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On the use of variance reducing multipliers in Monte Carlo computations of a global sensitivity index

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Abstract

First report of an attempt to apply variance reducing multipliers in Monte Carlo estimations of global sensitivity indices.

Keywords: Sensitivity index; Monte Carlo method; Variance reduction; Quasi-Monte Carlo

1. Global sensitivity indices

Assume that the model under investigation is described by a square-integrable function $f(x)$, where $x = (x_1, \ldots, x_n)$ and each x_i varies from 0 to 1. So $x \in I^n$ – an n-dimensional unit cube. All the multidimensional integrals below are from 0 to 1 for each variable.

Denote by y a specified set of m variables $x_{i_1}, \ldots, x_{i_m}$ and let z be the set of $n-m$ complementary variables, so that $x = (y, z)$, $y \in I^m$, $z \in I^{n-m}$. Let x' be another point $x' \in I^n$, $x' = (y', z')$.

Global sensitivity indices for y and z were introduced in [1], also in [2–4]. Their definition includes four integrals,

$$f_0 = \int f(x)\,dx\,, \qquad D_y = \int f(x) f(y, z')\,dx\,dz' - f_0^2\,,$$

$$D = \int f^2(x)\,dx - f_0^2\,, \qquad D_z = \int f(x) f(y', z)\,dx\,dy' - f_0^2\,,$$

that, in most general situations, can be estimated by the Monte Carlo method [5].

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Definition

$$S_y = D_y/D\,, \qquad S_z = D_z/D$$

and

$$S_y^{\text{tot}} = 1 - S_z\,, \qquad S_{yz} = 1 - S_y - S_z\,.$$

We recall that $0 \le S_y \le S_y^{\text{tot}} \le 1$, and that $S_y = S_y^{\text{tot}} = 0$ means that $f(x)$ does not depend on y while $S_y = S_y^{\text{tot}} = 1$ means that $f(x)$ depends on y only and does not depend on z.

Remark. An equivalent definition was given in [6]. Consider uniformly distributed independent random points η, η' in I^m and ζ, ζ' in I^{n-m}. Then the global sensitivity indices are equal to correlation coefficients,

$$S_y = r[f(\eta,\zeta), f(\eta,\zeta')]\,, \qquad S_z = r[f(\eta,\zeta), f(\eta',\zeta)]\,.$$

2. Variance reducing multipliers

Consider the problem of numerical estimation of an absolutely convergent n-dimensional integral,

$$I = \int_G \varphi(x)p(x)\,dx\,,$$

where $p(x)$ is a given distribution density (that is, $p(x) \ge 0$ and $\int_G p(x)\,dx = 1$). Let ξ be a random point defined in G with density $p(x)$. Then the integral is equal to the mathematical expectation $I = \mathbf{M}\varphi(\xi)$ and a crude Monte Carlo estimator,

$$\theta_N = \frac{1}{N}\sum_{i=1}^{N} \varphi(\xi_i)\,,$$

can be used for evaluating I. Here $\xi_1, \ldots, \xi_N$ are independent copies of ξ; the stochastic convergence $\theta_N \xrightarrow{P} I$ as $N \to \infty$ follows from the law of large numbers.

We assume that the variance $\mathbf{D}\varphi(\xi)$ is finite. Then according to the central limit theorem the variable θ_N is asymptotically normal and the probable error at large N is

$$w_N = 0.6745\,\left(\mathbf{D}\varphi(\xi)/N\right)^{1/2}.$$

We recall that w_N shows the order of magnitude of the approximation error $|\theta_N - I|$,

$$\mathbf{P}\{|\theta_N - I| < w_N\} \approx \mathbf{P}\{|\theta_N - I| > w_N\} \approx 0.50\,.$$

(In other words, $(\theta_N - w_N, \theta_N + w_N)$ is a 50% confidence interval for I.)

