Random Walk on Balls for a Boundary Value Problems with Mixed Boundary Conditions

Alexander S. Sipin[1,a)]

[1] *Vologda State University*

[a)] Corresponding author: cac1909@mail.ru

Abstract. New stochastic algorithms for solving a second-order elliptic equation with smooth coefficients are proposed. Boundary conditions of the third kind are considered.

INTRODUCTION

Monte Carlo methods are used to solve boundary value problems when other methods do not work, that is, in multidimensional problems with complex geometry. Modern Monte Carlo methods for solving boundary value problems are meshless, so there are no approximation errors. To build a stochastic algorithm, you need to choose the probability space and determine the unbiased estimator of the value of the solution of the boundary value problem at the selected point. Usually, the estimator is constructed on the trajectories of a random walk in the closure $\overline{D}$ of the bounded domain $D \in \mathbf{R}^m$ ($m \geq 3$), in which the boundary value problem is solved. Stochastic algorithms for solving important boundary value problems are presented in [1, 2].

Let

$$Mu = \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left(\varepsilon(x) \frac{\partial u}{\partial x_i} \right) \tag{1}$$

be an elliptic operator acting on $C^2(\overline{D})$. That is, the coefficient $\varepsilon \in C^1(\overline{D})$ and $\varepsilon(x) > 0$ for all $x \in \overline{D}$.

Let Γ be the boundary of the domain D, $\Gamma = \Gamma_1 \cup \Gamma_2$, $\Gamma_1 \cap \Gamma_2 = \emptyset$ and let Γ_1 be closed. We denote by n_x the external normal to Γ at point x. Consider the boundary value problem (BVP):

$$Mu(x) = -f(x), \quad x \in D; \qquad u(x) = \varphi(x), \quad x \in \Gamma_1; \qquad \frac{\partial u}{\partial n_x}(x) = \psi(x), \quad x \in \Gamma_2, \tag{2}$$

where $f \in C(\overline{D})$, $\varphi \in C(\Gamma_1)$ and $\psi \in C(\Gamma_2)$.

In case $\varepsilon(x) \equiv 1$, the unbiased estimators for $u(x)$ on trajectories of a Random Walk on Spheres were constructed in our previous paper [3]. Here we construct unbiased estimators for the solution of problem (2) on the trajectory of a Random Walk on Balls.

STOCHASTIC ALGORITHM

Let σ_m be the measure of the unit sphere in $\mathbf{R}^m$ and let $R(x)$ be a continuous function in $\overline{D}$ satisfying the inequalitie $R(x) \leq dist(x, \Gamma_1)$ for any $x \in \overline{D}$. Here, $dist(x, \Gamma_1)$ is the distance from point x to Γ_1. Let $B(x)$ denote the open ball of radius $R = R(x)$ centered at the point x, $T(x) = B(x) \cap D$, and $\gamma = \gamma(x) = B(x) \cap \Gamma_2$.

We define Levi function (see [1]) for operator M by equality

$$\mathcal{L}(y, x) = \frac{1}{R\sigma_m(m-2)\varepsilon(x)} \int_r^R \left(r^{2-m} - \rho^{2-m} \right) d\rho, \tag{3}$$

where $r = |y - x|$ - distance from point x to point y.

If $T(x) = B(x)$ then $\gamma(x) = \emptyset$, and using Green's formula we have integral representation for the solution of the BVP (2)

$$u(x) = \int_{T(x)} M_y \mathcal{L}(y,x) u(y) dy + \int_{T(x)} \mathcal{L}(y,x) f(y) dy, \tag{4}$$

where the operator M_y acts in the same way as the operator M, only with functions of the variable y.

In the case when $\gamma(x) \neq \emptyset$, we obtain the another representation

$$u(x) = \kappa \int_{T(x)} M_y \mathcal{L}(y,x) u(y) dy - \kappa \int_{\gamma(x)} \varepsilon(y) \frac{\partial \mathcal{L}(y,x)}{\partial n_y} u(y) d_y S + \kappa F(x), \tag{5}$$

where

$$F(x) = \int_{\gamma(x)} \varepsilon(y) \mathcal{L}(y,x) \psi(y) d_y S + \int_{T(x)} \mathcal{L}(y,x) f(y) dy, \tag{6}$$

$\kappa = 1$ for $x \in D$ and $\kappa = 2$ for $x \in \Gamma_2$.

After simple calculations, we get the value of the operator

$$M_y \mathcal{L}(y,x) = \frac{\varepsilon(y)}{R \varepsilon(x) \sigma_m r^{m-1}} \left(1 - (R - r) \sum_{i=1}^{m} \frac{\partial \ln \varepsilon(y)}{\partial y_i} \frac{\partial r}{\partial y_i} \right). \tag{7}$$

For sufficiently small R, the condition $R \cdot \sup_{y \in D} |\nabla \ln \varepsilon(y)| \leq 1$ is satisfied, and then the inequality $M_y \mathcal{L}(y,x) \geq 0$ is true for any $y \in T(x)$.

