STUDIA UNIV. "BABEŞ–BOLYAI", MATHEMATICA, Volume **XLVIII**, Number 3, September 2003

WEIGHTED UNIFORM SAMPLING METHOD BASED ON SPLINE FUNCTIONS

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Dedicated to Professor Gheorghe Micula at his 60^{th} *anniversary*

Abstract. The weighted uniform sampling method to reduce of variance is investigated by using the multivariate Schoenberg spline operator on the unit hypercube. The new estimators obtained for the random numerical integration are numerically compared with the crude Monte Carlo estimators.

1. Introduction

It is known that definite integrals can be estimated by probabilistic considerations, and these are rather when multiple integrals are concerned. The integral is interpreted as the mean value of certain random variable, which is an unknown parameter. To estimate this parameter, i.e. the definite integral, one regards the sample mean of the sampling from a suitable random variable. This sample mean is an unbiased estimator for the definite integral and is referred as *the crude Monte Carlo estimator*.

Generally, this method is not fast–converging ratio to the volume of sampling, and efficiency depends on the variance of the estimator, which is expressed by the variance of the integrand. Consequently, for improving the efficiency of Monte Carlo method, it must reduce as much as possible the variance of the integrated function. There is a lot of procedures for reducing of the variance in the Monte Carlo method. In the following we approach the reducing of variance by the so–called *weighted uniform sampling method*, using the multivariate Schoenberg spline operator on the unit hypercube.

Numerical experiments are considered comparatively with the crude Monte Carlo estimates.

2. Multivariate B-spline functions

Let $\boldsymbol{D}_n = [0,1]^n$ be the n–dimensional unit hypercube. We consider the fixed vectors $\boldsymbol{m} = (m_1, \ldots, m_n)$ and $\boldsymbol{k} = (k_1, \ldots, k_n)$, whose components are integer positive values, namely $m_i > 0$ and $k_i > 1$, $i = \overline{1,n}$.

Received by the editors: 09.04.2003.

An extended rectangular partition $\boldsymbol{\Delta}$ of the domain $\boldsymbol{D}_n$ is defined by the following one–dimensional extended partitions:

$$\Delta_i \colon t_1^{(i)} = \cdots = t_{k_i}^{(i)} = 0 < t_{k_i+1}^{(i)} \leqslant \cdots \leqslant t_{k_i+m_i-1}^{(i)} < 1 = t_{k_i+m_i}^{(i)} = \cdots = t_{2k_i+m_i-1}^{(i)},$$

for all $i = \overline{1,n}$, where $t_j^{(i)} < t_{k_i+j}^{(i)}$, $j = \overline{1, k_i + m_i - 1}$.

If one denotes the multi–index set

$$\boldsymbol{J} = \left\{ \boldsymbol{j} = (j_1, \ldots, j_n) \;\middle|\; j_i = \overline{1, m_i + 2k_i - 1},\, i = \overline{1,n} \right\},$$

the partition $\boldsymbol{\Delta}$ is given by the cartesian product

$$\boldsymbol{\Delta} = \Delta_1 \times \cdots \times \Delta_n = \left\{ \boldsymbol{t_j} = \left(t_{j_1}^{(1)}, \ldots, t_{j_n}^{(n)} \right) \;\middle|\; \boldsymbol{j} \in \boldsymbol{J} \right\}.$$

The points of $\boldsymbol{\Delta}$ are called *knots* of the partition.

Using the knots of the partition $\boldsymbol{\Delta}$, one defines *the* (n*–variate*) *B–spline functions*

$$\boldsymbol{M_{i,k}}(\boldsymbol{x}) = M_{i_1,k_1}^{(1)}(x_1) \cdots M_{i_n,k_n}^{(n)}(x_n), \quad \boldsymbol{x} = (x_1, \ldots, x_n) \in \boldsymbol{D}_n, \tag{1}$$

for every multi–index $\boldsymbol{i} = (i_1, \ldots, i_n) \in \boldsymbol{I}$, where

$$\boldsymbol{I} = \left\{ \boldsymbol{i} = (i_1, \ldots, i_n) \;\middle|\; i_j = \overline{1, m_j + k_j - 1},\, j = \overline{1,n} \right\}.$$

