Solving BVPs Using Quasirandom Walks on the Boundary

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Abstract. The "random walk on the boundary" Monte Carlo method has been successfully used for solving boundary-value problems. This method has significant advantages when compared to random walks on spheres, balls or a grid, when solving exterior problems, or when solving a problem at an arbitrary number of points using a single random walk. In this paper we study the properties of the method when we use quasirandom sequences instead of pseudorandom numbers to construct the walks on the boundary. Theoretical estimates of the convergence rate are given and numerical experiments are presented in an attempt to confirm the convergence results. The numerical results show that for "walk on the boundary" quasirandom sequences provide a slight improvement over ordinary Monte Carlo.

1 Introduction

The "random walk on the boundary" Monte Carlo method has been successfully used for solving various boundary-value problems of mathematical physics. This method is based on classical potential theory which makes it possible to convert the original problem (boundary-value problem) into an equivalent problem (boundary integral equation). The Monte Carlo technique is then used to solve numericaly the integral equation. This method was first published in [13], and then applied to solving various boundary-value problems.

The major drawback of the conventional Monte Carlo approach is the statistical rate of convergence: computational error behaves as $O(N^{-1/2})$, where N is the number of random walks. Computer simulation of randomness is usually based on

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the generation of a sequence of standard pseudorandom numbers that mimic the theoretical behavior of "real" random numbers. One possible way to improve the convergence is to change the type of random numbers used. Quasi-Monte Carlo methods (QMCMs) use quasirandom (also known as low-discrepancy) sequences instead of pseudorandom numbers. The quasi-Monte Carlo method for integration in s-dimensions has a convergence rate of approximately $O((\log N)^s N^{-1})$. While numerical integration is the major application area of quasirandom sequences, there are many other problems where quasi-Monte Carlo methods also give better results than the Monte Carlo methods. There are many papers on using quasirandom numbers on differential equations. The curious reader should consult, for example, [10, 3, 12, 8, 9].

Here, we recall some basic concepts of QMCMs, [1]. First, for a sequence of N points $\{x_n\}$ in the s-dimensional half-open unit cube I^s define

$$R_N(J) = \frac{1}{N}\#\{x_n \in J\} - m(J)$$

where J is a rectangular set and $m(J)$ is its volume. Then define two discrepancies

$$D_N = \sup_{J \in E} |R_N(J)|, \quad D_N^\star = \sup_{J \in E^\star} |R_N(J)|,$$

where E is the set of all rectangular subsets in I^s and $E^\star$ is the set of all rectangular subsets in I^s with one vertex at the origin.

The basis for analyzing QMC quadrature error is the Koksma-Hlawka inequality:

Theorem (Koksma-Hlawka, [1]): For any sequence $\{x_n\}$ and any function f of bounded variation (in the Hardy-Krause sense), the integration error is bounded as follows

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(x_n) - \int_{I^s} f(x)\, dx \right| \leq V(f) D_N^\star. \tag{1}$$

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 in s dimensions can be as low as $O(N^{-1}(\log N)^{s-1})$ (see, e.g. [1, 11]). Most notably there are the constructions of Hammersley, Halton, Sobol', Faure, and Niederreiter for producing quasirandom numbers. Description of these can be found, for example, in Niederreiter's monograph [11].

In this paper, we present quasirandom walks on the boundary for solving some boundary-value problems. The paper is organized as follows. The formulation of the problems are given in §2. The random walk on the boundary method is described in §3. In §4 the use of quasirandom sequences is discussed, and some numerical results are presented.

2 Formulation of the Problem

Consider the problem of computing the electrostatic potential, u, in the interior of a compact dielectric G surrounded by another dielectric media. Let $\rho(x)$ be the density of this charge distribution. Then we have

$$\Delta u(x) = -\frac{\rho(x)}{\epsilon} \ , \ x \in G \ (\text{or } x \in \mathbb{R}^3 \setminus \overline{G}) \ , \tag{2}$$

and $u(x)$ satisfies the continuity conditions on the boundary of the domain:

$$u_i(y) = u_e(y) \ , \ \epsilon_i \frac{\partial u_i}{\partial n(y)} = \epsilon_e \frac{\partial u_e}{\partial n(y)} \ , \ y \in \partial G. \tag{3}$$

Here, u_i and u_e are the limit values of the solution from inside and outside respectively, ϵ_i and ϵ_e are the corresponding constant dielectric permittivities.