Assume that a function $\alpha(x)$ is similar to $f(x)$ and $\mathbf{M}\alpha(\xi) = 1$, $\mathbf{D}\alpha(\xi) < \infty$. Sometimes $\alpha(x)$ is called an "easy function" or a "reference function". The new estimator investigated in [7] is

$$\theta_N^* = \theta_N \kappa_N\,,$$

with

$$\kappa_N = \lambda + (1-\lambda)\frac{1}{N}\sum_{i=1}^{N}\alpha(\xi_i)\,.$$

Clearly, for any λ the estimator is consistent: $\theta_N^* \xrightarrow{P} I$ as $N \to \infty$; but it is biased,

$$\mathbf{M}\theta_N^* = I + O\left(N^{-1}\right).$$

However, a special choice of λ implies a reduction of variance,

$$N\,\mathbf{D}\theta_N^* = (1-r^2)\mathbf{D}\varphi(\xi) + O\left(N^{-1}\right),$$

instead of

$$N\,\mathbf{D}\theta_N = \mathbf{D}\varphi(\xi)\,,$$

where r is the correlation coefficient $r = r(\varphi(\xi), \alpha(\xi))$.

The best value of λ is

$$\lambda = 1 + \frac{A_0 - 1}{\mathbf{D}\alpha(\xi)} \quad \text{with} \quad A_0 = \frac{\mathbf{M}\,\varphi(\xi)\alpha(\xi)}{\mathbf{M}\,\varphi(\xi)}\,.$$

For large N, this choice cannot be worse than $\lambda = 0$ or $\lambda = 1$.

The constant A_0 can be estimated from a relatively small number of trials N_0,

$$A_0 \approx \sum_{j=1}^{N_0}\varphi(\xi_j)a(\xi_j) \Bigg/ \sum_{j=1}^{N_0}\varphi(\xi_j)\,.$$

Remark. A variance reducing technique called weighted uniform sampling suggests a consistent estimator

$$\widetilde{\theta}_N = \theta_N/\kappa_N \quad \text{with } \lambda = 0\,.$$

According to [8], for this estimator at large N,

$$N\mathbf{D}\widetilde{\theta}_N = \mathbf{D}\left[\varphi(\xi) - I\alpha(\xi)\right] + O(N^{-1})\,.$$

Assertion. An inequality holds,

$$\mathbf{D}\left[\varphi(\xi) - I\alpha(\xi)\right] \geq (1-r^2)\mathbf{D}\varphi(\xi)\,.$$

Proof. We begin with an evident relation

$$(r\sqrt{\mathbf{D}\varphi} - I\sqrt{\mathbf{D}\alpha})^2 \geq 0\,,$$

which is equivalent to

$$r^2\,\mathbf{D}\varphi - 2rI\sqrt{\mathbf{D}\varphi}\,\sqrt{\mathbf{D}\alpha} + I^2\mathbf{D}\alpha \geq 0\,.$$

On the right and on the left add $(1-r^2)\mathbf{D}\varphi$. Then

$$\mathbf{D}\varphi - 2rI\sqrt{\mathbf{D}\varphi}\sqrt{\mathbf{D}\alpha} + I^2\mathbf{D}\alpha \geq (1-r^2)\mathbf{D}\varphi\,.$$

The left-hand side is equal to $\mathbf{D}[\varphi - I\alpha]$.

3. Computation scheme for global sensitivity indices

In order to avoid losses of accuracy, it was recommended in [1] to precompute roughly f_0, and to consider $f(x) - f_0$ instead of $f(x)$. Then the new f_0 will be near zero. In this situation the variance reducing multipliers (as well as the weighted uniform sampling or the importance sampling) are inefficient. Therefore we have decided to use one and the same easy function $a(x)$ that is similar to $f(x)$ for setting up three reference functions for computing the integrals in D_y, D_z and D, while f_0 is estimated by crude Monte Carlo. These reference functions are proportional to $a(x)a(y,z')$, $a(x)a(y',z)$ and $a^2(x)$, respectively. And integrals of these functions as well as integrals of their squares must be known.

