Bull. Nov. Comp. Center, Num. Anal., 10 (2001), 11–17

The Monte Carlo method for conjugate stationary diffusion equation with special item*

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1. The basic estimator

Consider the three-dimensional Dirichlet problem for the equation

$$\Delta u + (v, \operatorname{grad} u) + cu = -g, \quad u|_\Gamma = \psi \tag{1.1}$$

in a domain Ω with the boundary Γ, which is assumed simply connected and piecewise smooth. We suppose the functions v, c, and g to satisfy the Hölder condition in $\overline{\Omega}$, and the function ψ to be continuous on Γ. Let Γ_ε be ε-neighborhood of Γ, let $D(r)$ be the maximal ball with center at the point r, which lies in $\overline{\Omega}$, and let $S(r)$ be the corresponding sphere of the radius $d = d(r)$. For the function $u(r)$ we can write down the corresponding integral equation which has the following form in $\Omega \setminus \Gamma_\varepsilon$ [2]:

$$u_1(r) = \frac{1}{4\pi d^2(r)} \int\limits_{S(r)} u_1(r'(s))\, ds + \int\limits_{D(r)} G_r(r') c(r') u_1(r')\, dr' + \int\limits_{D(r)} G_r(r')(v(r'), \operatorname{grad} u_1(r'))\, dr' + \int\limits_{D(r)} G_r(r') g(r')\, dr'. \tag{1.2}$$

Where

$$G_r(r') = \frac{1}{4\pi}\left(\frac{1}{|r - r'|} - \frac{1}{d}\right)$$

is the "central" Green's function for the ball $D(r)$. We consider $u_1 \equiv u$ for $r \in \Gamma_\varepsilon$. Denote the unit vector in the direction of the velocity v by l, i.e., $l = v/|v|$. Using "non-central" Green's function we can derive the following integral equation for the function $(\operatorname{grad} u_1(r))_l \equiv \partial u_1/\partial l$ (see, e.g. [2]):

*Supported by the scientific program "Russian Universities – Basic Research" (3759) and FCP "Integration" (274).

$$\frac{\partial u_1}{\partial l}(r) = \int\limits_{S(r)} \frac{3a_l(r,r'(s))u_1(r'(s))}{4\pi d^3(r)}\,ds + \int\limits_{D(r)} \frac{\partial G_l}{\partial l}(r,r')c(r')u_1(r')\,dr' +$$
$$\int\limits_{D(r)} \frac{\partial G_l}{\partial l}(r,r')(v(r'),\operatorname{grad} u_1(r'))\,dr' + \int\limits_{D(r)} \frac{\partial G_l}{\partial l}(r,r')g(r')\,dr'. \quad (1.3)$$

Where $a_l(r,r') = (r'-r,l)/|r'-r|$ is the cosine of the angle between unit vector l and the vector $r'-r$. Note that the functions

$$F_0(r,r') = \frac{6G_r(r')}{d^2(r)} \quad \text{and} \quad F(r,r') = \frac{4}{3d(r)a_l}\frac{\partial G_l}{\partial l}(r,r') = \frac{d^3-|r-r'|^3}{3\pi d^4|r-r'|^2}$$

are probability densities in the ball $D(r)$. To construct the algorithms of the Monte Carlo method, we henceforth combine (1.2) and (1.3) into a single integro-algebraic equation by means of a special extension of the phase space. Here it is reasonable to consider $(v,\operatorname{grad} u)$ in the moving coordinate system with the basis vector $l(r) = v(r)/|v(r)|$, in this system $(v,\operatorname{grad} u) = v\cdot\frac{\partial u}{\partial l}$. Moreover, we pass from the function $\frac{\partial u}{\partial l}(r)$ to the function $\frac{d(r)}{3}\frac{\partial u}{\partial l}(r)$.

