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A TWO-STAGE ALGORITHM OF NUMERICAL EVALUATION OF INTEGRALS IN NUMBER-THEORETIC METHODS*1)

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Abstract

To improve the numerical evaluation of integrals in Number-Theoretic Methods, we give a two-stage algorithm. The main idea is that we distribute the points according to the variations of the quadrature on the subdomains to reduce errors. The simulations results are also given.

Key words: Numerical integration, Monte Carlo method, Number-theoretic method.

1. Introduction

The Number-Theoretic Method (NTM) is a special method which represents a combination of number theory and numerical analysis. The widest range of applications and indeed the historical origin of this method is found in numerical integration. Also related problems such as interpolation and the numerical solutions of integral equations and differential equations, optimization and experimental design in statistics can be dealt with successfully. [1–4] give a comprehensive review in bibliographic setting.

In this paper we consider the problem of evaluating integration. Let D be a domain in R^s (s-dimension) and $f(\boldsymbol{X})$ be a continuous function defined on D. We want to calculate the definite integral

$$I(f) = \int_D f(\boldsymbol{X}) d\boldsymbol{X} \tag{1}$$

There are two main approaches in evaluation of $I(f)$. One is Monte Carlo method (MCM) developed by S. Ulam and J. Von Neumann. The basic idea of the Monte Carlo method is to replace an analytic problem by a probabilistic problem with the same solution, and then investigate the latter problem by statistical simulation. For

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simplicity, we consider $D = [0,1]^s$ first. Suppose that $\boldsymbol{X}$ is a random vector which is uniformly distributed on $[0,1]^s$. Then

$$E(f(\boldsymbol{X})) = \int_D f(\boldsymbol{X})d\boldsymbol{X} = I(f)$$

with

$$\sigma(f(\boldsymbol{X})) = \Big[\int_D f^2(\boldsymbol{X})d\boldsymbol{X} - (Ef(\boldsymbol{X}))^2\Big]^{1/2}$$

if they exist. Let $\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_n$ be independent samples of $\boldsymbol{X}$ and

$$I(f,n) = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{X}_i) \tag{2}$$

By the strong law of large numbers, $I(f,n)$ converges to $I(f)$ with probability one as $n \to \infty$. Moreover, $I(f,n)$ is approximately normally distributed when n is large by the central limit theorem. Also the law of the iterated logarithm shows that with probability one

$$\lim_{n\to\infty}\sup\sqrt{\frac{n}{2\ln(\ln n)}}\Big|\frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{X}_i) - I(f)\Big| = \sigma^2(f(\boldsymbol{X}))$$

Another approach is the use of the number-theoretic method (NTM). The number-theoretic method for evaluation of the integral is based on the theory of the uniform distribution. Let $P_n = \{\boldsymbol{X}_k, k = 1, 2, \cdots, n\}$ be an NT-net on $[0,1]^s$ with low discrepancy (cf. Fand and Wand (1994)). Then we may use

$$I(f, P_n) = \frac{1}{n}\sum_{k=1}^{n} f(\boldsymbol{X}_k) \tag{3}$$

as an approximation for $I(f)$.

Definition. *Let $(n; h_1, h_2, \cdots, h_s)$ be a vector with integral components satisfying $1 \le h_i < n$, $h_i \ne h_j$ $(i \ne j)$, $s < n$ and the greatest common divisors $(n, h_i) = 1$, $i = 1, \cdots, s$. Let*

$$\begin{cases} g_{ki} = kh_i (mod\, n) \\ x_{ki} = (2g_{ki} - 1)/2n \end{cases} \quad k = 1, 2, \cdots, n,\ i = 1, 2, \cdots, s \tag{4}$$

where we use the usual multiplicative operation module n such that g_{ki} is confined by $1 \le g_{ki} \le n$. Then the set $P_n = \{\boldsymbol{X}_k, k = 1, 2, \cdots, n\}$ is called the lattice point set of the generating vector $(n; h_1, h_2, \cdots, h_s)$. If the set P_n has the discrepancy $o(n^{-\frac{1}{2}})$, then the set P_n is called a glp set. It can be seen that x_{ki} defined in (4) can be easily calculated by