For a Monte Carlo trial we select $2n$ standard random numbers $\gamma_1,\ldots,\gamma_{2n}$ and put $x = (\gamma_1,\ldots,\gamma_n)$, $x' = (\gamma_{n+1},\ldots,\gamma_{2n})$. At these points we compute all the integrands and reference functions, their squares (for variance estimation) and products (for estimating the λ-s). Sums of all these quantities are accumulated and after N_0 trials we estimate $\lambda_1, \lambda_2, \lambda_3$ and f_0.

Then the trials are repeated with $f(x) - f_0$ rather then $f(x)$, and continued for large N. For the integrands $a(x)a(y,z')$, $a(x)a(y',z)$, $a^2(x)$ both estimators θ_N and θ_N^* are computed; for the new $f(x)$ only θ_N is applied.

Quasi-Monte Carlo scheme. For a quasi-Monte Carlo trial number j we select the jth point of a quasi-random sequence in I^{2n}. Let $(q_{j,1},\ldots,q_{j,2n})$ be its Cartesian coordinates. Then put $x = (q_{j,1},\ldots,q_{j,n})$, $x' = (q_{j,n+1},\ldots,q_{j,2n})$ and proceed as above.

In our computations Sobol's LP_τ-sequences were used [9].

4. Exponential model function

For all $1 \le m \le n$ denote

$$I_m = \prod_{i=1}^{m} \frac{e^{b_i} - 1}{b_i}, \qquad H_m = \prod_{i=1}^{m} \frac{e^{2b_i} - 1}{2b_i}, \qquad R_m = \frac{H_m}{I_m^2}.$$

The exponential function

$$f(x) = \exp \sum_{i=1}^{n} b_i x_i - I_n + c_0$$

was studied, where each $0 \le x_i \le 1$. Here the constants b_i can be varied for tuning the importance of the corresponding variables x_i.

For this function the integral $f_0 = c_0$. However, in our experiments the value f_0 was estimated numerically and the computations confirmed that small changes in c_0, $0 \le c_0 \le 1$, had no influence on the results. For this model,

$$D = H_n - I_n^2$$

and all the sensitivity indices can be computed analytically.

To simplify the notations, assume that $y = (x_1,\ldots,x_m)$, $z = (x_{m+1},\ldots,x_n)$. Then

$$S_y = \frac{R_m - 1}{R_n - 1}, \qquad S_z = \frac{(R_n/R_m) - 1}{R_n - 1}, \qquad S_{yz} = \left(\frac{R_n}{R_m} - 1\right) S_y.$$

Substituting I_m and H_m in R_m, the following expression can be obtained:

$$R_m = \prod_{i=1}^{m} \frac{b_i}{2} \coth \frac{b_i}{2} .$$

Models with prescribed indices. For arbitrary positive S_y and S_z that satisfy the requirement $S_y + S_z \leq 1$, one can find that

$$R_m = (1 - S_y)/S_z , \qquad R_n = R_m(1 - S_z)/S_y .$$

Assume that there are two groups of equally important variables: $b_1 = \cdots = b_m = b'$ and $b_{m+1} = \cdots = b_n = b''$. Then b' and b'' can be computed from equations

$$\frac{b'}{2} \coth \frac{b'}{2} = \left(\frac{1 - S_y}{S_z} \right)^{1/m} , \qquad \frac{b''}{2} \coth \frac{b''}{2} = \left(\frac{1 - S_z}{S_y} \right)^{1/(n-m)} .$$

The approximate model. As a function similar to $f(x)$ we have considered a linear function

$$a(x) = \sum_{i=1}^{n} b_i (x_i - \tfrac{1}{2}) .$$

For this model, $\tilde{f}_0 = \int a(x)\,dx = 0$ and all the necessary constants can be found analytically.