Extend the phase space by adding a discrete variable j: $j=0$ or $j=1$. Put $w=(r,j)$ and introduce the following notations:

$$U(w) = U(r,j) = \begin{cases} u(r), & j=0; \\ \dfrac{d(r)}{3}\dfrac{\partial u}{\partial l}(r), & j=1, \end{cases} \qquad k(w,w') = \begin{cases} \dfrac{F_0(r,r')}{2}, & j=0, \\ \dfrac{F(r,r')}{2}, & j=1, \end{cases}$$

$$H(w) = \begin{cases} \displaystyle\int\limits_{D(r)} G_r(r')g(r')\,dr', & j=0, \\ \dfrac{d(r)}{3}\displaystyle\int\limits_{D(r)} \frac{\partial G_l}{\partial l}(r,r')g(r')\,dr', & j=1, \end{cases} \qquad a(w,w') = \begin{cases} 1, & j=0, \\ a_l(r,r'), & j=1, \end{cases}$$

$$M(w,w') = \begin{cases} \dfrac{2c(r')}{c_0}, & j=0,\ j'=0, \\ \dfrac{6v(r')}{c_0 d(r')}, & j=0,\ j'=1, \\ \dfrac{3c(r')a_l(r,r')}{c_0}, & j=1,\ j'=0, \\ \dfrac{9v(r')a_l(r,r')}{c_0 d(r')}, & j=1,\ j'=1. \end{cases} \quad (1.4)$$

Here c_0 is a constant satisfying the inequality $c_0 d_{\max}^2 < 6$. Using these notations, write down the system of integral equations (1.2), (1.3) in the form

$$U_1(w) = H(w) + \left[1 - \frac{c_0 d^2(r)}{6}\right] \int\limits_{S(r)} \frac{a(w, r'(s), 0)}{1 - c_0 d^2/6} \frac{U_1(r'(s), 0)}{4\pi d^2(r)} \, ds +$$

$$\left[\frac{c_0 d^2(r)}{6}\right] \sum_{j'=0}^{1} \int\limits_{D(r)} M(w, w') k(w, w') U_1(w') \, dr', \quad r \in \Omega \setminus \Gamma_\varepsilon, \tag{1.5}$$

$$U_1(w) \equiv U(w), \quad r \in \Gamma_\varepsilon.$$

According to (1.5), the estimator of the Monte Carlo method for $U(w)$ is constructed as follows.

With the probability $1 - c_0 d^2(r_n)/6$, the new point r_{n+1} is chosen uniformly at random on the sphere $S(r_n)$, the weight Q_n is multiplied by $[1 - c_0 d^2(r_n)/6]^{-1} a(w_n, w_{n+1})$, and j_{n+1} is set to equal 0.

With the probability $c_0 d^2(r_n)/6$ the point r_{n+1} is chosen at random in the ball $D(r_n)$ with the density $2k(w_n, w')$. Next, j_{n+1} takes one of the values 0 or 1 with equal probabilities. Finally, the weight Q_n is multiplied by $M(w_n, w_{n+1})$.

In the process of modeling, this "walk on spheres and balls", when the point occurs in Γ_ε at a random step N, the chain terminates and the estimator of solution, multiplied by the weight, is added to the counter. As a result we obtain the following estimator for $U(w_0)$:

$$\xi(w_0) = \sum_{n=0}^{N} Q_n H(w_n),$$

where

$$Q_n = \prod_{i=1}^{m_n} M(w_{k_i - 1}, w_{k_i}) \prod_{i=1}^{n - m_n} \frac{a(w_{t_i - 1}, w_{t_i})}{1 - c_0 d^2(r_{t_i - 1})/6}.$$

Here $\{r_{t_i}\}$, $i = 1, \ldots, n - m_n$, are points chosen on spheres, and $\{r_{k_i}\}$, $i = 1, \ldots, m_n$, are points chosen in balls. The function $H(w) = H(r, j) = h_j(r)$ can be estimated by the Monte Carlo method for one "random knot" [1].