$$x_{ki} = \Big\{\frac{2kh_i - 1}{2n}\Big\} \tag{5}$$

where $\{x\}$ stands for the fraction part of x. In one dimension case $P_n = \{(2k-1)/2n$, $k = 1, 2, \cdots, n\}$. The convergence rate of $I(f, P_n)$ can reach $O(n^{-1}(\log n)^s)$ which is *better than Monte Carlo method. This is why the error of $I(f, P_n)$ is smaller than that of $I(f, n)$. Example 1 gives the comparison.*

Example 1. Let $f(x) = \frac{1}{2\pi} e^{-\frac{1}{2}(x_1^2+x_2^2)}$ which is normal density of $N(0, I_2)$. Of course, the true value of the integral on $[0, \infty]^2$ is 0.25. Table 1 gives the errors of evaluation of the integral by using NTM (glp) with different n and A, where we truncate $[0, \infty]^2$ by $[0, A]^2$. We list the errors of Monte Carlo method on Table 2. It is clear that NTM (glp) is better than MCM.

Table 1

$n\backslash A$	55	89	144	233	377	610	987	1597
2	−.02052	−.02071	−.02158	−.02165	−.02198	−.02201	−.02214	−.02215
3	.00043	.00121	−.00068	−.00038	−.00109	−.00098	−.00125	−.00121
4	−.00010	.00185	−.00006	.00067	−.00004	.00023	−.00004	.00007
5	−.00212	.00015	−.00083	.00003	−.00032	.00001	−.00012	.00000
6	−.00542	−.00244	−.00213	−.00099	−.00082	−.00038	−.00032	−.00015
7	−.01144	−.00601	−.00445	−.00234	−.00172	−.00090	−.00066	−.00035
8	−.02034	−.01045	−.00778	−.00404	−.00299	−.00155	−.00115	−.00059
9	−.03123	−.01580	−.01177	−.00608	−.00450	−.00233	−.00172	−.00089
10	−.04292	−.02209	−.01600	−.00846	−.00610	−.00324	−.00233	−.00124
11	−.05461	−.02933	−.02025	−.01118	−.00770	−.00428	−.00294	−.00164
12	−.06602	−.03757	−.02453	−.01426	−.00932	−.00546	−.00356	−.00209

Table 2

$n\backslash A$	55	89	144	233	377	610	987	1597
2	−.02437	−.00280	−.00698	−.01060	−.00971	−.01605	−.01799	−.02232
3	−.02562	.01603	.01276	.01210	.01389	.00494	.00210	−.00354
4	−.06736	−.00818	−.00665	−.00099	.00570	−.00023	−.00448	−.00896
5	−.11436	−.03963	−.03148	−.02290	−.00968	−.01069	−.01642	−.01889
6	−.15438	−.06759	−.05054	−.04436	−.02603	−.02310	−.03006	−.03012
7	−.18583	−.09100	−.06324	−.06298	−.04055	−.03524	−.04353	−.04136
8	−.20941	−.11033	−.07181	−.07882	−.05183	−.04549	−.05535	−.05186
9	−.22603	−.12591	−.07804	−.09239	−.05968	−.05335	−.06494	−.06139
10	−.23688	−.13844	−.08299	−.10419	−.06474	−.05916	−.07244	−.07000
11	−.24336	−.14890	−0.8733	−.11460	−.06800	−.06359	−.07837	−.07794
12	−.24691	−.15825	−.09153	−.12392	−.07044	−.06731	−.08331	−.08542

Even so, in this paper we shall discuss a Two-Stage Algorithm (TSA) of numerical evaluation of integrals on NTM. In Section 2 we shall give discussions of improvement. Two-Stage Algorithm of one dimension and s-dimension will be given in Section 3 and Section 4 respectively.

