NUMERICAL INTEGRATION

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Keywords: Approximate integration, quadrature formula, cubature formula

Contents

Summary

The principal statements of problems for computation of definite and multiple integrals by means of quadrature and cubature formulae are presented and the most interesting and often used results of the theory of quadrature formulae are considered. A review of basic trends of the theory of cubature formulae is given.

1. Statements of Problems

The notion of a definite integral is basic in mathematics, and the computation of the integral is often a hard problem. The Newton-Leibnitz formula for the computation of the definite integral of a function $f(x)$ over the interval $[a,b]$ includes the antiderivative $F(x)$:

$$I[f]=\int_a^b f(x)dx=F(b)-F(a).$$

This formula theoretically is a complete description of the problem. However, Newton had already understood that the computation of $F(x)$ is possible in rare cases, therefore he put into use the formulae for the approximate computation of $I[f]$, which have the form

$$I[f] \simeq \sum_{j=1}^{N} c_j f(x_j) = Q_N[f]. \tag{1}$$

Such formulae are called quadrature formulae, the sum $Q_N[f]$ is called a quadrature sum, the numbers x_j are the nodes, and the numbers c_j are the coefficients of a quadrature formula. Note that in papers of western authors the sum $Q_N[f]$ is usually named a quadrature formula. Note also that the definition of the Riemann integral is introduced, in essence, through quadrature sums.

An integrand is often represented in the form $w(x)\varphi(x)$, where $w(x)$ is a certain fixed function. Such a situation occurs, for example, when computing the Fourier coefficients or when separating out a peculiarity of some kind in the integrand. Therefore, for greater generality we consider quadrature formulae of the form

$$I_w[f] = \int_a^b w(x) f(x) dx \simeq Q_N[f] = Q_N[a,b,f] \tag{2}$$

where a fixed function $w(x)$ is called a weight function. Note that the interval of integration can be infinite. The nodes of a quadrature formula are considered to be mutually different. To the formula (2) we associate the linear functional of error $l(f) = I_w[f] - Q_N[f]$ where integrated functions are elements of a certain space B, which for simplicity can be considered as a certain set of continuous functions. A quadrature formula is said to be exact for a function $f(x)$ if $l(f) = 0$.

There are several main directions in the construction and study of quadrature formulae.

(b). . . . . ▪ ¢ **Algebraically Accurate Formulae**

Let $\varphi_0, \varphi_1, ..., \varphi_m \in B,\ I_w[\varphi_i] = b_i,\ 1 \le i \le m$. Accuracy conditions for a quadrature formula for functions $\varphi_i(x)$ can be written in the form of a system of equations

$$\sum_{j=1}^{N} c_j \varphi_i(x_j) = b_i, \quad 1 \le i \le m\ . \tag{3}$$

The solvability of the system (3) with respect to x_j and c_j determines the possibility of the construction of formulae of required accuracy under given conditions for nodes and coefficients. Let us give basic statements of problems for algebraically accurate formulae in the case when $\varphi_i(x)$ are polynomials of one variable. Denote the set of all polynomials of degree not greater than m by P_m.

A1. For a given system of nodes $x_1, x_2, ..., x_N$ it is required to find coefficients $c_1, c_2, ..., c_N$ so that the formula (2) is exact for all polynomials of P_m for m being as large as possible.

Such a requirement on accuracy looks natural for functions which can be approximated adequately by polynomials. For instance, let a function be represented by the Taylor expansion

$$f(x)=\sum_{k=0}^{r-1} f^{(k)}(a)\frac{(x-a)^k}{k!}+R_r(x)$$

where $R_r(x)$ is Taylor's remainder, and the formula (2) is of an algebraic accuracy $r-1$. Then the error of a quadrature formula depends on the value of a remainder, because

$$l(f)=l(R_r(x))$$

and for functions whose Taylor series converges fast such formulae give good results.

A2. For given N it is required to find coefficients c_j and nodes x_j, $1 \le j \le N$, so that the formula (2) is exact for all polynomials of P_m for m being as large as possible.

