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- Математическое моделирование высокотехнологичных систем;
- Математическое моделирование и задачи управления.

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Stable Algorithm of Integrating Rapidly Oscillating Functions

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Abstract. The work describes the new regularized algorithm for computing integrals of rapidly oscillating functions allowing effectively and accurately determine the required value in the presence of stationary points. In the case where the phase function has stationary points (its derivative vanishes on the interval of integration), the calculation of the corresponding integral is still a sufficiently difficult task even for the Levin method due to the degeneracy of the resulting system of linear equations. The basic idea of regularization, described in the article, is the simultaneous modification of the amplitude and phase functions, which does not change the integrand, but eliminates the degeneracy of the phase function on the interval of integration. The regularized algorithm presented in the work is based on the Levin collocation method and describes the stable method of integration of rapidly oscillating functions at the presence of stationary points. Performance and high accuracy of the algorithms are illustrated by various examples.

Keywords: regularization, integration of rapidly oscillating functions, Levin collocation method, Chebyshev differentiation matrix, stable methods for solving systems of linear algebraic equations.

1. Introduction

Let us consider the method for the evaluation of the oscillatory integral

$$I = \int_a^b f(x) e^{i\omega g(x)} dx \equiv \int_a^b F(x) dx, \quad (1)$$

assuming that the constant of oscillations $\omega \gg 1$ is a “large” value; and in the domain of integration the amplitude $f(x)$ and phase $g(x)$ are sufficiently smooth functions.

The integrals of this type can be effectively calculated using the following methods: the method of steepest descent [1]; for integrands with linear phase Filon method [2] and in general case the Levin method [3–5] are often used.

The Levin method of collocations [5] is suitable for finding the oscillatory integrals with more complex amplitude and phase functions. It

consists in moving on to finding the antiderivative $p(x)$ of the integrand satisfying the condition

$$\frac{d}{dx} \left[p(x)e^{i\omega g(x)} \right] = f(x)e^{i\omega g(x)}. \quad (2)$$

Knowing the function $p(x)$ on the interval of integration (or more precisely, at the end points of this interval), one can calculate the value of the integral of the oscillating function by the formula

$$I[f] = \int_a^b f e^{i\omega g} dx = \int_a^b \frac{d}{dx} [p e^{i\omega g}] dx = p(b)e^{i\omega g(b)} - p(a)e^{i\omega g(a)}. \quad (3)$$

In the collocation method the problem of calculating the integral is replaced by the “equivalent” problem of finding the values of the function antiderivative at two points at the ends of the integration interval $[a, b]$, allowing to calculate the value of the integral $I[f]$ by the formula (3). (Note that the method does not use the boundary conditions for the solution of the problem (2), because any particular solution allows to calculate the value of the definite integral.)

Thus, the problem of the approximate calculation of the integral (1) from rapidly oscillating function can be reduced to solving the equation (2) using the method of collocations after expanding $p(x)$ in terms of the Chebyshev polynomials. By an appropriate choice of the approximation points, i.e. their location within the range of integration and their number, it is possible to improve the accuracy of the solution.

2. Approximation of a (sought antiderivative) function by the Chebyshev polynomials. Differentiation matrix

Among many basis systems of polynomials used to approximate functions on finite intervals the Chebyshev polynomials of the first kind have proven well for practical calculations. We consider the Chebyshev polynomials of the first kind as basis functions and assume that the interval of integration is $[a, b] = [-1, 1]$. Suppose that we know the values of a polynomial of the n -th degree at $(n + 1)$ points x_0, \dots, x_n . Then these values define the polynomial uniquely and hence uniquely determine the values $p'(x) = dp(x)/dx$ of its derivatives at these points. Furthermore, the value of the derivative at every point can be represented as a linear combination of values of the polynomial at these points. This dependence can be written in matrix form as [6]:

$$\begin{pmatrix} p'(x_0) \\ \vdots \\ p'(x_n) \end{pmatrix} = \begin{pmatrix} d_{0,0} & \cdots & d_{0,n} \\ \vdots & \ddots & \vdots \\ d_{n,0} & \cdots & d_{n,n} \end{pmatrix} \begin{pmatrix} p(x_0) \\ \vdots \\ p(x_n) \end{pmatrix}. \quad (4)$$

The matrix $D = \{d_{j,k}\}$ is called the differentiation matrix in the physical space.

If the basis functions are the Chebyshev polynomials of the first kind, and grid points are the Gauss-Lobatto nodes

$$x_j = \cos \frac{j\pi}{N}, \quad j = 0, \dots, N,$$

then matrix is called the *Chebyshev differentiation matrix* in physical space.

