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**RANDOM WALKS
ON BOUNDARY
FOR SOLVING PDEs**

The monograph presents new probabilistic representations for classical boundary value problems of mathematical physics. When comparing with the well known probabilistic representations in the form of Wiener and diffusion path integrals, the trajectories of random walks in our representations are simulated on the boundary of the domain as Markov chains generated by the kernels of the boundary integral equations equivalent to the original boundary value problem. The Monte Carlo methods based on the walk on boundary processes have a series of advantages: (1) high-dimensional problems can be solved, (2) the method is grid-free and gives the solution simultaneously in arbitrary points, (3) external and internal boundary value problems are solved using one and the same random walk on boundary process, (4) when comparing with the classical probabilistic representations, there is no ε -error generated by the approximations in the ε -boundary, and (5) parallel implementation of the walk on boundary algorithms is straightforward and much easier.

This is the first book devoted to the walk on boundary algorithms. First introduced by K. Sabelfeld for solving the interior and exterior boundary value problems for the Laplace and heat equations, the method was then extended to all the main boundary value problems of the potential and elasticity theories.

For specialists in applied and computational mathematics, applied probabilists, for students and post-graduates studying new numerical methods for solving PDEs.

keywords : *Markov chains, double layer potentials, heat and elasticity potentials, boundary integral equations, random estimators, random walk on boundary .*

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Chapter 1

Introduction

It is well known that the random walk methods for boundary value problems (BVP) for high-dimensional domains with complex boundaries are quite efficient, especially if it is necessary to find the solution not in all the points of a grid, but only in some marked points of interest. One of the most impressive features of the Monte Carlo methods is the possibility to calculate probabilistic characteristics of the solutions to BVPs with random parameters (random boundary functions, random sources, and even random boundaries).

Monte Carlo methods for solving PDEs are based:

- (a) on classical probabilistic representations in the form of Wiener or diffusion path integrals,
- (b) on probabilistic interpretation of integral equations equivalent to the original BVP which results in representations of the solutions as expectations over Markov chains.

In the approach (a), diffusion processes generated by the relevant differential operator are simulated using numerical methods for solving ordinary stochastic differential equations (Friedmann, 1976). To achieve the desired accuracy, it is necessary to take the discretization step small enough, which results in long random trajectories simulated.

For PDEs with constant coefficients, however, it is possible to use the strong Markov property of the Wiener process and create much more efficient algorithms first constructed for the Laplace equation (Müller, 1956) known as the walk on spheres method (WSM).

This algorithm was later justified in the framework of the approach (b) by passing to an equivalent integral equation of the second kind with generalized kernel and using the Markov chain which "solves" this equation. This approach was developed to general second order scalar elliptic equations, high-order equations related to the Laplace operator and some elliptic systems (Sabelfeld, 1991). We now shortly present two different approaches for constructing and justifying the walk on spheres algorithm: the first, conventional, coming from the approach (a), and the second, based on a converse mean value relation.

Let us start with a simple case, the Dirichlet problem for the Laplace equation in a bounded domain $G \subset R^3$:

$$\Delta u(x) = 0, \quad x \in G, \tag{1.1}$$

$$u(y) = \varphi(y), \quad y \in \Gamma = \partial G. \tag{1.2}$$

We seek a regular solution to (1.1) and (1.2), i.e. $u \in C^2(G) \cap C(G \cup \Gamma)$.

Let $d^* := \sup_{x \in G} d(x)$, where $d(x)$ is the largest radius of the spheres $S(x, d(x))$ centered at x and contained in \bar{G} .

Let $w_x(t)$ be the Wiener process starting at the point $x \in G$, and let τ_Γ be the first passage time (the time of the first intersection of the process $w_x(t)$ with the boundary Γ). We suppose that the boundary Γ is regular so that (1.1) and (1.2) has a unique solution. Then (Dynkin, 1963)

$$u(x) = \mathbb{E}_x \varphi(w_x(\tau_\Gamma)). \quad (1.3)$$

Note that in (1.3), only the random points on the boundary are involved. We thus can formulate the following problem: how to find these points without explicit simulation of the Wiener process inside the domain G ?