For $1 \leq m \leq n$, denote

$$B_m = \tfrac{1}{12} \sum_{i=1}^{m} b_i^2 , \qquad C_m = \tfrac{1}{120} \sum_{i=1}^{m} b_i^4 .$$

Then

$$\widetilde{D}_y = B_m , \qquad \widetilde{D}_z = B_n - B_m , \qquad \widetilde{D} = B_n ,$$

and the sensitivity indices for the linear model are

$$\widetilde{S}_y = \widetilde{S}_y^{\text{tot}} = B_m/B_n , \qquad \widetilde{S}_z = 1 - \widetilde{S}_y , \qquad \widetilde{S}_{yz} = 0 .$$

The three reference functions suggested in Section 3 are

$$\alpha_1 = a(x)a(y, z')/B_m ,$$
$$\alpha_2 = a(x)a(y', z)/(B_n - B_m) ,$$
$$\alpha_3 = a^2(x)/B_n .$$

Their expectations $\mathbf{M}\alpha_1 = \mathbf{M}\alpha_2 = \mathbf{M}\alpha_3 = 1$ and their variances

$$\mathbf{D}\alpha_1 = (B_n^2 + B_m^2 - C_m)/B_m^2 ,$$
$$\mathbf{D}\alpha_2 = \left[B_n^2 + (B_n - B_m)^2 - (C_n - C_m)\right]/(B_n - B_m)^2 ,$$
$$\mathbf{D}\alpha_3 = (2B_n^2 - C_n)/B_n^2 .$$

Discussion of the model. If the coefficients b_i are small, then $a(x) \approx f(x) - c_0$ and there are strong correlations between the integrands and the reference functions. Therefore, there is a considerable gain in accuracy due to the variance reduction. However, as a rule, accuracy requirements for sensitivity indices are moderate and in this situation the indices for $f(x)$ and for $a(x)$ can be regarded as equal. Hence, the case is not very interesting for Sensitivity Analysis of Model Output.

On the other hand, if the coefficients b_i are large, there is no similarity between $f(x)$ and $a(x)$ and no variance reduction.

The most interesting is the intermediate case when the b_i-s are neither small nor large; you cannot replace sensitivity indices S_y, S_z for $f(x)$ by indices $\tilde{S}_y$, $\tilde{S}_z$ for $a(x)$; but you can use $a(x)$ for constructing reference functions and thus reduce the variances and increase the accuracy. Such examples were found in our numerical experiments.

5. Ishigami model function

A nonlinear function,

$$f(X_1, X_2, X_3) = \sin X_1 + A \sin^2 X_2 + B X_3^4 \sin X_1 ,$$

was considered, where X_1, X_2, X_3 are independent random variables uniformly distributed in the interval $-\pi < x < \pi$ [10]. The main peculiarity of the model is the dependence on X_3: the first-order sensitivity index $S_3 = 0$ but S_3^{tot} cannot be neglected (in the following example S_3^{tot} is almost 10%).

For this function $f_0 = 0$, $S_k = D_k/D$, where

$$D_1 = \frac{1}{2} + \frac{B\pi^4}{5} + \frac{B^2\pi^8}{50}; \qquad D_2 = \frac{A^2}{8};$$

$$D_{13} = \left(\frac{1}{18} - \frac{1}{50}\right) B^2\pi^8; \qquad D = \frac{1}{2} + \frac{A^2}{8} + \frac{B\pi^4}{5} + \frac{B^2\pi^8}{18}.$$

All the other indices vanish: $S_3 = S_{12} = S_{23} = S_{123} = 0$.

