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Modified Latin Hypercube Sampling Monte Carlo (MLHSMC) Estimation for Average Quality Index

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Abstract. The Monte Carlo (MC) method exhibits generality and insensitivity to the number of stochastic variables, but it is expensive for accurate Average Quality Index (AQI) or Parametric Yield estimation of MOS VLSI circuits or discrete component circuits. In this paper a variant of the *Latin Hypercube Sampling* MC method is presented which is an efficient variance reduction technique in MC estimation. Theoretical and practical aspects of its statistical properties are also given. Finally, a numerical and a CMOS clock driver circuit examples are given. Encouraging results and good agreement between theory and simulation results have thus far been obtained.

Key Words: Monte Carlo Simulation; Parametric Yield or Average Quality Estimation

1. Introduction

During the past decade, the feature sizes of VLSI devices have been scaled down rapidly. Despite the technological progress in patterning fine-line features, the fluctuations in etch rate, gate oxide thickness, doping profiles, and other fabrication steps that are critical to device performances have not been scaled down in proportion. Consequently, the Average Quality Index (AQI) [1] or its special case Parametric Yield is becoming increasingly critical in VLSI design. Circuit designers must ensure that their chips will have an acceptable AQI or parametric yield under all manufacturing process variations.

The Monte Carlo (MC) method [2] is the most reliable technique in AQI and yield estimation of electrical circuits. Nevertheless, it requires a large number of circuit simulations to have a valuable estimation, i.e. to have a low variance estimator. The well-known variance reduction techniques in MC yield estimation are [3]: 1) *importance sampling*, 2) *control variates*, and 3) *stratified sampling*. The two first methods require some knowledge about the circuit responses, and for the latter a partitioning scheme must be realized [10]. Furthermore, some of these techniques are based on the acceptability region [3], which is not defined in AQI. Therefore, these techniques are not applicable to AQI estimation.

The efficiency of Latin Hypercube Sampling (LHS) [4] in MC (LHSMC) yield and AQI estimation has been shown in our earlier work [5,6]. In LHSMC, instead of random sampling, the LHS approach is used. In this contribution, the modified LHS (MLHS) which is more efficient than the standard LHS (SLHS), is presented.

This paper is organized as follows. The following Section reviews the AQI definition. In Section 3, the general aspect of LHS generation is presented. The Modified LHS Monte Carlo (MLHSMC) estimators will be discussed in Section 4. Section 5 describes the successful application of the MLHSMC method in some numerical and circuit examples. Finally, concluding remarks will be given in Section 6.

2. Average Quality Index

The quality of a circuit can be defined in various ways. In a fabrication line, the circuit quality changes from one to another. This is why one needs to define an AQI for a circuit production. One of the important quantities of AQI is the manufacturing parametric yield of a circuit.

Assume that we have m circuit performances $y = [y_1, y_2 \ldots, y_m]$. For each performance y_i, a *membership function* $\eta_i = \eta_i(y_i)$ can be defined by using *fuzzy sets* [7]. η_i can be interpreted as a quality index measuring the goodness of performance y_i. A good circuit should have a high value of the quality index η_i for every corresponding performance. The circuit quality index can be defined as

$$\eta(\mathbf{y}) = \varphi[\eta_1(y_1), \eta_2(y_2), \ldots, \eta_m(y_m)] \tag{1}$$

where $\varphi[.]$ is an appropriate intersection operator [4].

In the case of integrated circuits, the circuit parameters can be modeled as functions of their deterministic nominal values, x, and a set of process disturbances, ξ, i.e. $\mathbf{p} = \mathbf{p}(x, \xi)$. In addition, the components of ξ can be considered mutually independent [8]. One can formulate AQI in disturbance space as

$$Q(\mathbf{x}) = \eta = \int_{R^n} \eta(\mathbf{y}(\mathbf{x}, \xi)) f_\xi(\xi) d\xi \tag{2}$$

where $f_\xi(.)$ is the joint probability density function (pdf) of the process disturbances, and R^n is disturbance space. Furthermore, the parametric yield is a special case of AQI where the quality index takes on only 1 or 0 value (pass/fail).

For statistical circuit design, we need to calculate AQI. It can be evaluated numerically using either the quadrature-based, or MC-based methods [2,3]. The quadrature-based methods have high computational costs that grow exponentially with the dimensionality of the statistical space (curse of dimensionality). The MC method is the most reliable technique for statistical analysis of electrical circuits. The unbiased Primitive MC (PMC) based estimator of AQI can be expressed as

$$\hat{Q}_{MC}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} \eta(\mathbf{x}, \xi^i) \tag{3}$$

where $\eta(\mathbf{x}, \xi^i)$ denotes $\eta(\mathbf{y}(\mathbf{x}, \xi^i))$, ξ^i's are independently drawn random samples from $f_\xi(\xi)$, and N is the sample size.

3. Latin Hypercube Sampling Monte Carlo (LHSMC)

The Latin Hypercube Sampling (LHS) [4] is an extension of *quota sampling* [19], and can be considered as an n-dimensional extension of *Latin square sampling* [20]. The sampling region is partitioned in a specific way by dividing the range of each component of the disturbance vector ξ. We will only consider the case where the components of ξ are independent or can be obtained from an independent basis by linear transformation. However, the sample generation for correlated components with Gaussian distribution can easily be achieved.

A. *Sampling Scheme*

The LHS method operates in the following manner to generate a sample size N from the n variables $\xi = [\xi_1, \xi_2, \ldots, \xi_n]$ with joint pdf $f_\xi(\xi)$. The range of each variable is partitioned into N non overlapping intervals of equal probability $1/N$. One value from each interval is selected at random according to the probability density in the interval. The N values thus obtained for ξ_1 are randomly paired with the N values of ξ_2. These N pairs are combined in a random manner with the N values of ξ_3 to form N triplets, and so on, until a set of N n-tuples is formed. This set of n-tuples is a Latin hypercube sample. Fig. 1 illustrates an LHS sample in a two-dimensional space with sample size $N = 3$.

