Speeding-up Monte Carlo: Nearest Neighbors estimates as Control Variates

François Portier

ENSAI, CREST

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Joint work with Rémi Leluc, Johan Segers and Aigerim Zhuman

CREST
CENTER FOR RESEARCH IN ECONOMICS AND STATISTICS

ENSAI
École nationale de la statistique et de l'analyse de l'information

Introduction : Why bother with random sampling?

A guided tour in Monte Carlo

- Sampling techniques
  - Importance sampling and MCMC
  - Quasi-Monte Carlo
  - Determinantal sampling
- Post-hoc scheme
  - Adaptive volume calculation
  - Control variates

Nearest neighbor as control functionals

- Control functional
- Nearest neighbor background
- Construction of the estimate

Numerical illustration

The underlying integration problem

Let μ be a probability measure on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$ and $\varphi : \mathbb{R}^d \to \mathbb{R}$ be integrable.

- **Goal** : Estimate

$$\mu(\varphi) = \int \varphi \, \mathrm{d}\mu$$

- **Constraint:** only based on $\varphi(x_1), \ldots, \varphi(x_n)$, where $x_1, \ldots, x_n$ are called nodes. Here φ might be black-box function[1].

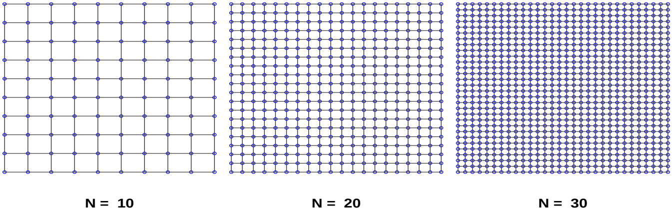
- **Central question:** number of nodes n necessary to obtain a given accuracy

[1] if φ has an explicit form, e.g., $\varphi(x) = \exp(-\|x\|^2)$, then some approximation techniques are probably more appropriate

Riemann's sums method for $\int_{[0,1]^d} \varphi(x)\,\mathrm{d}x$:

$$N^{-d} \sum_{x_i \in \text{Grid}} \varphi(x_i),$$

where $\text{Grid} = \{(i_1/N, \dots, i_d/N) \,:\, 1 \leq i_k \leq N,\ \forall k = 1, \dots, d\}$



Error bound

We have

$$\sup_{\varphi \in \Phi_d} \left| N^{-d} \sum_{x \in \text{Grid}} \varphi(x) - \int_{[0,1]^d} \varphi(x)\,\mathrm{d}x \right| \leq N^{-1}.$$

with $\Phi_d = \left\{ \varphi : [0,1]^d \mapsto \mathbb{R} \,:\, |\varphi(x) - \varphi(y)| \leq \max_{k=1,\dots,d} |x_k - y_k| \right\}$

Consider linear integration rules

$$\sum_{i=1}^{N^d} w_i \varphi(x_i).$$

The accuracy of the best algorithm over a class Φ_d is

$$e(N^d, \Phi_d) = \inf_{(w_i, x_i)_{i=1\ldots N^d}} \sup_{\varphi \in \Phi_d} \left| \sum_{i=1}^{N^d} w_i \varphi(x_i) - \int_{[0,1]^d} \varphi(x)\, \mathrm{d}x \right|$$

Complexity results (Novak, 2016)

$$e(N^d, \Phi_d) = \left(\frac{d}{2d+2} \right) N^{-1}$$

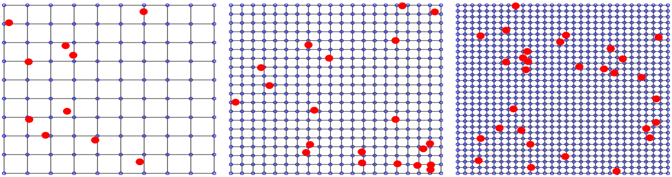
The midpoint rule is the optimal algorithm[2].

[2] If $\Phi_{k,d} = \{\varphi : [0,1]^d \to \mathbb{R}\,,\ \|D_\alpha \varphi\|_\infty \leq 1, \forall |\alpha| \leq k\}$, then $e(N^d, \Phi_{k,d}) \simeq N^{-k}$.

