A Quasi-Monte Carlo Method for Elliptic Boundary Value Problems

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Abstract

In this paper we present and analyze a quasi-Monte Carlo method for solving elliptic boundary value problems. Our method transforms the given partial differential equation into an integral equation by employing a well known local integral representation. The kernel in this integral equation representation can be used as a transition density function to define a Markov process used in estimating the solution. The particular process, called a *random walk on balls* process, is subsequently generated using quasirandom numbers. Two approaches of using quasirandom numbers for this problem, which uses an acceptance-rejection method to compute the transition probabilities, are presented. We also estimate the accuracy and the computational complexity of the quasi-Monte Carlo method. Finally, results from numerical experiments with Sobol and Halton quasirandom sequences are presented and are compared to the results with pseudorandom numbers. The results with quasirandom numbers provide a slight improvement over regular Monte Carlo methods. We believe that both the relatively high effective dimension of this problem and the use of the acceptance-rejection method impede significant convergence acceleration often seen with some quasi-Monte Carlo methods.

1 Introduction

Monte Carlo methods (MCMs) are powerful tools for solving multidimensional problems defined on complex domains. MCMs are based on the creation of statistics whose expected values are equal to computationally interesting quantities. As such, MCMs are used for solving a wide variety of elliptic and parabolic boundary value problems (BVPs), [20, 4, 12]. While it is often preferable to solve a partial differential equation with a deterministic numerical method, there are some circumstances where MCMs have a distinct advantage. For example, when the geometry of a problem is complex, when the required accuracy is moderate, when a geometry is defined only statistically, [7], or when a linear functional of the solution, such as a solution at a point, is desired, MCMs are often the most efficient method of solution.

Despite the universality of MCMs, a serious drawback is their slow convergence. The error of MCMs is stochastic, and the uncertainty in an average taken from N samples is $O(N^{-1/2})$ by virtue of the central limit theorem. One generic approach to improving the convergence of MCMs has been the use of highly uniform, quasirandom, numbers (QRNs) in place of the usual pseudorandom numbers (PRNs). While PRNs are constructed to mimic the behavior of truly random numbers, QRNs are

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constructed to be distributed as evenly as mathematically possible. Quasi-MCMs use quasirandom sequences, which are deterministic, and may have correlations between points, and they were designed primarily for integration. For example, with QRNs, the convergence of numerical integration can sometimes be improved to $O(N^{-1})$. In fact, quasi-Monte Carlo approaches to integral equations have been studied, but much less than the problem of finite dimensional quadrature, and there are several examples of quasi-MCM success in solving transport problems, [9, 14, 15, 21]. However, the effective use of QRNs for convergence acceleration when the probability density of a Monte Carlo statistic is defined via a Markov chain is problematic. The problem we consider in this paper is of this type.

In this paper we continue the process of studying the applicability of QRNs for Markov chainbased MCMs, [10, 11]. We consider an elliptic BVP and investigate a quasi-MCM version of the *random walk on balls* method, see [6]. The paper is organized as follows. In §2 we present a brief overview of QRNs. In §3 we than present an elliptic BVP and describe a MCM based on the walk on balls process for its solution. In §4 we discuss how the MCM can be realized using QRNs. Using one of the methods described, we then, in §5, present some numerical results that confirm that our quasi-MCM solves the problem and behaves consistent with the previously presented theoretical discussion. Finally, in §6 we draw some conclusions, and discuss opportunities for related future work.

2 QRNs and Integration

QRNs are constructed to minimize a measure of their deviation from uniformity called discrepancy. There are many different discrepancies, but let us consider the most common, the star discrepancy. Let us define the star discrepancy of a one-dimensional point set, $\{x_n\}_{n=1}^N$, by

$$D_N^{\star} = D_N^{\star}(x_1, \dots, x_N) = \sup_{0 \le u \le 1} \left| \frac{1}{N} \sum_{n=1}^N \chi_{[0,u)}(x_n) - u \right|$$
(1)

where $\chi_{[0,u)}$ is the characteristic function of the half open interval [0, u). In statistical terms, the star discrepancy is the largest absolute deviation of the empirical distribution of $\{x_n\}_{n=1}^N$ from uniformity. The mathematical motivation for quasirandom numbers can be found in the classic Monte Carlo application of numerical integration. We detail this for the trivial example of one-dimensional integration for illustrative simplicity.

