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ON THE APPLICATION OF QUADRATURE FORMULAS FOR CALCULATING INTEGRALS OF ARBITRARY MULTIPLICITY

Abstract. In this paper, we consider the calculation of integrals of arbitrary multiplicity by the methods of non-uniform grids, Monte Carlo and optimal coefficients. A comparative analysis of these numerical methods for integrating multiple integrals was made. It was established that the method of optimal coefficients had an advantage compared to other methods. It is shown that the use of uneven and parallelepipedal grids is the basis of almost all results obtained in the field of application of theoretic – numerical methods to the problems of approximate analysis. It is established that interpolation of functions of several variables by theoretic-numerical grids allows to receive interpolation formulas, accuracy of which rises with increase of smoothness of functions. The number of variables in this case has no significant effect on the order of the residual member. The use of the function $f \in E_s^{\alpha}$ to Fourier coefficients allows to obtain an interpolation formula from the quadrature formulas, which are constructed with the help of the parallelepipedal grids. This formula is accurate for trigonometric polynomials, the degree of which does not exceed the value of $\sqrt{N}\ln^{\frac{s}{2}} N$.

Key words: theoretic-numerical method, quadrature formula, method of optimal coefficients, multiple integrals.

1. Introduction

There are three types of problems in which theoretic – numerical approaches lead to general results: application of quadrature formulas for calculating integrals of arbitrary multiplicity, approximate solution of integral equations and interpolation of functions of several variables.

The paper considers the connection between the theory of uniform distribution and the number-theoretic method in approximate analysis. The main types of theoretic – numerical grids, non-uniform and parallelepipedal, are analyzed. The problems of finding the optimal coefficients for parallelepipedal grids are presented.

Theoretic – numerical algorithms of numerical integration are essential in the calculation of interaction integrals in quantum chemistry and in the calculation of nanoscale ferromagnetic heterosystems, and also in high-energy physics.

2. Materials and methods of research

2.1 Approximate calculation of multiple integrals

Integration of multiple integrals of functions of the class E_s^{α}.

The function of the form:

$$f(x_1,\ldots,x_s)=\sum_{m_1,\ldots,m_s=-\infty}^{\infty} C(m_1,\ldots,m_s)e^{2\pi i(m_1x_1+\ldots m_sx_s)} \tag{1}$$

belongs to the class E_s^{α} if $C(m_1,\ldots,m_s)=O\left(\left(\overline{m_1},\ldots,\overline{m_s}\right)^{-\alpha}\right)$, where $\overline{m_v}=\max(1,|m_v|)$ and the value of $\alpha>1$ characterizes the smoothness of functions.

The class E_s^{α} has periodic functions that have continuous derivatives of the form $\frac{\partial^{\alpha s} f}{\partial x_1^{\nu_1} \ldots \partial x_s^{\nu_s}}$, where $\nu_1,\ldots,\nu_s$ is an arbitrary permutation of fixed integers $\alpha_1,\ldots,\alpha_s$ selected from the interval $[0,\alpha s]$, so that $\alpha_1 + \ldots + \alpha_s = \alpha s$. In particular, for integer α, functions that have a derivative $\frac{\partial^{\alpha s} f}{\partial x_1^{\alpha} \ldots \partial x_s^{\alpha}}$ will belong to the class E_s^{α}.

It is not necessary for the function to be periodic. There are simple ways of transition from non-periodic functions to periodic functions [1-3]. The replacement of variables that do not disrupt the smoothness of the functions and does not lead to significant complication of calculations can also be used for the periodization of the function.

Let R be the error of the simplest quadrature formula

$$\int_0^1 \ldots \int_0^1 f(x_1,\ldots,x_s)dx_1 \ldots dx_s = \frac{1}{N}\sum_{k=1}^{N} f[\xi_1(k),\ldots,\xi_s(k)] - R, \tag{2}$$

where the collection of points $M_k = [\xi_1(k),\ldots,\xi_s(k)]$ is called a grid.

In the case of uniform grids, arising from partition of the unit s-dimensional cube into $N = n^s$ equal small cubes, the following estimate is valid for the functions of the class E_s^{α}:

$$R = O\left(\frac{1}{N^{\frac{\alpha}{s}}}\right), \tag{3}$$

achievable in this class; this estimate is not improved when using quadrature formulas with arbitrary weights. The disadvantage of quadrature formulas with uniform grids is the decrease in their accuracy with the increase of the number of measurements.