With the assumption that ∂G is smooth enough and there are only point charges inside G, $q_m, m = 1, \ldots, M$, it is possible to represent the solution in the form [5, 4]

$$u(x) = g(x) + \int_{\partial G} \frac{1}{2\pi} \frac{1}{|x-y|} \mu(y) d\sigma(y) \equiv g(x) + u_0(x) \ , \tag{4}$$

where $g(x) = \sum_{m=1}^{M} \frac{q_m}{4\pi\epsilon_i} \frac{1}{|x - x_m|}$, and x_m are the positions of the point charges.

Taking into account boundary conditions (3) and discontinuity properties of the single-layer potential's normal derivative [5], we arrive at the integral equation for the unknown density, μ:

$$\mu = -\lambda_0 \mathcal{K} \mu + f \ , \tag{5}$$

which is valid almost everywhere on ∂G. Here, $\lambda_0 = \frac{\epsilon_e - \epsilon_i}{\epsilon_e + \epsilon_i}$, and the kernel of the integral operator $\mathcal{K}$ is $\frac{1}{2\pi} \frac{\cos \phi_{yy'}}{|y - y'|^2}$, where $\phi_{yy'}$ is the angle between the external normal vector $n(y)$ and $y - y'$. The free term of this equation equals $\lambda_0 \frac{\partial g}{\partial n(y)}$, and it can be computed analytically. Since $\lambda_0 < 1$, the Neumann series for (5) converges (see, e.g. [5, 4]), and it is possible to calculate the solution as

$$u_0(x) = \sum_{i=0}^{\infty} (h_x, (-\lambda_0 \mathcal{K})^i f) \ , \tag{6}$$

where $h_x(y) = \frac{1}{2\pi} \frac{1}{|x-y|}$. Usually, however, $\epsilon_e \gg \epsilon_i$ and, hence, $||\lambda_1| - 1| = \frac{2\epsilon_i}{\epsilon_e + \epsilon_i} \ll 1$. Here, $\lambda_1 = -1/\lambda_0$ is the smallest characteristic value of the operator $-\lambda_0 \mathcal{K}$. This means that convergence in (6) is rather slow.

The situation is even worse when we consider a grounded body, G. In this case the original problem reduces to an internal Dirichlet problem for the Laplace equation:

$$\Delta u_0 = 0 \ , \quad u_0\Big|_{\partial G} = \psi \ . \tag{7}$$

The double-layer potential representation of its solution $u_0(x) = (\mu^*, h_x^*)$ leads to the following integral equation for the unknown density, μ^*:

$$\mu^* = -\mathcal{K}^*\mu^* + \psi \ . \tag{8}$$

Here, $h_x^*(y) = \dfrac{1}{2\pi}\dfrac{\cos\phi_{yx}}{|y-x|^2}$, the operator $\mathcal{K}^*$ is the adjoint of $\mathcal{K}$, and has the same characteristic values (see [5, 4]). This means that $\lambda_1^* = -1$ and the Neumann series for solving (8) does not converge.

To speed up the convergence in (6), and to calculate the solution of (8), we apply the method of spectral parameter substitution (see, e.g., [7], and [14, 15] for Monte Carlo algorithms based on this method). This means that we consider the parameterized equation $\mu_\lambda = \lambda(-\lambda_0\mathcal{K})\mu_\lambda + f$ and analytically continue its solution given by the Neumann series for $|\lambda| < |\lambda_1|$. This goal can be achieved by substituting in λ its analytical expression in terms of another complex parameter, η, and representing μ_λ as a series in powers of η.