A3. For given nodes $x_1, x_2, ..., x_{N_1}$, where $1 \le N_1 \le N$, it is required to find coefficients $c_1, c_2, ..., c_N$ and nodes $x_{N_1+1}, ..., x_N$ so that the formula (2) is exact for all polynomials of P_m for m being as large as possible.

A4. For given N and with the condition $c_1 = c_2 = ... = c_N$ it is required to find nodes $x_1, x_2, ..., x_N$ so that the formula (2) is exact for all polynomials of P_m for m being as large as possible.

Example 1. Let us construct quadrature formulae with the weight function $w(x)\equiv 1$ and the number $N = 1, 2, 3$ of nodes in the statement (A1) on the interval [0, 1]. Assume that $\varphi_i(x)= x^i$, $i \ge 0$. At first, let $N = 1$ and $x_1 = 1/2$. It is easy to check that in this case the system (3) is solvable only for $i \le 2$, and here $c_1 = 1$. The obtained quadrature formula

$$\int_0^1 f(x)dx \simeq f(1/2)$$

is exact for polynomials of degree not greater than one; it is called the rectangular formula (rectangle rule). If $N = 2$, $x_1 = 0$, $x_2 = 1$ then it is easy to verify that the system (3) is solvable only for $i = 1, 2$ as well, and here $c_1 = c_2 = 1/2$. The obtained formula

$$\int_0^1 f(x)dx \simeq \frac{1}{2}\left[f(0)+f(1)\right]$$

is called the trapezoidal formula (trapezoidal rule). If $N=3, x_1=0,\ x_2=1/2,\ x_3=1,$ from the system (3) for $i=0,1,2$ one can obtain the prismoidal formula (Simpson rule)

$$\int_0^1 f(x)dx \simeq \frac{1}{6}\left[f(0)+f(1/2)+f(1)\right].$$

It is exact not only for polynomials of the second degree, but also for those of the third degree.

It is evident that improving an accuracy of the quadrature formula (2) leads to an increase of the number of unknowns of the system (3), and the use of the latter for the construction of the formula becomes unpractical. Therefore to obtain formulae for exact integration of polynomials of high degree other methods are used, some of them are described below.

(b). Statements of Problems of Numerical Integration in Terms of Functional Analysis

It seems natural to characterize the quality of a quadrature formula by the value $|l(f)|$. Indeed, for a concrete given function the choice of a quadrature formula for which $|l(f)|$ takes a minimal value is natural. Though, if we seek a quadrature formula which provides satisfactory quality of the computation of an integral for some set of functions, then for characterization of quality of integration it is natural to take a quantity which depends on this set only. Such a quantity in Banach function spaces is the norm of the functional (2).

Assume that the functional (2) is linear and bounded on a Banach space B, i.e., it is an element of the conjugate space B^*. In this case the following problems are most often studied.

B1. To find $\|l\|_{B^*}$ for a given quadrature formula.

B2. To find a quadrature formula, which has the minimal norm $\|l\|_{B^*}$ for a given number of nodes.

Up to now, the solution of the problem (B2) is a question for many known functional spaces. Quadrature formulae satisfying the statement (B2) are called *the best ones*. Considerable progress has been made for some weakened statements of problems on the construction of the best formulae with a fixed set of nodes. Such formulae are called *optimal*.

B3. To find an optimal quadrature formula among all the formulae with a given fixed set of nodes.

B4. To find a sequence of quadrature formulae with functionals ρ^N of error where the index N denotes the number of nodes of a quadrature formula, such that for any other sequence of formulae with the same set of nodes and functionals l^N the following inequality holds:

$$\liminf_{N\to\infty} \left(\| l_N \|_{B^*} / \| \rho_N \|_{B^*} \right) \geq 1.$$

The sequences satisfying the statement (B4) are called *asymptotically optimal*.

The sequences of quadrature formulae for which l_N tends to zero as $N \to \infty$ play an important role in the theory of computations.

