

A probabilistic representation for systems of elliptic equations

K.K. Sabelfeld

New probabilistic representations for systems of elliptic equations are constructed in the form of expectations over the Markov chains. It is shown that this approach gives the effective Monte Carlo algorithms even in the cases, where the classical probabilistic representation based on the Wiener and diffusion processes fails. As an important example, we consider the system of Lamé equations. Construction of the method is based on the direct and inverse mean value theorems which we prove, in particular, for the Lamé equation. We derive accurate estimations for the exponential moments for the case of ε -spherical process (the “walk on spheres” process).

1. Introduction

It is well-known [1] that for the Dirichlet problem for elliptic and parabolic second order equations it is possible to construct two kinds of probabilistic representations: in the first one, the solution is represented as an expectation over the diffusion processes generated by the corresponding differential operator (e.g., in the case of the Laplace equation, the Wiener process is used). In the second approach, the Markov chains whose transition densities are related to the equation under study, are used.

It should be noted that the representations based on the Markov chains are known only for problems and equations for which the classical probabilistic representations based on the diffusion processes exist.

In this paper we present a probabilistic representation using the Markov chains for systems of elliptic equations with constant coefficients – it is well-known (see, e.g., [2]) that the classical probabilistic representations in these cases do not work.

To be more specific, we give simple illustration.

Let $G \subset R^3$ be a bounded domain with a boundary ∂G such that the Dirichlet problem

$$\begin{aligned}\Delta u &= 0, & x &\in G, \\ u(y) &= \varphi(y), & y &\in \partial G,\end{aligned}\tag{1.1}$$

has a unique solution $u(x) \in C^2(G) \cap C(\overline{G})$. Let w_x be a Wiener process starting at x , then the following classical probabilistic representation holds:

$$u(x) = E_x \varphi(w_x(\tau)), \quad (1.2)$$

where τ is the first passage time (i.e., $w_x(\tau)$ is the point of the boundary first reached by $w_x(t)$).

Now we define a Markov chain called the "walk on spheres" process [1]

$$x_0 = x, \quad x_{n+1} = x_n + d(x_n)w_n, \quad n = 0, 1, \dots,$$

where $d(x_n)$ is the distance from x_n to the boundary, $\{w_n\}_{n=0}^\infty$ is a set of independent unit isotropic vectors in R^3 . It is known [1] that $x_n \rightarrow y \in \partial G$ as $n \rightarrow \infty$, and the solution to (1.1) can be represented as

$$u(x) = E_x \varphi(y). \quad (1.3)$$

Moreover, to compute the solution to within accuracy ε , the cost is estimated by $T_\varepsilon \sim \frac{|\ln \varepsilon|}{\varepsilon^2}$ (see, e.g., [1]).

We generalize now the representation of the form (3) on the systems of elliptic equations.

2. A system of diffusion equations

Let us begin with the following system. We seek a regular solution to the boundary value problem in a domain $G \subset R^3$ with a regular boundary ∂G

$$\Delta u(x) + \gamma \frac{\partial \theta}{\partial x_i} = 0, \quad \Delta \theta(x) = 0, \quad (2.1)$$

$$u|_{\partial G} = \varphi_1, \quad \theta|_{\partial G} = \varphi_2. \quad (2.2)$$

Let $S(x, r) \subset \overline{G}$ be an arbitrary sphere and let s be a unit vector in R^3 with components s_i , $i = 1, 2, 3$. We denote by Ω the unit sphere $\Omega = \{s : |s| = 1\}$.

Theorem 1. *For each regular solution to (2.1) the following mean value relation holds:*

$$u(x) = N(u) + \frac{\gamma r}{8\pi} \int_{\Omega} s_i \theta(x + rs) d\Omega(s), \quad (2.3)$$

$$\theta(x) = N(\theta),$$

where N is the averaging operator

$$N(u) = \int_{S(x,r)} u(x + rs) d\Omega(s).$$

Proof. Since $\Delta^2 u(x) = 0$ we get (see, e.g., [1])

$$u(x) = N(u) - \frac{r^2}{6} \Delta u(x) = N(u) + \frac{r^2 \gamma}{6} \cdot \frac{\partial \theta}{\partial x_i}. \quad (2.4)$$

For each harmonic function

$$\frac{\partial \theta}{\partial x_i} = \frac{3}{4\pi} \int_{\Omega} s_i \theta(x + rs) d\Omega(s). \quad (2.5)$$

Indeed, since θ_{x_i} is harmonic, we get

$$\frac{\partial}{\partial x_i} \theta(x) = \frac{3}{4\pi R^3} \int \frac{\partial \theta}{\partial x_i} dV.$$

Integration by parts gives (2.5). From (2.4), (2.5) we get (2.3). \square

Now we show that (2.3) is a characteristic property of (2.1).