This problem was solved in (Müller, 1956) using the following considerations. In sphere $S(x, d(x))$ representation (1.3) gives:

$$u(x) = \mathbb{E}_x u(w_x(\tau_{S(x, d(x))})). \quad (1.4)$$

The same representation is valid for all points $y \in S(x, d(x))$, so we can use the strong Markov property and write the conditional expectation:

$$u(x) = \mathbb{E}_x \{ \mathbb{E}_y u(w_y(\tau_{S(y, d(y))})) | x = w(0); y = w(\tau_{S(x, d(x))}) \}. \quad (1.5)$$

We can iterate this representation many times and remark that only random points lying on the spheres $S(x, d(x))$, $S(y, d(y))$, \dots , are involved. It is well known that the points $w_x(\tau_{S(x, d(x))})$ are uniformly distributed over the sphere $S(x, d(x))$.

Thus we came to the definition of the walk on spheres process starting at x : it is defined as the homogeneous Markov chain $WS = WS\{x_0, x_1, \dots, x_k, \dots\}$ such that $x_0 = x$ and

$$x_k = x_{k-1} + d(x_{k-1})\omega_k, \quad k = 1, 2, \dots,$$

where $\{\omega_k\}$ is a sequence of independent unit isotropic vectors. It is known (Müller, 1956) that $x_k \rightarrow y \in \Gamma$ as $k \rightarrow \infty$, however the number of steps of the Markov chain WS is infinite with probability one. Therefore, an ε -spherical process is introduced as follows. Let $N_\varepsilon = \inf\{n : d(x_n) \leq \varepsilon\}$, then the ε -spherical process $WS_\varepsilon = \{x_0, x_1, \dots, x_{N_\varepsilon}\}$ is obtained from WS by stopping after N_ε steps.

Let \bar{x}_{N_ε} be any point on $S(x_{N_\varepsilon}, d(x_{N_\varepsilon})) \cap \Gamma$, then we set

$$\hat{\xi}(x) = u(x_{N_\varepsilon}), \quad \xi(x) = \varphi(\bar{x}_{N_\varepsilon}). \quad (1.6)$$

The unbiasedness $u(x) = \mathbb{E}_x \hat{\xi}(x)$ follows from (1.4), (1.5). An important question is what happens when $\varepsilon \rightarrow 0$. We remark that

$$\mathbb{E}\{u(x_{n+1}) | x_1, \dots, x_n\} = \mathbb{E}\{u(x_{n+1}) | x_n\} = u(x_n)$$

by the spherical mean value theorem. It means that $\{u(x_0), \dots, u(x_n), \dots\}$ is a martingale with respect to x_1, \dots, x_n, \dots . Since $\{u(x_0), \dots, u(x_{N_\varepsilon})\}$ is a stopped process constructed from $\{u(x_0), \dots, u(x_n), \dots\}$, it is also a martingale with respect to x_1, \dots, x_n (Motoo, 1959). Especially,

$$\mathbb{E}\{\hat{\xi}(x) | x_1, \dots, x_k; N_\varepsilon \geq k\} = \mathbb{E}\{u(x_{N_\varepsilon}) | x_k, N_\varepsilon \geq k\} = u(x_k),$$

and

$$\mathbb{E}_x \hat{\xi}(x) = u(x).$$

Let

$$L = \sup_{x, y \in G} \|x - y\|, \quad M = \sup_{x \in \Gamma} \varphi(x)$$

and assume that $u(x)$ satisfies the condition

$$|u(x) - u(y)| \leq c||x - y||, \quad x, y \in \bar{G}.$$

It is not difficult to show (Motoo, 1959) that

$$\mathbb{E}_x\{(\hat{\xi}(x) - u(x))^2\} \leq c^2L$$

and for the estimator $\xi(x)$ the following estimation is true:

$$\mathbb{E}_x(\xi - u)^2 \leq c^2\varepsilon^2 + 4Mc\varepsilon + c^2L^2,$$

and

$$\mathbb{E}_x \left\{ \frac{1}{n} \sum_{k=1}^n \xi_k(x) - u(x) \right\}^2 \leq c^2\varepsilon^2 + \frac{1}{n}(4Mc\varepsilon + c^2L^2),$$

where ξ_n are independent ξ -estimators of $u(x)$.

We now turn to the second approach.

It is well known that every solution to (1.1) satisfies the mean value relation:

$$u(x) = N_r u(x) := \frac{1}{\omega_m} \int_{S(x,r)} u(x+rs) d\Omega(s) \quad (1.7)$$

for each $x \in G$ and for all spheres $S(x,r)$ contained in \bar{G} ; ω_m is the surface area of the unit sphere $S(x,1)$ in R^m . Besides, the mean value relation (1.7) characterizes the solutions to (1.1). We need a stronger result, which presents an equivalent formulation of the problem (1.1), (1.2).

