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# Parametric estimate of the solution of the boundary value problem by the Monte Carlo method

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## Introduction

One of advantages of the Monte Carlo methods consists in capability to evaluate various functionals by weighting estimates, for instance, it is possible to evaluate the eigenvalues by using the estimate of the parametric derivations of the solution. The other significant application of weight estimates consists in capability of parametric extension of the solution in the case when a solution of the problem and its estimate are analytic functions.

In the present paper, applications of parametric estimates of the Monte Carlo method are illustrated on various numerate examples for the boundary value problem

$$\begin{aligned} \Delta u + \lambda u &= -g, \quad \boldsymbol{r} \in D, \\ \alpha u + \beta \frac{\partial u}{\partial \ell} &= \varphi, \quad \boldsymbol{r} \in \Gamma. \end{aligned} \tag{1}$$

In articles [1, 2], an algorithm of resolving the boundary value problem (1) was constructed by using the process "walking on spheres" with reflection from border. This algorithm has obtained rigorous vindication only for $\lambda \le 0$. If the first eigenvalue $c^*$ of problem (1) is greater than zero, then it is possible to extend the area of utilizing the algorithm in the case of $\lambda > 0$ via analytical continuation of the resolve. Let us represent a solution of problem (1) as the series

$$u(\boldsymbol{r}, \lambda) = \sum_{p=0}^{\infty} \frac{v_p(\boldsymbol{r}, \lambda)}{p!} (\lambda - \lambda_0)^p, \tag{2}$$

where the partial derivatives $v_p = u^{(p)} = \frac{\partial^p u}{\partial \lambda^p}$. Choosing $\lambda_0 < 0$ we can obtain an estimate of the solution for $0 < \lambda < c^*$. In the present article, it is shown numerically that it is possible to obtain the estimate of a solution of problem (1) for $0 < \lambda < c^*$ directly, do not resorting to the calculation of the parametric derivatives $v_p$ and to the construction of the series (2) on its basis.

# 1. The main problem and the estimate of the solution

Consider the boundary value problem (1) for $\lambda = -c \leq 0$ in the bounded domain $D \subset R^3$ with the boundary $\Gamma$. The vector field $\boldsymbol{\ell}$ satisfies the following conditions:

$$(\boldsymbol{\ell}(\boldsymbol{r}), \boldsymbol{n}(\boldsymbol{r})) \geq \theta_0 > 0, \quad \|\boldsymbol{\ell}(\boldsymbol{r})\| = 1, \quad \boldsymbol{r} \in \Gamma,$$

where $\boldsymbol{n}(\boldsymbol{r})$ is an outward normal vector to $\Gamma$ at $\boldsymbol{r}$. Let $\alpha$ and $\beta$ satisfy the conditions:

$$0 \leq \alpha(\boldsymbol{r}) \leq \alpha_{\max}, \quad 0 \leq \beta(\boldsymbol{r}) \leq \beta_{\max}, \quad \alpha(\boldsymbol{r}) + \beta(\boldsymbol{r}) \geq 1, \quad \boldsymbol{r} \in \Gamma. \qquad (3)$$

Henceforward, we suppose the functions $\alpha$, $\beta$, $g$, $\varphi$, the vector field $\boldsymbol{\ell}$, and the boundary $\Gamma$ satisfy the regularity conditions that guarantee the existence and the uniqueness of the solution $u(\boldsymbol{r})$ of the considered problem, and also the possibility of using the integral representation with the Green function for a ball inscribed in $D$ [4, 5].

Let us give the exact definition of the process of "random walk on spheres" with reflection from the boundary. The Markov chain $\{\boldsymbol{r}_k\}_{k=0,1,\dots,L}$ is specified by the following characteristic: $\pi(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_0)$ is the density of initial distribution (i.e., the chain goes out of the point $\boldsymbol{r}_0$); $p(\boldsymbol{r}, \boldsymbol{r}')$ is the density of transition function from $\boldsymbol{r}$ to $\boldsymbol{r}'$ which is defined by the expression:

$$p(\boldsymbol{r}, \boldsymbol{r}') = \begin{cases} s(c_0, d)\delta_{S(\boldsymbol{r})}(\boldsymbol{r}'), & \boldsymbol{r} \in D \setminus \Gamma_\varepsilon, \\ q(\boldsymbol{r})\delta_{\boldsymbol{r}-h\boldsymbol{\ell}}(\boldsymbol{r}'), & \boldsymbol{r} \in \Gamma_\varepsilon, \end{cases}$$