2. Unbiasedness of the estimator and boundedness of the variance

Lemma 1. *Suppose that the conditions*

$$|c(r)| \le \frac{c_0}{3}, \quad |v| \le \frac{c_0}{9} d(r), \tag{2.1}$$

are satisfied for $c_0 < 6c^*/\pi^2$, *where* $-c^*$ *is the first eigenvalue of the Laplace operator in* Ω. *Then the Neumann series for equation* (1.5) *converges.*

Proof. Consider the function

$$f(x) = \frac{6}{x^2}\left(1 - \frac{\sin x}{x}\right) = 1 - \frac{6}{5!}x^2 + \frac{6}{7!}x^4 - \frac{6}{9!}x^6 + \dots .$$

It is easy to see that the function $f(x)$ decreases from 1 to $6/\pi^2$ on the interval $[0, \pi]$. On the other hand, the inequality $c_0/c^* < f(x)$ implies that

$$\frac{1}{1 - c_0 d_i^2/6} < \frac{d_i\sqrt{c^*}}{\sin d_i\sqrt{c^*}}, \tag{2.2}$$

where

$$x = d_i\sqrt{c^*} \leq d_{\max}\sqrt{c^*} \leq \pi.$$

In view of (2.1), relation (2.2) means that $\xi(w_0)$ termwise dominated by some (not necessarily maximal) standard estimator ζ of a "walk on spheres" for which the Neumann series converges [2]. □

For specific types of domains, the condition $c_0/c^* < 6/\pi^2 \approx 0.6079$ can be weakened on accounting for the exact value of $d_{\max}$. For example, for a cube with the edge b we have $c^* = 3\pi^2/b^2$, $d_{\max} = b/2$, $c_0/c^* \leq 0.6888$.

Lemma 2. *Let U_0 and K_0 be respectively the Neumann series and the integral operator of equation* (1.5) *for $a_l \equiv 1$, $c \equiv c_0/3$, $0 < c_0 < 6c^*/\pi^2$, $g \equiv g_0 > 0$, and $v_0(r) = \frac{c_0 d(r)}{9}\frac{v}{|v|}\operatorname{sgn} U_0(r, 1)$. Moreover, assume be satisfied the following conditions in Γ_ε: $U_0(r, 1) = C^0$ and $U_0(r, 0) = u_0$, where*

$$\Delta u_0 + c u_0 = -g_0, \quad u_0|_\Gamma = C^0. \tag{2.3}$$

Then $\lim\limits_{n\to\infty} K_0^n U_0(w) = 0$ and $U_0(w) \geq C^0$.

Proof. The first claim of the lemma follows from the representation

$$U_0(w) = \sum_{i=0}^{n} K_0^i H_0 + K_0^{n+1} U_0(w)$$

relating to the fact that, under the conditions of the lemma, the Neumann series converges (see the proof of Lemma 1) and satisfies the equation

$$U_0(r, 0) = \int\limits_{S(r)} \frac{U_0(r'(s), 0)}{4\pi d^2(r)}\, ds + \frac{c_0 d^2}{18} \int\limits_{D(r)} F_0[U_0(r', 0) + |U_0(r', 1)|]\, dr' + \frac{d^2 g_0}{6}.$$

On the other hand, the function $u_0(r)$ in $\Omega \setminus \Gamma_\varepsilon$ satisfies the equation

$$u_0(r) = \int\limits_{S(r)} \frac{u_0(r'(s))}{4\pi d^2(r)}\,ds + \frac{c_0 d^2(r)}{18} \int\limits_{D(r)} F_0 u_0(r')\,dr' + \frac{d^2 g_0}{6}.$$

Hence,

$$U_0(r,0) \geq u_0(r) \geq C^0.$$

Using this estimate for $U_0(r,0)$ together with the integral equation for $U_0(r,1)$, we obtain

$$U_0(r,1) = \int\limits_{S(r)} \frac{U_0 ds}{4\pi d^2} + \frac{c_0 d^2}{12} \int\limits_{D(r)} F[U_0(r',0) + |U_0(r',1)|]\,dr' + \frac{d^2 g_0}{4} \geq C^0,$$

which completes the proof of the second claim of the lemma. □

Theorem 1. *Under the conditions of Lemma 1, there exists a unique bounded solution to* (1.7) *which is representable by the Neumann series; moreover,* $U_1(r,0) = u(r)$, $U_1(r,1) = \frac{d(r)}{3}\frac{\partial u}{\partial l}(r)$.