Theorem (Koksma-Hlawka, [8]): If f(x) has bounded variation, V(f), on [0, 1), and $x_1, \ldots, x_N \in [0, 1]$ have star discrepancy D^* , then:

$$\left|\frac{1}{N}\sum_{n=1}^{N}f(x_{n}) - \int_{0}^{1}f(x)\,dx\right| \le V(f)D_{N}^{\star},\tag{2}$$

The star discrepancy of a point set of N truly random numbers in one dimension is $O(N^{-1/2}(\log \log N)^{1/2})$, while the discrepancy of N quasirandom numbers can be as low as $O(N^{-1})^1$. In s > 3 dimensions it is rigorously known that the discrepancy of a point set with N elements can be no smaller than a constant depending only on s times $N^{-1}(\log N)^{(s-1)/2}$. This remarkable result of Roth, [19], has motivated mathematicians to seek point sets and sequences with discrepancies as close to this lower bound as possible. Since Roth's remarkable results, there have been

¹Of course, the N optimal quasirandom points in [0,1) are the obvious: $\frac{1}{(N+1)}, \frac{2}{(N+1)}, \dots, \frac{N}{(N+1)}$.

many constructions of low discrepancy point sets that have achieved star discrepancies as small as $O(N^{-1}(\log N)^{s-1})$. Most notably there are the constructions of Hammersley, Halton, Sobol, Faure, and Niederreiter, description of which can be found in Niederreiter's monograph [17].

While QRNs do improve the convergence of applications like numerical integration, it is by no means trivial to enhance the convergence of all MCMs. In fact, even with numerical integration, enhanced convergence is by no means assured in all situations with the näive use of quasirandom numbers, [1], [16].

3 Random Walks on Balls

In this section we give the formulation of the elliptic BVP under consideration, and a MCM for its solution. A full description of the MCM can be found in [6, 4, 3].

3.1 Formulation of the problem

Let $G \subset \mathbb{R}^3$ be a bounded domain with boundary ∂G . Consider the following elliptic BVP:

$$Mu \equiv \sum_{i=1}^{3} \left(\frac{\partial^2}{\partial x_i^2} + b_i(x)\frac{\partial}{\partial x_i}\right)u(x) + c(x)u(x) = -\phi(x), \qquad x \in G$$
(3)

$$u(x) = \psi(x), \qquad x \in \partial G.$$
 (4)

Assume that the data, $\phi(x)$, $\psi(x)$, and the boundary ∂G satisfy conditions ensuring that the solution of the problem (3), (4) exists and is unique, [13]. In addition, assume that $\nabla \cdot b(x) = 0$. The solution, u(x), has a local integral representation for any standard domain, T, lying completely inside the domain G, [13]. To derive this representation we proceed as follows. The adjoint operator of M has the form:

$$M^* = \sum_{i=1}^{3} \left(\frac{\partial^2}{\partial x_i^2} - b_i(x)\frac{\partial}{\partial x_i}\right) + c(x)$$

In the integral representation we use Levy's function defined as:

$$L_p(y,x) = \mu_p(R) \int_r^R (1/r - 1/\rho) p(\rho) d\rho, \ r < R,$$

where

$$\mu_p(R) = (4\pi q_p)^{-1}, \ q_p(R) = \int_0^R p(\rho) d\rho,$$

p(r) is a density function, and $r = |x - y| = \left(\sum_{i=1}^{3} (x_i - y_j)^2\right)^{1/2}$. Then the following integral representation holds, [6]:

$$\begin{split} u(x) &= \int_{T} [u(y)M_{y}^{*}L(y,x) + L(y,x)\phi(y)]dy \\ &+ \int_{\partial T} \sum_{j=1}^{3} \nu_{j} \left[\left(L(y,x)\frac{\partial u(y)}{\partial y_{j}} - u(y)\frac{\partial L(y,x)}{\partial y_{i}} \right) - b_{j}(y)u(y)L(y,x) \right] d_{y}S, \end{split}$$

where $\nu = (\nu_1, \nu_2, \nu_3)$ is the exterior normal to the boundary ∂G , and T is any closed domain in G.

