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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

HIGH DIMENSIONAL INTEGRATION: NEW WEAPONS FIGHTING THE CURSE OF DIMENSIONALITY

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The approximate computation of the definite integral of a function of several variables is one of the basic problems of numerical analysis. The problem is hard because of the so-called curse of dimensionality. This curse consists in the following: applying an integration rule with N nodes to a univariate function, we will get an integration error, say, $\varepsilon > 0$. Applying the corresponding Cartesian product rule to an s-variate function, we will need $N^{**}s$ nodes for the same integration error $\varepsilon > 0$. In mechanics we deal with at least six-dimensional functions, but in contemporary financial mathematics there occur 300-variate functions. The probabilistic Monte-Carlo methods provide error estimates independent of the dimensionality of the problem. Unfortunately, these methods are both slow in convergence and suffer from a lack of effectiveness as well. The quasi-Monte-Carlo methods, based on the number theory, work fast and effectively, at least in the case of finite and smooth integrands. Unfortunately, in reality multivariate functions with singularities do occur. The scope of the present paper is numerical integration of multivariate functions with singularities. In many cases the proposed methods are best possible with respect to the order of convergence. Best possible means an exact order of the error term, essentially not worse than in the univariate case.

Приближенное вычисление определенного интеграла функции нескольких переменных является одной из основных проблем численного анализа. Проблема с трудом поддается решению из-за так называемого «проклятия размерностей». Она заключается в следующем: интегрирование по N узлам одномерной функции приводит к ошибке интегрирования $\varepsilon > 0$. При соответствующем интегрировании функции s-переменных необходимы $N^{**}s$ узлов с той же самой ошибкой интегрирования $\varepsilon > 0$. В механике мы имеем дело по меньшей мере с 6-мерными функциями, но в современной прикладной математике используются функции 300 переменных. Вероятностные методы Монте-Карло позволяют оценивать ошибку независимо от проблемы размерностей. К сожалению, эти методы характеризуются медленной сходимостью и низкой эффективностью. Квази-Монте-Карло-методы, основанные на теории чисел, работают быстро и эффективно, по крайней мере для ограниченных и гладких подынтегральных выражений. К сожалению, в реальных вычислениях приходится иметь дело с функциями многих переменных с сингулярностями. Целью данной статьи является описание численного интегрирования функций многих переменных с сингулярностями. Во многих случаях представленные методы являются наилучшими из возможных относительно порядка сходимости, когда известен точный порядок слагаемого ошибки, который существенно не хуже, чем в одномерном случае.

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Dedicated to the memory of N. M. Korobov

1. THE PROBLEM SETTING

Consider functions $f(x_1, x_2, \ldots, x_s) = y$, $0 \leqslant x_\rho \leqslant 1$, $\rho = 1, \ldots, s$. Let $I^s = (0,1)^s$ the open unit cube, and $\bar{I}^s = [0,1]^s$ the closed s-dimensional unit cube. We are concerned with the numerical approximation of the integral of the function f by means of finite sums. Given a finite set of points in I^s or $\bar{I}^s$, $(x_1^{(1)}, x_1^{(2)}, \ldots, x_1^{(s)}), \ldots, (x_n^{(1)}, x_n^{(2)}, \ldots, x_n^{(s)}), \ldots$, $(x_N^{(1)}, \ldots, x_N^{(s)})$, we consider the integration method

$$R_N = \frac{1}{N} \sum_{n=1}^{N} f(x_n^{(1)}, \ldots, x_n^{(s)}) - \int_0^1 \ldots \int_0^1 f(x_1, \cdots, x_s) dx_1 \cdots dx_s. \tag{1}$$

One is interested in small values of R_N, of course. Some known results: If the pointed $(x_n^{(1)}, \ldots, x_n^{(s)})$, $n = 1, \ldots, N$, is a set of uniform distributed and independent random variables, one obtains the domical estimation of Monte-Carlo integration:

$$R_N = \mathrm{O}\left(\frac{1}{\sqrt{N}}\right). \tag{2}$$

This convergence rate is rather poor, but independent of the dimensionality of the problem and independent of the smoothness of the function $f(x_1, \ldots, x_s)$. Nothing is said about the constants involved.