The integral formulation of problem (2.1), (2.2)

Theorem 2. Suppose that (2.3) is uniquely solvable for each continuous φ_1 and φ_2 , and assume that for each $x \in G$ continuous functions $\hat{u}(x)$ and $\hat{\theta}(x)$ from $C(G \cup \partial G)$, $\hat{u}|_{\partial G} = \varphi_1$, $\hat{\theta}|_{\partial G} = \varphi_2$ satisfy (2.3) for all $x \in G$, for at least one sphere $S(x, r) \subset \bar{G}$. Then the functions $\hat{u}(x)$, $\hat{\theta}(x)$ solve problem (2.1), (2.2).

Proof. From the inverse mean value theorem for the harmonic equations (see [4]) we get that $\hat{\theta}(x)$ is harmonic in G , thus coincides with $\theta(x)$ in (2.1). Since (2.3) holds for $u(x)$, $\theta(x)$, the subtraction gives

$$(u - \hat{u})(x) = N(u - \hat{u}) + \frac{\gamma R}{8\pi} \int_{\Omega} s_i (\theta - \hat{\theta}) d\Omega(s),$$

which implies that $u - \hat{u}$ is harmonic in G . But $u|_{\partial G} = \hat{u}|_{\partial G} = \varphi_1$, thus $u \equiv \hat{u}$ in G .

Now we introduce the ε -spherical process, – the “walk on spheres” process

$$X_x^N = \{x_0, \dots, x_N\},$$

where x_N is the last state (such that $d(x_N) < \varepsilon$). On this process we define the random estimators

$$\hat{\xi}(x) = u(x_N) + \frac{\gamma}{2}\theta(x_N) \sum_{k=0}^{N-1} d(x_k) s_i^{(k)}, \quad (2.6)$$

$$\xi(x) = \varphi_1(\bar{x}_N) + \frac{\gamma}{2}\varphi_2(\bar{x}_N) \sum_{k=0}^{N-1} d(x_k) s_i^{(k)}, \quad (2.7)$$

where $\{s_i^{(k)}\}_{k=0}^{N-1}$ are the i -th components of the k -th unit isotropic vector, which are mutual independent for $k = 0, 1, \dots, N-1$. \square

Theorem 3. *The estimator $\hat{\xi}(x)$ is unbiased*

$$u(x) = E\hat{\xi}(x),$$

while the cost of the estimator $\xi(x)$ has the asymptotics

$$T_\varepsilon = \frac{c(\ln \varepsilon)^2}{\varepsilon^2}, \quad (2.8)$$

as $\varepsilon \rightarrow 0$.

Proof. The unbiasedness follows from the recurrent application of (2.3). The cost of the algorithm is

$$T_\varepsilon = \sqrt{D\xi} \cdot \frac{m_\varepsilon}{\varepsilon^2},$$

where m_ε is the average number of steps of the ε -spherical process, and is given by $m_\varepsilon \sim |\ln \varepsilon|$ [1]. Using the scheme of the proof for m_ε from [1], it is not difficult to show that $EN^2 \sim C_1 |\ln \varepsilon|^2 + C_2 |\ln \varepsilon|$. From this, keeping in mind in (2.6) that $d(x_k) < L$ (L is the diameter of the domain G) we get (2.8).

Note that the kernel of (2.3) allows a different random estimator. Indeed, let us define N new independent Markov chains on the trajectory X_x^N

$$Y_+^{N+}(j) = \{x_j, y_1^+(j), \dots, y_{N_+(j)}^+(j)\}, \quad j = 0, 1, \dots, N-1,$$

where

$$y_1^+(j) = x_j + s^+ d(x_j), \quad j = 0, 1, \dots, N-1,$$

s^+ has the density

$$p_+(s) = \frac{1}{\pi} s_3 = \frac{1}{2\pi} \sin 2\psi, \quad 0 < \psi < \pi/2,$$

in the semisphere $\{s_3 \geq 0\}$, and $y_2^+(j), \dots, y_{N_+(j)}^+(j)$ are constructed as in the standard isotropic ε -spherical process

$$N_+(j) = \inf\{n : d(y_n^+(j)) \leq \epsilon\}, \quad j = 0, 1, \dots, N-1.$$

Analogously,

$$Y_-^{N-}(j) = \{x_j, y_1^-(j), \dots, y_{N_-(j)}^-(j)\}, \quad y_1^-(j) = x_j - s^+ d(x_j), \\ j = 0, 1, \dots, N-1. \quad \square$$