In order to have a mathematical notation, LHS can be described as follows. The ranges of each of the n components of ξ are partitioned into N intervals of probability $1/N$. The Cartesian product of these intervals partitions the disturbance space S into N^n cells each of probability N^{-n}. Each cell can be labeled by a set of n cell coordinates $\boldsymbol{m_i} = [m_{i1}, m_{i2}, \ldots, m_{in}]$ where m_{ij} is the interval number of component ξ_j represented in cell i. A Latin hypercube sample of size

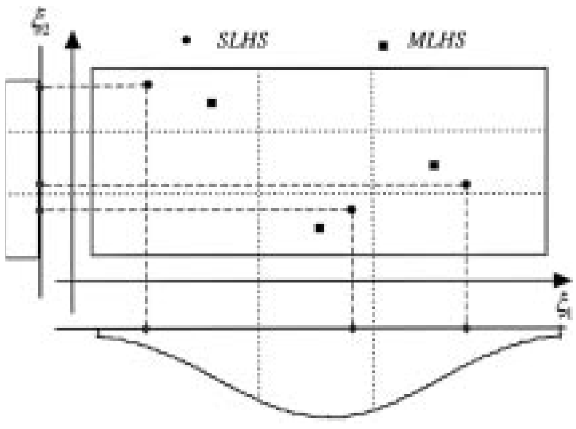


Fig. 1. SLHS sample generation for $N = 3$.

N is obtained from a random selection N of the cells $m_1, m_2, \ldots, m_N$, with the condition that for each j the set $[m_{ij}]_{i=1}^{N}$ be a permutation of the integers 1,2, ..., N. Then one sample in each selected cell is generated by using its conditional joint pdf. Let C_m denote cell m which is determined by $m = [m_1, m_2, \ldots, m_n]$. Then the conditional joint pdf of ξ, given ξ belongs to $_m$, is

$$f_{C_m}(\xi) = \begin{cases} N^n f_\xi(\xi) & \xi \in C_m \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

B. *Practical Implementation of LHS Generator*

In order to generate an N-point LHS sample, one should first create N correlated sample for each variable in the way pointed out in the previous subsection. Generally, the sample generator can be based on the following methods [2]:

1. inverse transform method,
2. composition method,
3. acceptance-rejection method.

Here, the ‘‘*Inverse Transform Method*’’ is used. In this method the inverse *Cumulative Distribution Function* (cdf) must be known analytically or numerically. The sample generation for each variable is as follow. The interval [0,1] is divided into N equal intervals. Then in each interval a sample is drawn with uniform pdf. Then these values are mapped to the ξ axis by the corresponding inverse cdf $(F^{-1}(\xi))$. Fig. 2 illustrates the sample generation for $N = 3$. The samples of each variable are randomly ordered. By juxtaposing these vectors, the LHS sample is achieved.

4. Modified Latin Hypercube Sampling (MLHS)

The LHS generation method pointed out in the previous section is called Standard LHS (SLHS). In this section, a variant of the SLHS method is presented. First the sample generation will be described, and then the statistical properties of its estimator are discussed.

A. *MLHS Generator*

In MLHS, after partitioning the range of each variable into N intervals of equal probability, the *mean* value of the conditional random variable of each interval is chosen as a sample of the interval. The rest are the same as in the LHS procedure (Fig. 1). After determining the upper and lower limits of each partition, we can calculate the mean values. For instance, consider the truncated Gaussian partition shown in Fig. 3. It can be shown that the mean value is given by (see Appendix A)

$$\bar{\xi}_1^i = \frac{N}{\sqrt{2\pi}}\left(e^{-\frac{(a-\mu)^2}{2\sigma^2}} - e^{-\frac{(b-\mu)^2}{2\sigma^2}}\right) + \mu \tag{5}$$

Suppose that the ‘‘*Inverse Transform Method*’’ is used for sample generation, in which the inverse of the cdf $F^{-1}(\xi)$ must be numerically evaluated. The computational complexities of SLHS and MLHS for an m-sample are given in Table 1. Generally, the inverse cdf evaluation is the dominant part of the sample generation time. It is seen that if MLHS is used in an optimization procedure with the number of iterations $m = 100$ and $n = 7$ with Gaussian pdf, (which is case of integrated circuits), then MLHS is

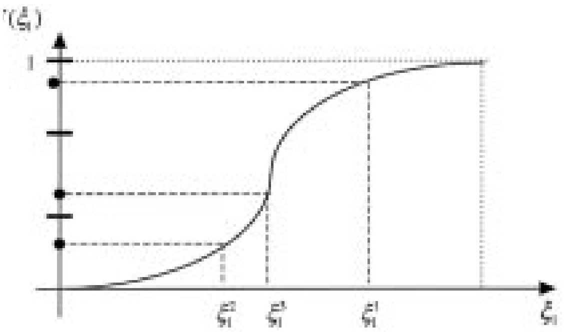


Fig. 2. Sample generation by the *Inverse Transform Method.*

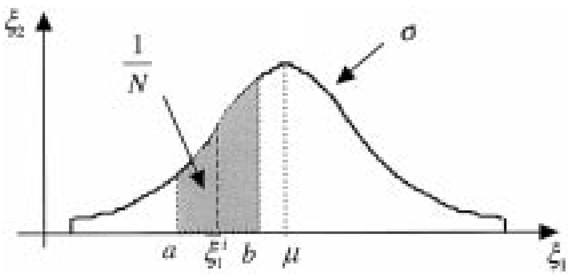


Fig. 3. A truncated Gaussian partition.

Table 1. Complexities of the SLHS and MLHS methods.

	Type	# Uniform R. V.	# F^{-1} evaluation
	SLHS	$2nmN$	nmN
MLHS	dif. pdf	nmN	nN
	same pdf	nmN	N

700 times as fast as the LHS generator. Therefore, the MLHS approach is more adapted for AQI or yield optimization procedure.

If an analytical form of the mean value of each interval is not available, one can use the *median* of the interval conditional pdf instead of its *mean* value. The sample generation can be stated as follows. First, the interval of $[0, 1]$ is divided into N equal intervals. Then the midpoint of each interval is determined. The components of this vector are mapped to the variable axis by the corresponding inverse cdf. The elements of this vector are randomly disordered. By repeating this procedure for all variables and juxtaposing the resulting vector, the MLHS sample with median type is generated. This type of MLHS takes less computational time than that of the *mean* value type. The sample value differences between median and mean types for a Gaussian pdf with $(0, 1/9)$ is shown in Fig. 4(a). The maximum sample value differences vs. sample size is illustrated in Fig. 4(b). It is seen that for large values of sample size the differences between the two types of MLHS can be ignored. In what follows the *mean* type MLHS is considered.