For the special case when the domain is a ball $T = B(x) = y : |y - x| \le R(x)$ with center x and radius $R(x), B(x) \subset \overline{G}$, and for $p(r) = e^{-kr}, k \ge b^* + Rc^*$ ($b^* = \max_{x \in G} |b(x)|, c^* = \max_{x \in G} |c(x)|$, the above representation can be simplified, [4]:

$$u(x) = \int_{B(x)} M_y^* L_p(y, x) u(y) dy + \int_{B(x)} L_p(y, x) \phi(y) dy.$$
(5)

Moreover, $M_y^* L_p(y, x) \ge 0$, $y \in B(x)$ for the above parameters k, b^* and c^* , and so it can be used as a transition density in a Markov process.

3.2 The Monte Carlo Method

Consider a Fredholm integral equation of the second type:

$$u(x) = \int_{G} k(x, y)u(y)dy + f(x), \text{ or } u = Ku + f,$$
(6)

and a MCM for calculating a linear functional of its solution:

$$J(u) = (h, u) = \int_G u(x)h(x)dx.$$
(7)

To solve this problem via a MCM^2 , we construct random walks, using h to select initial spatial coordinates for each random walk, and the kernel k, suitably normalized, to decide between termination and continuation of each random walk, and to determine the location of next point. There are numerous ways to accomplish this.

Consider the following random variable (RV) whose mathematical expectation is equal to J(u):

$$\theta[h] = \frac{h(\xi_0)}{\pi(\xi_0)} \sum_{j=0}^{\infty} Q_j f(\xi_j),$$
(8)

where $Q_0 = 1$; $Q_j = Q_{j-1} \frac{k(\xi_{j-1}, \xi_j)}{p(\xi_{j-1}, \xi_j)}$, j = 1, 2, ... Here $\xi_0, \xi_1, ...$ is a Markov chain (random walk) in the domain G with initial density function $\pi(x)$ and transition density function p(x, y), which is equal to the normalized integral equation kernel.

The Monte Carlo estimate of $J(u) = E[\theta]$ is

$$J(u) = E[\theta] \approx \frac{1}{N} \sum_{s=1}^{N} \{\theta_{k_s}\}_s,\tag{9}$$

where $\{\theta_{k_s}\}_s$ is the *s*-th realization of the RV θ on a Markov chain with length k_s , and N is the number of Markov chains (random walks) realized. The statistical error is $err_N \approx \sigma(\theta) N^{-\frac{1}{2}}$ where $\sigma(\theta)$ is the standard deviation of our statistic, θ .

We can consider our problem (5) as an integral equation (6) with kernel:

$$k(x,y) = \begin{cases} M_y^* L_p(y,x) & \text{, when } x \notin \partial G \\ 0 & \text{, when } x \in \partial G, \end{cases}$$

²We develop the solution in a Neumann series under the condition $||K^{n_0}|| < 1$ for some $n_0 \ge 1$

and the right-hand side given by

$$f(x) = \begin{cases} \int_{B(x)} L_p(y, x)\phi(y)dy & , \text{ when } x \notin \partial G \\ \psi(x) & , \text{ when } x \in \partial G. \end{cases}$$

However, for the above choice of k(x, y), ||K|| = 1, and to ensure the convergence of the MCM, a biased estimate can be constructed (see [6]) by introducing an ε -strip, ∂G_{ε} , of the boundary, ∂G , $\partial G_{\varepsilon} = \{x \in G : d(x) < \varepsilon\}$ where d(x) is the distance from x to the closest point of the boundary, ∂G . We now construct a MCM for this integral equation (8), (9), and a finite Markov chain with the transition density function:

$$p(x,y) = k(x,y) = M_y^* L_p(y,x) \ge 0,$$
(10)

 $|x-y| \leq R$, where R is the radius of the maximal ball with center x, and lying completely in G. In terms of (8) this transition density function defines a random walk $\xi_1, \xi_2, \ldots, \xi_{k_{\varepsilon}}$ such that every point $\xi_j, j = 1, \ldots, k_{\varepsilon} - 1$ is chosen in the maximal ball $B(x_{j-1})$, lying in G, in accordance with density (10). The Markov chain terminates when it reaches ∂G_{ε} , so that $\xi_{k_{\varepsilon}} \in \partial G_{\varepsilon}$.