Theorem 4. *Let*

$$Z_x^N = \{X_x^N; Y_+^{N+}(j), Y_-^{N-}(j), j = 0, 1, \dots, N-1\},$$

and let

$$\hat{\xi}_1(x) = u(x_N) + \frac{\gamma}{8} \sum_{j=0}^{N-1} d(x_j) [\Theta(y_{N_+(j)}^+(j)) - \Theta(y_{N_-(j)}^-(j))], \\ \xi_1(x) = \varphi_1(\bar{x}_N) + \frac{\gamma}{8} \sum_{j=0}^{N-1} d(x_j) [\varphi_2(\bar{y}_{N_+(j)}^+(j)) - \varphi_2(\bar{y}_{N_-(j)}^-(j))]. \quad (2.9)$$

Then

$$u(x) = E\hat{\xi}_1(x),$$

and estimations (5), (6) are true.

Note that the variances of estimators (2.9) are less than the variances of (2.6), (2.7) if the absolute value of $\Theta \in \Gamma_\epsilon$ is large and $\frac{\partial \Theta}{\partial n}$ is small.

Let us consider now the following boundary value problem:

$$\Delta u(x) + \gamma \frac{\partial^2 \Theta}{\partial x_i \partial x_j} = 0, \quad x \in G \subset R^3, \\ \Delta \Theta(x) = 0, \\ u|_\Gamma = \varphi_1, \quad \Theta|_\Gamma = \varphi_2. \quad (2.10)$$

Theorem 5. *Any regular solution to (2.10) satisfies the mean value relation*

$$u(x) = N(u) + \frac{5}{8\pi} \int_{\{s\}} \left[s_i s_j - \frac{\delta_{ij}}{3} \right] \Theta(s) d\Omega(s), \\ \Theta(x) = N(\Theta), \quad (2.11)$$

where δ_{ij} is the Kronecker symbol.

Integral formulation of problem (2.10)

Theorem 6. Assume that problem (2.10) has a unique solution for arbitrary continuous functions φ_1, φ_2 , and suppose that for all $x \in G$ the functions $\hat{u}, \hat{\Theta}$ from $C(G \cup \Gamma)$, $\hat{u}|_\Gamma = \varphi_1, \hat{\Theta}|_\Gamma = \varphi_2$ satisfy the mean value relation (2.11) at least for one sphere $S(x, r) \subset \bar{G}$. Then the functions $\hat{u}, \hat{\Theta}$ give the unique solution to (2.10).

Now we define the random estimators on the ε -spherical process

$$\begin{aligned}\hat{\xi}(x) &= u(x_N) + \frac{5\gamma}{2} \Theta(x_N) \sum_{k=1}^{N-1} \left(s_i^{(k)} s_j^{(k)} - \frac{\delta_{ij}}{3} \right), \\ \xi(x) &= \varphi_1(\bar{x}_N) + \frac{5\gamma}{2} \varphi_2(\bar{x}_N) \sum_{k=1}^N \left(s_i^{(k)} s_j^{(k)} - \frac{\delta_{ij}}{3} \right).\end{aligned}$$

Theorem 7. The following relations hold:

$$\begin{aligned}u(x) &= M\hat{\xi}(x), \\ M\hat{\xi}^2(x) &< (C_1 + C_2 |\ln \varepsilon|)^2, \\ |u(x) - M\xi(x)| &\leq A\varepsilon + B\gamma\varepsilon |\ln \varepsilon|,\end{aligned}$$

as $\varepsilon \rightarrow 0$, where C_1, C_2, A, B are constants, which do not depend on ε .

3. Lamé equations

We consider now the first boundary value problem of the elasticity theory

$$\begin{aligned}\mu \Delta u_i(x) + (\lambda + \mu) \frac{\partial}{\partial x_i} (\operatorname{div} u) &= 0, \quad i = 1, 2, 3, \quad x \in G \subset R^3, \\ u|_\Gamma &= \vec{\varphi} = (\varphi_1, \varphi_2, \varphi_3),\end{aligned}\tag{3.1}$$

or in short form

$$u_{i,jj} + \alpha u_{j,ji} = 0, \quad i, j = 1, 2, 3,\tag{3.2}$$

$\alpha = (\lambda + \mu)/\mu$, λ, μ are constants. We define the integral matrix operator, which takes the average on the sphere $N^1 : R^3 \rightarrow R^3$

$$N^1 u = \frac{1}{4\pi} \int_{\Omega} (a\delta_{ij} + bs_i s_j) u_j d\Omega(s), \quad i = 1, 2, 3,\tag{3.3}$$

a, b are arbitrary constants.