2.2 The first theoretic – numerical method for constructing quadrature formulas

This method is based on the use of non-uniform grids of the form [1]

$$M_k = \left(\left\{\frac{k}{N}\right\},\ldots,\left\{\frac{k^s}{N}\right\}\right), \tag{4}$$

where N is the prime number, $\left\{\frac{k^v}{N}\right\}$ is the fractional proportion of the number $\frac{k^v}{N}$.

In the case of non-uniform grids, the error estimate of the quadrature formula (2) takes the form

$$R = O\left(\frac{1}{\sqrt{N}}\right). \tag{5}$$

Non-uniform grids are obviously free from the main drawback of uniform grids – unlike estimate (3) the order of estimate (5) remains unchanged with the increase of the number of measurements.

Along with the above-mentioned advantage of non-uniform grids, these grids have a significant disadvantage – the accuracy of the results obtained using the corresponding quadrature formulas does not increase with increasing smoothness of the considered functions.

2.3 The second theoretic – numerical method for constructing quadrature formulas

This method is based on the use of parallelepipedal grids of the form

$$M_k = \left(\left\{\frac{ka_1}{N}\right\},\ldots,\left\{\frac{ka_s}{N}\right\}\right), \tag{6}$$

where $a_1,\ldots,a_s$ are integer numbers selected in a special way (optimal coefficients). This method does not have the disadvantage of non-uniform grids [5]. For parallelepipedal grids, the error estimate in formula (2) takes the form

$$R = O\left(\frac{\ln^{\alpha s} N}{N^{\alpha}}\right). \tag{7}$$

There are no grids that give better estimate R on the class E_s^{α} than $O\left(\frac{1}{N^{\alpha}}\right)$ [6]. This estimate cannot be improved for the case of quadrature formulas of the most general form as well [7]. Thus, grids of the form (6) lead to quadrature formulas, in which the error estimate does not allow further significant improvement.

When $s = 1$, there exists a single parallelepipedal grid, which coincides with the uniform grid, obtained by dividing the segment $[0,1]$ into N equal parts, i.e.

$$M_k = \left(\left\{\frac{k}{N}\right\}\right), \text{ where } k = 1,2,...,N \tag{8}$$

When $s = 2$, it is not difficult to show that the integers $a_1 = 1$, $a_2 = a$ will be optimal coefficients for any $a = a(N)$, in which incomplete partial relations $\frac{a}{N}$ will be limited to a value increasing with the growth of N not more than some degree of $\ln N$. In particular, when $N = u_n$, where u_n is a general term of the Fibonacci sequence (the Fibonacci sequence is defined as follows: $u_0 = 1$, $u_1 = 1$, $u_n = u_{n-1} + u_{n-2}$, $n = 2,3,...$), the integers $a_1 = 1$, $a_2 = u_{n-1}$ will be optimal coefficients and points

$$M_k = \left(\left\{\frac{k}{u_n}\right\}, \left\{\frac{ku_{n-1}}{u_n}\right\}\right), \text{ where } k = 1,2,...,u_n \tag{9}$$

form a two-dimensional parallelepipedal grid.

When $s \geq 3$, various sufficient optimality conditions can be used to calculate the optimal coefficients.

Let at $v = 1,2,...,s$ for integers z_v from the segment $[1, N-1]$ the functions $H(z_1,...,z_v)$ are determined by the equality [4]:

$$H(z_1,...,z_v) = \sum_{k=1}^{N-1}\left[1 - 2\ln\left(2\sin\pi\left\{\frac{kz_1}{N}\right\}\right)\right]\cdots\left[1 - 2\ln\left(2\sin\pi\left\{\frac{kz_s}{N}\right\}\right)\right].$$

The integers $a_1,...,a_s$ will be optimal coefficients if $a_1 = 1$ and for given $a_1,...,a_{v-1}$ $(v \geq 2)$ the value a_v is equal to any of the values z_v, at which the minimum of the function $H(a_1,...,a_{v-1},z_v)$ is reached.

Another sufficient condition for optimality according to [1] – the integers $a_1,...,a_s$ are optimal coefficients if the minimum multiplication $\overline{m_1},\cdots,\overline{m_s}$ for non-trivial solutions of the comparison $a_1m_1 + ... + a_sm_s \equiv 0 (\mathrm{mod}\, N)$ satisfies the condition $\overline{m_1},\cdots,\overline{m_s} > BN\ln^{-\gamma} N$, where $B > 0$ and $\gamma \geq 0$ are constants depending only on s.