The factors from the right side of the formula (1) are *the* (*one–variate*) *B–spline functions*, i.e.

$$M_{i_j,k_j}^{(j)}(x_j) = \left[t_{i_j}^{(j)}, \ldots, t_{i_j+k_j}^{(j)}; k_j (t - x_j)_+^{k_j-1} \right], \; i_j = \overline{1, m_j + k_j - 1}, \; j = \overline{1,n},$$

where $[z_0, z_1, \ldots, z_r; f(t)]$ denotes the r-th divided difference relative to the knots z_0, z_1,..., z_r of the function $f(t)$.

The normalized (n*–variate*) *B–spline* functions are defined by

$$\boldsymbol{N_{i,k}}(\boldsymbol{x}) = N_{i_1,k_1}^{(1)}(x_1) \cdots N_{i_n,k_n}^{(n)}(x_n), \quad \boldsymbol{x} = (x_1, \ldots, x_n) \in \boldsymbol{D}_n, \tag{2}$$

for every $\boldsymbol{i} = (i_1, \ldots, i_n) \in \boldsymbol{I}$, where

$$N_{i_j,k_j}^{(j)}(x_j) = \frac{t_{i_j+k_j}^{(j)} - t_{i_j}^{(j)}}{k_j} M_{i_j,k_j}^{(j)}(x_j)$$

are *the* (*one–variate*) *normalized B–spline functions.* We recall the following properties of B–spline functions:

(i) $\boldsymbol{N_{i,k}}(\boldsymbol{x}) \geqslant 0,$

(ii) $\boldsymbol{N_{i,k}}(\boldsymbol{x}) = A_{\boldsymbol{i,k}} \boldsymbol{M_{i,k}}(\boldsymbol{x}), \quad A_{\boldsymbol{i,k}} = \prod_{j=1}^{n} \frac{t_{i_j+k_j}^{(j)} - t_{i_j}^{(j)}}{k_j},$

(iii) $\sum_{\boldsymbol{i} \in \boldsymbol{I}} \boldsymbol{N_{i,k}}(\boldsymbol{x}) = 1,$

(iv) $\int_{\boldsymbol{D}_n} \boldsymbol{M_{i,k}}(\boldsymbol{x})\, \boldsymbol{dx} = 1.$

3. Schoenberg spline operator

Using the knots of partition $\boldsymbol{\Delta}$, one defines *the nodes*

$$\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}} = \left(\xi^{(1)}_{i_1,k_1}, \ldots, \xi^{(n)}_{i_n,k_n}\right), \quad \boldsymbol{i} = (i_1, \ldots, i_n) \in \boldsymbol{I},$$

where

$$\xi^{(j)}_{i_j,k_j} = \frac{t^{(j)}_{i_j+1} + \cdots + t^{(j)}_{i_j+k_j-1}}{k_j - 1}, \quad i_j = \overline{1, m_j + k_j - 1},\ j = \overline{1,n}.$$

We remark that $0 = \xi^{(j)}_{1,k_j} < \xi^{(j)}_{2,k_j} < \cdots < \xi^{(j)}_{m_j+k_j-1,k_j} = 1, \quad j = \overline{1,n}$, and consequently the nodes $\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}$, $\boldsymbol{i} \in \boldsymbol{I}$, belong to $\boldsymbol{D}_n$.

The (n*–variate*) *Schoenberg spline* operator relative to a real function f defined on $\boldsymbol{D}_n$ is given by

$$S_{\boldsymbol{\Delta}}(f)(\boldsymbol{x}) = (S_{\boldsymbol{\Delta}} f)(\boldsymbol{x}) = \sum_{\boldsymbol{i} \in \boldsymbol{I}} \boldsymbol{N}_{\boldsymbol{i},\boldsymbol{k}}(\boldsymbol{x})\, f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right), \quad \boldsymbol{x} \in \boldsymbol{D}_n. \tag{3}$$

Some important properties are recalled here:

(i) $S_{\boldsymbol{\Delta}}(f)(\boldsymbol{x})$ is a polynomial spline of degree k_i in the i-th variable,