Proof. Let $u(r)$ be a solution such that

$$|u(r)| \leq C_1 \quad \text{and} \quad \left|\frac{d(r)}{3}\frac{\partial u}{\partial l}\right| \leq C_1.$$

Then

$$U_1 = \sum_{i=0}^{n} K^i H + K^{n+1} U_1, \quad |K^{n+1} U_1| \leq \frac{C_1}{C^0} K^{n+1} U_0.$$

This yields a representation for U_1 in the form of a Neumann series. The remaining assertions of the theorem are valid in view of uniqueness of a bounded solution to the original differential problem. □

Remark. To estimate the derivative of a solution u in an arbitrary direction μ (rather than only in the direction of the velocity v), at the first step of the algorithm we should use for $\frac{d(r)}{3}\frac{\partial u}{\partial \mu}$ a representation similar to (1.5):

$$\frac{d(r)}{3}\frac{\partial u}{\partial \mu}(r) = h_\mu(r) + \left[1 - \frac{c_0 d^2(r)}{6}\right] \int\limits_{S(r)} \frac{a_\mu u(r'(s))}{1 - c_0 d^2/6} \frac{ds}{4\pi d^2(r)} +$$

$$\left[\frac{c_0 d^2(r)}{6}\right] \int\limits_{D(r)} \left(\frac{3a_\mu c(r')}{2c_0} u(r') + \frac{3a_\mu v(r')}{2c_0} \frac{\partial u}{\partial l}(r')\right) F(r,r')\,dr'. \quad (2.4)$$

After the above-described randomization of representation (2.4), we implement the modeling algorithm that relates to the basis vector $l(r)$.

Since the values $U(w)$ are unknown in Γ_ε, we construct estimators for these values as follows. For $j_N = 0$ we can put $H(r_N, 0) = u(r_N) = \psi(r_N^*)$, where

$$r_N^* \in \Gamma, \quad r_N \in \Gamma_\varepsilon, \quad |r_N - r_N^*| = d(r_N).$$

Assume that the first-order derivatives of a solution are bounded in Ω, i.e.,

$$\frac{d(r)}{3}\frac{\partial u}{\partial l} = \mathrm{O}(\varepsilon) \quad \text{for} \quad r \in \Gamma_\varepsilon.$$

Then for $j_N = 1$ we can take approximately $H(r_N, j_N) = 0$. As a result, we obtain a biased estimator $\xi_\varepsilon(w_0)$ for a solution.

Theorem 2. *Suppose that the first-order derivatives of the function $u(r)$ are bounded in Ω and that the conditions of Lemma 1 are satisfied. Then $\mathrm{E}\,\xi_\varepsilon(r, 0) = u_\varepsilon(r)$ exists, and*

$$|u(r) - u_\varepsilon(r)| \le C_2\varepsilon, \;\; \varepsilon > 0, \;\; r \in \Omega.$$

Moreover, $\mathrm{E}\,\xi_\varepsilon(r, 1) = f_{l\varepsilon}(r)$ exists, and

$$\left|\frac{d(r)}{3}\frac{\partial u}{\partial l} - f_{l\varepsilon}(r)\right| \le C_3\varepsilon, \quad \varepsilon > 0, \quad r \in \Omega.$$

Proof. Obviously,

$$|\xi - \xi_\varepsilon| = |Q_N[U(r_N, j) - \psi(r_N^*)(1 - j)]| \le Q_N^{(0)}\varepsilon C_4,$$

where $Q_N^{(0)}$ is the weight corresponding to some standard estimator of a walk on spheres for the case $c < c^*$, $g \equiv 0$. □