B. Statistical Properties of MLHSMC

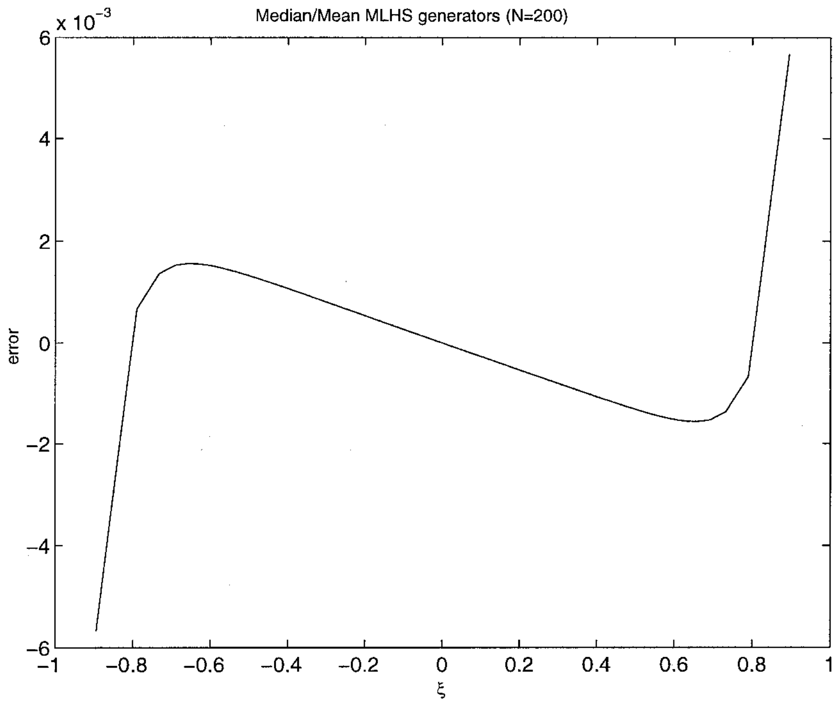
The MLHSMC estimator with sample size N is given by

$$T_{ML} = \frac{1}{N}\sum_{i=l}^{N} \eta(\xi^i) \tag{6}$$

where ξ^i's are generated by the MLHS method. Since the probability of selecting ξ^i from cell C_m is N^{-n}, and is the same for all cells, we have

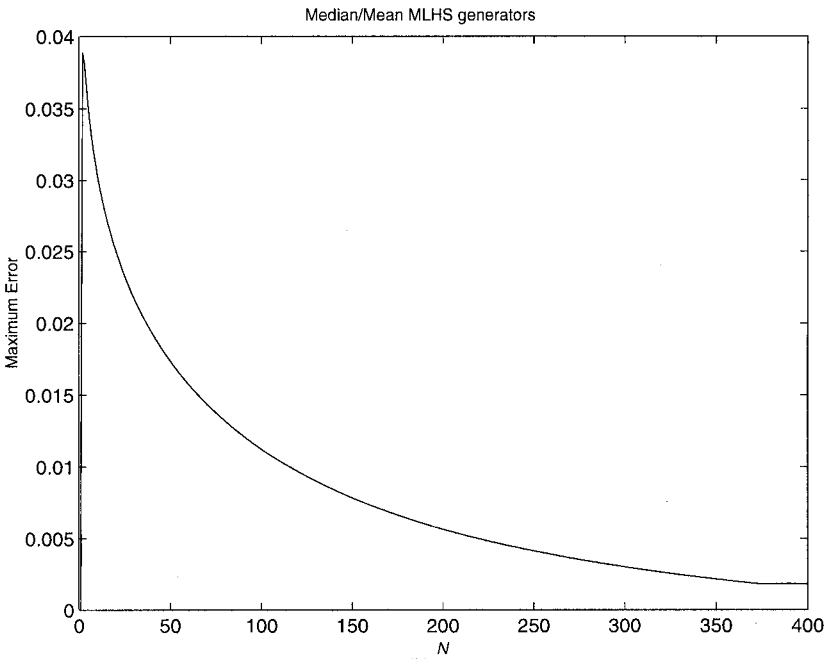
$$E[\eta(\xi^i)] = \sum_{\mathbf{m}\in R} \eta(\bar{\xi}_{\mathbf{m}})\Pr(\xi^i \in C_{\mathbf{m}}) = \frac{1}{N^n}\sum_{\mathbf{m}\in R} \eta(\bar{\xi}_{\mathbf{m}}) \tag{7}$$

where $E[.]$ stands for the expectation, $\Pr(.)$ is the probability, R denotes the space of all cells, and $\bar{\xi}_{\mathbf{m}}$ is



(a)

Fig. 4. Differences between mean and median types MLHS.



(b)

Fig. 4. (Continued)

the expectation of ξ in cell $C_{\mathbf{m}}$, expressed as

$$\bar{\xi}_{\mathbf{m}} = E[\xi | \xi \in C_{\mathbf{m}}] \tag{8}$$

Furthermore, the expectation of the MLHSMC estimator can be described as

$$\begin{aligned} E[T_{ML}] &= \frac{1}{N}\sum_{i=1}^{N} E[\eta(\xi^i)] \\ &= \frac{1}{N^n}\sum_{\mathbf{m}\in R} \eta(\bar{\xi}_{\mathbf{m}}) \\ &= \frac{1}{N^n}\sum_{\mathbf{m}\in R} \{E[\eta|\xi \in C_{\mathbf{m}}] \\ &\quad - E[\eta|\xi \in C_{\mathbf{m}}] + \eta(\bar{\xi}_{\mathbf{m}})\} \\ &= \frac{1}{N^n}\sum_{\mathbf{m}\in R} \left[\int_{C_{\mathbf{m}}} \eta(\xi) N^n f_{\xi}(\xi) d\xi\right] \\ &\quad + E_{C_{\mathbf{m}}}[\eta(\bar{\xi}_{\mathbf{m}}) - E[\eta|\xi \in C_{\mathbf{m}}]] \end{aligned} \tag{9}$$