From relations (4), (8) and (9) it can be seen that non-uniform grids with any s and parallelepipedal grids with $s \leq 2$ are indicated quite effectively with the help of simple formulas. When $s \geq 3$, different algorithms have to be used to find parallelepipedal grids. Consideration of algorithms, in which the number of operations necessary to specify the grid is not too large compared to the number of calculations in the corresponding quadrature formulas, can be practically effective.

The first of the above methods for finding optimal coefficients is practically effective, since the number of elementary operations in the calculations arising in it has order N^2. By slightly modifying this algorithm, it is possible to reduce the number of operations to $O(N^{1+\varepsilon})$, where $\varepsilon > 0$ is arbitrarily small.

Almost all the results obtained using parallelepipedal grids, it is possible to use practically effective algorithms. However, in some cases [1], the indication of the corresponding grids is still possible only with the help of $O(N^s)$ operations, where $s > 2$ is ineffective.

From the two grids leading to the following error estimates $|R| < C_1 N^{-\alpha_1} \ln^{\beta_1} N$ and $|R| < C_2 N^{-\alpha_2} \ln^{\beta_2} N$, it is natural to consider the first one, which is better if $\alpha_1 > \alpha_2$. However, the advantage of the first grid can be revealed only at very large values of N. Therefore, in computational practice, when choosing a quadrature formula, appropriate experiments are necessary.

3 Comparison of numerical methods for integrating multiple integrals

The multiple integral over the unit volume of some function $f(x_1, x_2, x_3, x_4)$ is replaced by the finite sum:

$$\int_0^1\int_0^1\int_0^1\int_0^1 f(x_1,x_2,x_3,x_4)dx_1dx_2dx_3dx_4 = \frac{1}{pq}\sum_{k=1}^{pq} f\left(\left\{\frac{a_0k}{pq}\right\},\left\{\frac{a_1k}{pq}\right\},\left\{\frac{a_2k}{pq}\right\},\left\{\frac{a_3k}{pq}\right\}\right),$$

where $pq = 4097$, and a_0, a_1, a_2, a_3 are optimal coefficients. The integrals of the following functions are calculated:

1. $\dfrac{x_1x_2x_3x_4}{0.0625}$; 2. $\dfrac{x_1 + x_2 - x_3 + 2x_4}{1.5}$; 3. $\dfrac{x_1^3x_2^2x_3e^{x_1x_2x_3x_4}}{0.051615162}$;
4. $1 + \cos 2\pi(x_1 + x_2 + x_3 + x_4)$;
5. $1 + \sin a\pi(x_1 + x_2 - x_3 + 2x_4)$ for $a = 10;30;60;100;200$;
6. $\dfrac{\prod_{i=1}^{4}\left(\dfrac{1}{1-x_i}\right)^2 e^{-a\left(\frac{x_i}{1-x_i}\right)^2}}{\dfrac{\pi^2}{16a^2}}$ for $a = 1;10;30;60;100$.

In integrals, non-periodic integrands were periodized and the integrals of them are equal to 1.

The following table shows the results of calculating the integrals in different ways. It shows that the method of optimal coefficients has an advantage over the calculation by other methods. And also in most cases, a significant advantage of parallelepipedal grids over other grids is revealed even with a very small value of N [15].

Table - Results of calculating integrals by different methods

Functions		Method of non-uniform grids	Monte Carlo methods				Method of optimal coefficients
			1	2	3	4	
1		0.38	0.78	1.05	1.02	1.01	0.999995
2		0.74	0.94	0.99	1.008	1.008	0.999999
3		0.80	0.75	1.07	1.04	0.99	1.000186
4		1.01	1.009	1.002	0.99	1.01	1.000000
5	10	1.01	1.008	0.99	0.99	0.99	1.00000000
	30	1.01	0.98	0.99	0.99	0.99	1.00000002
	60	1.01	0.98	0.99	1.008	1.003	1.00000004
	100	1.02	1.02	1.003	0.99	0.99	1.00000013
	200	0.98	1.01	0.99	1.0001	1.02	1.00000021
6	1	1.03	1.23	1.03	0.93	0.99	0.999682
	10	1.39	1.65	1.13	0.84	0.77	1.002806
	30	3.22	2.48	0.87	0.91	0.95	0.940240
	60	7.48	3.87	0.53	0.54	1.16	1.583021
	100	16.2	5.99	0.22	0.19	1.28	3.977712

All the obtained sets of optimal coefficients and the values of five, ten, fifteen-fold integrals calculated by the method of optimal coefficients with parallelepipedal grids for non-periodic functions are given in [8-14]. It was shown that the calculation of integrals with good accuracy was also possible for the small number of nodes of the quadrature formula N. A comparative characteristic of the calculated sets of optimal coefficients and values of multiple integrals by the theoretic - numerical methods, taking into account the number of nodes of the quadrature formula, was also given.