Theorem 3. *Suppose that* (2.8) *is satisfied, $c_0 \le 0.488c^*$, and $g \equiv 0$. Then $\mathrm{D}\,\xi_\varepsilon < C_d < +\infty$ for all $\varepsilon > 0$.*

Proof. Put $y = c_0/c^*$, $t = d\sqrt{c^*}$. Direct calculations show that the value

$$\max\left\{y > 0: \;\left(\frac{1}{1 - yt^2/6}\right)^2 \le \frac{t}{\sin t}\right\}$$

is attended at a point y^* such that $0.488 < y^* < 0.489$; moreover, the value of $\frac{t}{\sin t}(1 - yt^2/6)^2$ is minimal and equal to unity for $t \approx 2.175$. Hence, ξ_ε^2 is dominated in the same way as ξ in the proof of Lemma 1. □

To relax the boundedness condition on variance, we carry out the following modification of the estimator. We calculate the function $H(r, j)$ only at the step $(r, j) \to (r', 0)$, i.e., at the step to a sphere, but with the weight $[1 - c_0 d^2(r)/6]^{-1}$. Thus, $H(r, j) \to \tilde{H}(r, j)$:

$$\tilde{H}(r_{k_i-1},j)=0,\quad \tilde{H}(r_{t_i-1},j)=\frac{1}{1-c_0d^2(r_{t_i-1})/6}H(r_{t_i-1},j).$$

In the place of the estimator ξ_ε, we thereby consider the estimator $\xi_{\varepsilon,1}$ for which $\mathrm{E}\,\xi_\varepsilon=\mathrm{E}\,\xi_{\varepsilon,1}$.

Theorem 4. *Under the conditions of Theorem 3 the following estimates hold for* $g\not\equiv 0$: $\mathrm{D}\,\xi_{\varepsilon,1}<C_{d,1}<+\infty$ *for all* $\varepsilon>0$.

Proof. Assuming the conditions of the theorem, we have

$$\frac{d\sqrt{c^*}}{\sin(d\sqrt{c^*})}-1>\left(\frac{1}{1-c_0d^2/6}\right)^2-1\geq C_5d^2.$$

Also, observe that $H(r,j)=\mathrm{O}(d^2(r))$. Put $s(c,d)=\frac{d\sqrt{c}}{\sin(d\sqrt{c})}$. Termwise dominating $|\xi_{\varepsilon,1}|$ by the standard estimator $\eta^{(0)}$ of a "walk on spheres" for the case $c\equiv c_0/3<0.488c^*/3$ with the replacement $H\to\tilde{H}$, $3c/c_0\to 1$, $a(w,w')\to 1$, we have

$$\begin{aligned}|\xi_{\varepsilon,1}|&\leq\sum_{n=0}^{N}|Q_n|\,|\tilde{H}(w_n)|\leq C_6\sum_{i=0}^{N-m_N}\tilde{Q}_id_i^2\\&\leq\frac{C_6}{C_5}\sum_{i=0}^{N-m_N}\left[\prod_{j=0}^{i-1}s(c,d_j)\right](s(c,d_i)-1)\\&=\frac{C_6}{C_5}\sum_{i=1}^{N-m_N}(\tilde{Q}_i-\tilde{Q}_{i-1})=C_7(Q_N^{(0)}-1),\end{aligned}\qquad(2.5)$$

Hence, $|\xi_{\varepsilon,1}|\leq\eta^{(0)}$ for all $\varepsilon>0$; moreover $\mathrm{D}\,\eta^{(0)}<+\infty$. □

References

[1] Ermakov S.M., Mikhailov G.A. Statistic Modeling. – Moscow: Nauka, 1982 (in Russian).

[2] Mikhailov G.A. New Monte Carlo methods for solving the Helmholtz equation // Dokl. Akad. Nauk. – 1992. – Vol. 326, № 6. – P. 943–947.