Monte Carlo method for $\int_{[0,1]^d} \varphi(x)\,\mathrm{d}x$:

Let $(X_1, \ldots, X_n) \stackrel{iid}{\sim} \mathcal{U}[0,1]^d$, compute

$$n^{-1} \sum_{i=1}^{n} \varphi(X_i)$$



n= 10 n= 20 n= 30

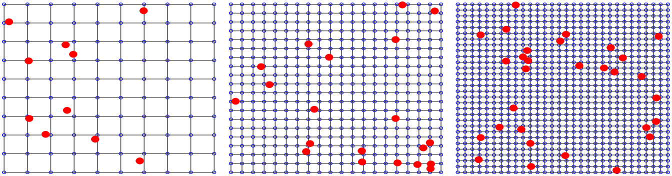
Uniform results (Talagrand, 1996; McDiarmid, 1998; Giné and Guillou, 2001)

with probability larger than $1-\delta$,

$$\sup_{\varphi\in\Phi} \left| n^{-1} \sum_{i=1}^{n} \varphi(X_i) - \int_{[0,1]^d} \varphi(x)\,\mathrm{d}x \right| \leq 2\mathbb{E}|R_n(\Phi)| + \sqrt{\frac{2\log(2/\delta)}{n}}$$

If for instance, Φ is of VC-type, $\mathbb{E}|R_n(\Phi)| \simeq n^{-1/2}$.

Summary



n= 10 n= 20 n= 30

	determisitic	random	Monte Carlo
$e(n, \Phi_d)$	$n^{-1/d}$	$n^{-1/d}$ $n^{-1/2}$	$n^{-1/2}$
$e(n, \Phi_d^k)$	$n^{-k/d}$	$n^{-k/d}$ $n^{-1/2}$	$n^{-1/2}$

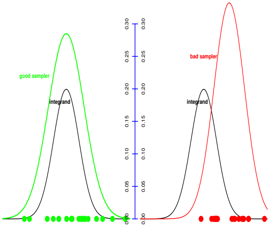
Monte Carlo

- Draw $X_1, \dots, X_n \overset{iid}{\sim} \mu$
- Compute $\frac{1}{n}\sum_{i=1}^{n} g(X_i)$

MCMC

- Draw $X_1, \dots, X_n \rightsquigarrow \mu$
- Compute $\frac{1}{n}\sum_{i=1}^{n} g(X_i)$

Importance sampling, stratified sampling...



Control variates

- Use the knowledge of $\int h_j d\mu = 0$ for functions $h_1, \dots, h_m$

Others

- Quasi-Monte Carlo
- DPP sampling

Books : Evans and Swartz (2000), Robert and Casella (2004), Glasserman (2003), Owen (2013a)

Sampling tool 1 (Importance sampling and MCMC)

A similar idea: sampling near target distribution

- (MCMC) $X_1, \ldots, X_n$ a Markov chain such that $(X_n) \rightsquigarrow \mu$

$$n^{-1} \sum_{i=1}^{n} g(X_i)$$

- (AIS) $X_i \sim q_{i-1}$ such that $q_i \to f$

$$n^{-1} \sum_{i=1}^{n} g(X_i)/q_{i-1}(X_i)$$

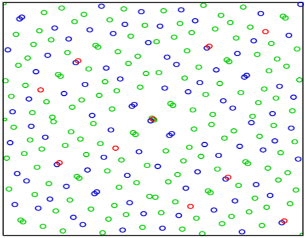
Highlights

- Relevant to Bayesian statistics
- the rate of convergence is not improved (only the asymptotic variance) (Robert and Casella, 2004; Evans and Swartz, 2000)

Sampling tool 2 (QMC)

Highlights

- Low-discrepancy sequences
- Using the Hardy-Krause variation of f
- Randomized version exists
- rate : $n^{-1}\log(n)^{d-1}$ (not under the same function class)



Issues

- Deterministic methods for the uniform measure $d\mu = \mathbb{I}_{[0,1]^d}$
- The bound decreases only when n is $\exp(d)$
- Hardy-Krauss variation is difficult to handle in practice

Sampling tool 3 (DPP)

A "random" quadrature rule

- Suppose that you have h_k such that $\int \varphi_k \varphi_j d\mu = \delta_{k,j}$ and define

$$K_n(x,y) = \sum_{i=1}^{n} \varphi_i(x)\varphi_i(y)$$

- $X_1, \dots, X_n$ follows a DPP with kernel K_N and reference measure μ. The estimate is

$$\sum_{i=1}^{n} \frac{g(X_i)}{K_N(X_i, X_i)}$$

Results (Bardenet and Hardy, 2020)

