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A Comparative Analysis of Monte Carlo Integrations and Numerical Quadrature for Multi-Dimensional Functions

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Abstract

Multidimensional integrals can be used in physics, machine learning, and engineering. However, they are difficult to solve correctly because the integrands are complex and the cost of calculation increases with the dimensionality. This research compares Monte Carlo Integration (MCI), Quasi- Monte Carlo (QMC) and numerical quadrature (NQ) techniques of solving multi-dimensional integrals that are chosen as benchmark functions. The objective of this research is to compare the methods with the benchmark function as the accuracy, computational efficiency, and convergence rate measure. Both MCI and QMC are consistently accurate, and MCI is more successful in high-dimensional problems because of its dimension-independent convergence. QMC is better at low dimensions but not higher-dimensional problems. NQ performs almost perfectly in low dimensionality and is computationally efficient with increasing dimensionality. Four more benchmark functions are used to evaluate the convergence behaviour, including smooth exponential, poly-separable, oscillatory, and nonsmoothed indicator functions. The findings show that MCI is converging with a steady rate for all integrands. QMC is seen to be more effective in smooth and separable functions, whilst convergence is compromised in oscillatory and nonsmoothed integrands. NQ shows second-order convergence to smooth integrals in low-dimensions, but it cannot do nonsmoothed functions. These results give an idea of the advantages and disadvantages of each technique based on the dimension and nature of integrand.

1. Introduction

Multidimensional integrals are one of the most important problems that must be assessed properly in a wide variety of scientific and engineering applications such as physics, machine learning and finance, where analytical solutions are frequently impractical because of the complexity of the integrands or the sheer number of dimensions of the problem. Conventional techniques such as numerical quadrature (NQ) work well in low dimensions are computationally costly and ineffective as the dimensionality increases because of the curse of dimensionality which is proportional to the increase in the number of required function evaluations to the dimensionality [1]. By applying the law of large numbers to approximate integrals, Monte Carlo Integration (MCI) and its Quasi-Monte Carlo Integration (QMC) which applies random and low-discrepancy sampling methods respectively to provide solutions to high-dimensional integrals, respectively. Specifically, MCI is dimension-independent such that the convergence rate is independent of the number of dimensions. This proves that MCI is particularly suitable to high-dimensional problems, but it can have high variance, particularly with smooth integrands [2][3]. MCI does well with multidimensional problems because its error rate does not change with the number of dimensions [6]. Although classical MCI has a dimension independent convergence rate, QMC can achieve a faster rate at which rapid convergence depends on the structure and smoothness of the integrand [3]. As a result of this, MCI becomes unbelievably valuable in problems like those seen in statistical physics and finance, as classical methods fail because of the dimensionality [7].

QMC is an improvement of MCI where low-discrepancy sequences such as Sobol or Halton sequences, are used to distribute the sample points more uniformly over the domain, and this minimizes the error relative to random sampling, especially when the integrand is smooth and separable [4][5]. Nevertheless, high dimensions or oscillatory integrands can lead to poor performance of QMC as the advantages of low-discrepancy sequences are compromised under these conditions [5]. Although MCI are useful, they can move slowly toward convergence and have high variation, especially on more regular functions. In such situations, using traditional quadrature results in greater accuracy and uses less evaluations, mainly when the problem is low-dimensional. QMC with smooth integrands can frequently be more effective than standard MCI in exploiting regularity with the help of low-discrepancy sampling, providing better accuracy with fewer function evaluations and smaller differences between performance of sampling-based algorithms and classical quadrature [3].

NQ helps to estimate the area under a curve by using predetermined methods with only a set of values. There are many kinds of numerical integration such as the trapezoidal rule, Simpson's rules, Gaussian quadrature, Widdle's rule, and other variants, and each one has different properties in terms of converging and computing quickly [7]. The method checks the integrand at different selected positions and adds together each contribution, weighted according to its position. As a result of being precise, predictable, and structured, this technique is regularly applied in scientific computing and does well for smooth functions in one or two dimensions [1]. If the problem has more than two dimensions, the accuracy of NQ gets much lower. Those methods are easy to use in low-dimensional settings, but their accuracy decreases when the number of dimensions is high [2].