Therefore, we have

$$E[T_{ML}] = E[\eta(\xi)] + E_{C_{\mathbf{m}}}[\eta(\bar{\xi}_{\mathbf{m}}) - E[\eta|\xi \in C_{\mathbf{m}}]] \tag{10}$$

From (10), it is seen that the MLHSMC estimator is not generally an unbiased estimator. It will be an unbiased estimator if the second term of the right hand side of equation (10) is equal to zero. In fact, the difference between the standard LHSMC (SLHSMC) and MLHSMC estimators is the use of the following approximation

$$E[\eta(\xi)|\xi \in C_{\mathbf{m}}] \approx \eta(E[\xi|\xi \in C_{\mathbf{m}}]) = \eta(\bar{\xi}_{\mathbf{m}}) \tag{11}$$

Now consider the following proposition concerning the bias of the MLHSMC estimator.

Proposition 1: *Assume that in each cell C_m the function η can be expressed as a multilinear function of ξ (linear in each ξ_i while other ξ_i's are fixed). Then the MLHSMC estimator is an unbiased estimator.*

The proof of this proposition is given in Appendix B. It is important to note that the class of multilinear functions is much larger than the class of linear functions. Furthermore, the multilinear property must be satisfied in each small cell, but does not need to be satisfied all over the disturbance space.

The behavior of the MLHSMC estimator bias in the general case is described in the following theorem.

Theorem 1: *It is assumed that the set of discontinuity points of the quality index function η over disturbance space is of the zero Lebesgue [11] measure. Then the bias of the MLHSMC estimator converges to zero as the sample size approaches infinity ($N \to \infty$).*

The proof of *Theorem 1* is given in Appendix B. It should be emphasized that the assumption of *Theorem*

1 holds for all realistic quality index functions and is not a restrictive condition. In practical circuit applications, it is found that the bias of the MLHSMC estimator is negligible for $N > 10$. Thus the bias of the estimator is not a restriction for this method.

One of the important properties of an estimator is its variance. The variance of the MLHSMC estimator (6) can be described as (see Appendix B)

$$\mathrm{Var}(T_{ML}) = \frac{1}{N}\mathrm{Var}(\eta_{\mathbf{m}}) + \frac{N-1}{N}\mathrm{Cov}(\eta_{\mathbf{1}}, \eta_{\mathbf{m}}) \qquad (12)$$

where $\eta_{\mathbf{1}} = \eta(\bar{\xi}_{\mathbf{1}})$, $\eta_{\mathbf{m}} = \eta(\bar{\xi}_{\mathbf{m}})$, and the two cells C_1 and $C_{\mathbf{m}}$ have no cell coordinates in common. Consider the following proposition.

Proposition 2: *If the quality index function η is a multilinear function in each cell C_m, then the variance of the MLHSMC estimator is less than that of the SLHSMC estimator.*

The proof of *Proposition 2* is given in Appendix C. It should be noted that the multilinear property does not imply the monotonicity condition. We now consider the following theorem about the variance of the MLHSMC estimator in the general case.

Theorem 2: *Suppose that the set of discontinuity points of the quality index function η over disturbance space is of the zero Lebesgue measure. Then the variance of the MLHSMC estimator approaches the variance of the SLHSMC estimator when $N \to \infty$.*

The proof of this theorem is described in Appendix C. Simulation results have shown that variance efficiency gain with respect to SLHSMC can be obtained for $10 < N < 100$. This is a very interesting property for the AQI or yield optimization by ''Stochastic Approximation Approach'' [9], where AQI or yield is estimated by a small sample size.

5. Numerical and Circuit Examples

Here we present a CMOS clock driver circuit and a 3-dimensional quadratic performance function to show the advantages of the MLHSMC estimator over those of PMC.

In order to compare two different estimation methods, an efficiency measure is introduced which is the product of the ratio of the respective variances and the ratio of the respective computation times [3]

$$\gamma = \frac{\sigma_R^2 \tau_R}{\sigma_L^2 \tau_L} \qquad (13)$$

where τ_R and σ_R^2 denote the computation time and the variance of the PMC estimator, and τ_L and σ_L^2 are the computation time and the variance of the LHSMC estimator, respectively.

Example 1: *CMOS Clock Driver Circuit* [1]

A CMOS clock driver is shown in Fig. 5. The clock driver provides two outputs V_{out1} and V_{out2} in opposite phase. The nominal response of the circuit is shown in Fig. 6. The performance of interest is the clock skew as shown in Fig. 6. The specifications are that the skew belongs to the interval $[-1, 1]$ ns.

OMEGA [15] is an open electric simulator which

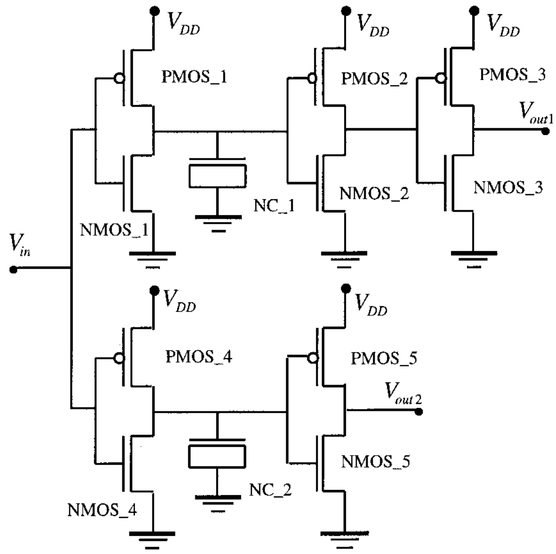


Fig. 5. Schematic circuit of a CMOS clock driver.