where $\delta_{S(\boldsymbol{r})}$ is the generalized $n$-dimensional density that corresponds to uniform distribution on the sphere $S(\boldsymbol{r})$, and $\delta_{\boldsymbol{r}-h\boldsymbol{\ell}}$ is the generalized density corresponding to transition from the point $\boldsymbol{r} \in \Gamma_\varepsilon$ to the point $\boldsymbol{r} - h\boldsymbol{\ell}(\boldsymbol{b})$ with probability 1, where $\boldsymbol{b} = \boldsymbol{b}(\boldsymbol{r})$; $p(\boldsymbol{r})$ is the probability of chain termination at a point $\boldsymbol{r}$, which is defined by the expression

$$p(\boldsymbol{r}) = 1 - \int_D p(\boldsymbol{r}, \boldsymbol{r}')\, d\boldsymbol{r}' = \begin{cases} 1 - s(c_0, d), & \boldsymbol{r} \in D \setminus \Gamma_\varepsilon, \\ 1 - q(\boldsymbol{r}), & \boldsymbol{r} \in \Gamma_\varepsilon, \end{cases}$$

where $d = d(\boldsymbol{r})$, $\varepsilon_r = |\boldsymbol{b} - \boldsymbol{r}|$, $0 \leq c_0 \leq c$, and $L$ is the number of the final state (the moment of terminating the trajectory).

In [1, 2], the estimates of the average number E$R$ of reflections and the average number E$L$ of transitions are obtained.

Write the collision estimate $\xi(\boldsymbol{r})$ for $\boldsymbol{r} = \boldsymbol{r}_0 \in D$ in recurrent form [1, 2]:

$$\xi_i = Q(\boldsymbol{r}_i)\xi_{i+1} + f_i, \quad i = 0, \dots, L-1, \tag{4}$$

$$Q(\boldsymbol{r}_i) = \begin{cases} \dfrac{s(c, d_i)}{s(c_0, d_i)}, & \boldsymbol{r}_i \in D \setminus \Gamma_\varepsilon, \\ 1, & \boldsymbol{r}_i \in \Gamma_\varepsilon. \end{cases}$$

Here

$$s(c, d) = \frac{d\sqrt{c}}{\mathrm{sh}(d\sqrt{c})}, \qquad q(\boldsymbol{r}) = \frac{\beta + \alpha\varepsilon_r}{\beta + \alpha\varepsilon_r + \alpha h}.$$

Having calculated with the probability $1 - p(\boldsymbol{r}_i)$ the estimate $\xi_{i+1}$ is calculated at the next point $\boldsymbol{r}_{i+1}$ of the chain and the estimate of the function $f(\boldsymbol{r})$ is added to it. With the complementary probability $p(\boldsymbol{r}_i)$ the chain terminates. Obviously, the inequality $p(\boldsymbol{r}) < 1$ must hold if the corresponding weight is nonzero.

For $\boldsymbol{r} \in D \setminus \Gamma_\varepsilon$ the quantities $f_i = f(\boldsymbol{r}_i)$ are estimated in randomize form in accordance with the expression

$$\begin{aligned} f(\boldsymbol{r}) &= \frac{1}{4\pi}\int_\Omega d\omega \int_0^d x\left(1 - \frac{x}{d}\right)\frac{s(c,d)}{s(c, d-x)} g(x, \omega)\, dx \\ &= \frac{d^2}{6}\,\mathrm{E}\left\{\frac{s(c,d)}{s(c, d-\xi)} g(\xi, \omega)\right\}, \end{aligned} \tag{5}$$

where $\omega$ is an isotropic $n$-dimensional unit vector, the value $\xi$ is distributed in the interval $(0, d)$ with the density

$$p(x) = \frac{6x(1 - x/d)}{d^2}.$$

In $\Gamma_\varepsilon$, the quantities $f_i = f(\boldsymbol{r}_i)$ are calculated exactly:

$$f(\boldsymbol{r}) = \frac{h}{\beta + \alpha(\varepsilon_r + h)}\varphi(\boldsymbol{r}) + \phi(\boldsymbol{r}). \tag{6}$$

There is the unknown error function $\psi(\boldsymbol{r})$ in expression (6). For this reason, we have to pass to the actual biased estimate $\xi_{r,h}$, in which $\phi(\boldsymbol{r})$ is replaced by zero:

$$\xi(\boldsymbol{r}_0) = \sum_{i=0}^{L}\left(\prod_{j=0}^{i-1} Q(\boldsymbol{r}_j)\right) f(\boldsymbol{r}_i).$$

In [1], the following main theorem for the estimate was proved:

**Theorem 1.** *If the second-order derivatives of a solution of* (1) *are bounded in* $\Gamma_{\varepsilon+h}$ *and one of the conditions:* $\alpha(\boldsymbol{r}) \geq \alpha_0 > 0$ *or* $c > 0$ *is satisfied, then the mathematical expectation* $\mathrm{E}\xi_{r,h} = u_h(\boldsymbol{r})$ *exists,* $\|\mathrm{E}\xi_{r,h}\| < \infty$, $\|\mathrm{D}\xi_{r,h}\| < \infty$, *and* $|u(\boldsymbol{r}) - u_h(\boldsymbol{r})| \leq C\,h$, $\boldsymbol{r} \in D$, $h > 0$.