Although the high-dimensional integrals have been adequately studied using MCI, QMC, and NQ being applied to low-dimensional problems, the relative performance of these solvers in terms of accuracy, computational efficiency, and convergence behaviour, particularly across a variety of integrand types and dimensions, has not been studied. This research seeks to fill this gap by comparing the accuracy and computational efficiency of MCI, QMC and NQ in solving multi-dimensional integrals, but also comparing the convergence rates of the three by using other benchmark functions (smooth exponential, poly-separable, oscillatory and nonsmoothed indicator). In this way, the research aims to give information on the advantages and limitations of these approaches, as well as offer a practical advice on the application of the most appropriate technique, depending on the dimensionality of the problem and the nature of integrand applied. In this paper, 4 sections are provided. The Introduction provides the background, problems of the research and aims of the research. Methodology provides a description of the experimental design, functions benchmarking and evaluation criteria. The Results and Discussion give the findings on the accuracy, efficiency and convergence behaviour. Lastly, the Conclusion will sum up the most important findings, implications, and recommendations on further research and implementation.

2. Methodology

This section provides the methodology approach to comparing MCI, QMC and NQ to solve multi-dimensional integrals. This paper is largely devoted to the assessment and comparison of these procedures according to their accuracy, computational efficiency, and convergence behavior with the help of numerous benchmark functions. Such approaches are especially significant to the calculation of integrals in higher-dimensional spaces, where even conventional approaches such as NQ can be computationally expensive and ineffective because of the curse of dimensionality [1]. The exponential decay function is taken as the benchmark function, because it can easily be compared to the exact solution. Also, all other benchmark functions (smooth exponential, poly-separable, oscillatory and nonsmoothed indicator functions) are provided to test the convergence rates of the methods. This section will provide a description of the choice of benchmark functions, flowchart, tools and implementation environment and the criteria in each method.

2.1 Selection of Benchmark Function

The study is systematic and adheres to an experimental design to assess the effectiveness of MCI, QMC and NQ techniques. The main task is to test the accuracy, the efficiency of the computation, and the convergence behavior of these methods of multi-dimensional integrals. The exponential decay function was selected as the standard of analyzing accuracy and computational efficiency in which the results were evaluated in the dimensions of $d = 2$ up till $d = 10$.

$$f(x) = exp\left(-\sum_{i=1}^{d} x_i\right),\ x = (x_1, x_2, \ldots, x_d) \tag{1}$$

Four benchmark functions were selected as the standard of analysing convergence rates which are smooth exponential, poly-separable, oscillatory and nonsmoothed indicator functions.

$$f(x) = exp\left(-\sum_{i=1}^{d} x_i\right) \tag{2}$$

$$f(x) = \prod_{i=1}^{d} x_i^2 \tag{3}$$

$$f(x) = \sin\left(2\pi \sum_{i=1}^{d} x_i\right) \tag{4}$$

$$f(x) = \begin{cases} 1, \ if \ \sum_{i=1}^{d} x_i < 0.5 \times d \\ 0, \ if \ \sum_{i=1}^{d} x_i \geq 0.5 \times d \end{cases} \tag{5}$$

MCI and QMC were tested on samples of size N of 100 to 100,000 and grid resolutions n of NQ varied correspondingly. Convergence rate was examined by the plotting of the error versus sample size of MCI and QMC, grid resolution of NQ. The experimental setup was made in such a way that it can compare the three methods fully in various dimensionalities and integrand types.

2.2 Flowchart

To make the experimental design easier to comprehend, the following flowchart shows the steps to be followed in the study:

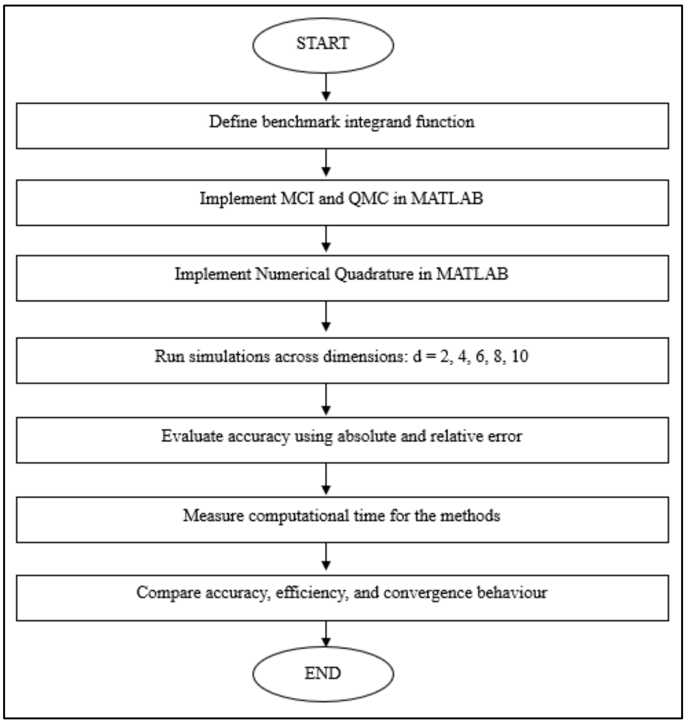


Fig. 1 Flowchart of the methodology

2.3 Tools and Implementation Environment

Numerical experiments were all performed in MATLAB R2023b which offers credible instruments of numerical integration and performance measurement. Monte Carlo Integration was created with the help of pseudo-random sampling created by the MATLAB rand function and Quasi-Monte Carlo Integration was created with the help of low-discrepancy Sobol sequences created by the sobolset function. In low-dimensional cases, Numerical Quadrature was applied using integral and integral2 adaptive integration functions of MATLAB. The computation efficiency of the formula was determined by the timeit function in MATLAB in order to have the same and repeatable run time. Numerical stability, reproducibility, and reproducibility are obtained through the use of built in MATLAB functions.

2.4 Monte Carlo and Quasi-Monte Carlo Integration

In the case of MCI and QMC, the integration was estimated by determining the value of the integrand at the sampled points in the unit hypercube and taking the sample mean. Samples in MCI were created randomly, and deterministic low-discrepancy sequences were utilized in QMC to enhance the domain coverage. The sample sizes were also systematically augmented to study their impact on the accuracy and convergence. Both were tested on various dimensions to determine the scalability, and especially the behaviour of error and runtime with increasing dimensionality.

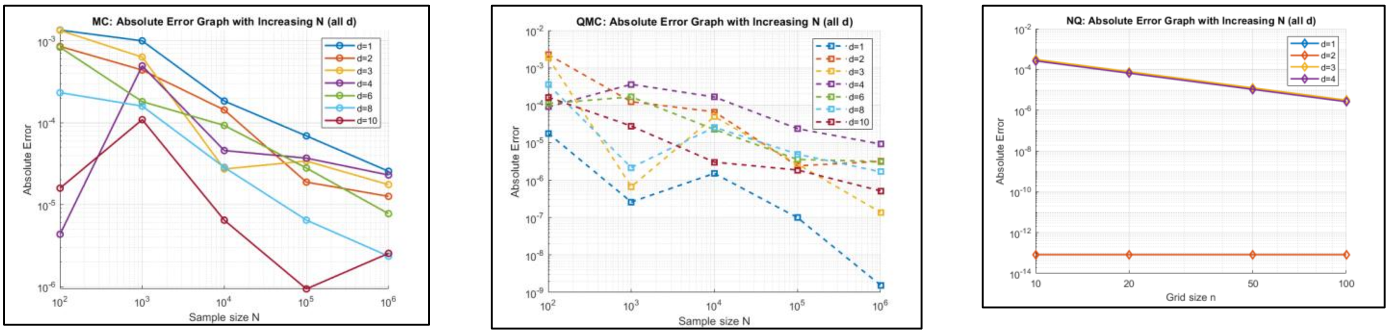
2.5 Numerical Quadrature

The application of NQ in lower dimensional setting was mainly because of its computational cost in higher dimensionality. Approximations of the integrals were done by adaptive quadrature schemes by refining the evaluation grid according to the behaviour of the integrand. The grid resolution was gradually enhanced to examine the impact of the resolution on accuracy and convergence. This application underscores the weaknesses of NQ in problems of high dimensionality and offers a good benchmark against which to compare in the low-dimensional ones.