(ii) $S_{\boldsymbol{\Delta}}(f)$ defines a positive linear operator,

(iii) If $m_i = 1$, then $S_{\boldsymbol{\Delta}}(f)(\boldsymbol{x})$ is a polynomial of degree $k_i - 1$ in the i-th variable, and consequently if $m_i = 1$, for all $i = \overline{1,n}$, the $S_{\boldsymbol{\Delta}}(f)(\boldsymbol{x})$ is the multivariate Bernstein polynomial,

(iv) $S_{\boldsymbol{\Delta}}(f) = f$, for all $f(\boldsymbol{x}) = x_1^{s_1} \ldots x_n^{s_n}, \quad s_i = 0, 1,\ i = \overline{1,n}$,

(v) If $f \in C(\boldsymbol{D}_n)$, then $S_{\boldsymbol{\Delta}}(f)$ converges uniformly to the function f as $\frac{\|\Delta_1\|}{k_1} + \cdots + \frac{\|\Delta_n\|}{k_n} \to 0$, where $\|\Delta_i\|$ denotes the norm of the partition Δ_i.

Taking into account that

$$N^{(j)}_{i_j,k_j}(0) = \delta_{1,i_j}, \quad N^{(j)}_{i_j,k_j}(1) = \delta_{m_j+k_j-1,i_j}, \quad i_j = \overline{1, m_j + k_j - 1},\ j = \overline{1,n},$$

where $\delta_{r,s}$ denotes the Kronecker symbol, we have $S_{\boldsymbol{\Delta}}(f)(\boldsymbol{e}) = f(\boldsymbol{e})$, for all the vertices $\boldsymbol{e}$ of the hypercube $\boldsymbol{D}_n$.

4. Crude Monte Carlo method

Let $\boldsymbol{X}$ be an n–dimensional random variable having the probability density function $\rho\colon \mathbb{R}^n \to \mathbb{R}$. In the random numerical integration the multidimensional integral

$$I[\rho; f] = \int_{\mathbb{R}^n} \rho(\boldsymbol{x})\, f(\boldsymbol{x})\, \boldsymbol{dx} \tag{4}$$

is interpreted as the mean value of the random variable $f(\boldsymbol{X})$, where $f\colon \mathbb{R}^n \to \mathbb{R}$ usually belongs to $L^2_\rho(\mathbb{R}^n)$, in other words $\int_{\mathbb{R}^n} \rho(\boldsymbol{x})\, f^2(\boldsymbol{x})\, \boldsymbol{dx}$ exists, and therefore the mean value $I[\rho; f]$ exists.

Using a basic statistical technique, the mean value given by (4) can be estimated by taking N independent samples (random numbers) $\boldsymbol{x}_i$, $i = \overline{1,N}$, with the probability density function ρ. These random numbers are regarded as values of the independent identically distributed random variables $\boldsymbol{X}_i$, $i = \overline{1,N}$, i.e. sample variables with the common probability function ρ.

We use the same notation $\bar{I}_N[\rho;f]$ for the sample mean of random variables $f(\boldsymbol{X}_i)$, $i=\overline{1,N}$, and respectively for its value, i.e.

$$\bar{I}_N[\rho;f]=\frac{1}{N}\sum_{i=1}^{N}f(\boldsymbol{X}_i),$$

$$\bar{I}_N[\rho;f]=\frac{1}{N}\sum_{i=1}^{N}f(\boldsymbol{x}_i).$$

The estimator $\bar{I}_N[\rho;f]$ satisfies the following properties:

$$E\left(\bar{I}_N[\rho;f]\right)=I[\rho;f],\quad \text{(unbiased estimator of } I[\rho;f]\text{)},$$

$$Var\left(\bar{I}_N[\rho;f]\right)\to 0,\quad N\to\infty,$$

$$\bar{I}_N[\rho;f]\to I[\rho;f],\quad N\to\infty,\quad \text{(with probability 1)}.$$