Theorem 1: (Steklov). The inequality

$$\lim_{N\to\infty} Q_N[f] = I[f] \tag{4}$$

holds if and only if the following conditions are satisfied:
(a) the equality (4) holds for any polynomial f;
(b) there is a number k such that
$$\sum_{j=1}^{N} |c_j| \leq k, \quad N = 1, 2, \dots .$$
Let us note that these conditions are satisfied, if quadrature formulae $I[f] \simeq Q_N[f]$ are exact for $f(x) \equiv 1$ and the coefficients of quadrature formulae are positive.

1.3 Multi-dimensional Case

Now, let us make some remarks concerning a multi-dimensional case. An expression of the form

$$I_\Omega^\omega[f] = \int_\Omega \omega(x_1, \dots, x_n) f(x_1, \dots, x_n) dx_1 \dots dx_n \simeq$$
$$\sum_{j=1}^{N} c_j f(x_1^j, \dots, x_n^j) = \sum_{j=1}^{N} c_j f(x^j) = Q_N(f) \tag{5}$$

where $\Omega \subset R^n$ is said to be a *cubature formula*. All the definitions and statements of problems for cubature formulae are analogous to those for quadrature formulae. It should be noticed that increasing the dimension of a space essentially complicates analysis; in particular, the system (3) often becomes practically unsolvable for a formula of accuracy of order ≥ 4 even in the two-dimensional case. Besides, a new parameter, namely, the form of the integration domain Ω, plays an important role here.

Here we will not consider the third fundamental direction in the theory of approximate integration, based on probabilistic statistical methods, for instance, on the Monte Carlo method, restricting ourselves to certain aspects of the theory of approximate integration by means of quadrature and cubature formulae.

2. Quadrature Formulae

Historically, the theory of approximate integration has its origin in the study of algebraically accurate formulae, though the founders of integral calculus did not use such a terminology. We say that a positive integer d is the *algebraic degree of accuracy of a quadrature formula* (2), if this formula is exact for all functions of P_d and is not exact for at least one polynomial of P_{d+1}. The following theorem gives the estimate of accuracy of a quadrature formula with N nodes.

Theorem 2: If $\omega(x) \geq 0,\ x \in [a,b]$, and there exist moments

$$\mu_k = \int_a^b \omega(x) x^k dx, \quad \mu_0 > 0 ,$$

then the algebraic degree d of accuracy of a quadrature formula (2) with N nodes satisfies the inequality $d \leq 2N - 1$.

2.1. Interpolatory Quadrature Formulae

In the theory of quadrature formulae, the so-called interpolatory quadrature formulae play an important role. Let $x_1, \ldots, x_N$ be mutually different points and a function $f(x)$ be determined in some domain of a complex variable which contains these points. Denote the polynomial $(x - x_1) \cdot \ldots \cdot (x - x_N)$ by $\omega_N(x)$ and put

$$l_k(x) = \omega_N(x) / (x - x_k)\omega'_N(x).$$

Then the *polynomial*

$$P(x) = \sum_{j=1}^{N} l_j(x) f(x_j)$$

is called an *polynomial interpolation* of degree not higher than $N - 1$. The polynomial $P(x)$ has the following remarkable properties. First, the equality

$$P(x_j) = f(x_j), \quad 1 \leq j \leq N ,$$

is valid, and second, if $f(x)$ is a polynomial of degree not higher than $N - 1$, then $P(x) = f(x)$.

The quadrature formula (2) is called interpolatory quadrature formula, if its coefficients are determined by equalities

$$c_j = \int_a^b \omega(x) l_j(x) dx .$$

The following is an important theorem.

Theorem 3: The quadrature formula (2) is interpolatory quadrature formula, if and only if it is exact for an arbitrary polynomial of degree not higher than $N-1$.

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Biographical Sketch

Mikhail V. Noskov was born in Perm, Russia. He completed his Diploma in Mathematics at the Krasnoyarsk State Pedagogical Institute in 1969. In 1984 he took the Russian degree of Candidate in Physics and Mathematics at the Novosibirsk State University. In 1992 he was awarded the Russian degree of Doctor in Physics and Mathematics from S.- Peterburg State University for his thesis “Some problems of approximate integration of periodic functions”. In 1994 he took Professor Diploma at the Chair “Applied Mathematics”. Since 1972 he is working at the Krasnoyarsk State Technical University. M. V.

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