If we are interested in the solution at the point ξ_0 , we choose $h(x) = \delta(x - \xi_0)$ in (8). Then $u(\xi_0) = E[\theta(\xi_0)]$, where

$$\theta(\xi_0) = \sum_{j=0}^{k_{\varepsilon}-1} \int_{B(\xi_j)} L_p(y,\xi_j)\phi(y)dy + \psi(\xi_{k_{\varepsilon}}).$$
(11)

3.3 The Algorithm

The Monte Carlo algorithm for estimating $u(\xi_0)$ consists of simulating N Markov chains with a transition density given in (10), scoring the corresponding realizations of $\theta[\xi_0]$ and accumulating them. This algorithm is known as the *random walks on balls* algorithm and is described in detail in [4, 3]. Direct simulation of random walks with the density function p(x, y) given by (10) is problematic due to the complexity of the expression for $M_y^*L(y, x)$. It is computationally easier to represent p(x, y) in spherical coordinates as $p_1(r)p_2(\mathbf{w}|r)$. Thus, given ξ_{j-1} , the next point is $\xi_j = \xi_{j-1} + r\mathbf{w}$, where the distance, r, is chosen with density

$$p_1(r) = (ke^{-kr})/(1 - e^{-kR}),$$
 (12)

and the direction, \mathbf{w} , is chosen according to:

$$p_2(\mathbf{w}/r) = 1 + \frac{\sum_{i=1}^3 b_i(x+r\mathbf{w})w_i + c(x+r\mathbf{w})r}{e^{-kr}} \int_r^R e^{-k\rho} d\rho - \frac{c(x+r\mathbf{w})r^2}{e^{-kr}} \int_r^R \frac{e^{-k\rho}}{\rho} d\rho.$$
(13)

To simulate the direction, \mathbf{w} , the acceptance-rejection method (ARM) is used with the following majorant:

$$h(r) = 1 + \frac{b^*}{e^{-kr}} \int_r^R e^{-k\rho} d\rho.$$
 (14)

Thus the algorithm for a single random walk with $\theta = 0$, $\xi = \xi_0$ initially is:

- **1.** Calculate $R(\xi)$.
- **2.** Simulate the distance r with density $p_1(r)$ as given in (12).
- **3.** Simulate the direction **w** using the ARM:
 - **3.1.** Calculate the function h(r) via (14).
 - **3.2.** Generate random w uniformly on the unit 3-dimensional sphere.
 - **3.3.** Calculate $p_2(\mathbf{w}|r)$ according to (13).
 - **3.4.** Generate γ uniformly in [0, 1].
 - **3.5.** If $\gamma h(r) \leq p_2(\mathbf{w}|r)$ go to step 4 (acceptance), if not, go to step 3.2 (rejection).
- 4. Compute the next point as $\xi = \xi + r\mathbf{w}$.
- **5.** Update $\theta(\xi)$ using 11.
- **6.** If $\xi \in \partial G_{\varepsilon}$ then **stop**, if not, **go to** step **1** and continue.

The computational complexity of this MCM is equal to

$$S = NE[k_{\varepsilon}](t_0 + S_0^{-1}t_1 + t_2),$$

where N is the number of walks (Markov chains), $E[k_{\varepsilon}]$ is the average number of steps in a single random walk, S_0 is the efficiency of the ARM, t_0 is the number of operations to simulate r and to compute h(r), t_1 is the number of operations to simulate **w** and to compute p_2 , and t_2 is the number of operations to compute $\theta(\xi)$. If the radius, r, of every ball is fixed then according to [20] the average number of steps in the random walk is: $E[k_{\varepsilon}] \approx \frac{4R^2|ln\varepsilon|}{r^2}$. Here R is the radius of the maximal ball lying in G with center at ξ_0 . The conditions for $E[r] \in (\alpha R, 0.5R)$, for $\alpha \in (0, 0.5)$ can be found in [3]. Combining these results we obtain:

$$E[k_{\varepsilon}] \approx \frac{1}{\alpha^2} |ln\varepsilon|.$$

We now estimate S_0 , the efficiency of the ARM. For a general ARM, let us assume that the density, $u_1(x)$, has an easily computable majorant function, $u_2(x)$, with $0 \le u_1(x) \le u_2(x)$, for all x, and $U_1 = \int_G u_1(x) dx$ and $U_2 = \int_G u_2(x) dx$. Let η be a random variable distributed via $u_2(x)/U_2$ and let γ be uniformly distributed in [0, 1]. It has been shown [5] that if $\gamma u_2(\eta) \le u_1(\eta)$, then η is distributed with density $u_1(x)/U_1$. The value $S_0 = U_1/U_2$ is called the *efficiency* of the ARM, and so S_0^{-1} is the average number of attempts to obtain a single realization of $u_1(x)/U$. Thus, in our case