Taking into account these results, the crude Monte Carlo integration formula is defined by

$$I[\rho;f]=\int_{\mathbb{R}^n}\rho(\boldsymbol{x})f(\boldsymbol{x})\,\boldsymbol{dx}\approxeq\frac{1}{N}\sum_{i=1}^{N}f(\boldsymbol{x}_i). \tag{5}$$

It must remark that in (4) the domain of integration is only apparently the whole n–dimensional Euclidean space. Thus, it is possible that the density $\rho(\boldsymbol{x})=0$, $\boldsymbol{x}\notin\boldsymbol{D}$, where $\boldsymbol{D}$ is a region of the n–dimensional Euclidean space $\mathbb{R}^n$, therefore the integral (4) becomes

$$I[\rho;f]=\int_{\boldsymbol{D}}\rho(\boldsymbol{x})f(\boldsymbol{x})\,\boldsymbol{dx},$$

and the crude Monte Carlo method must be interpreted in an appropriate manner.

5. **Weighted uniform sampling method**

This method was given in [8], reconsidered in [11], and recently in [6] it was compared with other methods for reducing of the variance.

Let us consider the integral

$$I[f]=\int_{\boldsymbol{D}}f(\boldsymbol{x})\,\boldsymbol{dx}=V\int_{\boldsymbol{D}}\frac{1}{V}f(\boldsymbol{x})\,\boldsymbol{dx},$$

where $\boldsymbol{D}\subset\mathbb{R}^n$ and $V=\text{Volume}(\boldsymbol{D})$.

The crude Monte Carlo estimator for $I[f]$ is

$$\bar{I}_N^c[f]=\frac{V}{N}\sum_{i=1}^{N}f(\boldsymbol{X}_i),$$

with the sampling variables $\boldsymbol{X}_i$, $i=\overline{1,N}$, independent uniformly in the region $\boldsymbol{D}$, i.e. these have the common density probability function

$$\rho(\boldsymbol{x})=\begin{cases}\dfrac{1}{V}, & \text{if } \boldsymbol{x}\in\boldsymbol{D},\\[2mm] 0, & \text{if } \boldsymbol{x}\notin\boldsymbol{D}.\end{cases}$$

The method of weighted uniform sampling consists in the considering a function $g\colon \boldsymbol{D} \to \mathbb{R}$ such that

$$\int_{\boldsymbol{D}} g(\boldsymbol{x})\, \boldsymbol{dx} = 1,$$

and the corresponding sampling function

$$\bar{I}_N^w[g;f] = \left(\sum_{i=1}^{N} f(\boldsymbol{X}_i)\right) \Big/ \left(\sum_{i=1}^{N} g(\boldsymbol{X}_i)\right),$$

where $\boldsymbol{X}_i$, $i = \overline{1,N}$, are the same above sampling variables.

If one denotes by Θ_N and $\tilde{\Theta}_N$, the sample means of $f(\boldsymbol{X}_i)$ and respectively of $g(\boldsymbol{X}_i)$, $i = \overline{1,N}$, we have

$$\bar{I}_N^w[g;f] = \frac{\Theta_N}{\tilde{\Theta}_N} \cdot$$

Taking into account that the sample means

$$\Theta_N = \frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{X}_i) = \bar{I}_N^c[f]/V,$$

$$\tilde{\Theta}_N = \frac{1}{N}\sum_{i=1}^{N} g(\boldsymbol{X}_i) = \bar{I}_N^c[g]/V$$

are unbiased estimators for $I[f]$ and $I[g] = 1$ respectively, it results that

$$\frac{E(\Theta_N)}{E\left(\tilde{\Theta}_N\right)} = I[f] \cdot$$

However $\bar{I}_N^w[g;f]$ is a biased estimator for $I[f]$, satisfying only asymptotical relation

$$E\left(\bar{I}_N^w[g;f]\right) \approxeq I[f].$$

For the variance of the estimator $\bar{I}_N^w[g;f]$ we have [6]:

$$Var(\bar{I}_N^w[g;f]) = \frac{V^2}{N} Var[f(\boldsymbol{X}) - I[f]\, g(\boldsymbol{X})] + O\left(\frac{1}{N^2}\right),$$

that is

$$Var(\bar{I}_N^w[g;f]) \approxeq \frac{V^2}{N} Var[f(\boldsymbol{X}) - I[f]\, g(\boldsymbol{X})].$$