The use of non-uniform and parallelepipedal grids forms the basis of almost all the results obtained in the field of application of theoretic – numerical methods to the problems of approximate analysis.

For a multiple Fredholm integral equation of 2nd kind:

$$\varphi(P) = \lambda \int_{G_s} k(P,Q)\varphi(Q)dQ + f(P), \tag{10}$$

where integration is extended to a unit s – dimensional cube G_s. We will assume that the free term and the core of this equation belong to the classes E_s^{α} and E_{2s}^{α} respectively, and that the denominator of Fredholm $D(\lambda)$ is non – zero. Using theoretic - numerical grids M_k, one can obtain [5] an approximate solution of equation (10) in the form

$$\varphi(P) = \frac{\lambda}{N}\sum_{k=1}^{N} K(P,M_k)\tilde{\varphi}(M_k) + f(P) + R,$$

where values of $\tilde{\varphi}(M_k)$ are determined from a system of linear algebraic equations:

$$\tilde{\varphi}(M_k) = \frac{\lambda}{N}\sum_{l=1}^{N} K(M_k,M_l)\tilde{\varphi}(M_l) + f(M_k), \text{ where } k = 1,2,...,N;$$

moreover, the error R, depending on the choice of grids, has the same order as in the calculation of multiple integrals of functions belonging to the class E_s^{α}.

For an arbitrarily small $\varepsilon > 0$ and sufficiently small λ, using the method of iterations and non-uniform grids of the form (4) to calculate the increasing multiplicity integrals, we can obtain an explicit approximate expression for $\varphi(P)$:

$$\varphi(P) = f(P) + \frac{1}{N}\sum_{k=1}^{N}\sum_{v=1}^{n} \lambda^v K(P,M_{1,k})..K(M_{v-1,k},M_{v,k})f(M_{v,k}) + O\left(N^{-\frac{1}{2}+\varepsilon}\right).$$

Here $M_{v,k} = \left(\left\{\frac{k^{s(v-1)+1}}{N}\right\},...,\left\{\frac{k^{sv}}{N}\right\}\right)$, $n = [y\ln N]$ is the integer part of the quantity $y\ln N$ and y is some constant depending on ε and the character of decreasing Fourier coefficients of the kernel of equation (10).

Using parallelepipedal grids and slightly changing the definition of classes E_s^{α} [6], it is possible in the analytical expression for $\varphi(P)$ to improve the residual term to $O(N^{-\alpha+\varepsilon})$. The same methods can be applied [15] to solving multiple Volterr equations and equations of the mixed type, in which some of the integrations are constant and some of them are in variable limits. In [16], questions of the numerical solution of nonlinear Volterr integral equations of the first kind with a differentiable kernel, which degenerates at the initial point of the diagonal, are considered. It is shown that this equation reduces to the Volterr integral equation of the third kind and a numerical method is developed on the basis of the regularized equation. The convergence of the numerical solution to the exact solution of the Volterr integral equation of the first kind is proved, the estimates of the error and the recursive formula of the computational process are obtained.

In questions of interpolation of functions of many variables, the theoretic – numerical grids make it possible to obtain interpolation formulas, the accuracy of which increases with increasing smoothness of functions, and the number of variables does not significantly affect the order of smallness of the remainder

term. Applying quadrature formulas constructed using parallelepipedal grids to the Fourier coefficients of the function $f \in E_s^{\alpha}$, we obtain the interpolation formula

$$f(x_1,...,x_s)=\frac{1}{N}\sum_{k=1}^{N} f\left(\frac{ka_1}{N},...,\frac{ka_s}{N}\right)\psi_k(x_1,...,x_s)+O\left(N^{-\frac{\alpha-1}{2}}\ln^{\frac{\alpha+1}{2}s-1}N\right),$$

where functions $\psi_k(x_1,...,x_s)$ are defined by equality

$$\psi_k(x_1,...,x_s)=\sum_{\overline{m}_1,...,\overline{m}_s<\sqrt{N}\ln^{-\frac{s}{2}}N} e^{2\pi i\left[m_1\left(x_1-\frac{ka_1}{N}\right)+...+m_s\left(x_s-\frac{ka_s}{N}\right)\right]}.$$

This formula is exact for trigonometric polynomials, the degree of which does not exceed the value $\sqrt{N}\ln^{-\frac{s}{2}}N$.