The approximate model. We have selected an approximate model that does not depend on X_3,

$$a(X_1, X_2) = C \sin X_1 + A w(X_2) ,$$

with $C = 1 + 0.2B\pi^4$ and

$$w(x) = \begin{cases} 4\left|\dfrac{x}{\pi}\right|^2 - \dfrac{1}{3}, & \text{for } |x| \le \dfrac{\pi}{2}, \\ 4\left(1 - \left|\dfrac{x}{\pi}\right|^2\right) - \dfrac{1}{3}, & \text{for } \dfrac{\pi}{2} \le |x| \le \pi. \end{cases}$$

For the approximate model, $\tilde{S}_1 = \tilde{D}_1/\tilde{D}$, $\tilde{S}_2 = \tilde{D}_2/\tilde{D}$ where $\tilde{D}_1 = \frac{1}{2}C^2$, $\tilde{D}_2 = \frac{4}{45}A^2$, $\tilde{D} = \tilde{D}_1 + \tilde{D}_2$. All the other indices vanish.

Three auxiliary functions were introduced,

$$\alpha_1 = a(x, y)a(x, y')/\tilde{D}_1 ,$$

$$\alpha_2 = a(x, y)a(x', y)/\tilde{D}_2 ,$$

$$\alpha_{\text{sq}} = a^2(x, y)/\tilde{D} .$$

Table 1
Convergence of S_y and S_y^{tot} (Example 6.1)

$\log_2 N$	$1000\,S_y$				$1000\,S_y^{\text{tot}}$			
	MC		Q-MC		MC		Q-MC	
	crude	mult	crude	mult	crude	mult	crude	mult
8	405	264	363	349	483	554	356	353
9	334	283	314	309	478	534	405	405
10	331	295	288	286	444	475	391	392
11	310	286	304	303	453	430	384	382
12	286	287	295	295	396	390	385	384
13	272	283	291	291	382	375	394	393
14	278	284	287	287	400	392	396	396
15	280	285	286	286	402	398	396	396
∞		287				396		

The expectations $\mathbf{M}\alpha_1 = \mathbf{M}\alpha_2 = \mathbf{M}\alpha_{\text{sq}} = 1$ and the variances

$$\mathbf{D}\alpha_1 = \left(\frac{1}{\widetilde{D}_1}\right)^2 \left[\tfrac{3}{8}C^4 + \tfrac{4}{15}C^2A^2 + \left(\tfrac{4}{45}\right)^2 A^4\right] - 1\,,$$

$$\mathbf{D}\alpha_2 = \left(\frac{1}{\widetilde{D}_2}\right)^2 \left[\tfrac{1}{4}C^4 + \tfrac{4}{45}C^2A^2 + \frac{16}{3\cdot 5\cdot 7\cdot 9}A^4\right] - 1\,,$$

$$\mathbf{D}\alpha_{\text{sq}} = \left(\frac{1}{\widetilde{D}}\right)^2 \left[\tfrac{3}{8}C^4 + \tfrac{4}{15}C^2A^2 + \frac{16}{3\cdot 5\cdot 7\cdot 9}A^4\right] - 1\,.$$

Each of these auxiliary functions was used as a reference function twice,

α_1 – for $f(x,y,z)f(x,y',z')$ and for $f(x,y,z)f(x,y',z)$;
α_2 – for $f(x,y,z)f(x',y,z')$ and for $f(x,y,z)f(x',y,z)$;
α_{sq} – for $f(x,y,z)f(x,y,z')$ and for $f^2(x,y,z)$.

Integrands $f(x,y,z)$ and $f(x,y,z)f(x',y',z)$ were treated by crude Monte Carlo.

6. Numerical experiments

Example 6.1. The exponential model from Section 4 was computed with $n = 6$ variables, one of them dominant,

$$b_1 = 1.5\,, \qquad b_2 = \cdots = b_6 = 0.9\,, \qquad c_0 = 0\,.$$

For the first variable, $S_1 = 0.2870$, $S_1^{\text{tot}} = 0.3962$. If we consider $y = (x_1)$, $z = (x_2, \ldots, x_6)$, then $S_{yz} = 0.1092$. For the linear approximation, $\widetilde{S}_1 = \widetilde{S}_1^{\text{tot}} = 0.3571$, $\widetilde{S}_{yz} = 0$.