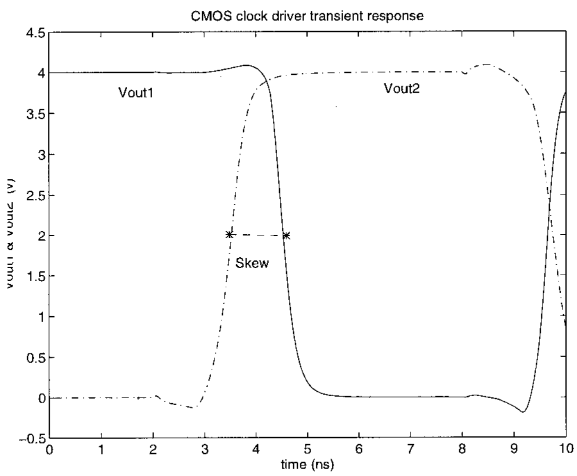


Fig. 6. Nominal response of the CMOS clock driver.

Table 2. Process noise factors.

i	ξ_i	$E(\xi_i)$	sigma σ_i	Description
1	ξ_1	1.074 μm	0.01 μm	PMOS Width Reduction
2	ξ_2	0.211 μm	0.01 μm	PMOS Length Reduction
3	ξ_3	0.142 V	0.1 V	PMOS Flat Band Voltage
4	ξ_4	15 nm	1 nm	Oxide Thickness
5	ξ_5	0.982 μm	0.01 μm	NMOS Width Reduction
6	ξ_6	0.152 μm	0.01 μm	NMOS Length Reduction
7	ξ_7	− 0.95 V	0.1 V	NMOS Flat Band Voltage

was developed at ''Ecole Supérieur d'Electricité'' (SUPELEC). OMEGA was used as the circuit simulator with BSIM transistor models, and Matlab [16] was as our programming environment. The interactions between OMEGA and Matlab are done through Interprocess Communications [17]. The model parameters used to characterize CMOS manufacturing process disturbances are listed in Table 2. These variables are considered independent, and to be of Gaussian probability distribution.

The bias of the MLHSMC yield estimator of this circuit is depicted in Fig. 7. One can see that the bias of the estimator can be ignored for practical values of sample size and it converges to zero as sample size approaches infinity. The results confirm the theoretical bases described in the previous section. It should be noted that the bias is estimated and it contains some uncertainty. That is why there are some fluctuations in the presented curves. The standard deviation (SD) of the MLHSMC and PMC estimators, as well as the efficiency of the MLHSMC yield estimator over the PMC estimator for this circuit are shown in Fig. 8. It is seen that the MLHSMC estimator is almost 3 times as fast as the PMC estimator.

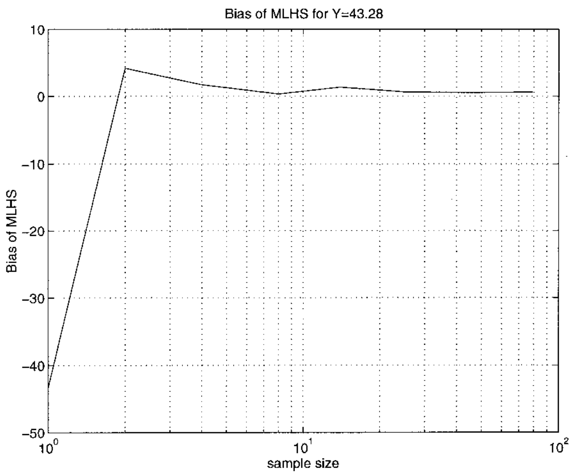


Fig. 7. Bias of the MLHSMC yield estimator for the CMOS clock driver.

Example 2: *Quadratic Performance Function*

Suppose that the behavior of a circuit performance can be expressed as a 3-dimensional quadratic function. The function for this example is taken as

$$y(\xi) = a_0 + \mathbf{J}\xi + \frac{1}{2}\xi^T\mathbf{H}\xi \tag{14}$$

where $a_0 = 3$, and the matrices J and H are as follows:

$$\mathbf{J} = \begin{bmatrix} -1 \\ 10 \\ 2 \end{bmatrix} \mathbf{H} = \begin{bmatrix} 1 & -4 & 5 \\ -4 & 3 & 4 \\ 5 & 4 & -2 \end{bmatrix} \tag{15}$$

The disturbances are considered to be independent with Gaussian pdf over the following region of tolerance

$$R_T = \{\xi||\xi_i - \xi_i^0| \leq t_i \; i = 1,2,3\} \tag{16}$$

where $\xi^0 = [0.5, 0.5, 0.5]^T$ and $t = [1, 1, 1]^T$ is the tolerance vector of disturbances. For quality index definition, a ''sigmoidal'' fuzzy membership function [1] is chosen.

The bias of MLHSMC for this example is given in Fig. 9. It is seen that the bias practically can be ignored for $N > 20$. In addition, the efficiency of MLHSMC and SLHSMC with respect to PMC are shown in Figs. 10 and 11, respectively. Fig. 12 shows the efficiency of the MLHSMC estimator over the SLHSMC estimator. It is seen that the MLHSMC method is more efficient than that of SLHSMC for $10 < N < 100$. This property can be used in

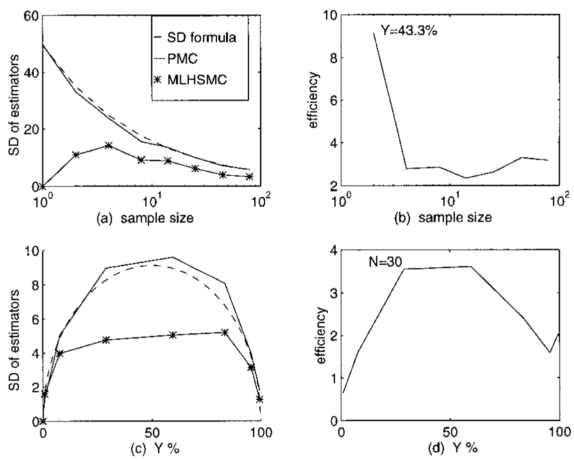


Fig. 8. Simulation results of the CMOS clock driver circuit.