In this particular case, it is possible to use the substitution $\lambda = \dfrac{2|\lambda_1|\eta}{1-\eta} \equiv \chi(\eta)$, and hence

$$u_0(x) = \sum_{i=0}^{n} l_i^{(n)}(-\lambda_0)^i \left(h_x, \mathcal{K}^i f\right) + O(q^{n+1}) \ , \tag{9}$$

where $q = \dfrac{1}{1+2|\lambda_1|} < \dfrac{1}{3}$, and $l_i^{(n)} = \sum\limits_{j=i}^{n} C_{j-1}^{i-1}(2|\lambda_1|)^i q^j$. The rate, q, of geometric convergence of the transformed series in powers of η at the point $\eta_0 = \chi^{-1}(1)$ is determined by the ratio of $|\eta_0|$ and $L = \min_i |\chi^{-1}(\lambda_i)|$. Here, λ_i are characteristic values of $\mathcal{K}$ (and $\mathcal{K}^*$), and $L = 1$ [5, 7].

Given a desired computational accuracy, we can calculate the number of terms needed in (9). Thus, the problem reduces to computing a finite number of multidimensional integrals.

The same representation is valid for the solution of the Dirichlet problem (7):

$$u_0(x) = \sum_{i=0}^{n} l_i^{(n)_*}(-1)^i \left(\mathcal{K}^{*i}\psi, h_x^*\right) + O(q_*^{n+1}) \ . \tag{10}$$

Here, $q_* = 1/3$, and $l_i^{(n)_*} = \sum\limits_{j=i}^{n} C_{j-1}^{i-1} 2^i q_*^j$ (see [15]).

3 Random Walks on the Boundary

To construct Monte Carlo estimates for $u_0(x)$, it is sufficient to calculate the integral functionals $I_i(x) = \left(h_x, \mathcal{K}^i f\right)$ and $I_i^*(x) = \left(\mathcal{K}^{*i}\psi, h_x^*\right)$ of iterations of the reciprocally adjoint integral operators. Here, the domain of integration is $[\partial G]^{i+1}$.

Let G be a convex domain. In this case, the kernel, $k(y, y')$, of $\mathcal{K}$ corresponds to the uniform in a solid angle distribution of the point y as viewed from the point y'. This means that the most convenient way to implement the random walk on the boundary algorithm here is to use direct estimates for $I_i(x)$ and adjoint estimates for $I_i^*(x)$ [15]. Therefore

$$I_i(x) = \mathbb{E}Q_i h_x(y_i) \ , \quad I_i^*(x) = \mathbb{E}Q_i^* \psi(y_i) \ , \tag{11}$$

where $Y = \{y_0, y_1, \ldots\}$ is the Markov chain of random points on the boundary ∂G, with the initial density p_0 and transition density $p(y_i \to y_{i+1}) = \frac{1}{2\pi} \frac{\cos\phi_{y_{i+1}y_i}}{|y_{i+1} - y_i|^2}$, and random weights are $Q_i = \frac{f(y_0)}{p_0(y_0)}$, $Q_i^* = \frac{h_x^*(y_0)}{p_0(y_0)}$, $i = 1, 2, \ldots, n$. Hence, biased estimators for u_0 are $\theta_1 = \sum_{i=0}^{n} l_i^{(n)} (-\lambda_0)^i \frac{f(y_0)}{p_0(y_0)} h_x(y_i)$ and $\theta_2 = \sum_{i=0}^{n} l_i^{(n)*} (-1)^i \frac{h_x^*(y_0)}{p_0(y_0)} \psi(y_i)$ (for the Dirichlet problem).

Construction of the Markov chain, Y, is based on its geometrical interpretation. Given a point, y_i, we simulate a random isotropic direction ω_i and find the next point y_{i+1} as the intersection of this direction with the boundary surface ∂G. It is well known that different procedures can be used to choose $\omega_i = (\omega_{i,1}, \omega_{i,2}, \omega_{i,3})$. We consider the procedure based on the direct simulation of the longitudiual angle. Normally, an acceptance-rejection method would be used. But since we plan to use quasirandom numbers, this is inadvisable (see, e.g. [6]). So we use the following algorithm: $\omega_{i,3} = 1 - 2\alpha_{i,1}$, $\varphi_i = 2\pi\alpha_{i,2}$, $d = \sqrt{1 - \omega_{i,3}^2}$, $\omega_{i,1} = \sin\varphi_i / d$, $\omega_{i,2} = \cos\varphi_i / d$, where the α_i are standard uniform pseudorandom numbers in the unit interval.