2. Discussions of the Accuracy in Evaluations by NTM

Although the NTM is a very good tool to solve the problems of numerical evaluation of multiple integrals, as we saw in Section 1. In some situations, the results are not accurate enough and we need some modifications.

(i) Suppose that the integrant function $f(\boldsymbol{X})$ is a continuous function defined on

$D = [0, \infty]^s$. We want to evaluate

$$I(f) = \int_D f(\boldsymbol{X}) d\boldsymbol{X}$$

by NTM. After choosing n, the number of points to evaluate the integrals, we should truncate $[0, \infty]^s$ by $D' = [0, A]^s$ or $D' = [0, A_1] \times [0, A_2] \times \cdots \times [0, A_s]$ and spread the points on it. It seems a dilemma: Since $I(f) < \infty$ and $f(x) \to 0$ as x_i $(i = 1, 2, \cdots, n)$ goes to ∞, if we pick small A (or A_i) we lose the integral on D/D' which can not be negligible, if we pick large A (or A_i), the large area leads the low density of the points, which may affect the accuracy of the integral since many points fall the area on which $f(x)$ almost vanishes. We may find that if we can choose a suitable pair of n and A, we can get the good evaluation. For instance, (55,4), (89, 5), (144, 4), (233, 5), (377, 4) in Table 1 are good pairs. On the other hand, large A leads poor evaluation. Pair (55, 4) is better than (1597, 7), that is we use more than 1500 points and get worse result if A is not suitable. The question here is how to choose n with a suitable A.

(ii) Suppose that $D = [a, b]^s$ with $-\infty < a < b < +\infty$ and $f(\boldsymbol{X})$ is a continuous function on D. If the variation of $f(\boldsymbol{X})$ is huge, only a few points of n are available for evaluating the integrals.

Example 2. Let $f(\boldsymbol{X}) = 50x_1^{20}x_2^{20}$ and $D = [0, 1]^2$. The values of $f(\boldsymbol{X})$ are small except $x_1 \cong 1$ and $x_2 \cong 1$. NTM distributes the points uniformly and $f(\boldsymbol{X})$ vanishes at most points. The remained points at which $f(\boldsymbol{X})$ is not near zero gives the poor results by NTM. Table 3 gives the poor results by MCM and NTM. The true value of $I(f)$ is 0.11338.

Table 3

n	h_2	MCM	NTM
55	34	.00544	.64713
89	55	.00348	.48143
144	89	.00562	.35306
233	144	.04543	.26534
377	233	.06712	.20787
610	377	.13816	.17195
987	610	.11869	.14944

(iii) NTM gives good evaluation of integral on whole D but not on the subdomains of it.

Example 3. Let $f(\boldsymbol{X}) = 50(x_1^{20} + x_2^{20})$ and $D = [0, 1]^2$. We pick $n = 144$, $h_2 = 89$ and get the evaluation of the integral 4.75788 by NTM. It is quite well. The true value of integral is 4.76191. Now, we divide D into subdomains: $\left[0, \frac{1}{3}\right] \times \left[0, \frac{1}{3}\right]$, $\left[0, \frac{1}{3}\right] \times \left[\frac{1}{3}, \frac{2}{3}\right]$, $\left[0, \frac{1}{3}\right] \times \left[\frac{2}{3}, 1\right]$, $\left[\frac{1}{3}, \frac{2}{3}\right] \times \left[0, \frac{1}{3}\right]$, $\left[\frac{1}{3}, \frac{2}{3}\right] \times \left[\frac{1}{3} \times \frac{2}{3}\right]$, $\left[\frac{1}{3}, \frac{2}{3}\right] \times \left[\frac{2}{3}, 1\right]$, $\left[\frac{2}{3}, 1\right] \times \left[0, \frac{1}{3}\right]$, $\left[\frac{2}{3}, 1\right] \times \left[\frac{1}{3}, \frac{2}{3}\right]$, and $\left[\frac{2}{3}, 1\right] \times \left[\frac{2}{3}, 1\right]$. Then we evaluate the integral on subdomains.