Computations were carried out twice: with ordinary pseudorandom numbers [5] and with quasi-random points. In Table 1 the corresponding results are marked as MC and Q-MC. The line $N = \infty$ contains exact values.

From Table 1 one can see that the MC estimates for S_y were considerably improved due to multipliers; however the S_y^{tot} values were improved only when the number of trials was large, $N \geq 2^{11}$. The crude Q-MC estimates clearly outplayed the crude MC estimates but their improvement due to multipliers was not significant.

Table 2
Convergence of S_y and S_y^{tot} (Example 6.2)

$\log_2 N$	$1000\,S_y$				$1000\,S_y^{tot}$			
	MC		Q-MC		MC		Q-MC	
	crude	mult	crude	mult	crude	mult	crude	mult
10	607	609	669	700	745	761	704	695
11	617	644	701	700	771	777	736	736
12	650	650	669	669	761	748	732	734
13	639	641	658	658	743	749	731	731
14	643	639	644	644	743	743	734	733
15	639	645	642	642	735	739	729	729
16	635	640	643	643	736	736	733	733
∞		643				734		

In this example the correlation coefficients related to D_y, D_z and D were 0.72, 0.65 and 0.63. The model function's variation was $e^6 - 1 = 402.4$.

Example 6.2. The same exponential model was considered with $n = 20$ variables of two types,

$$b_i = \begin{cases} 0.6 & \text{for } 1 \le i \le 10, \\ 0.4 & \text{for } 11 \le i \le 20; \end{cases} \quad c_0 = 0.$$

For this model $S_i = 0.05616$, $1 \le i \le 10$; $S_i = 0.02504$, $11 \le i \le 20$.

Let $y = (x_1, \ldots, x_{10})$, $z = (x_{11}, \ldots, x_{20})$, so that $m = 10$. Then

$$S_y = 0.6432, \qquad S_y^{tot} = 0.7341, \qquad S_{yz} = 0.0908,$$

while for the linear approximation,

$$\widetilde{S}_y = 0.6932, \qquad \widetilde{S}_y^{tot} = 0.6932, \qquad \widetilde{S}_{yz} = 0.$$

In this example the correlation coefficients are 0.65, 0.71 and 0.60. However, the function $f(x)$ is worse: its variation is $e^{10} - 1 = 22025$. No wonder that the convergence in Table 2 is worse than that in Table 1.

Again the crude Monte Carlo estimates for S_y are improved due to multipliers but there is no clear improvement for S_y^{tot}. The crude Q-MC estimates outplay crude MC only at sufficiently large N. And the multipliers are inefficient in quasi-Monte Carlo.

Fig. 1 shows the computational errors in D_y, D_z, D, respectively: δ_1, δ_2, δ_3 for crude Monte Carlo and δ_1^*, δ_2^*, δ_3^* for MC with multipliers; N is the number of trials. These errors seem large but in fact are reasonable because $D_y = 1.16 \cdot 10^4$, $D_z = 4.79 \cdot 10^3$, $D = 1.80 \cdot 10^4$ are rather large.

From Fig. 1 one can see that as a rule, the multipliers lead to smaller errors in the D-s. Unfortunately, sometimes despite of the improvement in the values of D_z and D the ratio D_z/D is not improved.

Example 6.3. The Ishigami model function from Section 5 was considered with $A = 7.0$, $B = 0.05$. The exact sensitivity indices for this case are

$$S_1 = 0.219, \qquad S_2 = 0.687, \qquad S_3 = 0; \qquad S_{12} = S_{23} = 0, \qquad S_{13} = 0.0946; \qquad S_{123} = 0.$$

Hence $S_3^{tot} = S_3 + S_{13} + S_{23} + S_{123} = 0.0946$. For the approximate model $\widetilde{S}_1 = 0.309$, $\widetilde{S}_2 = 0.691$, all the other indices vanish: $\widetilde{S}_3 = \widetilde{S}_{12} = \widetilde{S}_{23} = \widetilde{S}_{13} = \widetilde{S}_{123} = 0$.