It is known (see, e.g., [1]) that the regular solutions to (3.1) satisfy the mean value relation (for all spheres $S(x, r) \subset \bar{G}$)

$$u(x) = N^1 u, \quad (3.4)$$

where

$$a = \frac{3(2-\alpha)}{2(3+\alpha)}, \quad b = \frac{15\alpha}{2(3+\alpha)}.$$

Integral formulation of problem (3.1)

Theorem 8. *Assume that problem (3.1) has a unique solution for arbitrary continuous function φ , and suppose that for all $x \in G$ the function $\hat{u}(x)$ from $\hat{u} \in C^3(G \cup \Gamma)$, $\hat{u}|_\Gamma = \varphi$ satisfies the mean value relation (3.4) at least for one sphere $S(x, r) \subset \bar{G}$. Then the function \hat{u} is the unique solution to (3.1).*

Let S_k be a matrix with entries

$$(S_k)_{ij} = 3s_i^{(k)}s_j^{(k)}, \quad i, j = 1, 2, 3.$$

On X_x^N we define the random estimators

$$\hat{\xi}(x) = \prod_{k=1}^N (pE + qS_k)u(x_N), \quad (3.5)$$

$$\xi(x) = \prod_{k=1}^N (pE + qS_k)\varphi(\bar{x}_N), \quad (3.6)$$

where

$$p = a = \frac{3(2-\alpha)}{2(3+\alpha)}, \quad q = \frac{5\alpha}{2(3+\alpha)}.$$

Theorem 9. *The random estimator $\hat{\xi}$ is unbiased, i.e.,*

$$M\hat{\xi}(x) = u(x).$$

4. Exponential moments of the “walk on spheres” process

In more general case, we need to estimate the exponential moment $\langle e^{\lambda N_\varepsilon} \rangle$. It is interesting to find the asymptotics of this expression as $\varepsilon \rightarrow 0$. For the half-space R_3^+ we prove the following result:

Theorem 10. *For $\lambda < \lambda_0 = \ln 2 - 1 - \ln \ln 2 \approx 0.0596$ the moment $\langle e^{\lambda N_\varepsilon} \rangle$ is finite and*

$$\langle e^{\lambda N_\varepsilon} \rangle \leq e^\lambda \frac{1}{2(1-\alpha)} \left(\frac{R_0}{\varepsilon} \right)^{\frac{\alpha}{\ln 2} - 1},$$

where $\alpha < 1$ is the solution of equation

$$\alpha e^{-\alpha} = \frac{\ln 2}{2} e^\lambda,$$

R_0 is the distance from the starting point x to ∂G .

For the mean number of steps of the ε -process the following estimate is true:

$$\langle N_\varepsilon \rangle \leq \frac{1}{2(1-\ln 2)} + \frac{\ln 2}{2(1-\ln 2)^3} + \frac{\ln \frac{R_0}{\varepsilon}}{2(1-\ln 2)^2}.$$

Proof. For arbitrary $\varepsilon > 0$, the exact representation of $P(N_\varepsilon = k)$, the probability that the number of steps is equal to k , $k > 1$ is

$$P(N_\varepsilon = k) = \frac{1}{2^k} \left(1 - \frac{\varepsilon}{2R_0} \right) \frac{\varepsilon}{R_0} \times \\ \int_{\varepsilon}^{2R_0} dR_1 \int_{\varepsilon}^{2R_1} dR_2 \dots \int_{\varepsilon}^{2R_{k-3}} dR_{k-2} \int_{\varepsilon}^{2R_{k-2}} dR_{k-1} \frac{1}{R_{k-1}} \prod_{j=1}^{k-2} \frac{1}{R_j} \left(1 - \frac{\varepsilon}{2R_j} \right).$$

Since $\varepsilon < 2R_j$ for all j , we get

$$\langle \exp \lambda N_\varepsilon \rangle \leq \exp(\lambda) \frac{\varepsilon}{2R_0} \sum_{i=0}^{\infty} \left(\frac{\exp \lambda}{2} \right)^i \frac{\ln^i \{2^i R_0 / \varepsilon\}}{i!} \\ = \exp(\lambda) \frac{\varepsilon}{2R_0} \sum_{i=0}^{\infty} \left(\frac{\ln 2 \exp \lambda}{2} \right)^i \frac{1}{i!} \left[i + \ln \left(\frac{R_0}{\varepsilon} \right)^{\frac{1}{\ln 2}} \right]^i \equiv f(a),$$