$$S_0 = \frac{1}{1 + \frac{b^*}{k}(1 - e^{-kR})} \ge \frac{1}{2}.$$

4 Quasi-Random Walks

In this section we discuss how to construct a quasi-MCM for the problem considered here. We will need to figure out how to use quasirandom sequences to simulate the previously defined random walks. We propose a method that combines pseudorandom and quasirandom elements in the construction of the random walks in order to take advantage of the superior uniformity of quasirandom numbers and the independence of pseudorandom numbers.

Error bounds arising in the use of quasi-MCMs for integral equations is based on Chelson's estimates. Below Chelson's results are rewritten in terms related to our particular problem:

$$\left| u(\xi_0) - \frac{1}{N} \sum_{1}^{N} \theta_s^*(\xi_0) \right| \le V(\theta^*) \ D_N^*(Q)$$
(15)

where Q is a sequence of quasirandom vectors in $[0, 1)^{dT}$, d is the number of QRNs in one step of a random walk, T is the maximal number of steps in a single random walk, and θ^* corresponds to θ for the random walk $\xi_0, \xi_1, \ldots, \xi_{k_{\varepsilon}}$ generated from Q by a one-by-one map. Space precludes more discussion of the work of Chelson, but the reader is referred to the original for clarification, [2].

This digestion of Chelson's results is the integral equation analog of the Koksma-Hlawka inequality. It ensures convergence, but it's rate is very pessimistic due to the high dimension of the quasirandom sequence. There are many other examples of the successful use of quasirandom sequences for solving particular integral equations, including transport problems, [9, 14, 15, 21]. In addition, Spanier proposed a hybrid method which combines features of both pseudorandom and quasirandom sequences that is similar to what we propose below.

The effectiveness of quasi-MCMs has some important limitations. First of all, quasi-MCMs may not be directly applicable to certain simulations, due to correlations between points of the quasirandom sequence. This problem can be overcome in many cases by rewriting the quantity which is statistically sampled as an integral or by judicious scrambling of the QRNs used, [18]. However, as the resulting integral is often of very high dimensional, this leads to a second limitation as the improved accuracy of quasi-MCMs applied to integrals is generally lost in very high dimensions. In the MCM described in this paper, a random walk is a trajectory

$$\xi_0 \to \xi_1 \to \ldots \to \xi_{k_{\varepsilon}},$$

where ξ_0 is the initial point and the transition probability from ξ_{j-1} to ξ_j is $p(\xi_{j-1}, \xi_j)$, (see (10)). Using quasirandom sequences in this problem is not so simple. One approach is to follow the methods proposed by Chelson and other authors, i. e., to use a $k_{\varepsilon}(1 + 3S_0^{-1}) \approx 7k_{\varepsilon}$ -dimensional sequence with length N for N random walks. Here k_{ε} is the length of a Markov chain and S_0 is the efficiency of the ARM. Here we interpret the trajectory as a point in $G \times \ldots \times G = G^{i+1}$, and the density of this point is:

$$p_i(\xi_0, \xi_1, \dots, \xi_i) = p(\xi_0, \xi_1) \dots p(\xi_{i-1}, \xi_i).$$
(16)

The difficulty here is that the dimension of such a sequence is very high (several hundreds) and, consequently, the discrepancy of such a high dimensional quasirandom sequence is approximately that of a pseudorandom sequence and therefore of no improvement over ordinary MCMs.

Another possibility is to assign a different one-dimensional sequence to each trajectory. The length of such sequence is $k_{\varepsilon}(1 + 3S_0)$. Without some kind of random scrambling, this will cause the trajectory to repeat the same pattern over and over, and the method will not converge. These difficulties can be avoided by using a single one-dimensional sequence of length $N(k_{\varepsilon}(1 + 3/S_0))$. Thus we assign the first $(k_{\varepsilon}(1 + 3/S_0))$ QRNs to the first trajectory, the next $(k_{\varepsilon}(1 + 3/S_0))$ QRNs go with the second trajectory, etc. This is another way to fill the $(k_{\varepsilon}(1 + 3/S_0))$ - dimensional unit cube with quasirandom points; however, there are large holes meaning large discrepancy and so the convergence is not any better than the previously mentioned method.