Calculating the normal derivative in formula (5), we obtain

$$-\frac{\partial \mathcal{L}(y,x)}{\partial n_y} = \frac{\varepsilon(y)(R - r) \cos \varphi_{x,y}}{R \varepsilon(x) \sigma_m r^{m-1}}, \tag{8}$$

where $y \in \gamma(x)$ and $\varphi_{x,y}$ is the angle between vectors n_y and $y - x$. It is obvious that $\cos \varphi_{x,y} \geq 0$ if $\gamma(x) \neq \emptyset$ and the domain $T(x)$ is convex. The inequalities imply the following statement

Theorem 1. *Let $\varepsilon \in C^1(\overline{D})$ and $\varepsilon(x) > 0$. Let the boundary be convex, i.e. for all $x, y \in \Gamma_2$ the segment (x, y) with ends at these points lies in D, then there exists a constant R_0, such that :*

1. *For the function $R(x) = \min(R_0, dist(x, \Gamma_1))$, the inequality $M_y \mathcal{L}(y,x) \geq 0$ is true for any $y \in T(x)$;*
2. *The kernel $M_y \mathcal{L}(y,x) dy$ of the equation (4) is stochastic ;*
3. *The kernel $\kappa M_y \mathcal{L}(y,x) dy - \kappa \frac{\partial \mathcal{L}(y,x)}{\partial n_y} d_y S$ of the equation (5) is stochastic;*
4. *$R(x) \geq c \cdot dist(x, \Gamma_1)$, for some $c > 0$.*

The last two statements of the theorem follow from the fact that $u(x) \equiv 1$ is a solution to the boundary value problem (2). As a constant c in the inequality $R(x) \geq c \cdot dist(x, \Gamma_1)$, we can take the ratio R_0/R_1, where $R_1 = \max_{x \in \overline{D}} dist(x, \Gamma_1)$.

Random Walk on Balls

We fix a constant R_0 so that the conditions of Theorem 1 are satisfied. We will use stochastic kernels from formulas (4) and (5) as transition functions of the Markov chain X_n $(n = 0, 1, 2...)$ with a fixed initial state $X_0 = x$, where $x \in D \cup \Gamma_2$. We call this Markov chain a Random Walk on Balls and denote its transition function $P(x, dy)$. Equations (4) and (5) can now be combined, namely

$$u(x) = \int_Q u(y) P(x, dy) + \kappa F(x), \tag{9}$$

where $Q = D \cup \Gamma_2$ is the state space of the random walk. On the trajectories of a random walk, the *standard* sequence of unbiased estimators for the solution of the equation (9) is defined,

$$\eta_n = \sum_{i=0}^{n-1} \kappa(X_i) F(X_i) + u(X_n), \quad (n = 0, 1, 2, ...).$$

To study the random walk and equation (9), we use the probability potential theory. The definitions and statements required for this are contained in [4]. Let's formulate some of them.

The measurable function u is said to be excessive for Markov chain if $\int_Q u(y)P(x,dy) \le u(x)$ everywhere in Q. The solution of the equation (9) is an excessive function if and only if $F(x) \ge 0$ everywhere in Q. Conditions $f(x) \ge 0$ everywhere in D, and $\psi(x) \ge 0$ everywhere in Γ_2 are sufficient for this.

Theorem 2. *Let $u(x)$ be a bounded excessive solution of equation (9). Then*

1. *The standard sequence of unbiased estimators is a uniformly integrable martingale with respect to the σ-algebras flow generated by the walk;*
2. *For any finite Markov moment τ, the random variable η_τ is an unbiased estimator for $u(x)$.*

The function $v_k(x)$ is called the coordinate function if $v_k(x) = x_k$ for any $x = (x_1, x_2, ..., x_m) \in \mathbf{R}^m$.

Lemma 1. *Let, for each coordinate function $v_k(x)$, $(k = 1, 2, ...m)$, there exist an excessive solution $w_k(x)$ of the equation (9) such that $v_k(x) + w_k(x)$ or $v_k(x) - w_k(x)$ are excessive. Then the Random Walk on Balls converges with probability 1 to a random point $X_\infty \in \overline{\Gamma_1}$.*

The following theorem is an analogue of Lemma 6 from [3].