## 2. Extension of the estimates on the case of solving the equation $\Delta u + cu = -g$ with $c > 0$

In the present section, the numerical investigation of possibility of extending the estimate on the case of solving problem (1) for the equation $\Delta u + cu = -g$ with positive $c$ is carried out. Earlier, a stochastic estimate of a solution to the Dirichlet problem for the equation $\Delta u + cu = -g$ with positive $c$ has been constructed in article [6]. The approach used in this article is based on a probabilistic representation of a solution of the Dirichlet problem which is true for $c < c^*$, where $-c^*$ is the first eigenvalue of the Laplace operator for the domain $D$ on the class of functions satisfied the boundary condition $u|_\Gamma = 0$. In the case of the second and the third boundary value problems, a probabilistic representation of a solution has been constructed for $c < 0$ only [8]. Nevertheless, the region of application of the constructed algorithm could be expanded on the case of the problem

$$\begin{aligned} &\Delta u + cu = -g, \quad \boldsymbol{r} \in D, \\ &\alpha u + \beta \frac{\partial u}{\partial \ell} = \varphi, \quad \boldsymbol{r} \in \Gamma, \end{aligned} \tag{7}$$

with positive parameter $c$. If we suggest that a solution $u(\boldsymbol{r}, c)$ of problem (7) is an analytical function up to $c < c_1^*$, then the function $\mathrm{E}\,\xi(\boldsymbol{r}, c)$ is an analytical function of $c$ also, and the equality $\mathrm{E}\,\xi(\boldsymbol{r}, c) = u(\boldsymbol{r}, c)$ holds for $c < 0$ and $\forall \boldsymbol{r} \in D$. Since two analytical functions coincide for $c < 0$, then this parity will hold up to $c < c_1^*$.

Consider the boundary value problem in the unit cube $D \subset R^3$:

$$\begin{aligned} &\Delta u + cu = 0, \qquad \boldsymbol{r} \in D, \\ &\alpha u + \beta \frac{\partial u}{\partial \boldsymbol{n}} = \varphi, \quad \boldsymbol{r} \in \Gamma. \end{aligned} \tag{8}$$

Let the boundary condition in (8) either satisfy the requirement $\alpha \geq \alpha_0 > 0$, or have the mixed form:

$$\begin{aligned} &\alpha u + \beta \frac{\partial u}{\partial l} = \varphi_1, \quad \boldsymbol{r} \in \Gamma_1, \\ &u = \varphi_2, \qquad\qquad \boldsymbol{r} \in \Gamma_2, \end{aligned}$$

where $\Gamma_1$ is an open subset of $\Gamma$ and the subset $\Gamma_2 = \Gamma \setminus \Gamma_1$ is nonempty.

In this case, the first eigenvalue $c^*$ of the uniform problem (8) is greater than zero. To obtain the integral representation corresponding to problem (8) for $c > 0$ the Green spherical function for the Helmholtz equation should be used [5, 7]. The expression of the weight $s(c, d)$ (in $R^3$) is the following:

$$s(c,d) = \begin{cases} \dfrac{d\sqrt{|c|}}{\operatorname{sh}(d\sqrt{|c|})}, & c \le 0; \\ \dfrac{d\sqrt{c}}{\sin(d\sqrt{c})}, & c \ge 0. \end{cases}$$

It is clear that the general form of estimate (4) remains the same. The weight $s(c,d) \ge 1$ for $c > 0$, so we will consider only the case with breaking in $\varepsilon$-neighbourhood of the border (i.e., $p(\boldsymbol{r}) = 0$ for $\boldsymbol{r} \notin \Gamma_\varepsilon$).