3. Results and Discussion

3.1 Accuracy Analysis

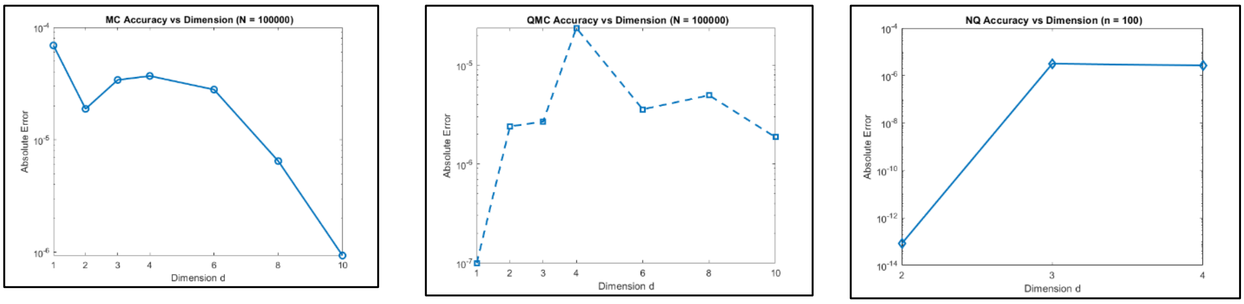
Figure 2 reflects the impact of sample refinement on accuracy for MCI, QMC, and NQ. In MCI, the absolute error is found to diminish steadily with the size of the sample in all the dimensions under test with only slight variations at smaller sample sizes and this behaviour is expected to be dimension-independent convergence behaviour. QMC also has a similar decreasing behaviour with sample size but with even smaller error rates than MCI, especially in lower dimensions. At intermediate sample sizes, small non-monotonic fluctuations are seen because of its uniformly distributed low discrepancies. Conversely, NQ is much faster in the reduction of errors with grid refinement in cases of low dimension, and nearly machine-precision accuracy can be obtained even on moderate grid resolutions. The results suggest that MCI is the best method with increased refinement, QMC is the best method with smooth problems and NQ with the best method in the low-dimensional setting.



(a) (b) (c)

Fig. 2 Effect of sample refinement on accuracy (a) MCI; (b) QMC; (c) NQ

Besides effect of sample refinement, effect of dimensionality on accuracy also took place in this study. The impact of dimensionality on accuracy is explained by the change in absolute error with the increase in dimension at a constant sample size. As illustrated in the Figure 3(a), MCI displays relatively steady error values across dimensions, but does not have significant variations and instead, there are moderate variations with no apparent systematic deterioration in accuracy with increase in dimension. Quasi-Monte Carlo (QMC) is less accurate at higher dimensions but less variable and in general, it is less accurate than lower dimensions and this demonstrates that low-discrepancy sampling is less effective in high-dimensional spaces. On the other hand, Numerical Quadrature is very accurate in a two-dimensional case and the error increases drastically when the dimension is raised to three and four, indicating high sensitivity to dimensionality. Overall, this suggests that MCI is least sensitive to increasing dimension, QMC works best under low-dimensional problems, whereas NQ can only be used under very low-dimensional problems.



(a) (b) (c)

Fig. 3 Effect of dimensionality on accuracy (a) MCI; (b) QMC; (c) NQ

3.2 Computational Efficiency Analysis

The computational efficiency was provided by comparing the run time of MCI, QMC and NQ operated under identical refinement conditions as shown in Figure 4. MCI and QMC are the only algorithms which are effectively computable even in higher dimensions ($d > 4$), and the cost of NQ grows exponentially with dimension. MCI has low runtime across the dimensions that have been tested, which implies that it is highly scaled in high-dimensional problems. QMC is more costly in terms of runtime due to the additional overhead of low-discrepancy sequence generation yet, computation is not more expensive than MCI. The only instance of the curse of dimensionality is NQ, which is only low-dimensional, overhead is low and performance increases exponentially with the dimension. Overall, the results indicate that MCI is the most scalable technique, QMC is more precise and expensive, and NQ can be used on tasks of small dimensions only.