More accurate results in the interpolation of functions of many variables can be obtained in another way, based on the representation of a function by some finite sum of integrals and then applying the corresponding quadrature formulas to these integrals.

4. Conclusion

The application of theoretic – numerical methods to the problems of approximate analysis is reduced to the use of non-uniform and parallelepipedal grids. Theoretic – numerical grids make it possible to obtain interpolation formulas, the accuracy of which increases with increasing smoothness of functions. The number of variables does not significantly affect the order of smallness of the residual term.

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ЕРКІН ЕСЕЛІ ИНТЕГРАЛДАРДЫ ЕСЕПТЕУ ҮШІН КВАДРАТУРАЛЫҚ ФОРМУЛАЛАРДЫ ҚОЛДАНУ ТУРАЛЫ

Аннотация. Бұл мақалада біркелкі емес торлар, Монте-Карло және оңтайлы коэффициенттер әдісте-рімен еркін еселі интегралдарды есептеу қарастырылды. Көп өлшемді интегралдарды есептеудің көрсетілген сандық әдістеріне салыстырмалы талдау жасалды. Оңтайлы коэффициенттер әдісі басқа әдістермен салыстырғанда артықшылыққа ие екендігі анықталды. Шамамен талдау мәселелеріне теориялық-сандық әдістерді қолдану саласында біркелкі емес және параллелепипедалды торларды пайдалану нәтижелердің көшпілігінің негізі болып табылатыны көрсетілген. Көп айнымалылы функцияларды теориялық-сандық торлармен интерполяциялау функциялардың тегістігін арттырумен өсетін интерполяциялық формулаларды алуға мүмкіндік беретіні анықталды. Бұл жағдайда айнымалылардың саны қалдық мүшенің аздығы тәртібіне елеулі әсер етпейді. Фурье коэффициенттеріне $f \in E_s^{\alpha}$ функцияны пайдалану параллелепипедалды торлар арқылы құрылатын квадратуралық формулалардан интерполяциялық формуланы алуға мүмкіндік береді. Мұндай формула дәрежесі $\sqrt{N}\ln^{-\frac{s}{2}}N$ мәннен аспайтын тригонометриялық полиномдар үшін дәл болып табылады.

Түйін сөздер: теориялық-сандық әдісі, квадратуралық формула, оңтайлы коэффициенттер әдісі, көп өлшемді интегралдар.

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О ПРИМЕНЕНИИ КВАДРАТУРНЫХ ФОРМУЛ ДЛЯ ВЫЧИСЛЕНИЯ ИНТЕГРАЛОВ ПРОИЗВОЛЬНОЙ КРАТНОСТИ

Аннотация. В данной работе рассмотрено вычисление интегралов произвольной кратности методами: неравномерных сеток, Монте-Карло и оптимальных коэффициентов. Был сделан сравнительный анализ указанных численных методов интегрирования многократных интегралов. Установлено, что метод оптимальных

коэффициентов обладает преимуществом по сравнению с остальными методами. Показано, что использование неравномерных и параллелепипедальных сеток составляет основу большинства результатов, полученных в области применения теоретико-числовых методов к вопросам приближенного анализа. Установлено, что интерполяция функций многих переменных теоретико-числовыми сетками позволяет получить интерполяционные формулы, точность которых возрастает с увеличением гладкости функций. Число переменных в этом случае не оказывает существенного влияния на порядок малости остаточного члена. Использование функции $f \in E_s^{\alpha}$ к коэффициентам Фурье позволяет получить интерполяционную формулу из квадратурных формул, которые построены с помощью параллелепипедальных сеток. Такая формула точна для тригонометрических полиномов, степень которых не превосходит величины $\sqrt{N}\ln^{-\frac{s}{2}} N$.

Ключевые слова: теоретико-числовой метод, квадратурная формула, метод оптимальных коэффициентов, многократные интегралы.

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