4 Quasirandom Walks on the Boundary

In this section we discuss how to use quasirandom numbers for solving the boundary-value problems (2), (3) and (7). To construct Monte Carlo estimates, in §2, we reformulated the original problem into the problem of solving integral equations (5) and (8). So, in order to make use of these representations when constructing quasirandom estimates, we have to refer to a Koksma-Hlawka type inequality for integral equations, [2]:

$$\left| u[Y^*] - \frac{1}{N} \sum_{1}^{N} \theta^*[Y^*] \right| \le V(\theta^*) \ D_N^*(Q) \ , \tag{12}$$

where Q is a sequence of quasirandom vectors in $[0,1)^s$, $s = d \times T$, and 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 an estimate $\theta[Y]$ based on the random walk Y^* generated from Q by a one-to-one map. Space precludes more discussion of the work of Chelson, but the reader is referred to the original for clarification, [2].

This inequality ensures convergence when θ^* is of bounded variation in the Hardy-Krause sense, which is a very serious limitation. But even when this condition is satisfied, the predicted rate of convergence is very pessimistic due to the high (and, strictly speaking, possibly unbounded) dimension of the quasirandom sequence in the general Monte Carlo method for solving these integral equations, (e.g. (6)). To avoid this limitation, we consider variants of the method with each random walk having fixed length. Clearly, the smaller the dimension of Q, the better the rate estimate in (12).

Guided by this reasoning, we used the representations (9) and (10), and the correspondent random estimators θ_1 and θ_2, to construct quasirandom solutions to the original boundary-value problems.

It is essential to note that despite the improved rate of convergence of our quasirandom-based calculations, constants in the error estimates are hard to calculate. On the contrary, the statistical nature of Monte Carlo solutions makes it possible to determine confidence intervals almost exactly.

5 Numerical Tests

We performed numerical tests with two problems.

The first one is the Dirichlet problem for the Laplace equation inside a sphere with an exact analytic solution.

To solve this problem with quasirandom sequences, we fix the length of series to be $n = 4$. That provides a 1% bias, and use $2(n+1)$-dimensional Sobol, Halton and Faure sequences. We compared the approximate value of the solution at different points computed using MCM and QMCM. The QMCM solution shows a slightly better rate of convergence for Sobol and Halton sequences.

Table 1. Test problem 1. Exact and approximate solution at different points

x	$u(x)$	URAND	SOBOĹ	FAURE	HALTON
(0.9,0,0)	0.124339	0.125317	0.124259	0.123183	0.125915
(0,0.9,0)	0.074873	0.079288	0.074843	0.081115	0.075192
(0,0,0.9)	0.074873	0.077072	0.075623	0.085194	0.074769

The second problem is (2), (3) with G being the unit cube with the only one unit point charge inside, $\epsilon_i = 4.0$, $\epsilon_e = 78.5$. To calculate u_0, defined by (4), we use the estimator θ_1 and compute point values for the same order of bias (number of terms, $n = 4$) and different sample number.

Both tables show that we achieve a better acuracy when we replace pseudorandom numbers with quasirandom sequences. We performed numerical tests with Sobol, Halton and Faure sequences.

Table 2. Test problem 2. Exact and approximate solution at the point $(0.95, 0.95, 0.95)$ using different number of walks

$Ntr.$	$u(x)$	URAND	SOBOĹ	FAURE	HALTON
100	-0.02446	-0.04086	-0.02234	-0.02102	-0.02537
1000	-0.02446	-0.02947	-0.02635	-0.02476	-0.02418
10000	-0.02446	-0.02634	-0.02470	-0.02436	-0.02448

6 Conclusions

In this paper we presented a successful application of quasirandom sequences to the walks on the boundary method for solving boundary-value problems. The success is due to the following reason: instead of solving the original integral equation arising from integral representation of the solution, we parameterized the equation, analytically continued the solution, and used a special substitution to accelerate the convergence significantly. In this way, the problem was reduced to solving a small number of multidimensional integrals. This is the key point for the successive use of quasirandom sequences - they are designed to solve multidimensional integrals with a better rate of convergence than arises from pseudorandom numbers.

We tested our approach by solving two problems using pseudorandom numbers and the Sobol, Halton and Faure sequences. The accuracy of the quasirandom walks on the boundary method is better and the advantage of this method is significant for the second test problem.

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