On the other hand we have

$$Var(\bar{I}_N^c[f]) = \frac{V^2}{N} Var[f(\boldsymbol{X})] \cdot$$

In this manner, the comparison of the variances of the two estimators $\bar{I}_N^c[f]$ and $\bar{I}_N^w[g;f]$ is reduced to compare the variances $Var[f(\boldsymbol{X})]$ and $Var[f(\boldsymbol{X}) - I[f]\, g(\boldsymbol{X})]$.

Because

$$Var[f(\boldsymbol{X})] - Var[f(\boldsymbol{X}) - I[f]\, g(\boldsymbol{X})] = I[f]\left[2Cov(f(\boldsymbol{X}), g(\boldsymbol{X})) - I[f]\,\sigma^2[g]\right],$$

the covariance $Cov\left(f\left(\boldsymbol{X}\right), g\left(\boldsymbol{X}\right)\right)$ controls the magnitude of difference of the two variances, it must that g has the same monotonicity as f.

In the following we consider the function g from the weighted uniform sampling method given by the multivariate spline function corresponding to the integrand f defined by Schoenberg spline operator.

If the integration region is the unit hypercube $\boldsymbol{D}_n$, the crude Monte Carlo estimator is

$$\bar{I}_N^c\left[f\right] = \frac{1}{N}\sum_{i=1}^{N} f\left(\boldsymbol{X}_i\right),$$

where the sampling variables $\boldsymbol{X}_i$, $i = \overline{1, N}$, are independent uniformly distributed on $\boldsymbol{D}_n$.

The function g from presented weighted uniform sampling method is the following

$$g\left(\boldsymbol{x}\right) = K \cdot \left(S_{\boldsymbol{\Delta}} f\right)\left(\boldsymbol{x}\right),$$

where $\left(S_{\boldsymbol{\Delta}} f\right)\left(\boldsymbol{x}\right)$ is given by (3) and the constant K is such that

$$\int_{\boldsymbol{D}_n} g\left(\boldsymbol{x}\right)\boldsymbol{dx} = 1.$$

From this condition we have that

$$g\left(\boldsymbol{x}\right) = \frac{\left(S_{\boldsymbol{\Delta}} f\right)\left(\boldsymbol{x}\right)}{\sum_{\boldsymbol{i}\in\boldsymbol{I}} A_{\boldsymbol{i},\boldsymbol{k}} f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right)} = \frac{\sum_{\boldsymbol{i}\in\boldsymbol{I}} \boldsymbol{N}_{\boldsymbol{i},\boldsymbol{k}}\left(\boldsymbol{x}\right) f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right)}{\sum_{\boldsymbol{i}\in\boldsymbol{I}} A_{\boldsymbol{i},\boldsymbol{k}} f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right)}.$$

Finally, the random numerical integration formula is given by

$$\bar{I}_N^w\left[g; f\right] = \frac{\left[\sum_{\boldsymbol{i}\in\boldsymbol{I}} A_{\boldsymbol{i},\boldsymbol{k}} f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right)\right]\left[\sum_{i=1}^{N} f\left(\boldsymbol{x}_i\right)\right]}{\sum_{i=1}^{N}\left[\sum_{\boldsymbol{i}\in\boldsymbol{I}} \boldsymbol{N}_{\boldsymbol{i},\boldsymbol{k}}\left(\boldsymbol{x}_i\right) f\left(\boldsymbol{\xi}_{\boldsymbol{i},\boldsymbol{k}}\right)\right]}. \tag{6}$$

The random points $\boldsymbol{x}_i$, $i = \overline{1, N}$, are independent uniformly distributed in the hypercube $\boldsymbol{D}_n$.

We must remark that the spline functions give a more flexible method than Bernstein polynomials, which have been used in [3], for the same uniform sampling method. This is because the nodes in the Schoenberg spline operator are not necessarily equidistant, like in the Bernstein operator. Consequently, if some smoothness informations for the integrand f are known, we can require more nodes in the domain of integration where the function f has a bed smoothness.