- unbiased
- rate : $n^{-1/2} n^{-1/2d}$

Issues

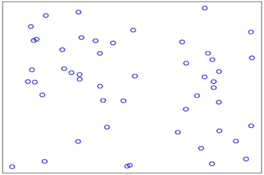
- Hard to sample from DPP (n^3 operations last time I checked)
- φ_k might not be known as it depends on μ

Post-hoc scheme 1: volume calculation

Integration problem

- $x_1, \ldots, x_n$ random points
- Observe $(x_1, g(x_1)), \ldots, (x_n, g(x_n))$
- Goal : Evaluate $\int g(x)dx$

$x_1, \ldots, x_n$ in $[0,1]^2$ with uniform law



Monte-Carlo: $n^{-1} \sum_{i=1}^{n} g(x_i)$

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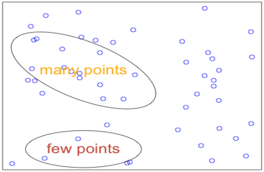

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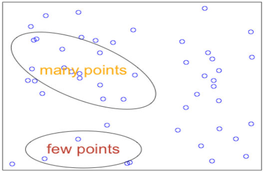
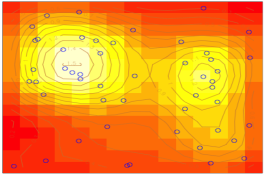


Monte-Carlo: $n^{-1} \sum_{i=1}^{n} g(x_i)$

$\widehat{f}(x) = n^{-1} \sum_{i=1}^{n} K(x - x_i)$



$n^{-1} \sum_{i=1}^{n} \frac{g(x_i)}{\widehat{f}(x_i)}$

(Delyon and Portier, 2016)

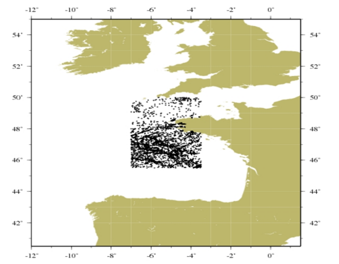
Advantages

- x_i's distribution is not used
- fast rates $n^{-1/2} n^{-(k-d)/2(k+d)}$
- robust to dependent x_i's

Difficulties

- computing time is n^2
- choice of the bandwidth
- dimension curse $k > d$

Evaluate average temperature of oceans (Azaïs et al., 2018)



Initial project was: use Voronoi cells volume to build the estimate (rate in $n^{-k/d}$)

Post-hoc scheme 2: Control variate

Idea Glasserman (2004); Owen (2013b)

- Use the knowledge of $h_1, \ldots, h_m$ such that

$$\int h_k d\mu = 0 \qquad k = 1, \ldots, m$$

- Let $X_1, \ldots, X_n$ be iid with common distribution μ

$$n^{-1} \sum_{i=1}^{n} \{g(X_i) - \sum_{k=1}^{m} \beta_k h_k(X_i)\}$$

First properties

- Unbiased property
- variance reduction up to $\min_{\beta \in \mathbb{R}^m} \mathbb{E}[(g(X_1) - \sum_{k=1}^m \beta_k h_k(X_1))^2]$

Issues

- Construction of h_k
- Computation of $\beta_1, \ldots, \beta_m$

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Numerical illustration

Control functional (Oates et al., 2017; Portier and Segers, 2019)

(i) building a function $\hat{g}$ of which the integral $\mu(\hat{g})$ is known
(ii) using this function to derive an enhanced Monte-Carlo estimate with the centered random variables $[\hat{g}(X_i) - \mu(\hat{g})]$ as

$$\hat{\mu}_n^{(CV)}(g) = \frac{1}{n} \sum_{i=1}^{n} \{g(X_i) - (\hat{g}(X_i) - \mu(\hat{g})\} .$$

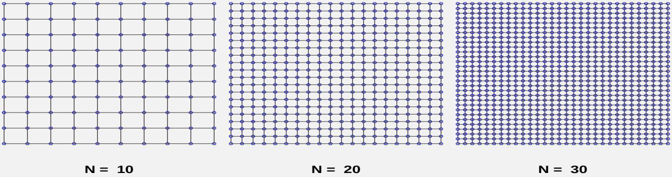
First property

Whenever the function $\hat{g}$ is constructed from another sample $\tilde{X}_1, \ldots \tilde{X}_n$ being either independent from $X_1, \ldots X_n$ or not random,

$$\mathbb{E}[(\hat{\mu}_n^{(CV)}(g) - \mu(g))^2] = \frac{1}{n} \int \mathbb{E}[(g - \hat{g})^2] d\mu$$