However, one can also try to use QRN-PRN hybrid to generate the walks. We have N points in the first ball because every trajectory starts at its center, ξ_0 . This means that it is most important to sample the next N points, $(\xi_1)_s$, which are located in this ball, with the density p(). The first possibility is to use a 7-dimensional QRN sequence with length N to find the next point, ξ_1 ,

for each of the N walks. We can extend this approach for the first M balls in every walk by using QRNs for them and PRNs for the other balls further along in the walk. Thus we can reduce the error if the internal contribution in $\theta(\xi_j)$ for $j = 1, \ldots M$ is relatively large, which can only occur when $\psi \neq 0$. We can also use QRNs to simulate unit isotropic vectors with the ARM and can use PRNs for uniform random variable needed in the rejection decision. This is motivated by the fact that it is more important for the vector to be uniformly distributed than to be independent. However, for the random number used for comparison it is more important that it be independent. The length of every walk depends on ε , and on the coefficients of the considered BVP (b^* and c^*). In addition, the efficiency of ARM depends again on these coefficients. So, a careful analysis of this problem has to be made in order to choose the best way to use QRN sequences.

5 Numerical Results

We consider the following problem in the unit cube G

$$Mu = \Delta u + \sum_{j=1}^{3} b_j \frac{\partial}{\partial x_j} u + c(x)u = 0$$
, in $G = [0, 1]^3$

with the boundary conditions

$$u(x_1, x_2, x_3) = e^{c_0(x_1 + x_2 + x_3)}, \ (x_1, x_2, x_3) \in \partial G$$

Here $b_1 = b_0(x_2 - x_3)$, $b_2 = b_0(x_3 - x_1)$, $b_3 = b_0(x_1 - x_2)$, and so the condition $\nabla \cdot b(x) = 0$ is satisfied, and $c(x) = -3.0c_0^2$.

We performed numerical tests of compare our MCM to our proposed quasi-MCM. In the MCM, the algorithm is implemented using PRNs. The quasi-MCM version of the algorithm uses N PRNs to simulate the distance r and a 3-dimensional Sobol sequence of length 2N to simulate the direction **w** via the ARM. We used QRNs in this way because in our particular numerical example the right-hand side of the BVP is 0. If this were not so, the first hybrid strategy would have been used. Relative errors of the MCM and the quasi-MCM in the solution at the center (0.5, 0.5, 0.5) are presented on Fig. 1. In addition, the average length of random walks versus ε are presented on Fig. 2. The results show that even in this complicated case the quasirandom sequences can be used successfully and that the quasi-MCM has a better accuracy and a faster convergence than the MCM.

6 Conclusions

In this paper we presented a quasi-Monte Carlo algorithm for the solution a 3-dimensional elliptic BVP. Our method, based on the *random walks on balls* method, converts the partial differential equation into an equivalent integral equation. The method then uses functions derived in the conversion to integral equation form to define a Markov process and statistic on paths defined by that Markov process whose expected value equals a linear functional of solution of the original problem. We then presented several approaches for the use of QRNs to generate samples of the statistic in question, and used one of these strategies to numerically solve a particular elliptic BVP with a quasi-MCM. Our quasi-MCM was slightly more accurate and less costly than the corresponding MCM. This result is quite encouraging, as the effective dimension of this problem



Figure 1: Relative errors in the solution of the MCM and the quasi-MCM at the center point: (0.5, 0.5, 0.5).



Figure 2: The average length of the random walk versus ε .

is quite high. So high, in fact, that it was doubtful if quasi-MCMs had any real chance of beating MCMs.