On the other hand, we consider the Cartesian product rules: Let $x_1, x_2, \ldots, x_N \in \bar{I}^s$ and $y = f(x)$ be a continuous function on $\bar{I} = [0,1]$. So we have a one-dimensional integration rule

$$R_N^{(1)} = \frac{1}{N} \sum_{n=1}^{N} f(x_n) - \int_0^1 f(x) dx. \tag{3}$$

The principle of the Cartesian product rules consists in a repeated application of the one-dimensional rule to an s-variate function:

$$R_{N^s}^{(s)} = \frac{1}{N^s} \sum_{n_1=1}^{N} \cdots \sum_{n_s=1}^{N} f(x_{n_1}, \ldots, x_{n_s}) - \int_0^1 \cdots \int_0^1 f(x_1, \ldots, x_s) dx_1 \cdots dx_s. \tag{4}$$

The error term $R_{N^s}^{(s)}$ will not be better than $R_N^{(1)}$, in general. But the computational complexity is N^s. This fact is the well-known curse of dimensionality. There are two remedies: the Hlawka–Koksma inequality and Korobov's method:

Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N \in \bar{I}^s$. Let $I(\mathbf{a}) = \mathbf{x} : 0 \leqslant x_\rho \leqslant a_\rho, \rho = 1, \ldots, s, \mathbf{a} \in \bar{I}^s$.

Definition.

$$D_N^* := \sup_{\mathbf{a}} \left| \frac{\#\{x_n \in I(\mathbf{a})\}}{N} - a_1 a_2 \cdots a_s \right| \tag{5}$$

is called the *-discrepancy (star discrepancy) of the finite point set $\mathbf{x}_1, \ldots, \mathbf{x}_N$.

The following theorem is essentially due to H. Weyl: Weyl's criterion: The infinite sequence $(\mathbf{x}_n)_{n=1}^{\infty}$, $\mathbf{x}_n \in \bar{I}^s$, is uniform distributed if one of the following conditions holds:

(a) for all continuous functions $f : \bar{I}^s \to \mathbb{C}$ holds

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) = \int_{\bar{I}^s} f(\mathbf{x}) d\mathbf{x}; \tag{6}$$

(b) for all $\mathbf{m} \in \mathbb{Z}^s$ holds

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \mathrm{e}^{2\pi i \mathbf{m}\mathbf{x}_n} = \begin{cases} 0, & \mathbf{m} \neq \mathbf{0}, \\ 1, & \mathbf{m} = \mathbf{0}; \end{cases} \tag{7}$$

(c)

$$\lim_{N\to\infty} D_N^* = 0.$$

Weyl's criterion is the guideline for numerical application of number theoretical methods. At first we cite the Hlawka–Koksma inequality:

Theorem. (Hlawka): Let $f(\mathbf{x})$ be a function with bounded variation in the sense of Hardy–Krause, $V(f(\mathbf{x})) < \infty$. Then holds the inequality

$$|R_N(f)| = \left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}) - \int_{\bar{I}^s} f(\mathbf{x}) d\mathbf{x} \right| \leqslant D_N^* V(f). \tag{8}$$

There is a huge number of estimations of the discrepancy of special sequences. We give only two examples.

Example 1. Let $\mathbf{x}_{n_1,\ldots,n_s} = \left(\frac{n_1}{N}, \frac{n_2}{N}, \ldots, \frac{n_s}{N}\right), n_1, \ldots, n_s = 1, \ldots, N$. Then $D_{N^s}^* \leqslant \frac{2^s}{N}$. This also means the curse of dimensionality.

Example 2. Let $(a_1, \ldots, a_s) \in \mathbb{Z}^s$ be optimal coefficients modulo N in the sense of Korobov. Let $\mathbf{x}_n = \left(\frac{na_1}{N}, \ldots, \frac{na_s}{N}\right) \bmod n, n = 1, \ldots, N$. Then

$$D_N^* = \mathrm{O}\left(\frac{(\ln N)^{\beta}}{N}\right), \ \beta \leqslant s \tag{9}$$

holds. Apart from the logarithmic factor this estimation is independent of the dimensionality of the problem. Unfortunately, the Hlawka–Koksma inequality does not take into account additional smoothness conditions of the function $f(\mathbf{x})$.