Example 1

Partitioning estimate



- μ is the uniform measure on $[0,1]^d$ and $\mathcal{G}$ is a regular grid with $n = N^d$ elements
- Define

$$\hat{g} = \text{pieceswise constant over elements of the grid}$$

Standard results give $\sqrt{\int (g - \hat{g})^2 \mathrm{d}\mu} = O(n^{-1/d})$

- implying an integration method with rate

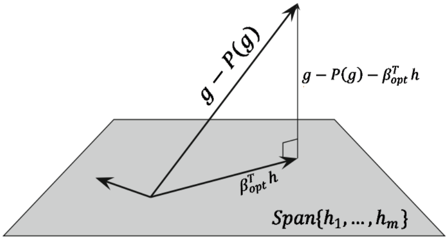
$$n^{-1/2} n^{-1/d}$$

(restrictive constraint $n = N^d$ plus $2n$ evaluations are needed)

Example 2

Ordinary least-squares

- Relying on two different samples, (Oates et al., 2017) propose to (a) build an RKHS control variate $\hat{g}$ and (b) compute the Monte Carlo average requires twice the number of request to g
- Using the same sample to $X_1, \ldots, X_n$ to approximate $\hat{g}$ has been investigated in Leluc et al. (2021) OLS is used to fit g with m basis functions. Theory says that the rates is in $n^{-1/2}m^{-1/d}$.
- Unfortunately, a constraint on m is needed (see for instance Remark 12 in Leluc et al. (2021)) which in general prevents from using $m = n$ control variates.



Definition (Nearest neighbor and distance)

Given a set of points $X_1, \ldots, X_n$ and any point $x \in \mathbb{R}^d$, define $\hat{N}_n(x)$ as the nearest neighbor of x among $X_1, \ldots, X_n$ and $\hat{\tau}_n(x)$ the associated distance, i.e.,

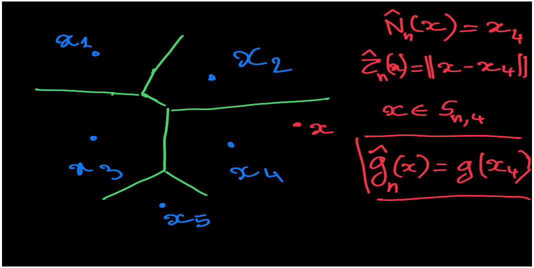
$$\hat{N}_n(x) \in \underset{Y \in \{X_1, \ldots, X_n\}}{\arg\min} \|x - Y\|, \qquad \hat{\tau}_n(x) = \|\hat{N}_n(x) - x\|.$$

Definition (Voronoï cells and volumes)

The Voronoï cells associated to $(X_i)_{i \geq 1}$ are given by

$$S_{n,i} = \{x \in \mathbb{R}^d : \hat{N}_n(x) = X_i\}.$$

Their volume with respect to μ is denoted by $V_{n,i} = \mu(S_{n,i})$.



Construction of the estimate

Definition (1-NN estimate of g)

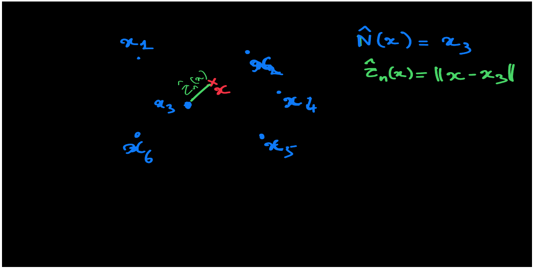
$$\forall x \in \mathbb{R}^d, \quad \hat{g}_n(x) = g(\hat{N}_n(x))$$

It is piece-wise constant on the Voronoï partition

$$\hat{g}_n(x) = \sum_{i=1}^{n} g(X_i) \mathbb{1}_{S_{n,i}}(x)$$

Main idea

- g is accessible without noise (no variance term) $\Rightarrow$ We take the 1-NN



PB 1

- The use of $\hat{g}_n$ as control functional leads to unsatisfactory strategy due to the over-fitting equation
$$\hat{g}_n(X_i) = g(X_i)$$

Solution 1

- Use the leave-one-out $\hat{g}_n^{(i)}(X_i)$ defined as the standard 1-NN except that the i-th observation has been removed