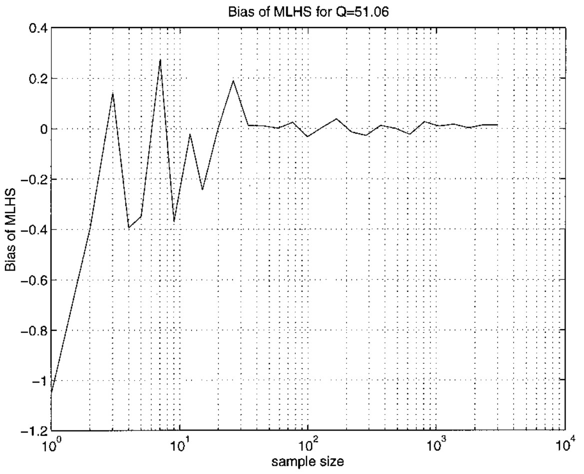


Fig. 9. Bias of MLHSMC in the case of the quadratic function.

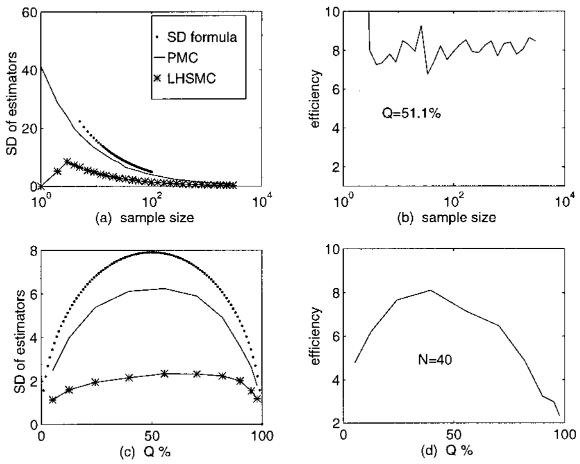


Fig. 10. Efficiency of MLHSMC in the case of the quadratic function.

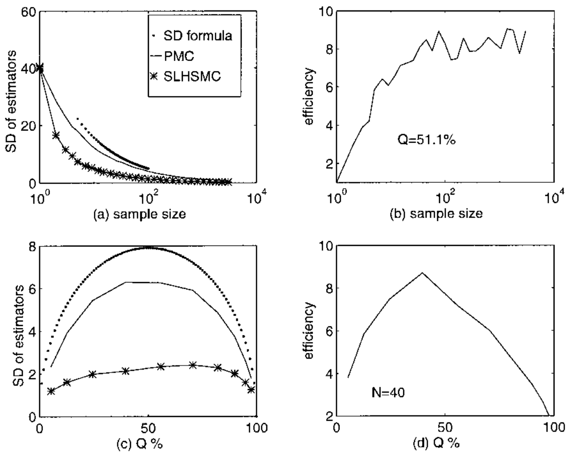


Fig. 11. Efficiency of SLHSMC for the quadratic function.

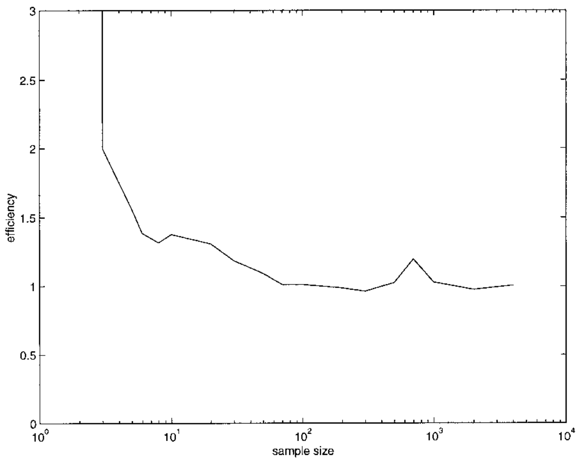


Fig. 12. Efficiency of MLHSMC over SLHSMC for the quadratic function.

estimators with small sample size, such as the yield gradient estimator in the *Stochastic Approximation* approach [9]. It should be noted that the efficiency here is related to the ratio of two variances, and the efficiency of sample generation was not taken into account.

In order to estimate the variance of each estimator, we repeated the estimation process 1000 times. In Fig. 10(a) and (c), one can see that the standard deviation of the AQI estimator using MLHSMC is less than that of the PMC estimator with respect to sample size and AQI value, respectively. The dashed line is the theoretical standard deviation of the PMC yield estimator with the same value of AQI. Also, the efficiency of SLHSMC is shown in Fig. 11(b) and (d). In Fig. 10(b), it is seen that the MLHSMC method is almost 7.5 times as fast as PMC with the same degree of confidence on results. Furthermore, the results of several applications have shown that the efficiency of the MLHSMC approach in AQI estimation is greater than in yield estimation.

6. Conclusions

In this paper, a variant of the Latin hypercube sampling, called MLHS, is presented. The MLHS approach is a variance reduction technique in MC yield or AQI estimation methods. It has the following advantages over the SLHSMC estimator in practical problems: 1) fast sample generation, particularly in an optimization procedure, and 2) more precise estimator (smaller estimation variance) with the same computational time. The theoretical properties of MLHSMC were also described. Finally, simulation results of a CMOS clock driver circuit and a 3-dimensional quadratic performance function were given to show the efficiency of the MLHSMC approach. Good agreement between theory and simulation was achieved.

Furthermore, it is felt that the MLHSMC estimator is a well-adapted estimator in AQI or yield optimization by the *Stochastic Approximation* approach [9] or the *Centers of Gravity* algorithm [18]. Further research in this area is in progress.

Appendix A. Mean Value of Truncated Gaussian PDF

For the sake of simplicity, we first consider a standard Gaussian pdf with zero mean and $\sigma = 1$. We suppose that this pdf is partitioned into N intervals of equal probability. An interval with limits a and b is considered (Fig. 3). The conditional pdf of this interval is given by

$$f_{ab}(\xi) = \begin{cases} \frac{N}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} & \xi \in [a, b] \\ 0 & \text{otherwise} \end{cases} \tag{A1}$$

The mean value is obtained by

$$\bar{\xi} = \int \xi f_{\xi}(\xi) d\xi = \int_a^b \xi \frac{N}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} d\xi \tag{A2}$$

and after some manipulations, we have

$$\bar{\xi} = \frac{N}{\sqrt{2\pi}} \left(e^{-\frac{a^2}{2}} - e^{-\frac{b^2}{2}} \right) \tag{A3}$$