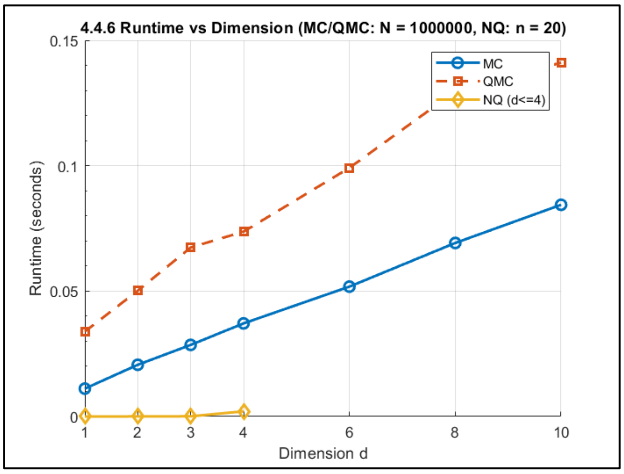
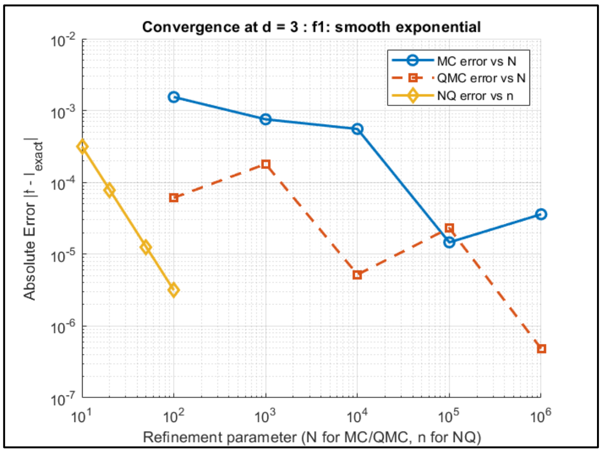


Fig. 4 Runtime comparison of MCI, QMC and NQ under fixed refinement condition

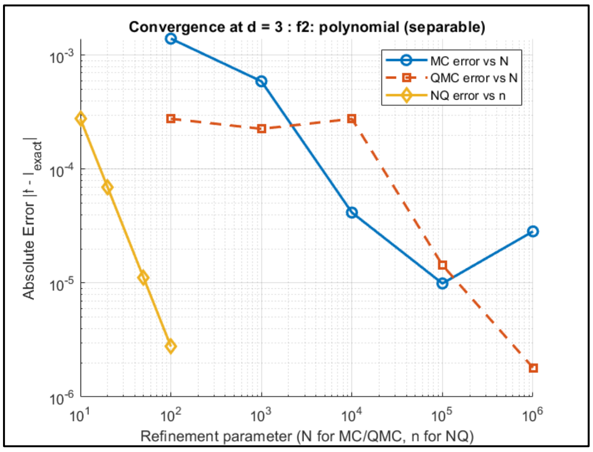
3.3 Convergence Rate Analysis

Fig. 5 shows the convergence behaviour of MCI, QMC and NQ at the specified fixed dimension $d = 3$ on four chosen benchmark functions. MCI shows a consistent decrease in error as the smooth exponential and smooth separable polynomial functions are refined. QMC tends to achieve a higher rate of error reduction and lower overall error with increased refinement, due to more uniform sampling. NQ has a very rapid rate of convergence to these smooth problems with very small errors at coarse grid resolutions. On the other hand, convergence of MCI and QMC is slower, and more intermittent in the oscillatory case, since the oscillation in signs of the integrand increases the variance, but NQ is much more problem dependent. MCI will accept the smooth decrease in error when the indicator function is non-smooth, whereas QMC will fail to show a significant gain in convergence, and

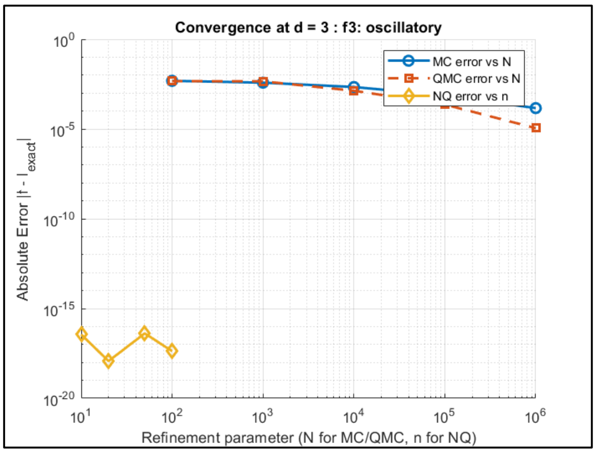
NQ will not increase with smoothness, which shows the regularity of the integrand. In general, the findings indicate that convergence performance is very sensitive to the smoothness of the integrand. MCI will be the most stable in every case, whereas QMC and NQ will prove strong at convergence of smooth functions.