Following the previous idea we introduce

$$\hat{\mu}_n^{(\mathrm{NN-loo})}(g) = \frac{1}{n}\sum_{i=1}^{n}\{g(X_i) - (\hat{g}_n^{(i)}(X_i) - \mu(\hat{g}_n^{(i)}))\}, \tag{1}$$

Construction of the estimate

PB 2

- $\mu(\hat{g}_n^{(i)})$ implies to compute many integrals

Solution 2

- $\mu(\hat{g}_n^{(i)}) \simeq \mu(\hat{g}_n)$

The working estimate is then

$$\hat{\mu}_n^{(\mathrm{NN})}(g) = n^{-1} \sum_{i=1}^{n} \{g(X_i) - (\hat{g}_n^{(i)}(X_i) - \mu(\hat{g}_n))\}. \quad (2)$$

Degree and expected degree (isolation of point)

Denote by $S_{n,j}^{(i)}$ ($V_{n,j}^{(i)}$) (the volume of) the j-th Voronoï cell obtained from the sample $\mathcal{X}^{(i)} = \{X_1, \ldots, X_n\} \backslash X_i$.

Definition

The degree of point X_j is defined as

$$\hat{d}_j = \sum_{i \neq j} \mathbb{1}_{S_{n,j}^{(i)}}(X_i).$$

The expected degree is

$$\hat{c}_j = \sum_{i \neq j} V_{n,j}^{(i)}.$$

Proposition (Quadrature rules)

The estimate $\hat{\mu}_n^{(NN-loo)}(g)$ can be expressed as a linear estimates of the form

$$\hat{\mu}_n^{(\mathrm{NN-loo})}(g) = \sum_{i=1}^{n} w_{i,n}^{(\mathrm{NN-loo})} g(X_i)$$

where $w_{i,n}^{(\mathrm{NN-loo})} = (1 + \hat{c}_i - \hat{d}_i)/n$ (the weights does not depend on g)

Convergence rate

Proposition

Assume that $g : \mathbb{R}^d \to \mathbb{R}$ *is L-Lipschitz,* $\inf_{x \in \mathcal{X}} f(x) > b$ *and* $\sup_{x \in \mathcal{X}} f(x) < U$*. Then we have*

$$\mathbb{E}\Big[\big(\hat{\mu}_n^{(\mathrm{NN-loo})}(g) - \mu(g)\big)^2\Big] \leq C n^{-1} n^{-2/d}$$

Method implementation

The method CVNN returns the value of $\hat{\mu}_n^{(NN)}(g)$ for which the integral $\int \hat{g}_n d\mu$ is replaced by a Monte Carlo estimate that uses $M = n^2$ generation. That is

$$\int \hat{g}_n d\mu \simeq M^{-1} \sum_{i=1}^{M} \hat{g}_n(\tilde{X}_i),$$

where $\tilde{X}_i$ are i.i.d draws according to μ.

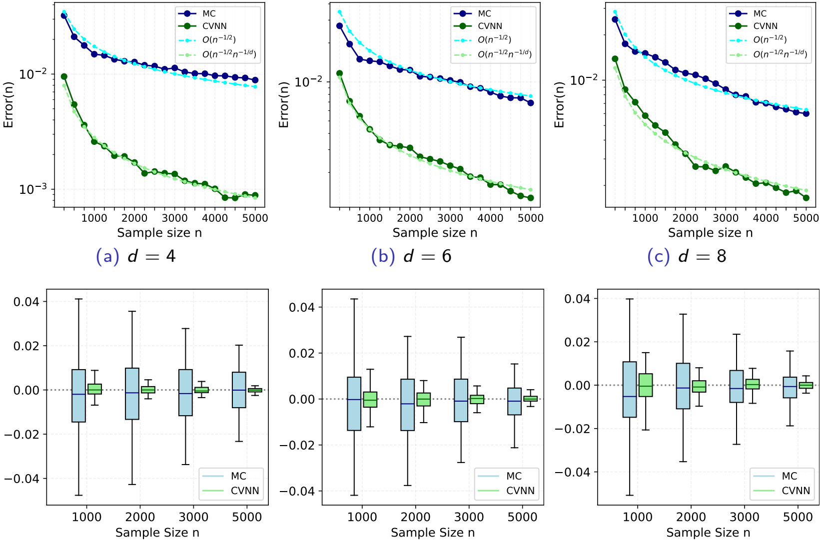
Integrand

$$g_1(x) = 1 + \sin(\pi(2d^{-1} \sum_{i=1}^{d} x_i - 1)) \qquad g_2(x) = \prod_{i=1}^{d} \log(2)2^{1-x_i},$$