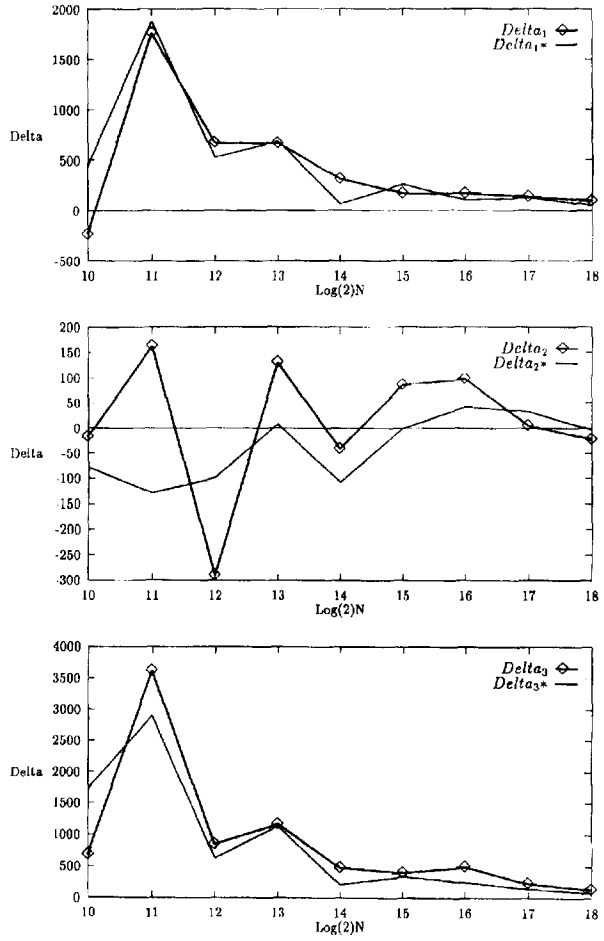

Fig. 1. Example 6.2. Monte Carlo computation errors for D_y, D_z, D.

Table 3
Convergence of S_1 and S_3^{tot} (Example 6.3)

$\log_2 N$	1000 S_1				1000 S_3^{tot}			
	MC		Q-MC		MC		Q-MC	
	crude	mult	crude	mult	crude	mult	crude	mult
5	508	215	273	182	47	38	62	60
7	296	251	203	196	28	27	88	88
9	264	261	226	221	69	74	91	92
11	251	247	224	221	77	77	94	94
13	221	226	218	218	90	90	94	94
15	223	223	219	218	92	92	94	94
∞		219				95		

From Table 3 one can see that the multipliers improved Monte Carlo estimates of S_1, especially at small N. But in quasi-Monte Carlo calculations the multipliers were inefficient, though crude quasi-Monte Carlo is clearly superior to crude Monte Carlo.

Correlation coefficients in this example vary from 0.54 to 0.79.

7. Conclusions

Variance reduction or quasi-Monte Carlo? In our experiments quasi-Monte Carlo computations are more efficient than ordinary Monte Carlo with variance reduction. We think that this situation is characteristic for problems where the exact and the approximate models are more-or-less of one type.

However, the situation may be different if the main model is rather complex (e.g., it includes partial differential equations or an integro-differential transport equation) while the approximate model is much easier (e.g., an algebraic system).

So we believe that further experiments in this direction could be suggestive.

On multipliers in quasi-Monte Carlo. We have found that the multipliers improve Monte Carlo estimates but are useless in quasi-Monte Carlo. However, it was demonstrated in [7] that such multipliers may be useful in quasi-Monte Carlo also. We have noticed that the correlation coefficients for the examples in [7] were much larger than in Section 6, $r > 0.90$. Maybe this is the reason of different conclusions.

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