Further we will consider the boundary value problem (8) with the following exact solution

$$u(\boldsymbol{r}) = \begin{cases} \operatorname{ch}\left(r_1\sqrt{\frac{|c|}{3}}\right)\operatorname{ch}\left(r_2\sqrt{\frac{|c|}{3}}\right)\operatorname{ch}\left(r_3\sqrt{\frac{|c|}{3}}\right), & c < 0; \\ \cos\left(r_1\sqrt{\frac{c}{3}}\right)\cos\left(r_2\sqrt{\frac{c}{3}}\right)\cos\left(r_3\sqrt{\frac{c}{3}}\right), & c > 0. \end{cases} \tag{9}$$

Two boundary conditions were considered. In the first problem, the condition on $\Gamma$ had the form $u + \frac{\partial u}{\partial n} = \psi$ (Table 1). In the second case, the problem with the mixed boundary condition:

$$u|_{\Gamma_1} = \psi_1, \quad \left.\frac{\partial u}{\partial \boldsymbol{n}}\right|_{\Gamma_2} = \psi_2$$

was solved, where $\Gamma_1$ consists of the cube faces $r_1 = 0$, $r_2 = 0$, $r_3 = 0$, and $\Gamma_2$ consists of the cube faces $r_1 = 1$, $r_2 = 1$, $r_3 = 1$ (Table 2). The view of the function $\psi$ is obtained by substitution the exact solution $u(\boldsymbol{r})$ (9) in the formula of the corresponding boundary condition.

The evaluation of $c^*$ for the first problem is approximately estimated: $c^* \approx 5.1$. For the other problem there is the explicit value: $c^* = 0.75\pi^2 \approx 7.4$.

Let us consider now the computation results. The solution was estimated for different values $c$ in the cube center. The obtained results are reflected

**Table 1.** The problem with the third boundary condition

| $c$ | $u(\boldsymbol{r},c)$ | $u_N \pm \sigma_N$ | $\sigma^2$ | $N$ | $h$ |
|---|---|---|---|---|---|
| − 10.00 | 3.0261 | $3.0318 \pm 0.0171$ | 14.6 | $5 \cdot 10^4$ | .001 |
| −5.00 | 1.7966 | $1.7990 \pm 0.0078$ | 3.1 | $5 \cdot 10^4$ | .001 |
| −1.00 | 1.1312 | $1.1284 \pm 0.0045$ | 1.0 | $5 \cdot 10^4$ | .001 |
| 1.00 | 0.8809 | $0.8748 \pm 0.0050$ | 1.3 | $5 \cdot 10^4$ | .001 |
| 2.00 | 0.7732 | $0.7653 \pm 0.0076$ | 2.9 | $5 \cdot 10^4$ | .001 |
| 3.00 | 0.6759 | $0.6597 \pm 0.0202$ | 20.5 | $5 \cdot 10^4$ | .001 |
| 4.00 | 0.5883 | $0.4888 \pm 0.1403$ | 984.3 | $5 \cdot 10^4$ | .001 |
| 5.00 | 0.5097 | $0.5674 \pm 0.3719$ | 69152.7 | $5 \cdot 10^5$ | .01 |
| 5.25 | 0.4914 | $0.2421 \pm 0.7848$ | 307996.2 | $5 \cdot 10^5$ | .01 |

**Table 2.** The problem with the mixed boundary condition

| $c$ | $u(r, c)$ | $u_N \pm \sigma_N$ | $\sigma^2$ | $N$ | $h$ |
|---|---|---|---|---|---|
| $-10.00$ | 3.0261 | $3.0413 \pm 0.0075$ | 5.08 | $9 \cdot 10^4$ | .001 |
| $-5.00$ | 1.7966 | $1.8018 \pm 0.0027$ | 0.66 | $9 \cdot 10^4$ | .001 |
| $-1.00$ | 1.1312 | $1.1320 \pm 0.0004$ | 0.02 | $9 \cdot 10^4$ | .001 |
| 1.00 | 0.8809 | $0.8802 \pm 0.0005$ | 0.02 | $9 \cdot 10^4$ | .001 |
| 3.00 | 0.6759 | $0.6733 \pm 0.0018$ | 0.28 | $9 \cdot 10^4$ | .001 |
| 5.00 | 0.5097 | $0.4947 \pm 0.0060$ | 3.26 | $9 \cdot 10^4$ | .001 |
| 6.00 | 0.4394 | $0.3863 \pm 0.0103$ | 9.64 | $9 \cdot 10^4$ | .001 |
| 6.50 | 0.4071 | $0.3498 \pm 0.0312$ | 971.15 | $1 \cdot 10^6$ | .01 |
| 7.00 | 0.3767 | $0.2295 \pm 0.0352$ | 1238.87 | $1 \cdot 10^6$ | .01 |

in Tables 1, 2. Here $u_N$ is the solution estimate, $\sigma_N$ is the estimate of the corresponding mean square error, $\sigma^2$ is the estimate of $\mathrm{D}\xi_h$, $N$ is the number of trajectories, $h = \varepsilon$ is the length of rebound.