Theorem 3. *Let Γ_1 contain a closed subset Γ_3 with a positive measure, and the distance from which to $\overline{\Gamma_2}$ is positive. Then the Random Walk on Balls converges with probability 1 to a random point $X_\infty \in \overline{\Gamma_1}$.*

Theorem 3 follows from Lemma 1. The function $w_k(x)$ required for this is a solution of the Neumann problem

$$Mw_k(x) = -\left|\frac{\partial \varepsilon}{\partial x_k}\right|, \quad x \in D; \qquad \frac{\partial w_k}{\partial n_x}(x) = 1, \quad x \in \Gamma_2. \tag{10}$$

The function $w_k(x)$ is obviously excessive. The inequalities

$$M(w_k(x) + v_k(x)) = -\left|\frac{\partial \varepsilon}{\partial x_k}\right| + \frac{\partial \varepsilon}{\partial x_k} \le 0, \quad \frac{\partial (w_k + v_k)}{\partial n_x} = 1 + n_{k,x} \ge 0$$

show that $w_k(x) + v_k(x)$ is excessive function. Here $n_{k,x}$ is the k-th coordinate of the normal vector at the point x. Let us check that problem (10) has a solution. The conditions of the theorem ensure that there exists a non-negative functions $\psi_1, \psi_2 \in C(\Gamma)$ such that $\psi_1(x) = 1$, $\psi_2(x) = 0$ for any $x \in \overline{\Gamma_2}$, and $\psi_1(x) = 0$, $\psi_2(x) = 1$ for any $x \in \Gamma_3$. From the condition for the existence of a solution of the Neumann problem with the normal derivative $\psi(x) = \psi_1(x) - \lambda\psi_2(x)$ and the right-hand side $f(x) = |\partial\varepsilon/\partial x_k|$, we have

$$\int_D f(y)dy + \int_\Gamma \varepsilon(y)\psi_1(y)d_yS - \lambda \int_\Gamma \varepsilon(y)\psi_2(y)d_yS = 0.$$

The parameter λ is uniquely determined from this equality, because

$$\int_\Gamma \varepsilon(y)\psi_2(y)d_yS \ge \int_{\Gamma_3} \varepsilon(y)\psi_2(y)d_yS > 0.$$

Therefore, there exist the functions $w_k(x)$ $(k = 1, 2, ..., m)$, satisfying the conditions of Lemma 1, and the random walk X_n converges with probability 1 to some random vector X_∞.

Now it is obvious that there exist a solution $w(x)$ of the equation $Mw(x) = -1$ with normal derivative $\psi(x) \equiv 1$ for any $x \in \Gamma_2$. This solution is a bounded excessive function. Using Theorem 2, it is easy to show that $F(X_n) \to 0$ almost surely. The function $F(x)$ is continuous in $\overline{D}$, equal to zero on Γ_1, and positive in $\overline{D} \setminus \Gamma_1$. Hence, $X_\infty \in \Gamma_1$ with probability 1.

Remark. To simulate the Random Walks on Balls, you can use von Neumann acceptance-rejection technique.

Estimators

For $\delta > 0$ we define Γ_δ as δ-neighborhood of the set Γ_1, and $\tau = \tau_\delta$ as the hitting time to Γ_δ by the random walk. Due to Theorem 3, $P\{\tau_\delta < +\infty\} = 1$. Hence, τ_δ is finite Markov moment. Due to Theorem 2, random variable

$$\eta_\delta = \sum_{i=0}^{\tau_\delta - 1} \kappa(X_i)F(X_i) + u(X_{\tau_\delta})$$

is unbiased estimator for BVP solution $u(x)$. Using $\widehat{X}_{\tau_\delta} \in \Gamma_1$, such that $|X_{\tau_\delta} - \widehat{X}_{\tau_\delta}| < \delta$, we define $\varepsilon(\delta)$-biased estimator

$$\widehat{\eta}_\delta = \sum_{i=0}^{\tau_\delta - 1} \kappa(X_i) F(X_i) + \varphi(\widehat{X}_{\tau_\delta}),$$

where $\varepsilon(\delta)$ is modulus of continuity function $u(x)$. In practical use of the estimator $\widehat{\eta}_\delta$, it is necessary to replace the values of $F(X_i)$ by their unbiased estimators.

Case $T(x) = B(x)$.

$$F(x) = \int_{B(x)} \mathcal{L}(y, x) f(y) dy = \frac{R^2(x)}{\varepsilon(x) 6m} E f(x + R\rho\omega),$$

where ω is unit vector of random direction, and the random variable ρ has the probability density

$$p(s) = \frac{6m}{m-2} s^{m-1} \int_s^1 (s^{2-m} - t^{2-m}) dt$$

on the segment$[0, 1]$.

Case $T(x) \neq B(x)$ is reduced to the previous one.

$$F_1(x) = \int_{T(x)} \mathcal{L}(y, x) f(y) dy = \int_{B(x)} \mathcal{L}(y, x) \widetilde{f}(y) dy,$$

where $\widetilde{f}(y) = 0$ for any $y \in B(x) \setminus T(x)$, and $\widetilde{f}(y) = f(y)$ for any $y \in T(x)$.

The integral

$$F_2(x) = \int_{\gamma(x)} \varepsilon(y) \mathcal{L}(y, x) \psi(y) d_y S$$

is estimated in the same way as the potential of a simple layer when solving the Neumann problem for the Poisson equation (see [1]).

CONCLUSION

We have developed a new stochastic algorithm for solving a boundary value problem with conditions of the third kind for a second order elliptic equation. The proven convergence theorem for a random walk on balls became the basis for justifying the algorithm.

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