Proposition 1.1 Integral Formulation. *We suppose that the problem (1.1), (1.2) has a unique solution for any continuous function φ . Suppose that there exists a function $v \in C(G \cup \Gamma)$, $u|_{\Gamma} = \varphi$, $v(x) = u(x)$ in Γ_ε ($\varepsilon \geq 0$) such that the mean value relation holds at every point $x \in G \setminus \Gamma_\varepsilon$ for the sphere $S(x,d(x))$. Then $v(x)$ is the unique solution to the problem (1.1), (1.2).*

Proof. The proof uses the maximum property (Courant and Hilbert, 1989). Since u also satisfies the mean value relation for every sphere contained in G , we conclude that the function $u - v$ satisfies the mean value relation at every point $x \in G \setminus \Gamma_\varepsilon$. Let F be a closed set of points $x \in G \setminus \Gamma_\varepsilon$ where $u - v$ attains its maximum M . Let x_0 be a point of F which has the minimal distance from the surface $Y = \{y : d(y) = \varepsilon\}$. If x_0 were an interior point of $x \in G \setminus \Gamma_\varepsilon$, we could find a sphere $S(x_0, r_0) \subset G$ for which the mean value relation holds, thus $u - v = M$ inside $S(x_0, r_0)$. Therefore, x_0 should belong to Y . We repeat the same argument for the minimum of $u - v$. Since $(u - v)|_Y = 0$, we have $v \equiv u$ in G . \square

Using this proposition, we rewrite an integral equation equivalent to the problem (1.1), (1.2).

Let $\delta_x(y)$ be a generalized density describing the uniform distribution on a sphere $S(x, d(x))$, and let us define the kernel function as follows:

$$k_\varepsilon(x, y) = \begin{cases} \delta_x(y) & \text{if } x \in G \setminus \Gamma_\varepsilon, \\ \mathbf{0} & \text{if } x \in \Gamma_\varepsilon. \end{cases} \quad (1.8)$$

We define also a function $f_\varepsilon(x)$ in G :

$$\mathbf{f}_\varepsilon(\mathbf{x}) = \begin{cases} \mathbf{0} & \text{if } \mathbf{x} \in G \setminus \Gamma_\varepsilon, \\ \mathbf{u}(\mathbf{x}) & \text{if } \mathbf{x} \in \Gamma_\varepsilon. \end{cases}$$

By the proposition, we can write an equivalent integral equation :

$$\mathbf{u}(\mathbf{x}) = \mathbf{K}_\varepsilon \mathbf{u}(\mathbf{x}) + \mathbf{f}_\varepsilon(\mathbf{x}), \quad (1.9)$$

where the integral operator \mathbf{K}_ε is defined by

$$\mathbf{K}_\varepsilon \psi(\mathbf{x}) = \int_G \mathbf{k}_\varepsilon(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) d\mathbf{y} \quad (1.10)$$

for each $\psi(\mathbf{x}) \in C(G)$.

Proposition 1.2. *For any $\varepsilon > 0$, integral equation (1.9) has the unique solution given by*

$$\mathbf{u}(\mathbf{x}) = \mathbf{f}_\varepsilon(\mathbf{x}) + \sum_{i=1}^{\infty} \mathbf{K}_\varepsilon^i \mathbf{f}_\varepsilon(\mathbf{x}). \quad (1.11)$$

Besides, this solution coincides with the solution to (1.1), (1.2).

Proof. Let ε be fixed. To show the convergence of the series

$$\mathbf{f}_\varepsilon(\mathbf{x}) + \sum_{i=1}^N \mathbf{K}_\varepsilon^i \mathbf{f}_\varepsilon(\mathbf{x}), \quad (1.12)$$

it is sufficient to prove that $\|\mathbf{K}_\varepsilon^2\|_{L^\infty} < 1$ (this fact also implies the uniqueness of the solution to (1.11)). Let $\nu(\varepsilon) = \varepsilon^2/4(d^*)^2$. For $\mathbf{x} \in G \setminus \Gamma_\varepsilon$ we have

$$\begin{aligned} \int_G \mathbf{k}_\varepsilon(\mathbf{x}, \mathbf{y}) \int_G \mathbf{k}_\varepsilon(\mathbf{y}, \mathbf{y}') d\mathbf{y}' d\mathbf{y} &= \int_{G \setminus \Gamma_\varepsilon} \delta_{\mathbf{x}}(\mathbf{y}) \left(\int_G \delta_{\mathbf{y}}(\mathbf{y}') d\mathbf{y}' \right) d\mathbf{y} = \\ &= \int_{G \setminus \Gamma_\varepsilon} \delta_{\mathbf{x}}(\mathbf{y}) d\mathbf{y} \leq 1 - \nu(\varepsilon) < 1. \end{aligned}$$