The received results indicate that the estimate of the Monte Carlo method for $c > 0$ is close to the exact solution (taking into consideration the mean square error $\sigma_N$), moreover, in the case of the problem with the third boundary condition good accuracy is obtained up to $c = c^*$.

## 3. Estimating spectral parameter derivatives of the solution

We want to clarify the possibility of evaluation of the parametric derivatives $u^{(m)}(\cdot, c)$ by the estimates $\xi_r^{(m)}(c)$. Further the notations

$$\lambda = -c \quad \text{and} \quad s_0(\lambda, d) = s(-\lambda, d)$$

will be used. Let us examine the situation when $\lambda < 0$, and estimate (4) is simulated on the chain with absorptions as inside $D$ as in neighbourhood of the boundary, i.e., $c_0 > 0$.

The main result of [3] is presented below.

**Theorem 2.** *If $g \equiv 0$, $\varphi \equiv 1$, $\lambda < 0$ and $0 < c_0 \le c$ then the following inequalities hold:*

$$|u^{(m)}(\boldsymbol{r}) - \mathrm{E}\xi_{r,h}^{(m)}| \le C_m h, \quad \boldsymbol{r} \in D, \quad m = 1, 2, \dots .$$

*Moreover, the values $\mathrm{E}\left(\xi_{r,h}^{(m)}\right)^2$ are limited uniformly for all $\boldsymbol{r} \in D$ and $h > 0$, i.e., $\mathrm{E}\left(\xi_{r,h}^{(m)}\right)^2 \le D_m < +\infty$.*

In the former section, the numerical algorithm for estimating the initial eigenvalues of the Laplace operator will be presented. It should note that the simplest algorithm is obtained for $\lambda = 0$, but for all that the stating $s(\lambda, \boldsymbol{r}) = s(0, \boldsymbol{r}) \equiv 1$ holds and fulfillment of the inequality $\rho(K) < 1$ is guaranteed only for the third boundary value problem, when $\alpha(\boldsymbol{r}) \geq \alpha_0 > 0$, $\boldsymbol{r} \in \Gamma$. In this case, it should simulate the breaking trajectories in $\Gamma_\varepsilon$ with the probability $p(\boldsymbol{r}) = 1 - q(\boldsymbol{r})$ only. It is clear that all obtained results will transfer on this case.

## 4. Computing eigenvalues

Computing parametric derivatives of a solution of the problem

$$\Delta u - cu = 0, \quad \alpha u + \beta \frac{\partial u}{\partial \ell}\bigg|_\Gamma = 1$$

realizes the iterations of the resolvent operator $[\Delta - c]^{-1}$ at uniform boundary condition. Consequently, the following expression holds:

$$\frac{m u^{(m-1)}(\boldsymbol{r}_0)}{u^{(m)}(\boldsymbol{r}_0)} \underset{m \to \infty}{\longrightarrow} c^* + c, \quad \forall \boldsymbol{r}_0 \in D, \tag{10}$$

where $(-c^*)$ is the first eigenvalue of the Laplace operator for the domain $D$ on the class of functions which satisfy to the uniform condition $\alpha u + \beta \frac{\partial u}{\partial \ell}|_\Gamma = 0$.

Using relation (10) the algorithm of the Monte Carlo method for estimating the value $c^*$ can be obtained:

$$c^* \approx \frac{m \,\mathrm{E}\, \xi_{r,h}^{(m-1)}(c)}{\mathrm{E}\, \xi_{r,h}^{(m)}(c)} - c, \tag{11}$$

where $\xi_{r,h}^{(m)}(c)$ is the biased estimate of the $m$-th parametric derivatives of the solution.

Let us proceed to constructing algorithm of calculating parametric derivatives by the Monte Carlo method. As it is seen from the type of the estimate, it is enough to define an algorithm of calculating the derivatives $Q_\lambda^{(m)}$, where

$$Q = \prod_{j=0}^{i-1} \frac{s(c, d_j)}{s(c_0, d_j)}.$$

Introduce the notation $a = \sqrt{c}$. Differentiating on the variable $a$ via the logarithmic derivative

$$Q'_a = Q(\ln Q)'_a,$$

the recurrent expression can be obtained:

$$Q_a^{(m)} = \sum_{k=1}^{m} t_k Q_a^{(m-k)} \frac{(m-1)!}{(k-1)!(m-k)!}, \quad Q_a^{(0)} = Q,$$