Furthermore, for a Gaussian pdf with mean μ and variance σ^2, the mean value is described as

$$\bar{\xi} = \frac{N}{\sqrt{2\pi}} \left(e^{-\frac{(a-\mu)^2}{2\sigma^2}} - e^{-\frac{(b-\mu)^2}{2\sigma^2}} \right) + \mu \tag{A4}$$

Appendix B. Bias of MLHSMC Estimators

In this section, the bias property of the MLHSMC estimator is mathematically described. The MLHSMC estimator, which is an estimator of $\bar{\eta} = E[\eta(\xi)]$, is expressed as

$$T_{ML} = \frac{1}{N} \sum_{i=1}^{N} \eta(\xi^i) \tag{B1}$$

where ξ^i's are generated by the MLHS method. After some algebra, the expectation of this estimator can be written as

$$E[T_{ML}] = \bar{\eta} + E_{C_{\mathbf{m}}} \left[\eta(\bar{\xi}_{\mathbf{m}}) - E[\eta | \xi \in C_{\mathbf{m}}] \right] \tag{B2}$$

where $C_{\mathbf{m}}$ denotes a cell in the disturbance space, and $\bar{\xi}_{\mathbf{m}}$ is the mean value of ξ in the cell $C_{\mathbf{m}}$,

$$\bar{\xi}_{\mathbf{m}} = E[\xi | \xi \in C_{\mathbf{m}}] \tag{B3}$$

Now, consider the following proposition.

Proposition 1: *Assume that in each cell $C_{\mathbf{m}}$ the function η can be expressed as a multilinear function of ξ (linear in each ξ_i while other ξ_i's are fixed). Then the MLHSMC estimator is an unbiased estimator.*

Proof: From the multilinear assumption, the quality index function η in each cell $C_{\mathbf{m}}$ can be written as

$$\eta(\xi) = \sum_{j_1=0}^{1} \sum_{j_2=0}^{1} \cdots \sum_{j_n=0}^{1} a^m_{j_1 j_2 \ldots j_n} \xi_1^{j_1} \xi_2^{j_2} \ldots \xi_n^{j_n} \tag{B4}$$

In addition, in SLHS and MLHS sample generation it is supposed that the disturbance random variables are independent. Thus by using (B4), the following result is straightforward

$$E[\eta(\xi) | \xi \in C_{\mathbf{m}}] = \eta(E[\xi | \xi \in C_{\mathbf{m}}]) = \eta(\bar{\xi}_{\mathbf{m}}). \tag{B5}$$

By substituting (B5) into (B2), the proposition is proved. ■

Now we consider the following lemma before describing the asymptotic behavior of the estimator bias in the general case.

Lemma 1: *Suppose that the cell $C_{\mathbf{m}}$'s are obtained from the LHS method. Then for all cells in which the function quality index η is continuous, we have*

$$\lim_{N \to \infty} E[\eta(\xi) | \xi \in C_{\mathbf{m}}] = \lim_{N \to \infty} \eta(\bar{\xi}_{\mathbf{m}}) \tag{B6}$$

Proof: Let $\xi^{\mathbf{m}}_{Min}$ and $\xi^{\mathbf{m}}_{Max}$ denote the point where η has its maximum and minimum in the cell $C_{\mathbf{m}}$, respectively. Then it is obvious that

$$\eta(\xi^{\mathbf{m}}_{Min}) \le E[\eta(\xi) | \xi \in C_{\mathbf{m}}] \le \eta(\xi^{\mathbf{m}}_{Max})$$
$$\eta(\xi^{\mathbf{m}}_{Min}) \le \eta(\bar{\xi}_{\mathbf{m}}) \le \eta(\xi^{\mathbf{m}}_{Max}) \tag{B7}$$

The shape of each cell is hyperbox with dimensions approaching zero when sample size N approaches infinity. Therefore, if ξ^1 and ξ^2 are two arbitrary points within the cell C_m, then

$$\lim_{N\to\infty} d(\xi^1,\xi^2) = 0 \tag{B8}$$

where d stands for *Euclidean* distance. From (B8), and the continuity property of η over cell $C_{\mathbf{m}}$, one can conclude that

$$\lim_{N\to\infty} \eta(\xi^{\mathbf{m}}_{Min}) = \lim_{N\to\infty} \eta(\xi^{\mathbf{m}}_{Max}) \tag{B9}$$

By taking the limit of (B7) and using (B9), the proof is completed. ■

In the general case, the behavior of the MLHSMC estimator bias is described as the following theorem.

Theorem 1: *It is assumed that the set of discontinuity points of the quality index function η over disturbance space is of the zero Lebesgue [11] measure. Then the bias of the MLHSMC estimator converges to zero when the sample size approaches infinity ($N \to \infty$).*

Proof: From (B2), the bias of the MLHSMC estimator (B_{mlhs}) can be expressed as

$$B_{mlhs} = E_{C_{\mathbf{m}}}[\Delta_{\mathbf{m}}] \tag{B10}$$

where $\Delta_{\mathbf{m}}$ is defined as

$$\Delta_{\mathbf{m}} = \eta(\bar{\xi}_{\mathbf{m}}) - E[\eta|\xi \in C_{\mathbf{m}}] \tag{B11}$$

Suppose that N approaches infinity. Then the right hand side of (B10) can be expressed as an integral. According to *Lemma 1*, one can conclude that the limit of $\Delta_{\mathbf{m}}$ is equal to zero over the points where η is continuous. To the contrary, $\Delta_{\mathbf{m}}$ can be non zero over the point where η has discontinuity points ($\Delta_{\mathbf{m}} \in [0,1]$). From the assumption of zero *Lebesgue* measure over the discontinuity points of η, it can be concluded that the set of non zero $\Delta_{\mathbf{m}}$ is of the zero *Lebesgue* measure. Therefore, the related integral (right hand side of B(10)) is equal to zero. Hence the MLHSMC estimator approaches an unbiased estimator when $N \to \infty$. ■

Appendix C. Variance of MLHSMC Estimators

In this section the variance of the MLHSMC estimator is mathematically discussed in comparison with the SLHSMC estimator.