Let $\mathbf{v}(\mathbf{x}) := \mathbf{f}_\varepsilon(\mathbf{x}) + \sum_{i=1}^{\infty} \mathbf{K}_\varepsilon^i \mathbf{f}_\varepsilon(\mathbf{x})$. It is clear that \mathbf{v} satisfies

$$\mathbf{v}(\mathbf{x}) = \mathbf{K}_\varepsilon \mathbf{v}(\mathbf{x}) + \mathbf{f}_\varepsilon(\mathbf{x}).$$

□

Now we remark that, to use (1.9) for numerical purposes, it is necessary to know the solution to the boundary problem in Γ_ε . However, we obtain an approximation if we take in Γ_ε

$$\mathbf{u}(\mathbf{x}) = \bar{\mathbf{f}}_\varepsilon(\mathbf{x}) \approx \varphi(\bar{\mathbf{x}}), \quad \mathbf{x} \in \Gamma_\varepsilon, \quad (1.13)$$

where $\bar{\mathbf{x}}$ is the point of Γ nearest to \mathbf{x} , since $\mathbf{u} \in C(G \cup \Gamma)$. Instead of (1.13) we could use any continuous extension of φ to Γ_ε (the ideal case is the harmonic extension).

Thus, let us consider the equation

$$\mathbf{u}_\varepsilon(\mathbf{x}) = \mathbf{K}_\varepsilon \mathbf{u}_\varepsilon(\mathbf{x}) + \bar{\mathbf{f}}_\varepsilon(\mathbf{x}), \quad \mathbf{x} \in \mathbf{G} \setminus \Gamma_\varepsilon, \quad (1.14)$$

where $\bar{\mathbf{f}}_\varepsilon$ is an approximation of $\mathbf{u}(\mathbf{x})$ in Γ_ε , e.g., given by (1.13). Note that the solution to (1.14) is not harmonic, but it is clear that $|\mathbf{u}(\mathbf{x}) - \mathbf{u}_\varepsilon(\mathbf{x})| = O(\omega(\varepsilon))$ as $\varepsilon \rightarrow 0$, where $\omega(\varepsilon)$ is the continuity modulus of the function $\mathbf{u}(\mathbf{x})$ in Γ_ε . For example, for Lipschitz continuous functions we get

$$|\mathbf{u}(\mathbf{x}) - \mathbf{u}_\varepsilon(\mathbf{x})| \leq C\varepsilon.$$

Having (1.14) and the convergence of the Neumann series, it is possible to use the standard Monte Carlo estimators for the integral equations of the second kind (see e.g., Ermakov and Mikhailov, 1982). If we choose the transitional density in each sphere in accordance with the kernel (i.e., uniformly on the surface of a sphere), and introduce absorption in Γ_ε with probability one (no absorption in $\mathbf{G} \setminus \Gamma_\varepsilon$), we exactly obtain the unbiased estimators $\hat{\boldsymbol{\xi}}(\mathbf{x})$ and $\boldsymbol{\xi}(\mathbf{x})$. Estimations for the variance of the estimators of the solutions to the integral equations can be obtained from the analysis of kernel $\mathbf{k}_\varepsilon^2/\mathbf{p}$ where \mathbf{p} is a transitional density. This kernel in our case coincides with the kernel of the original integral equation, that leads to the convergence of the Neumann series representing the variance.

Thus we see that in the walk on spheres algorithms we have no necessity to simulate long trajectories of the Wiener process. Nevertheless, we have to construct a series of random points distributed inside the domain.

However, we would like to find probabilistic representations in the form of an expectation taken over Markov chains defined on the boundary of the domain. We will see that this is really possible to do using the boundary integral equations of the potential theory and special Monte Carlo estimators for solving integral equations.