where

$$t_k = (\ln Q)_a^{(k)} = \sum_{j=0}^{i-1} [\ln s(c, d_j)]_a^{(k)} = \sum_{j=0}^{i-1} t_k^{(j)},$$

and

$$\begin{aligned} Q_\lambda^{(1)} &= -Q_a^{(1)}/(2a), \quad Q_\lambda^{(m)} = (-2a)^{-m} \sum_{k=1}^{m} a_k^{(m)} a^{k-m} Q^{(k)}, \quad m > 1, \\ a_1^{(m)} &= (-1)^{(m-1)}(2m-3)!!, \quad a_m^{(m)} = 1, \\ a_k^{(m)} &= a_{k-1}^{(m-1)} - (2m-2-k) a_k^{(m-1)}, \quad 1 < k < m. \end{aligned}$$

The values $t_k^{(j)}$ are calculated for the $j$-th sphere by the following formulas:

$$t_k^{(j)} = (k-1)!(-1)^{k-1} a^{-k} + d_j^k f_k, \quad k = 1, 2, \ldots.$$

$$\begin{aligned} &f_1 = -\operatorname{ch}(d_j a)/\operatorname{sh}(d_j a), && f_2 = f_1^2 - 1, \\ &f_3 = 2 f_1 f_2, && f_4 = 2(f_2^2 + f_1 f_3), \\ &f_5 = 2(3 f_2 f_3 + f_1 f_4), && f_6 = 2(3 f_3^2 + 4 f_2 f_4 + f_1 f_5), \\ &f_7 = 2(10 f_3 f_4 + 5 f_2 f_5 + f_1 f_6), && f_8 = 2(10 f_4^2 + 15 f_3 f_5 + 6 f_2 f_6 + f_1 f_7). \end{aligned}$$

At $c = 0$ we have

$$Q_\lambda^{(m)} = \sum_{k=1}^{m} b_k t_k Q_\lambda^{(m-k)} \frac{(m-1)!}{(k-1)!(m-k)!}, \quad Q_\lambda^{(0)} = Q,$$

where

$$b_k t_k = \sum_{j=0}^{i-1} \lim_{c \uparrow 0} [\ln s(c, d_j)]_\lambda^{(k)} = b_k \sum_{j=0}^{i-1} t_k^{(j)}, \quad t_k^{(j)} = d_j^{2k},$$

and the constant coefficients $b_k$ come out by using obvious recursion from the presentation which holds for sufficiently small values $c$

$$\begin{aligned} \ln \left[ \frac{d\sqrt{c}}{\operatorname{sh}(d\sqrt{c})} \right] &= -\ln \left( \sum_{k=0}^{\infty} \frac{d^{2k}}{(2k+1)!} c^k \right) \\ &= \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \left( \sum_{k=0}^{\infty} \frac{d^{2k}}{(2k+1)!} c^k \right)^p = \sum_{k=1}^{\infty} d^{2k} b_k (-c)^k / k!. \end{aligned}$$

Give ten coefficients $b_k$:

$$b_1 = 1.666666667 \cdot 10^{-1}, \qquad b_6 = 1.298642568 \cdot 10^{-4},$$
$$b_2 = 1.111111111 \cdot 10^{-2}, \qquad b_7 = 7.893341227 \cdot 10^{-5},$$
$$b_3 = 2.116402116 \cdot 10^{-3}, \qquad b_8 = 5.598081415 \cdot 10^{-5},$$
$$b_4 = 6.349206349 \cdot 10^{-4}, \qquad b_9 = 4.537581858 \cdot 10^{-5},$$
$$b_5 = 2.565335899 \cdot 10^{-4}, \qquad b_{10} = 4.137766635 \cdot 10^{-5}.$$

Now consider the results of numerical tests. New algorithms are utilized for computing the parametric derivatives $u_\lambda^{(k)}$ $(\lambda = -c)$ of a solution of the boundary value problem

$$\Delta u - cu = 0, \quad \text{in} \quad D = \{0 \le r_i \le 1, \;\; i = 1,2,3\},$$
$$\left.\frac{\partial u}{\partial n}\right|_{\Gamma_1} = 0, \quad u|_{\Gamma_2} = 1,$$

where

$$\Gamma_1 = \{r \in \partial D \mid r_1 = 0 \vee r_1 = 1\}, \quad \Gamma_2 = \partial D \setminus \Gamma_1.$$

Calculations are performed at the cube center $r = (0.5, 0.5, 0.5)$ for $c = 5$, $h = \varepsilon = 0.001$, the number of trajectories $N = 50\,000$ (Table 3).