(both integrate to 1 on $[0,1]^d$)

Parameters

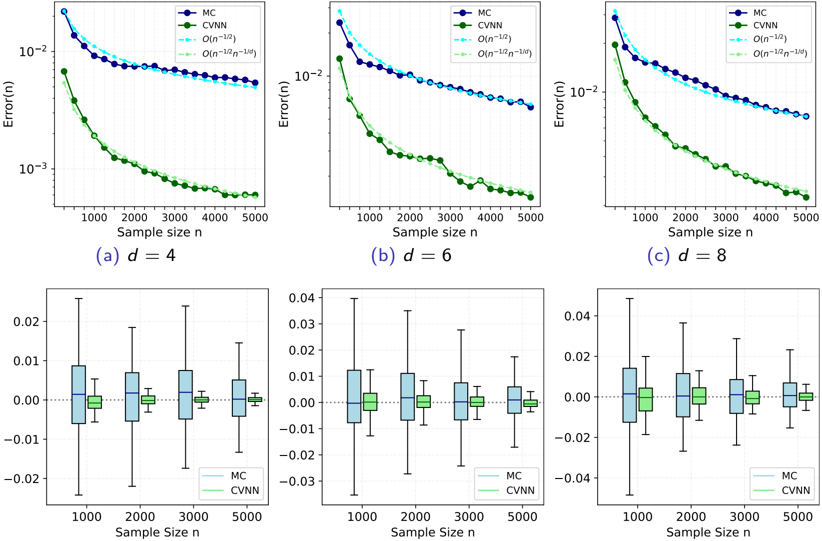
- dimensions $d \in \{4; 6; 8\}$,
- from $n = 250$ to $n = 5,000$
- performance measured with $\mathbb{E}[|\hat{\mu}_n^{(\mathrm{NN})}(g) - \mu(g)|^2]^{1/2}$



(a) $d = 4$ (b) $d = 6$ (c) $d = 8$

(d) $d = 4$ (e) $d = 6$ (f) $d = 8$

Figure: Boxplots obtained over 100 replications for function g_1 in dimension $d \in \{4; 6; 8\}$.



(a) $d = 4$ (b) $d = 6$ (c) $d = 8$

(d) $d = 4$ (e) $d = 6$ (f) $d = 8$

Figure: Boxplots obtained over 100 replications for function g_2 in dimension $d \in \{4; 6; 8\}$.

Integrand	Sample Size n / Method	500	$1,000$	$2,000$	$3,000$	$5,000$
g_1 $(d = 2)$	MC	9.4e-4	4.6e-4	1.9e-4	1.5e-4	1.1e-5
	QMC (Sobol)	4.1e-5	2.0e-5	3.6e-6	2.6e-6	1.0e-6
	NN-euclidean	6.7e-6	1.7e-6	3.7e-7	1.7e-7	5.3e-8
	NN-manhattan	7.0e-6	1.7e-6	4.4e-7	1.7e-7	5.7e-8
	NN-chebyshev	6.1e-6	1.7e-6	3.8e-7	2.3e-7	6.2e-8
g_2 $(d = 2)$	MC	5.0e-4	2.0e-4	1.1e-4	5.8e-5	3.1e-5
	QMC (Sobol)	6.3e-6	5.2e-6	1.7e-6	5.1e-7	2.1e-7
	NN-euclidean	9.2e-6	1.9e-6	5.0e-7	1.9e-7	1.0e-7
	NN-manhattan	8.5e-6	2.5e-6	5.3e-7	2.2e-7	9.7e-8
	NN-chebyshev	1.0e-5	1.9e-6	4.8e-7	1.8e-7	1.0e-7
g_3 $(d = 2)$	MC	1.8e-4	7.5e-5	3.4e-5	2.7e-5	2.1e-5
	QMC (Sobol)	5.7e-6	2.5e-6	5.4e-7	4.9e-7	1.7e-7
	NN-euclidean	7.9e-7	2.0e-7	3.9e-8	2.3e-8	7.7e-9
	NN-manhattan	8.2e-7	1.9e-7	4.0e-8	2.1e-8	6.7e-9
	NN-chebyshev	8.3e-7	2.2e-7	3.5e-8	2.4e-8	9.6e-9

Table: Mean Squared Error for integrands g_1, g_2, g_3 in dimension $d = 2$ obtained over 100 replications.

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The paper is not available yet but should be soon

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