Korobov's method overcomes this flaw:

Let $\bar{m} = \max(1, |m|), m \in \mathbb{Z}$. Consider the Korobov classes

$$E_s^\alpha(C) = \left\{ f(\mathbf{x}) : |C(\mathbf{m})| \leqslant \frac{C}{(\bar{m}_1, \ldots, \bar{m}_s)^\alpha}, \mathbf{m} \in \mathbb{Z}^s \right\}, \tag{10}$$

where $C(\mathbf{m})$ means the Fourier coefficients of $f(\mathbf{x})$:

$$C(\mathbf{m}) = \int\limits_{\bar{I}^s} f(\mathbf{x})\ \mathrm{e}^{-2\pi i \mathbf{m}\mathbf{x}} d\mathbf{x}. \tag{11}$$

Remark. If $f(\mathbf{x})$ is 1-periodic in each variable $x_1, \ldots, x_s$, and if $\dfrac{\partial^{\alpha s} f}{\partial^\alpha_{x_1}, \ldots, \partial^\alpha_{x_1}}$ is continuous and bounded by C, then $f \in E_s^\alpha(C)$. This can be shown by αs-fold partial integrations of formula (11).

Theorem. (Korobov): If $f(\mathbf{x}) \in E_s^\alpha(C)$and if $\mathbf{a} = (a_1, \ldots, a_s)$ consists of optimal coefficients in the sense of Korobov, then the estimation holds:

$$|R_N(f)| = \left| \frac{1}{N} \sum_{n=1}^{N} f\left(\frac{n\mathbf{a}}{N}\right) - \int\limits_{\bar{I}^s} f(\mathbf{x}) d\mathbf{x} \right| \leqslant \frac{C_1 C(\ln^{\alpha\beta} N)}{N^\alpha}, \tag{12}$$

with an explicit constant C_1 and some $\beta \leqslant s$. This estimation is best possible apart from logarithmic factors: There is always a function $f(\mathbf{x}) \in E_s^\alpha(C)$, such that

$$\left| \frac{1}{N} \sum_{n=1} N f\left(\frac{n\mathbf{a}}{N}\right) - \int\limits_{\bar{I}^s} f(\mathbf{x}) d\mathbf{x} \right| \geqslant \frac{C(s)\ \ln^{s-1}(N)}{N^\alpha}. \tag{13}$$

More generally, there is no integration rule with $R_N = \mathrm{o}\left(\dfrac{1}{N^\alpha}\right)$, if $f \in E_s^\alpha$.

All these methods are classical and can be found in Korobov [3], Drmota–Tichy [1] or Niederreiter [2].

The methods described are concerned only with proper integrals of bounded functions. Singularities are not allowed. From the theoretical and also from the practical point of view it is important to develop integration rules for unbounded functions as well:

Problem. Let $f(\mathbf{x})$: $\bar{I}^s \to \mathbb{C}$ or $I^s \to \mathbb{C}$. Find classes of unbounded functions f and integration rules $\displaystyle\sum_{n=1}^{N} g_{n,N} f(\mathbf{x}_n)$, such that

$$\lim_{N \to \infty} \sum_{n=1}^{N} g_{n,N} f(\mathbf{x}_n) = \int\limits_{I^s} f(\mathbf{x}) d\mathbf{x}. \tag{14}$$

Furthermore, give estimations for the error term

$$R_N = \sum_{n=1}^{N} g_{n,N} f(\mathbf{x}_n) - \int\limits_{I^s} f(\mathbf{x}) d\mathbf{x}. \tag{15}$$

2. SOLUTIONS OF THE PROBLEM

We distinguish between the two cases:

First case: The location of the singularities of $f(\mathbf{x})$ in $\bar{I}^s$ is unknown.

Second case: The location of the singularities is known. We assume that $f(\mathbf{x})$ is unbounded at most on the bonudary of $I^s = (0,1)^s$.

For the sake of completeness we refer to some of our own former results [4].