The improvement seen suggests opportunities for further work to obtain even greater gains in convergence rate with quasi-MCMs applied to boundary value problems. Clearly, the high effective dimension of the problem makes the use of QRNs very problematic. Thus, we feel that approaches to reduce this effective dimensionality should be explored. In addition, the use of the ARM removed quasirandom points from the QRN sequence. This is clearly not a good thing to do, as omissions in a QRN sequence leave holes that result in increased discrepancy. However, a general approach to quasirandom sampling from distributions while using the ARM is still a hard and open problem. Finally, it is important to recognize that the definitions of discrepancy and the Koksma-Hlawka inequality are so closed tied to numerical integration, that it is our belief that new measures of uniformity for random walks should be explored. Given such a tuned quantity, a more powerful way to generate and analyze uniform random walks may be possible. This would most assuredly lead to better convergence and more optimistic error estimates for a broad array of quasi-MCMs employing random walks.

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References

- R. E. CAFLISCH, "Monte Carlo and quasi-Monte Carlo methods," Acta Numerica, 7: 1–49, 1998.
- [2] P. CHELSON, "Quasi-Random Techniques for Monte Carlo Methods," *Ph.D. dissertation*, The Claremont Graduate School, 1976.
- [3] I. DIMOV, T. GUROV, "Estimates of the computational complexity of iterative Monte Carlo algorithm based on Green's function approach," *Mathematics and Computers in Simulation*, 47 (2-5): 183-199, 1998.
- [4] I. DIMOV, A. KARAIVANOVA, H. Kuchen, H. Stoltze, "Monte Carlo algorithms for elliptic differential equations. Data Parallel Functional Approach," *Journal of Parallel Algorithms* and Applications, 9: 39–65, 1996.
- [5] S.M. ERMAKOV, G.A. MIKHAILOV, Statistical Modeling, Nauka, Moscow, 1982.
- [6] S. ERMAKOV, V. NEKRUTKIN, V. SIPIN, Random Processes for solving classical equations of the mathematical physics, Nauka, Moscow, 1984.
- [7] C. O. HWANG, J. A. GIVEN AND M. MASCAGNI, "On the rapid estimation of permeability for porous media using Brownian motion paths," *Phys. Fluids*, **12(7)**: 1699-1709, 2000.
- [8] J. F. KOKSMA, "Een algemeene stelling uit de theorie der gelijkmatige verdeeling modulo 1," Mathematica B (Zutphen), 11: 7–11, 1942/43.
- [9] C. LECOT, I. COULIBALY, "A quasi-Monte Carlo scheme using nets for a linear Boltzmann equation," SIAM J. Num. Anal., 35: 51–70, 1998.

- [10] M. MASCAGNI AND A. KARAIVANOVA, "Are Quasirandom Numbers Good for Anything Besides the Integration?" Proceedings of PHYSOR2000, Pittsburgh, PA, 2000.
- [11] M. MASCAGNI AND A. KARAIVANOVA, "Matrix Computations Using Quasirandom Sequences," Proceedings of the Second International Conference on Numerical Analysis and Applications, Rousse, Bulgaria, 2000.
- [12] G. A. MIKHAILOV, New Monte Carlo Methods with Estimating Derivatives, Utrecht, The Netherlands, 1995.
- [13] C. MIRANDA, Equasioni alle dirivate parziali di tipo ellittico, Springer Verlag, Berlin, 1955.
- W. MOROKOFF, "Generating Quasi-Random Paths for Stochastic Processes," SIAM Rev., Vol. 40, No.4, pp. 765–788, 1998.
- [15] W. MOROKOFF AND R. E. CAFLISCH, "A quasi-Monte Carlo approach to to particle simulation of the heat equation," SIAM J. Numer. Anal., 30: 1558–1573, 1993.
- [16] B. MOSKOWITZ AND R. E. CAFLISCH, "Smoothness and dimension reduction in quasi-Monte Carlo methods," J. Math. Comput. Modeling, 23: 37–54, 1996.
- [17] H. NIEDERREITER, Random Number Generation and Quasi- Monte Carlo methods, SIAM, Philadelphia, PA, 1992.
- [18] A. OWEN, "Scrambling Sobol and Niederreiter-Xing points," Stanford University Statistics preprint, 1997.
- [19] K. F. ROTH, "On irregularities of distribution," Mathematika, 1: 73–79, 1954.
- [20] K. SABELFELD, Monte Carlo Methods in Boundary Value Problems, Springer Verlag, Berlin -Heidelberg - New York - London, 1991.
- [21] J. SPANIER, L. LI, "Quasi-Monte Carlo Methods for Integral Equations," Lecture Notes in Computer Statistics, Springer, 127: 382–397, 1998.