Table 4 tells us that on some D_i NTM underestimates the integrals $\left(\text{i.g. } \left[\frac{2}{3}, 1\right] \times \left[0, \frac{1}{3}\right]\right)$ and on some D_i NTM overestimates the integrals (i.g. $[2/3, 1], \times[2/3, 1]$). The total integral is evaluated very well but on some subdomains it is very bad, for instance on $[2/3,1]\times[2/3,1]$, the error is 0.5239911 over 33%. This also shows that NTM only views the whole pictures in average.

To overcome such difficulties, we suggest a Two-Stage method of NTM. The main idea is that we distribute the points according to the variations of the quadrature on the subdomains to detect the details.

Table 4

D_i	NTM	# (points)	True
$\left[0,\frac{1}{3}\right]\times\left[0,\frac{1}{3}\right]$	1.3643×10^{-10}	16	1.5174×10^{-10}
$\left[0,\frac{1}{3}\right]\times\left[\frac{1}{3},\frac{2}{3}\right]$	2.2884×10^{-4}	17	1.5912×10^{-4}
$\left[0,\frac{1}{3}\right]\times\left[\frac{2}{3},1\right]$	0.6024776	15	0.7934917
$\left[\frac{1}{3},\frac{2}{3}\right]\times\left[0,\frac{1}{3}\right]$	2.2884×10^{-4}	17	1.5912×10^{-4}
$\left[\frac{1}{3},\frac{2}{3}\right]\times\left[\frac{1}{3},\frac{2}{3}\right]$	2.0909×10^{-4}	15	3.1823×10^{-4}
$\left[\frac{1}{3},\frac{2}{3}\right]\times\left[\frac{2}{3},1\right]$	0.7206415	16	0.7936507
$\left[\frac{2}{3},1\right]\times\left[0,\frac{1}{3}\right]$	0.6024764	15	0.7934917
$\left[\frac{2}{3},1\right]\times\left[\frac{1}{3},\frac{2}{3}\right]$	0.7206495	16	0.7936507
$\left[\frac{2}{3},1\right]\times\left[\frac{2}{3},1\right]$	2.110974	17	1.586983
Total	4.75788	144	4.76191

3. One Dimension Case

We start with one dimension case. Let $f(x)$ be a continuous function on $[a,b]$. Two-Stage Algorithm:

Step 1. Distribute m points $\{x_i\}$ on $[a,b]$ uniformly, that is, $a=x_1<x_2<\cdots x_m<x_{m+1}=b$ with same $\Delta=x_{i+1}-x_i$ (If $a=-\infty$, we choose $x_1=a_0$ such that $f(a_0)$ is small enough. Similar thing happens if $b=+\infty$). Calculate the values of $f(x_i)$ $(x_i=1,2,\cdots,m+1)$.

Step 2. Investigate the variations of $f(x)$ in each interval. Let $h_i=|f(x_{i+1})-f(x_i)|$ as a measure of variation on $[x_i,x_{i+1}]$ and define $H=\sum_1^m h_i$, the "total variation". Furthermore, let

$$n_i=\begin{cases}\left[\dfrac{nh_i}{H}\right] & \text{if } \dfrac{nh_i}{H}\ge 1\\ 1 & \text{if } \dfrac{nh_i}{H}<1\end{cases}$$

where $[x]$ denotes the integer part of x.

Step 3. Use n_i as the number of points to evaluate the integral on $[x_i,x_{i+1}]$ by NTM.

Step 4. Sum up the values obtained in Step 3.

Remark. (i) The total number we used is $n^*=(n+1)+\sum_1^m n_i$;

(ii) It seems that the good evaluation will be gotten by increasing m as increasing n.

Example 4. Let $f(x)=50x^{20}$ on $[0,1]$, Table 5 compares the errors of evaluations of integral by MCM, NTM and TSA. The true value of integral is 2.380952.