6. **Numerical experiments**

Numerical examples are considered in the unidimensional ($n = 1$) and bidimensional ($n = 2$) cases for the estimator (6) with the integrand f given by $f\left(x\right) = \frac{1}{1+x}$ and $f\left(x, y\right) = \frac{1}{1+x+y}$ respectively. The interior knots for the variable x are $0.1, 0.3, 0.5, 0.7, 0.9$, and $0.2, 0.5, 0.8$ for the variable y. The numerical results comprised in the following two tables compare the estimates obtained by the weighted uniform sampling technique and the crude Monte Carlo method.

Each table contains: the sampling volume N, the orders k (or k_1, k_2) of the spline functions, the estimates given by the two methods $\bar{I}_N^c[f]$ and $\bar{I}_N^w[g;f]$, the error estimates Err^c and Err^w respectively, and the ratio Err^c/Err^w. We also remark that the estimations and the error estimates from each row of tables represent the mean values in one hundred of samplings.

$$I[f] = \log 2 = 0.69314718...$$

N	k	$\bar{I}_N^c[f]$	$\bar{I}_N^w[g;f]$	Err^c	Err^w	Err^c/Err^w
50	2	0.6911300	0.6931458	2.017e-03	1.394e-06	1447.4
100	2	0.6910238	0.6931734	2.123e-03	2.621e-05	81.0
300	2	0.6921497	0.6931548	9.975e-04	7.649e-06	130.4
500	2	0.6922726	0.6931520	8.745e-04	4.836e-06	180.9
50	3	0.6911300	0.6931688	2.017e-03	2.161e-05	93.3
100	3	0.6910238	0.6931799	2.123e-03	3.274e-05	64.9
300	3	0.6921497	0.6931633	9.975e-04	1.609e-05	62.0
500	3	0.6922726	0.6931567	8.745e-04	9.477e-06	92.3
50	5	0.6911300	0.6931639	2.017e-03	1.674e-05	120.5
100	5	0.6910238	0.6931832	2.123e-03	3.598e-05	59.0
300	5	0.6921497	0.6931694	9.975e-04	2.219e-05	44.9
500	5	0.6922726	0.6931605	8.745e-04	1.336e-05	65.5

$$I[f] = \log \frac{27}{16} = 0.5232481...$$

N	k_1	k_2	$\bar{I}_N^c[f]$	$\bar{I}_N^w[g;f]$	Err^c	Err^w	Err^c/Err^w
50	2	2	0.5208017	0.5233035	2.446e-03	5.539e-05	44.2
100	2	2	0.5216731	0.5232890	1.575e-03	4.082e-05	38.6
300	2	2	0.5225268	0.5232643	7.214e-04	1.615e-05	44.7
50	2	3	0.5208017	0.5233042	2.446e-03	5.610e-05	43.6
100	2	3	0.5216731	0.5232827	1.575e-03	3.452e-05	45.6
300	2	3	0.5225268	0.5232604	7.214e-04	1.227e-05	58.8
50	2	4	0.5208017	0.5233092	2.446e-03	6.108e-05	40.1
100	2	4	0.5216731	0.5232843	1.575e-03	3.618e-05	43.5
300	2	4	0.5225268	0.5232619	7.214e-04	1.380e-05	52.3
50	3	4	0.5208017	0.5233095	2.446e-03	6.133e-05	39.9
100	3	4	0.5216731	0.5232821	1.575e-03	3.393e-05	46.4
300	3	4	0.5225268	0.5232607	7.214e-04	1.260e-05	57.3
50	4	4	0.5208017	0.5233096	2.446e-03	6.146e-05	39.8
100	4	4	0.5216731	0.5232812	1.575e-03	3.310e-05	47.6
300	4	4	0.5225268	0.5232622	7.214e-04	1.403e-05	51.4
50	5	5	0.5208017	0.5233079	2.446e-03	5.980e-05	40.9
100	5	5	0.5216731	0.5232791	1.575e-03	3.097e-05	50.8
300	5	5	0.5225268	0.5232640	7.214e-04	1.582e-05	45.6

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