High Dimensional Integration: New Weapons Fighting the Curse of Dimensionality

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HIGH DIMENSIONAL INTEGRATION: NEW WEAPONS FIGHTING THE CURSE OF DIMENSIONALITY

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DEDICATED TO THE MEMORY OF N.M. KOROBOV

INTRODUCTION

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 of the following: applying an integration rule with N nodes to an univariate function, you will get an integration error, say, $\varepsilon > 0$. Applying the corresponding cartesian product rule to a s-variate function, you 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 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 end suffer of a lack of effectiveness as well. The Quasi-Monte-Carlo-Methods, based on number theory, are working 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.

1. THE PROBLEM SETTING

Consider functions $f(x_1, x_2, \ldots, x_s) = y$, $0 \le x_\rho \le 1$, $\rho = 1, \ldots, s$. 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

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

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 receives 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 an 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 of a repeated application of the one-dimensional rule to a s-variate function:

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

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 to remedies: The inequality of Hlawka-Koksma and Korobovs method:
Let $\vec{x_1}, \vec{x_2}, \ldots, \vec{x_N} \in \bar{I}^s$. Let $I(\vec{a}) = \vec{x} : 0 \le x_\rho \le a_\rho, \rho = 1, \ldots, s, \vec{a} \in \bar{I}^s$.

Definition:

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

is called the *-discrepancy (star discrepancy) of the finite point set $\vec{x_1}, \ldots, \vec{x_N}$.

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

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

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

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

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} e^{2\pi i \vec{m}\vec{x_n}} = \begin{cases} 0 & \vec{m} \ne \vec{0} \\ 1 & \vec{m} = \vec{0} \end{cases} \tag{7}$$

(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 $f(\vec{x})$ be a function with bounded variation in the sense of Hardy-Krause, $V(f(\vec{x})) < \infty$. Then holds the inequality

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

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

Example 1: Let $\vec{x}_{n_1,\ldots,n_s} = \left(\frac{n_1}{N}, \frac{n_2}{N}, \ldots, \frac{n_s}{N}\right), n_1, \ldots, n_s = 1, \ldots, N$. Then $D_{N^s}^* \leq \frac{2^s}{N}$. 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 $\vec{x_n} = \left(\frac{na_1}{N}, \ldots, \frac{na_s}{N}\right) \bmod n, n = 1, \ldots, N$. Then

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

holds. Apart of 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 $f(\vec{x})$.
Korobovs method overcomes this flaw:

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

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

where $C(\vec{m})$ means the Fouriercoefficients of $f(\vec{x})$:

$$C(\vec{m}) = \int_{\bar{I}^s} f(\vec{x}) e^{-2\pi i \vec{m}\vec{x}} d\vec{x} \tag{11}$$

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

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

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

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

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

More general, there is no integration rule with $R_N = \mathrm{o}\left(\frac{1}{N^\alpha}\right)$, if $f \in E_s^\alpha$.
All this 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 $f(\vec{x})$: $\bar{I}^s \to \mathbb{C}$ or $I^s \to \mathbb{C}$. Find classes of unbounded functions f and integration rules $\sum_{n=1}^N g_{n,N} f(\vec{x_n})$, such that

$$\lim_{N\to\infty} \sum_{n=1}^{N} g_{n,N} f(\vec{x_n}) = \int_{I^s} f(\vec{x}) d\vec{x}. \tag{14}$$

Furthermore, give estimations for the error term

$$R_N = \sum_{n=1}^{N} g_{n,N} f(\vec{x_n}) - \int_{I^s} f(\vec{x}) d\vec{x}. \tag{15}$$

2. SOLUTIONS OF THE PROBLEM

We distinguish the two cases:
First case: The location of the singularities of $f(\vec{x})$ in $\bar{I}^s$ is unknown.
Second case: The location of the singularities is known. We assume, that $f(\vec{x})$ is unbounded at most on the bonudary of $I^s = (0,1)^s$.

For the sake of completeness we refer some of 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

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

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

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

Definition: The class $C(\beta, \gamma)$ of s-variate functions $f(\vec{x}), 0 \leq \vec{x} \leq 1$, 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)

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

Here $V(.)$ means again the variation of a function in the sense of Hardy and Krause. For dimension $s = 1$ the definition coincide with the usual total variation of an 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 $f(\vec{x}) \in C(\beta, \gamma)$ and if the discrepancy of the set of nodes $\vec{x_1}, \vec{x_2}, \ldots, \vec{x_N}$ is D_N^*, then for $B = (D_N^*)^{\frac{-1}{(\beta+\gamma)}}$ the estimation holds:

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

Remark: We also proved, that the order of convergence stated in (20) is best possible even in the case $s = 1$, provided $f(\vec{x}) \in C(\beta, \gamma)$. Now we come to the 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 an 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 continuates 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 to 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

$$\begin{aligned} p(t) &= p_\gamma(t) = p_0 \int_0^t (\tau(1-\tau))^\gamma d\tau, \\ p_0 &= (\int_0^1 (\tau(1-\tau))^\gamma d\tau) \end{aligned} \tag{22}$$

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

(e) $p_\gamma \leq p_0 \sum_{i+2j=n} \frac{n!}{i!j!}$

(f) $\frac{1}{p(t)(1-p(t))} \leq \frac{4+2^{\gamma+1}(\gamma+1)}{p_0} \frac{1}{(t(1-t))^{\gamma+1}}$

(g) $p(t) \leq \frac{p_0}{\gamma+1} t^{\gamma+1}, 1 - p(t) \leq \frac{p_0}{\gamma+1}(1-t)^{\gamma+1}$ for $0 \leq t \leq 1$

Some proofs of the parts of the Lemma are straight forward, 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 $n_1, \ldots, n_s, 0 \leq n_\rho \leq \alpha, \rho = 1, \ldots, s$, holds:

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

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 ëxtremefunction $f(x) = (x(1-x))^{-\beta}, 0 < \beta < 1$. We remind (21) for general $s = 1, 2, \ldots$:

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

with

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

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 $\vec{a} = (a_1, \ldots, a_s)$ are optimal coefficients, $\vec{a} = \vec{a}(N)$, 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

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

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 can not be improved significantly, even in the case of boundedness of $f(\vec{x})$.

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, $(n\vec{\Theta})$, 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.

LITERATUR

Korobovs book is the classical reference, whereas Niederreiters book contains most of the resent developments in number theoretical numerics. Drmota-Tichy is the perhaps comprehensive book on uniform distribution of sequences, containing two thousands of references.

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