Example 5. Denote by $\Phi(x)$, the normal distribution function, that is

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2} du = \int_{-\infty}^{x} \phi(u) du$$

Table 5

n	MCM	NTM(gp)	TSA $(m = 3)$	n^*
10	−2.237063	−0.377930	−0.056817	11
15	−2.081293	−0.177232	−0.023938	16
20	0.042024	−0.101614	−0.013241	21
25	−0.432550	−0.065614	−0.008479	26
30	−0.756873	−0.045786	−0.005956	31
40	0.867197	−0.025880	−0.003503	41
50	1.217550	−0.016600	−0.002387	51
60	1.462220	−0.011541	−0.001790	61
80	0.709920	−0.006500	−0.001202	81
100	0.602445	−0.004162	−0.000933	101
150	−0.126244	−0.001850	−0.000669	151
200	0.082538	−0.001041	−0.000578	201

Table 6

$n = n^*$	MCM	NTM (gp)	TSA $(m = 3)$	$\sum_1^m n_i$
9	0.02706314	0.02137493	0.02188900	5
10	0.02435687	0.02163402	0.02216353	6
11	0.03733996	0.02182641	0.02231307	7
12	0.03427031	0.02197313	0.02240336	8
13	0.03163413	0.02208753	0.02246202	9
14	0.02937456	0.02217845	0.02250227	10
15	0.02749133	0.02225188	0.02253105	11
16	0.02577312	0.02231203	0.02255236	12
17	0.02425705	0.02236193	0.02256857	13
18	0.03112461	0.02240377	0.02258119	14
19	0.02948647	0.02243919	0.02259121	15
20	0.02807975	0.02246945	0.02259929	16
21	0.02674478	0.02249550	0.02260590	17
22	0.02552911	0.02251809	0.02261138	18
23	0.03105132	0.02253780	0.02261597	19
24	0.02975789	0.02255510	0.02261986	20
29	0.02506723	0.02261650	0.02263257	25
34	0.02156441	0.02265289	0.02263929	30
39	0.01946303	0.02267622	0.02264327	35
44	0.02431821	0.02269205	0.02264583	40
104	0.02254400	0.02273972	0.02265266	100

We want to evaluate $1-\Phi(2)$. Since $\phi(x)$ goes to zero as $u \to \infty$ quickly and $1-\Phi(7) < 10^{-9}$, we consider the interval[2, 7] and compute $\Phi(7)-\Phi(2)$ by MCM, NTM and TSA. Table 6 lists the results where we let $n^* = (m+1) + \sum_1^m n_i$. The value of $\Phi(7) - \Phi(2)$ is 0.02275 by the statistical table. Table 6 gives us the impression that for small n

(up to 29) TSA is better than NTM and MCM, but for large n NTM is better. Here we point out: we prefer choosing large m when n is a fixed large number. Although in this situation $\sum_{l}^{m} n_i$, the number of points which we use to evaluate the integral, is smaller relatively, the accuracy will be promoted. On the last line of Table 6, the value of TSA ($m = 3$) is 0.02265266. It is worse than that of NTM. But if we let $m = 20$, it is 0.02273807; and if we let $m = 30$, it is 0.02274179. It seems that there is a suitable $\alpha = \alpha(n) < 1$ and we can get good result by choosing $m \cong n\alpha$.

4. S-dimension Case

We develop the idea of Section 3 to s-dimension case. Let D be a domain in R^s and $f(\boldsymbol{X})$ be a continuous function on D. We want to calculate

$$I(f) = \int_D f(\boldsymbol{X}) d\boldsymbol{X}$$

First of all, we can find a rectangle of D, say D^*, on which $f(\boldsymbol{X})$ is bounded such that

$$\Delta = \int_{D/D^*} f(\boldsymbol{X}) d\boldsymbol{X} \tag{8}$$

can be negligible. Then we evaluate

$$I(f) = \int_{D^*} f(\boldsymbol{X}) d\boldsymbol{X} \tag{9}$$

Two-Stage Algorithm:

Step 1. Divide D^* into r rectangles and let the volumes of the rectangles as equal as possible.