Improvement of the algorithm for computing the elements of differentiation matrix can be achieved through the use of its antisymmetry property:

$$D_{ij} = -D_{n-i, n-j}, \quad i = n/2 + 1, \dots, n.$$

Approximation of the function by the Chebyshev polynomials of the first kind is remarkable by the fact that it allows to easily calculate the coefficients of the function derivative in the expansion in terms of the same polynomials. Thus, if $p(x) = \sum_{k=0}^n a_k T_k(x)$, then the coefficients b_k , $k = 0, \dots, n$ of the derivative of the function $p(x)$

$$\frac{d}{dx} \left(\sum_{k=0}^n a_k T_k(x) \right) = \sum_{k=0}^n b_k T_k(x)$$

can be calculated using recurrent relations $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$, $k = 2, 3, \dots$, together with the initial conditions $T_0(x) = 1$, $T_1(x) = x$, as the solution of the system of linear algebraic equations [7]:

$$Aa = b. \tag{5}$$

3. Relation between the differentiation matrices in the frequency and physical spaces

Let us write down the expression for the derivative of a function, approximated by the Chebyshev polynomials in the physical space:

$$\begin{pmatrix} p'(x_0) \\ \vdots \\ p'(x_n) \end{pmatrix} = \begin{pmatrix} d_{0,0} & \cdots & d_{0,n} \\ \vdots & \ddots & \vdots \\ d_{n,0} & \cdots & d_{n,n} \end{pmatrix} \begin{pmatrix} p(x_0) \\ \vdots \\ p(x_n) \end{pmatrix}. \tag{6}$$

Taking into account that in the frequency space the vector $p(x)$ can be represented as

$$\begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ \dots \\ p_n \end{bmatrix} = \begin{bmatrix} T_{0,0} & T_{1,0} & T_{2,0} & \vdots & T_{n,0} \\ T_{0,1} & T_{1,1} & T_{2,1} & \vdots & T_{n,1} \\ T_{0,2} & T_{1,2} & T_{2,2} & \vdots & T_{n,2} \\ \dots & \dots & \dots & \ddots & \dots \\ T_{0,n} & T_{1,n} & T_{2,n} & \vdots & T_{n,n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \dots \\ a_n \end{bmatrix},$$

and the derivative in the frequency space is calculated in accordance with the expression

$$\begin{bmatrix} p'_0 \\ p'_1 \\ p'_2 \\ \dots \\ p'_n \end{bmatrix} = \begin{bmatrix} T_{0,0} & T_{1,0} & T_{2,0} & \vdots & T_{n,0} \\ T_{0,1} & T_{1,1} & T_{2,1} & \vdots & T_{n,1} \\ T_{0,2} & T_{1,2} & T_{2,2} & \vdots & T_{n,2} \\ \dots & \dots & \dots & \ddots & \dots \\ T_{0,n} & T_{1,n} & T_{2,n} & \vdots & T_{n,n} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 3 & \dots \\ & 0 & 4 & 0 & \dots \\ & & 0 & 6 & \dots \\ & & & \ddots & \dots \\ 0 & & & & 0 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \dots \\ a_n \end{bmatrix},$$

then from the equation (6) it follows

$$TA = DT,$$

where T is matrix with elements $T_{i,j} = T_i(x_j)$.

4. The method of quadratures

In the case where the integration is set on the interval $x \in [a, b]$, then the transition to a standard domain $[-1, 1]$ of the Chebyshev polynomials of the first kind can be carried out by the change of variables $x = \frac{b-a}{2}t + \frac{b+a}{2}$, $t \in [-1, 1]$. The derivative of the required function is calculated by the formula

$$p'(x) = \frac{2}{b-a} p'(t). \quad (7)$$

According to the introduced linear transformation the Gauss-Lobatto nodes $t_j = \cos\left(\frac{j\pi}{n}\right)$ in the original coordinates have the form

$$x_j = \frac{b-a}{2} \cos\left(\frac{j\pi}{n}\right) + \frac{b+a}{2}, \quad j = 0, 1, \dots, n.$$

Vectors of the functions values and their derivatives at the Gauss-Lobatto nodes are calculated by the formulas

$$\begin{aligned} p &= [p(x_0), p(x_1), \dots, p(x_n)]^T, \\ p' &= [p'(x_0), p'(x_1), \dots, p'(x_n)]^T, \\ g' &= [g'(x_0), g'(x_1), \dots, g'(x_n)]^T, \\ f &= [f(x_0), f(x_1), \dots, f(x_n)]^T. \end{aligned}$$

Obviously, in accordance with the definition of the Chebyshev differentiation matrix, we can write p' in vector-matrix form of (7) taking into account (4):

$$p' = \frac{2}{b-a} Dp$$

and the system of equations in the method of collocations can now be written as

$$\frac{2}{b-a} Dp + i \cdot \text{diag}(\omega g') p = f,$$

or

$$(D + i\Lambda) p = \lambda f, \quad (8)$$

where $\lambda = (b-a)/2$, $\Lambda = \text{diag}(\lambda \omega g'(x_0), \lambda \omega g'(x_1), \dots, \lambda \omega g'(x_n))$ is diagonal matrix. The solution of the system (8) contains $p(b)$ and $p(a)$, whereas the required integral is calculated using the formula (3).