Utilizing the estimates of the solution and its parametric derivatives at $c = 5$, the value of the solution was evaluated for other values of $c$ via the Taylor series to compare with the corresponding solution estimates, which had been obtained directly. The mean square error was evaluated by the following manner:

$$\sigma\Big(\sum_{i=1}^{m} \xi_i\Big) \le \sum_{i=1}^{m} \sigma(\xi_i) = \tilde{\sigma}.$$

The numerical results are included in Table 4. The estimates $y_N$ of the solution for various values of $c$ were obtained by formula (4) at $h = \varepsilon = 0.001$,

**Table 3.** Estimates of the parametric derivatives

| $u_h$ | $u'_h \cdot 10^3$ | $u''_h \cdot 10^4$ | $u'''_h \cdot 10^5$ |
|---|---|---|---|
| $0.7133 \pm 0.0005$ | $44.64 \pm 0.057$ | $40.32 \pm 0.151$ | $50.18 \pm 0.359$ |

**Table 4.** Estimates with using Taylor series at $c = 5$

| $c$ | $y_N \pm \sigma_N$ | $y_N^{(5)} \pm \sigma_N$ | $y_N^{(10)} \pm \sigma_N$ |
|---|---|---|---|
| 0 | $1.0000 \pm 0.0000$ | $0.9999 \pm 0.0011$ | $1.0000 \pm 0.0011$ |
| 10 | $0.5318 \pm 0.0007$ | $0.5317 \pm 0.0011$ | $0.5318 \pm 0.0011$ |
| 15 | $0.4091 \pm 0.0007$ | $0.4051 \pm 0.0032$ | $0.4091 \pm 0.0037$ |
| 20 | $0.3221 \pm 0.0006$ | $0.2826 \pm 0.0093$ | $0.3262 \pm 0.0215$ |

the number of trajectories $N = 50\,000$. Here $y_N^{(5)}$ is the solution estimate, obtained on basis of the Taylor series with five derivatives, and the estimate $y_N^{(10)}$ is obtained by the Taylor series with ten derivatives, respectively.

The results of the numerical tests demonstrate that estimates of the solution, which are received by the algorithm "walking on spheres" with reflection, is in good accordance with the estimate on the basis of the Taylor series.

In the second numerical test, relation (11) was numerically realized in the center of the cube

$$D = \{0 \le r_i \le 1, \; i = 1,2,3\} \subset R^3$$

for the family of the boundary value problems

$$\Delta u + \lambda u = 0, \quad \left.\frac{\partial u}{\partial n}\right|_{\Gamma_1} = 0, \quad u|_{\Gamma_2} = 0. \tag{12}$$

Here $\Gamma_1$ and $\Gamma_2$ are parts of the surface $\Gamma = \Gamma_1 \cup \Gamma_2$ of the cube $D$ which are constituted from the cube sides. The exact values $c^*$ for such kind of problems (12) are known, and some of them are put in Table 5.

**Table 5.** Exact values of $c^*$

| Problem # | Equations of sides constituted $\Gamma_1$ | $c^*$ |
|---|---|---|
| 1 | $r_1 = 0$ | $2.25\pi^2 \approx 22.207$ |
| 2 | $r_1 = 0, \quad r_1 = 1$ | $2\pi^2 \approx 19.739$ |
| 3 | $r_1 = 0, \quad r_2 = 0, \quad r_3 = 0$ | $0.75\pi^2 \approx 7.402$ |
| 4 | $r_1 = 0, \quad r_1 = 1, \quad r_2 = 0, \quad r_3 = 0$ | $0.5\pi^2 \approx 4.935$ |

For the considering family of the problems there are two parameters having an influence on computational costs of estimates: the values $c$ and $c_0$. Carrying out calculations the following behaviour has been remarked. Foremost, growth of $c$ implies considerable diminution of the estimate of the mean square error of the value $c^*$, but at the same time to reach adequate accuracy it has to calculate higher order derivatives. Secondly, for $c_0 > 0$ the computation time was diminished, but the statistic error of the estimate increased and precision became worse, so as the optimal parameter was chosen $c_0 = 0$. Thirdly, during employment of the algorithm of computation $c^*$, which corresponds to $c = 0$, it was noticed that test time was less twice approximately in compare with the algorithm for $c > 0$, but the variance was considerably greater, what did not give advantage in total.