Given a function $f : \bar{I}^s \to \mathbb{C}$, so we define functions $f_B, \hat{f}_B$, $B > 0$ such that

$$\begin{aligned} f_B(\mathbf{x}) &= f(\mathbf{x}), \quad \text{if } |f(\mathbf{x})| \leqslant B, \\ &= 0, \qquad\quad \text{if } |f(\mathbf{x})| > B, \end{aligned} \tag{16}$$

$$\begin{aligned} \hat{f}_B(\mathbf{x}) &= 0, \qquad\quad \text{if } |f(\mathbf{x})| \leqslant B, \\ &= f(x), \quad \text{if } |f(\mathbf{x})| > B. \end{aligned} \tag{17}$$

So we have $f(\mathbf{x}) = f_B(\mathbf{x}) + \hat{f}_B(\mathbf{x})$. We gave a suitable class of functions in the following manner:

Definition. The class $C(\beta, \gamma)$ of s-variate functions $f(\mathbf{x}), 0 \leqslant \mathbf{x} \leqslant 1$, consists of all functions which fulfill $\forall B > 0$:

(a)

$$I(|\hat{f}_B|) = \mathrm{O}(B^{-\beta}) \text{ for some } \beta > 0, \tag{18}$$

(b)

$$V(f_B) = \mathrm{O}(B^{\gamma}) \text{ for some } \gamma \geqslant 1. \tag{19}$$

Here $V(.)$ means again the variation of a function in the sense of Hardy and Krause. For dimension $s = 1$ the definition coincides with the usual total variation of a univariate function. The use of $V(.)$ is natural because of the functional analytic connection between the spaces of continuous functions and the spaces of Radon measures, i.e., point measures and Lebesgue measure.

We proved the following theorem:

Theorem. If $f(\mathbf{x}) \in C(\beta, \gamma)$ and if the discrepancy of the set of nodes $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ is D_N^*, then for $B = (D_N^*)^{\frac{-1}{(\beta+\gamma)}}$ the estimation holds:

$$I(f) = \frac{1}{N} \sum_{n=1}^{N} f_B(\mathbf{x}_n) + \mathrm{O}\left((D_N^*)^{\frac{\beta}{(\beta+\gamma)}}\right). \tag{20}$$

Remark. We also proved that the order of convergence stated in (20) is best possible even in the case $s = 1$, provided $f(\mathbf{x}) \in C(\beta, \gamma)$. Now we come to case two, the new and much more efficient results concerning the case that the singularities of the integrand are concentrated on the boundary ∂I^s of the unit cube.

The idea of the method: Consider a univariate function $f(x)$, $f : (0,1) \to \mathbb{C}$, which has singularities at $x = 0$ or $x = 1$, and which fulfills some smoothness conditions in $(0,1)$. We ask for an integral-preserving transformation of $f(x)$ which also continues the differentiability conditions of $f(x)$ to $I = [0,1]$.

Let $p(t) = x$ be a function, which is strictly increasing in $[0,1]$ and which fulfills differentiability conditions of sufficient high order. Then we have for functions $p(t)$ with $p(0) = 0, p(1) = 1$:

$$\int_0^1 f(x)dx = \int_0^1 f(p(t))p'(t)dt = \int_0^1 g(t)\,dt. \tag{21}$$

If $p(t)$ does not tend too fast to $p(0) = 0$ and $p(1) = 1$, then one will be able to remove singularities at $x = 0, 1$ by means of (21). We propose the function

$$p(t) = p_\gamma(t) = p_0 \int_0^t (\tau(1-\tau))^\gamma d\tau, \quad p_0 = \left(\int_0^1 (\tau(1-\tau))^\gamma d\tau \right). \tag{22}$$

The connection of $p(t)$ with the incomplete beta integral is clear. We state some important properties of $p(t)$:

Lemma.

(a) $p(0) = 0, p(1) = 1$,

(b) $p'(0) = p'(1) = 0, p(t) > 0$ for $t \in (0,1)$,

(c) $p^{(n)}(0) = p^{(n)}(1) = 0$ for $n = 1, 2, \ldots, n_0 < \gamma$,

(d) $|p^{(n)}(t)| \leqslant p_\gamma (t(1-t))^{\gamma+1-n}$ for $1 \leqslant n < \gamma + 1$ and $0 \leqslant t \leqslant 1$,

(e) $p_\gamma \leqslant p_0 \sum\limits_{i+2j=n} \dfrac{n!}{i!j!}$,

(f) $\dfrac{1}{p(t)(1-p(t))} \leqslant \dfrac{4 + 2^{\gamma+1}(\gamma+1)}{p_0} \dfrac{1}{(t(1-t))^{\gamma+1}}$,

(g) $p(t) \leqslant \dfrac{p_0}{\gamma+1} t^{\gamma+1}, 1 - p(t) \leqslant \dfrac{p_0}{\gamma+1}(1-t)^{\gamma+1}$ for $0 \leqslant t \leqslant 1$.