Let us write down the equation (8) in the case of finding a solution in frequency space, taking into account that $D = TAT^{-1}$, and $p = Ta$:

$$\frac{2}{b-a} TAT^{-1}Ta + i \cdot \text{diag}(\omega g')Ta = f,$$

or

$$TAa + i \cdot \Lambda Ta = \lambda f, \quad (9)$$

Here, in order to reduce formulas the following designations are used: $T_{i,j} = T_i(x_j)$ and $\lambda_i = \lambda \omega g'(x_i)$. The solution to this system of linear algebraic equations for the expansion coefficients $a = (a_0, a_1, \dots, a_n)$ over the basis functions allows to determine the approximate value of the integral using the equation (3).

Equation (9) is still valid for an arbitrary set of different grid points. From this equation it follows that the matrix of the system becomes singular only when at least one of the values $g'(x_k) = 0$, $k = 0, \dots, n$ becomes zero.

The method of quadrature described above is well studied [1, 5, 7, 8] and works well in cases where the phase function has no stationary points. However, in the case where the phase function has stationary points (its derivative vanishes at the interval of integration), the system (9) can be

degenerate and calculating corresponding integral becomes ill-posed problem.

For solving this ill-posed problem, various methods are proposed [1, 5, 8–11], but their practical use is rather difficult.

5. Regularization of numerical integration method for rapidly oscillating functions

In order to avoid the singularity of the matrix $TA + i\lambda \cdot \text{diag}(\omega g')$ of the system (9), we modify the integrand, multiplying and dividing it by the same function $\exp(iCx)$, where C is a complex number. Then the integral (1) takes the form

$$\int_a^b f(x) e^{-iCx} e^{i(Cx + \omega g(x))} dx. \quad (10)$$

The exponential function $\exp(iCx)$ is continuous, therefore the value of the integral for such a replacement will not change.

Introducing the notations $\tilde{f}(x) = f(x)e^{-iCx}$ and $\tilde{g}(x) = Cx + \omega g(x)$, we get a new equation for the coefficients, similar to the equation (3):

$$[TA + i\tilde{g}T]a = \tilde{f}, \quad (11)$$

The required value of the integral (10) is then calculated by the formula

$$I[f] = \int_a^b \tilde{f} e^{i\tilde{g}} dx = \int_a^b \frac{d}{dx} [\tilde{p} e^{i\tilde{g}}] dx = \tilde{p}(b) e^{i\tilde{g}(b)} - \tilde{p}(a) e^{i\tilde{g}(a)},$$

where $\tilde{p}(x) = \sum_{k=0}^n \tilde{a}_k T_k(x)$.

The solution of the system (11) with respect to the coefficients of the solution expansion in terms of the Chebyshev polynomials makes it easy to calculate the values $\tilde{p}(a)$ and $\tilde{p}(b)$:

$$\begin{aligned} \tilde{p}(a) &= \sum_{j=0}^n a_j, \\ \tilde{p}(b) &= \sum_{j=0}^n (-1)^j a_j. \end{aligned}$$

Thus, the use of the regularization method¹ (the replacement of the integrand with the aim to solve the ill-posed problem) and the transition to the solution of the modified problem of integration allows to consistently calculate integrals of rapidly oscillating functions, including those with phase functions having stationary points.

¹Regularization in statistics, machine learning, theory of inverse problems is method of adding some further information to the statement of the problem with the aim to solve the ill-posed problem or prevent retraining.

Choosing the constant C in (11) in such a way that the inequality $\operatorname{Re}(C) > -\omega |g'(x)|$, $x \in [a, b]$ is true, allows to ensure all diagonal elements of the matrix of the linear algebraic equations system (11) being nonzero, and guarantees the existence and uniqueness of the system solution.

Ensuring sustainability is much more difficult due to the structure of the system (11), in which the elements with maximum absolute values are concentrated in the far right column of the matrix — see formula (5).

However, using this regularization method allows to improve the properties of the system (taking into account the number of approximation points), and to increase (in absolute value) the diagonal elements by choosing constant C , thus ensuring the predominance of the leading elements on the diagonal.

Conclusion

The article describes the new regularized algorithm for computing integrals of rapidly oscillating functions allowing effectively and accurately determine the required value in the presence of stationary points. In the case where the phase function has stationary points (its derivative vanishes on the interval of integration) the calculation of the corresponding integral is still a sufficiently difficult task even for the Levin method due to the degeneracy of the resulting system of linear equations. The basic idea of regularization, described in the article, is the simultaneous modification of the amplitude and phase functions, which does not change the integrand, but eliminates the degeneracy of the phase function in the interval of integration. Practically, this means a transition from calculating $\int_a^b f(x) e^{i\omega g(x)} dx$ to the integration of the new integrand $\int_a^b f(x) e^{-iCx} e^{i(Cx + \omega g(x))} dx$, where the constant C is chosen from the condition $|C + \omega g'(x)| \neq 0$, $x \in [a, b]$.

The numerical examples in the article show significant increase in integration accuracy when using regularization even in the absence of the stationary points. Properties of linear algebraic system are improved with increasing (by selecting constant C) of the diagonal elements of the matrix, providing the predominance of the leading elements on the diagonal.

A similar approach can be extended to the integrals in infinite limits using other (non-Chebyshev functions of the first kind) basis functions.

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