In Tables 6, 7, 8, some results of computation of values $c^*$ are presented. Calculations are made in the cube center $\boldsymbol{r} = (0.5, 0.5, 0.5)$ at $h = \varepsilon = 0.001$. Here, as $c_{N,0}^{*(m)}$, $c_{N,10}^{*(m)}$ and $c_{N,20}^{*(m)}$ are denoted the Monte Carlo method estimates of the value $c^*$, obtains at $c = 0$, $c = 10$, and $c = 20$ correspondingly

**Table 6.** Estimates of the value $c^* \approx 19.739$ for Problem 2 ($c_0 = 0$, $N = 2\,500\,000$ at $c = 0$ and $N = 1\,000\,000$ at $c > 0$)

| $m$ | $c_{N,0}^{*(m)} \pm \sigma_{N,0}^{*(m)}$ | $c_{N,10}^{*(m)} \pm \sigma_{N,10}^{*(m)}$ | $c_{N,20}^{*(m)} \pm \sigma_{N,20}^{*(m)}$ |
|---|---|---|---|
| 3 | $19.34 \pm 0.006$ | $18.38 \pm 0.003$ | $16.77 \pm 0.002$ |
| 4 | $19.62 \pm 0.016$ | $19.32 \pm 0.007$ | $18.63 \pm 0.004$ |
| 5 | $19.64 \pm 0.038$ | $19.61 \pm 0.014$ | $19.34 \pm 0.007$ |
| 6 | $19.56 \pm 0.083$ | $19.69 \pm 0.025$ | $19.59 \pm 0.012$ |
| 7 | $19.45 \pm 0.17$ | $19.72 \pm 0.042$ | $19.68 \pm 0.019$ |
| 8 | $19.35 \pm 0.31$ | $19.71 \pm 0.070$ | $19.71 \pm 0.028$ |
| 9 | $19.31 \pm 0.53$ | $19.67 \pm 0.12$ | $19.72 \pm 0.042$ |
| 10 | $19.36 \pm 0.82$ | $19.59 \pm 0.19$ | $19.74 \pm 0.060$ |

**Table 7.** Estimate of the value $c^* \approx 7.402$ for Problem 3 ($N = 3 \cdot 10^5$, $c_0 = 0$ for $c = 15$, and $N = 10^6$, $c_0 = 0$ for $c = 10$).

| $m$ | $c_{N,10}^{*(m)} \pm \sigma_{N,10}^{*(m)}$ | $c_{N,15}^{*(m)} \pm \sigma_{N,15}^{*(m)}$ |
|---|---|---|
| 3 | $8.74 \pm 0.007$ | $9.21 \pm 0.007$ |
| 4 | $8.22 \pm 0.014$ | $8.80 \pm 0.012$ |
| 5 | $7.82 \pm 0.023$ | $8.26 \pm 0.020$ |
| 6 | $7.60 \pm 0.036$ | $7.89 \pm 0.034$ |
| 7 | $7.51 \pm 0.054$ | $7.68 \pm 0.054$ |
| 8 | $7.48 \pm 0.077$ | $7.57 \pm 0.084$ |
| 9 | $7.48 \pm 0.11$ | $7.52 \pm 0.13$ |
| 10 | $7.52 \pm 0.15$ | $7.49 \pm 0.19$ |

**Table 8.** Estimate of the value $c^* \approx 4.935$ for Problem 4 ($c_0 = 0$, $N = 300\,000$).

| $m$ | $c_{N,10}^{*(m)} \pm \sigma_{N,10}^{*(m)}$ |
|---|---|
| 3 | $5.580 \pm 0.006$ |
| 4 | $5.318 \pm 0.011$ |
| 5 | $5.127 \pm 0.017$ |
| 6 | $5.029 \pm 0.026$ |
| 7 | $4.982 \pm 0.036$ |
| 8 | $4.956 \pm 0.050$ |
| 9 | $4.939 \pm 0.067$ |
| 10 | $4.926 \pm 0.088$ |

on the basis of relations (10), (11). The statistical error of estimates $c_N^{*(m)}$ was calculated by the expression

$$\sigma_{N,c}^{*(m)} = \frac{m\left(u_{N,c}^{(m-1)}\sigma_{N,c}^{(m)} + u_{N,c}^{(m)}\sigma_{N,c}^{(m-1)}\right)}{u_{N,c}^{(m)}\left(u_{N,c}^{(m)} - \sigma_{N,c}^{(m)}\right)}, \tag{13}$$

where $u_{N,c}^{(m)}$ is the estimate of the $m$-th parametric derivative, $u_c^{(m)}$, $\sigma_{N,c}^{(m)}$ is respective mean square error. Formula (13) is obtained from consideration of confidence intervals for values of kind (10), (11).

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