaries, but on the whole the obtained solution is in complete agreement with the true solution (Figs. 2b and 3b). Third, uncertainty in the prescription of $f^{(1)}(t_0)$ and $f^{(1)}(T)$ when calculating the second derivative results in substantial degradation of the results, even when information about $f^{(2)}(t_0)$ and $f^{(2)}(T)$ is used (Fig. 3a). We note that the uncertainty in prescribing the boundary conditions has an analogous effect on the accuracy of the solution of the system of linear algebraic equations using Tikhonov's method.[1] Thus numerical differentiation using the Fourier transform, as follows from the numerical examples 1 and 2, gives approximately the same accuracy in solving the problem as the accuracy obtained with the use of matrix methods. At the same time, the proposed method makes the calculations many times faster, especially for problems with large dimension, such as numerical differentiation of lidar signals.[8]

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