We now shortly present the idea of the walk on boundary algorithm for solving (1.1), (1.2). We suppose for simplicity that the domain is convex and the solution can be represented in the form of a double layer potential (Vladimirov, 1981):

$$\mathbf{u}(\mathbf{x}) = \int_{\Gamma} \frac{\cos \varphi_{\mathbf{y}\mathbf{x}}}{2\pi|\mathbf{x} - \mathbf{y}|^2} \boldsymbol{\mu}(\mathbf{y}) d\sigma(\mathbf{y}), \quad (1.15)$$

where $\varphi_{\mathbf{y}\mathbf{x}}$ is the angle between the vector $\mathbf{x} - \mathbf{y}$ and $\mathbf{n}_\mathbf{y}$, the interior normal vector at the point $\mathbf{y} \in \Gamma$, and $\boldsymbol{\mu}(\mathbf{y})$ is a continuous function satisfying the boundary integral equation:

$$\boldsymbol{\mu}(\mathbf{y}) = - \int_{\Gamma} \mathbf{p}(\mathbf{y}, \mathbf{y}') \boldsymbol{\mu}(\mathbf{y}') d\sigma(\mathbf{y}') + \boldsymbol{\varphi}(\mathbf{y}), \quad (1.16)$$

where

$$\mathbf{p}(\mathbf{y}, \mathbf{y}') = \frac{\cos \varphi_{\mathbf{y}'\mathbf{y}}}{2\pi|\mathbf{y} - \mathbf{y}'|^2}.$$

It is clear that

$$d\Omega_x = \frac{d\sigma(\mathbf{y}) \cos \varphi_{\mathbf{y}\mathbf{x}}}{|\mathbf{x} - \mathbf{y}|^2}$$

is a solid angle of view of the surface element $d\sigma(\mathbf{y})$ from the point $\mathbf{x} \in \mathbf{G}$. Thus the isotropic distribution of \mathbf{y} in angular measure Ω_x at the point \mathbf{x} corresponds to the distribution of \mathbf{y} on Γ with the density

$$p_0(x, y) = \frac{\cos \varphi_{yx}}{4\pi|x - y|^2}. \quad (1.17)$$

Since G is convex, $p_0 \geq 0$ and for arbitrary $x \in G$

$$\int_{\Gamma} p_0(x, y) d\sigma(y) = 1.$$

Thus we can rewrite (1.15) in the form of the expectation

$$u(x) = 2 \mathbb{E}_x \mu(Y_0), \quad (1.18)$$

where Y_0 is a random point on Γ which is obtained as the intersection of the ray $A_x = \{z : z = x + t\omega ; t \geq 0\}$ (ω is a unit isotropic vector), having random isotropic direction ω , with the boundary Γ . Note that if we could find $\mu(y)$ on Γ , we could use the representation (1.18) for numerical purposes. In Chapter 3 we shall see that $\mu(y)$ can be found from (1.16) by special iterations which leads to the following algorithm.

Let us define the following Markov chain on the boundary:

$WB_x\{Y_0, Y_1, \dots, Y_m\}$, where the first point Y_0 is obtained as described above, and

$$Y_{n+1} = Y_n + |Y_{n+1} - Y_n|\omega_n,$$

where $\{\omega_k\}_{k=0}^{m-1}$ is a sequence of independent unit isotropic vectors in R^3 . On the process $WB_x\{Y_0, Y_2, \dots, Y_m\}$ we can construct the following random estimator ($m \geq 2$):

$$\xi_m(x) = 2[\varphi(Y_0) - \varphi(Y_1) + \varphi(Y_2) + \dots] + (-1)^{m+1}\varphi(Y_m). \quad (1.19)$$

In Chapter 3 we shall show that

$$u(x) \approx \mathbb{E}\xi_m$$

and the larger m , the higher is the accuracy of this representation. More exactly, to achieve the accuracy ε , the cost is $O\left(\frac{|\ln \varepsilon|^2}{\varepsilon^2}\right)$ which shows that this algorithm has a high efficiency.

Remarkably, the same walk on boundary process can be used to solve interior and exterior Dirichlet, Neumann and the third boundary value problems. Note also that the method is grid-free but gives the solution simultaneously in arbitrary points prescribed. When comparing with the classical probabilistic representations, there is no ε -error coming from the approximation in Γ_ε . Note also that the parallelization of the walk on boundary algorithms is very simple, since the length of all the trajectories is one and the same.

In the present book we construct and justify the walk on boundary algorithms for three classes of PDEs: (1) classical stationary potential problems (Chapter 3), (2) heat equation (Chapter 4), and (3) spatial elasticity problems (Chapter 5). The basic Monte Carlo methods using Markov chains for solving integral equations are presented in Chapter 2. In Chapter 6 we discuss different aspects related to the walk on boundary algorithms (the Robin problem and the ergodicity theorem, evaluation of derivatives, etc.). Nonlinear problems are treated in Chapter 7.