Let $C_{P_1}, C_{P_2}, \ldots, C_{P_N}$ represent the cells from which $\xi^1, \xi^2, \ldots, \xi^N$ are sampled, respectively, and let

$$U = [C_{P_1}, C_{P_2}, \ldots, C_{P_N}] \tag{C1}$$

represent the ordered N-tuple of disjoint cells. There are $M = (N!)^n$ such ordered N-tuples. We will index U and the corresponding cells with superscripts, such as

$$U^i = [C^i_{P_1}, C^i_{P_2}, \ldots, C^i_{P_N}]\, i = 1,2,\ldots,M \tag{C2}$$

Each of these N-tuples are equally likely, that is

$$\Pr(U = U^i) = \frac{1}{M} \tag{C3}$$

Using the well-known formula [14], we have

$$\mathrm{Var}(T_{LM}) = E[\mathrm{Var}(T_{LM}|U^i)] + \mathrm{Var}(E[T_{LM}|U^i]) \tag{C4}$$

It can easily be shown that

$$\mathrm{Var}(T_{LM}|U^i) = 0 \qquad i = 1,2,\ldots,M \tag{C5}$$

and then

$$E[\mathrm{Var}(T_{LM}|U^i)] = 0 \tag{C6}$$

After some algebra, in the same way as in the ''*Result 5*'' of [13], the second term of (C4) can be expressed as

$$\mathrm{Var}(T_{ML}) = \frac{1}{N}\mathrm{Var}(\eta_{\mathbf{m}}) + \frac{N-1}{N}\mathrm{Cov}(\eta_{\mathbf{1}}, \eta_{\mathbf{m}}) \tag{C7}$$

where $\eta_{\mathbf{1}} = \eta(\bar{\xi}_{\mathbf{1}}), \eta_{\mathbf{m}} = \eta(\bar{\xi}_{\mathbf{m}})$, and the two cells $C_{\mathbf{1}}$ and $C_{\mathbf{m}}$ have no cell coordinates in common. In addition, the variance of the SLHSMC estimator can be written as [3]

$$\mathrm{Var}(T_{SL}) = \frac{1}{N}\mathrm{Var}(\eta) + \frac{N-1}{N}\mathrm{Cov}(\mu_{\mathbf{1}}, \mu_{\mathbf{m}}) \tag{C8}$$

where T_{SL} denotes the SLHSMC estimator, $\mu_{\mathbf{m}}$ is defined as

$$\mu_{\mathbf{m}} = E[\eta(\xi)|\xi \in C_{\mathbf{m}}] \tag{C9}$$

and the pairs $(\mu_{\mathbf{1}}, \mu_{\mathbf{m}})$ correspond to cells having no cell coordinates in common.

Proposition 2: *If the quality index function η is a multilinear function in each cell $C_{\mathbf{m}}$, then the variance of the MLHSMC estimator is less than that of the SLHSMC estimator.*

Proof: According to the multilinear assumption, equation (B5) holds and one can write

$$\mu_{\mathbf{m}} = E[\eta(\xi)|\xi \in C_{\mathbf{m}}] = \eta(\bar{\xi}_{\mathbf{m}}) = \eta_{\mathbf{m}} \tag{C10}$$

By inserting (C10) into (C7) and (C8), we have

$$\mathrm{Var}(T_{ML}) - \mathrm{Var}(T_{SL}) = \frac{1}{N}[\mathrm{Var}(\eta_{\mathbf{m}}) - \mathrm{Var}(\eta)] \tag{C11}$$

and by using the well-known formula,

$$\mathrm{Var}(\eta) = E[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})] + \mathrm{Var}(E[\eta(\xi)|\xi \in C_{\mathbf{m}}]) \tag{C12}$$

Furthermore, by substituting (C12) into (C11), the difference between the variance of the two estimators is given by

$$\mathrm{Var}(T_{ML}) - \mathrm{Var}(T_{SL}) = -\frac{1}{N}E[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})] \tag{C13}$$

Therefore, the proof of *Proposition 2* is completed. ■

The following theorem states the asymptotic behavior of the variance of the MLHSMC estimator in the general case.

Theorem 2: *Suppose that the set of discontinuity points of the quality index function η over disturbance space is of the zero Lebesgue measure. Then the variance of the MLHSMC estimator approaches the variance of the SLHSMC estimator when $N \to \infty$.*

Proof: Suppose that $N \to \infty$. Then from *Lemma 1*, over the point where η is continuous, we have

$$\lim_{N\to\infty} \eta_{\mathbf{m}} = \lim_{N\to\infty} \mu_{\mathbf{m}} \tag{C14}$$

In the theorem it is assumed that the set of discontinuity points of η is of the zero Lebesgue measure. In addition, the quality index η belongs to $[0, 1]$, so $\eta_{\mathbf{m}}$, and $\mu_{\mathbf{m}} \in [0, 1]$. From these properties, it can be shown that

$$\begin{aligned} &\lim_{N\to\infty} \mathrm{Var}(\eta_{\mathbf{m}}) = \lim_{N\to\infty} \mathrm{Var}(\mu_{\mathbf{m}}) \\ &\lim_{N\to\infty} \mathrm{Cov}(\eta_{\mathbf{l}}, \eta_{\mathbf{m}}) = \lim_{N\to\infty} \mathrm{Cov}(\mu_{\mathbf{l}}, \mu_{\mathbf{m}}) \end{aligned} \tag{C15}$$

By substituting (C15) into (C7) and (C8), we have

$$\lim_{N\to\infty} [\mathrm{Var}(T_{ML}) - \mathrm{Var}(T_{SL})] = -\lim_{N\to\infty} \left\{ \frac{1}{N}E[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})] \right\} \tag{C16}$$

In [12], it is shown that $\max[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})] = 0.25$, and then

$$\max\{E[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})]\} = 0.25 \tag{C17}$$

By using (C17) in (C16), it is seen that the right hand side of equation (C16) is equal to zero. Therefore, the result of Theorem 2 follows immediately.

Moreover, in [10] it is shown that

$$\lim_{N\to\infty} E[\mathrm{Var}(\eta(\xi)|\xi \in C_{\mathbf{m}})] = 0 \tag{C18}$$

Consequently, the difference between the variance of the MLHSMC and SLHSMC estimators converges to zero with a convergence rate greater than $1/N$. ■

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