Step 2. Let $E_1, E_2, \cdots, E_r$ be the rectangles in Step 1, we measure the variations of $f(\boldsymbol{X})$ in $E_i = [a_{i1}, b_{i1}] \times [a_{i2}, b_{i2}] \times \cdots \times [a_{is}, b_{is}]$ by

$$h_i = \max_{U,V} |f(\boldsymbol{U}) - f(\boldsymbol{V})| \quad (i = 1, 2, \cdots, s)$$

where $\boldsymbol{U}, \boldsymbol{V}$ are corner points of E_i, i.e., $\boldsymbol{U}, \boldsymbol{V}$ with the form of $(e_{i1}, e_{i2}, \cdots, e_{is})$ ($e_{ij} = a_{ij}$ or b_{ij}).

Step 3. Let $n_i = [nh_i/H] + 1$, where $H = \sum_{i=1}^{r} h_i$

Step 4. Use n_i as the number of points to evaluate the integral on E_i

Step 5. Sum up the values obtained in Step 4.

Example 6. We compute multivariate normal distribution for $s = 2$ with $\mu_1 = \mu_2 = 0$, $\sigma_1 = \sigma_2 = 1$ and $\rho_{12} = 0$. The probability that $\boldsymbol{X}$ falls on the first orthant is called the orthant probability. Gupta (1963) provided a comprehensive review. Steak (1962) gave a substantial review of the results pertaining to orthant probabilities in the equicorrelated case, and Johnson and Kotz (1972) presented some additional results and references. Here we choose $D = [0, 10] \times [0, 10]$ and believe that the probability $\boldsymbol{X}$ falls on $[0, \infty] \times [0, \infty]/[0, 10] \times [0, 10]$ is very small.

Table 7

$n(h_2)$		Evaluation
55	(34)	0.2070753
89	(55)	0.2279124
144	(89)	0.2340000
233	(144)	0.2415409
377	(233)	0.2439044
610	(377)	0.2467571
987	(610)	0.2476715

Table 7 lists the results by NTM (glp). It converges slowly to 0.25. If we use TSA, we only choose $n = 144$ and the evaluation is 0.2481206 which is better than NTM (glp) of $n = 987$.

The details are the following:

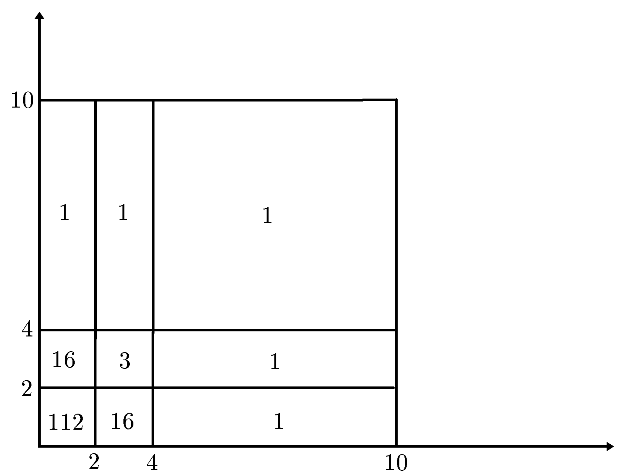

Figure 1

Let lines $x_1 = 2$, $x_1 = 4$, $x_2 =$ and $x_2 = 4$ divide $[0, 10] \times [0, 10]$ into 9 rectangles as Fig.1. Measure the variation of $\phi(x_1, x_2) = (2\pi)^{-1} \exp\left(-\frac{1}{2}x_1^2 - \frac{1}{2}x_2^2\right)$ in each rectangle and distribute 144 points according to c_i (see Fig.1). They almost concentrate on $[0, 2] \times [0, 2]$.

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