Some proofs of the parts of the Lemma are straightforward, some are not. We now introduce a suitable class of functions, having singularities on ∂I^s:

Definition. $H_s^{\beta,\alpha}(C)$ consists of all functions $f(x_1, \ldots, x_s), 0 < x_\rho < 1, \rho = 1, \ldots, s$, such that for all $n_1, \ldots, n_s, 0 \leqslant n_\rho \leqslant \alpha, \rho = 1, \ldots, s$, holds:

$$\left| \frac{\partial^{n_1 + \ldots + n_s} f(x_1, \ldots, x_s)}{\partial x_1^{n_1} \partial x_2^{n_2} \cdots \partial x_s^{n_s}} \right| \leqslant \frac{C}{\left(\prod_{\rho=1}^s (x_\rho(1-x_\rho))^{\beta+n_\rho} \right)}, \tag{23}$$

whereas all the derivatives are continuous, and $0 < \beta < 1$.

The introduction of the class $H_s^{\beta,\alpha}(C)$ was motivated by the univariate extreme function $f(x) = (x(1-x))^{-\beta}, 0 < \beta < 1$. We remind (21) for general $s = 1, 2, \ldots$:

$$\int_0^1 \cdots \int_0^1 f(x_1, x_2, \ldots, x_s)\, dx_1 dx_2 \cdots dx_s = \int_0^1 \cdots \int_0^1 g(t_1, \ldots, t_s)\, dt_1 dt_s \tag{24}$$

with

$$g(t_1, \ldots, t_s) = f(p(t_1), p(t_2), \ldots, p(t_s)) p'(t_1) p'(t_2) \cdots p'(t_s). \tag{25}$$

We consider now the reactors of nodes

$T_n = \left(\frac{1}{2N} + \frac{na_1}{N}, \frac{1}{2N} + \frac{na_2}{N}, \ldots, \frac{1}{2N} + \frac{na_s}{N}\right)$, mod N, where $\mathbf{a} = (a_1, \ldots, a_s)$ are optimal coefficients, $\mathbf{a} = \mathbf{a}(N)$, and $n = 1, \ldots, N$. We get the integration rule

$$I_N(f) := \frac{1}{N} \sum_{n=1}^{N} f(p(t_{1,n}), p(t_{2,n}), \ldots, p(t_{s,n})) p'(t_{1,n}), p'(t_{2,n}), \ldots, p'(t_{s,n}), \tag{26}$$

with $t_{\rho,n} = \frac{1}{2N} + \frac{na_\rho}{N}, \rho = 1, \ldots, s$.

Now we are able to state the

Theorem. If $f \in H_s^{\beta,\alpha}(C)$ and if $\gamma > \frac{\alpha + \beta}{1 - \beta}$, then

$$\left| \int_0^1 \ldots \int_0^1 f(x_1, \ldots, x_s) dx_1 \cdots dx_s - I_N(f) \right| \leqslant C_1(\alpha, \beta, \gamma, s) C \frac{(\ln N)^{\alpha,\beta}}{N^\alpha}, \tag{27}$$

where the constant $C_1(\alpha, \beta, \gamma, s)$ is explicit. The proof makes heavy use of the lemma and makes use of an explicit and complicated estimation of all of the derivatives of $g(t_1, \ldots, t_s)$.

Remark 1. According to (13), our theorem cannot be improved significantly, even in the case of boundedness of $f(\mathbf{x})$.

Remark 2. The use of the classical optimal coefficients is only one example of the application of number-theoretical methods to improper integrals.

We have further methods, using, e.g., the Weyl sequences, $(n\boldsymbol{\Theta})$, especially the sequences $n(e^{r_1}, e^{r_2}, \ldots, e^{r_s}), n = 1, 2, \ldots, r_i \neq r_k \in \mathbb{Q}$, $i \neq k$. Estimations of $R_N = \int f dx - I_N(f)$ via the Diaphony are available as well.

LITERATURE

Korobov's book is a classical reference, whereas Niederreiter's book contains most of the recent developments in number-theoretical numerics. The book by Drmota and Tichy is perhaps a comprehensive book on uniform distribution of sequences, containing two thousand references.

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