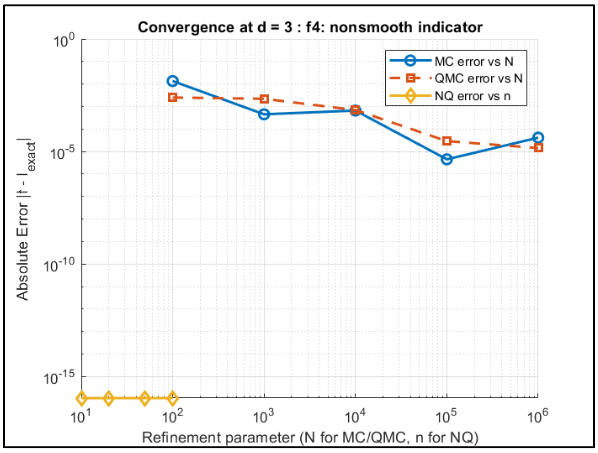
(a)



(b)



(c)



(d)

Fig. 5 Convergence rate analysis on (a) unsmooth exponential function; (b) separable polynomial function; (c) oscillatory function; (d)nonsmoothed indicator function

3.4 Result Summary

Table 1 is a summary of the comparative performance of MCI, QMC and NQ with respect to accuracy, computer efficiency and convergence behaviour.

Table 1 Summary of MCI, QMC and NQ Performance

Method	Accuracy	Computational Efficiency	Convergence Behaviour
MCI	Has constant stability of accuracy across dimensions and low sensitivity to dimensionality, thus it is	Highly scalable for high-dimensional problems, with execution time increasing approximately	Exhibits some convergence that is independent of dimension of all types of integrands and oscillatory

Table 1 Continued

	appropriate to high dimensional problems.	linearly with dimension and sample size.	functions whose convergence is more gradual because of greater variance.
QMC	Gives greater accuracy than MCI to smooth low to moderate dimensional problems but the accuracy is irregular and the advantage decreases as dimensionality increases.	Has increased computational cost than MCI because of low-discrepancy sequence generation and is still computationally feasible at moderate dimensional sizes.	Convergence is much higher than that of MCI with smooth and separable integrands but deteriorates with oscillatory and nonsmoothed functions.
NQ	Gives near machine accuracy on low dimensions but the error increases very fast with dimensionality such that it is not usable in high dimensional integration.	Very low dimensionality, highly efficient, however, the cost of computation increases exponentially with the dimensionality, making it infeasible on high dimensional problems.	Performs well in low dimensions with smooth integrands and badly with nonsmoothed or discontinuous functions, where grid refinement can do little to help.

4. Conclusion

In this paper, the numerical approximation to multi-dimensional integrations using MCI, QMC and NQ have been evaluated on a comparative basis in the unit hypercube. The findings reveal that there is a consistent and reliable accuracy of MCI over the increasing dimensions and convergence behaviour is not very sensitive to dimensionality. Hence, it is appropriate to use in high-dimensional problems. QMC reaches a better accuracy and convergence rate when smooth and separable integrands are involved in low to moderate dimensions, though the cost of its implementation is significantly higher because it produces low-discrepancy sequences. Conversely, NQ is more accurate and converges faster in low dimensional contexts, but when dimensionality grows NQ becomes computationally infeasible as dimensionality grows as a manifestation of the curse of dimensionality.

Computationally, MCI has been determined to be the most scalable and time-efficient of all the dimensions that were tried, and QMC had a distinct trade-off between better quality and longer run time. The convergence analysis also revealed a strong performance of method with integrand properties, MCI exhibits very strong behaviour in all type of functions, QMC performs well with smooth problems and NQ is highly sensitive to both dimension and smoothness. The given findings prove the idea that no one integration method can be considered universally optimal and that the choice of methods should be supported by the dimension of the problems and the regularity of integrands.

Future directions can include more advanced methods of QMC, including higher-order digital nets or scrambling strategies that adapt to non-smooth integrands, which can be better than the current method. Besides that, hybrid strategies involving a combination of Monte Carlo methods with deterministic quadrature strategies or variance reduction strategies could provide a promising accuracy-efficiency balance. The applicability of the present work could be further improved by extending the analysis to the practical application in other areas, including uncertainty quantification, financial mathematics, and physical simulations.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: ***study conception and design:*** *Nurfarhana Izzati Norul Annuar;* ***data collection:*** *Nurfarhana Izzati Norul Annuar;* ***analysis and interpretation of results*** *Nurfarhana Izzati Norul Annuar, Fazlina Aman* ***draft manuscript preparation:*** *Nurfarhana Izzati Norul Annuar, Fazlina Aman. All authors reviewed the results and approved the final version of the manuscript.*

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