where

$$a = \ln \left(\frac{R_0}{\varepsilon} \right)^{\frac{1}{\ln 2}}.$$

Direct calculations show that $f(a)$ satisfies the equation

$$\frac{\partial f}{\partial a} = \frac{\ln 2 \exp \lambda}{2} f(a+1),$$

whose solution has the form

$$f(\bar{a}) = f(0) \exp(\alpha a),$$

where α is the unique on the interval $(0, 1)$ solution to the equation

$$\alpha \exp(-\alpha) = \frac{\ln 2}{2} \exp \lambda.$$

The value $f(0)$ is

$$\begin{aligned} f(0) &= \exp(\lambda) \frac{\varepsilon}{2R_0} \sum_{i=0}^{\infty} \left(\frac{\ln 2 \exp \lambda}{2} \right)^i \frac{1}{i!} i^i \\ &= \exp(\lambda) \frac{\varepsilon}{2R_0} \left\{ 1 + \sum_{i=0}^{\infty} \left(\frac{\ln 2 \exp \lambda}{2} \right)^i \frac{1}{i!} i^i \right\} \\ &= \exp(\lambda) \frac{\varepsilon}{2R_0} \left\{ 1 + \frac{\alpha}{1-\alpha} \right\} = \frac{\exp(\lambda)}{1-\alpha} \cdot \frac{\varepsilon}{2R_0}. \end{aligned}$$

Thus,

$$\begin{aligned} \langle \exp \lambda N_\varepsilon \rangle &\leq f(a) = \frac{\varepsilon}{2R_0} \frac{\exp(\lambda)}{1-\alpha} \exp \left\{ \alpha \ln \left(\frac{R_0}{\varepsilon} \right)^{\frac{1}{\ln 2}} \right\} \\ &= \frac{\exp(\lambda)}{2(1-\alpha)} \left(\frac{R_0}{\varepsilon} \right)^{\frac{\alpha}{\ln 2} - 1}. \end{aligned}$$

Note that $f(0) < \infty$ iff $\ln 2 \exp(\lambda) < 2/e$, i.e., $f(0) < \infty$ if $\lambda < \lambda_0 = \ln 2 - 1 - \ln \ln 2 \approx 0.0596$.

The solution to $\alpha \exp(-\alpha) = \ln 2 \exp \lambda / 2$ on $(0,1)$ can be found numerically, e.g., for $\lambda = 0.05$ we get $\alpha = 0.86$, and

$$\langle \exp(\lambda N_\varepsilon) \rangle \leq 3.754 \left(\frac{R_0}{\varepsilon} \right)^{0.24}.$$

For the mean number of steps we get

$$\langle N_\varepsilon \rangle \leq \frac{\varepsilon}{2R_0} \sum_{i=0}^{\infty} \left(\frac{\ln 2}{2} \right)^i (i+1) \frac{1}{i!} (i+a)^i.$$

Indeed, let

$$F(\beta) = \frac{\varepsilon}{2R_0} \sum_{i=0}^{\infty} \left(\frac{\ln 2}{2} \right)^i \frac{1}{i!} \beta^{i+1} \left[i + \ln \left(\frac{R_0}{\varepsilon} \right)^{\frac{1}{\ln 2}} \right]^i.$$

Now

$$\langle N_\varepsilon \rangle = \frac{\partial F}{\partial \beta} \Big|_{\beta=1}.$$

But

$$F(\beta) = \frac{\beta}{2(1-\alpha)} \left(\frac{R_0}{\varepsilon} \right)^{\frac{1}{\ln 2} - 1},$$

where $\alpha \exp(-\alpha) = \frac{\beta \ln 2}{2}$. The derivative gives

$$\frac{\partial F}{\partial \beta} \Big|_{\beta=1} = \frac{1}{2(1-\ln 2)} + \frac{\ln 2}{2(1-\ln 2)^3} + \frac{\ln \frac{R_0}{\varepsilon}}{2(1-\ln 2)^2}. \quad \square$$

Note that the estimation obtained is not crude even if ε is not very small: for example, it gives a nonzero estimation when $R_0 = \varepsilon$.

References

- [1] K.K. Sabelfeld, Monte Carlo Methods in Boundary Value Problems, Springer-Verlag, Heidelberg, New York, 1991.
- [2] M.E. Muller, Some continuous Monte Carlo method for the Dirichlet problem, Ann. Math. Statistics, 27(3), 1956.
- [3] M. Freidlin, Functional Integration and Partial Differential Equations, Annals of Mathematics Studies, Princeton University, 1985.
- [4] R. Courant and D. Hilbert, Methods of Mathematical Physics, Vol. 2, John Wiley Sons, N.Y., 1989.