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## ESTIMATING THE DERIVATIVES OF A SOLUTION TO THE ELLIPTIC BVP BY STATISTICAL MODELLING METHOD

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Differential problem. Let us consider the problem of estimating the solution and the solution gradient at an arbitrary point r for the following BVP:

$$\Delta u(r) - c(r)u(r) + (v(r), \nabla u(r)) = -g(r), \ r \in \Omega \subset \mathbb{R}^3$$
(1)

$$u(y) = \psi_1(y), \ y \in \Gamma_1, \ (\nabla u(y), \gamma(y)) + \alpha(y)u(y) = \psi_2(y), \ y \in \Gamma_2, \ \Gamma_1 \bigcup \Gamma_2 = \partial \Omega$$
(2)

Suppose that there exists the unique and smooth enough solution u to the problem (1)–(2). We suggest to reduce the initial differential problem (1) to the integral equation of the second kind U = KU + G for unknown function

$$U(\mathbf{w}) \equiv U(r, j) = \begin{cases} u(r), & j = 0; \\ R(r)u'_v(r)/3, & j = 1; \end{cases}$$

here  $\mathbf{w} = (r, j) \in \mathbb{R}^3 \times \{0, 1\}$  is a point of extended phase space,  $u'_v = (v/|v|, \nabla u)$  and function R(r) is the distance from the point r to the boundary. Equivalent integral equation. We offer to rewrite equation (1) isolating diffusion operator

 $\mathcal{D}_{\kappa} \equiv \Delta - \kappa^2$  (for some positive constant  $\kappa^2$ ) on the left-hand side:

$$\Delta u(r) - \kappa^2 u(r) = -\left(\kappa^2 - c(r)\right)u(r) - \left(v(r), \nabla u(r)\right) - g(r).$$

Integral equations for the function u(r) and its spatial derivative  $u'_v(r)$  can be obtained using the mean-value theorem. We suggest to use non-central Green's functions  $\mathcal{G}^{\kappa}_{r_0}(r,r')$  for the diffusion operator  $\mathcal{D}_{\kappa}$  in the ball  $B(r_0, R(r_0))$  which is the largest one centered at  $r_0$  and contained in  $\overline{\Omega}$ :

$$\mathcal{G}_{r_0}^{\kappa}(r,r') = \frac{1}{4\pi} \left[ \frac{\sinh\left\{\kappa(R-|V|)\right\}}{\sinh\left\{\kappa R\right\}|V|} - \frac{\sinh\left\{\kappa\left(R-|W|\right)\right\}}{\sinh\left\{\kappa R\right\}|W|} \right], \quad V = r' - r; \quad W = \varrho(r' - r_0) - \frac{r - r_0}{\varrho}.$$

here  $\rho = R(r)/|r' - r_0|$ . Let  $\Gamma_{\varepsilon}$  be the  $\varepsilon$ -strip of the boundary  $\Gamma$  and  $R_{\max} = \max_{r \in \Omega} R(r)$ . To construct statistical algorithms, integral equations for u(r) and  $u'_v(r)$  are combined below into a unified integro-algebraic equation with  $r_0 = r$ . We choose the parameter  $c_0$  such that  $c_0 R_{\max}^2 < 6$  and use the variable  $p(r) = (1 - c_0 R^2(r)/6)$  for randomization of the unified equation:

$$U(r,j) = p(r) \int_{S(r,R)} F_S(r,r')U(r',0)Q_{j0}(r,r')dS_{r'} + G(r,j) +$$
(3)  
+(1-p(r))  $\int_{B(r,R)} F_j(r,r') \left[ p_1^c Q_{j1}^c(r,r')U(r',1) + p_0^c Q_{j0}^c(r,r')U(r',0) \right] dr',$ 

here  $S(r,R) = \partial B(r,R)$ ,  $Q_{ij'}^{(c)}$  are weights,  $p_0^c = p_0^c(r,r')$  and  $p_1^c = 1 - p_0^c$  are some probabilities. Having the equation (3), we construct the Random Walk on Spheres and Balls Algorithm which enables us to estimate both the solution u(r) and its gradient. The statistical estimator  $\zeta(\mathbf{w}_0)$  for  $U(\mathbf{w}_0)$  is derived according to (3) by standard Monte Carlo procedure.

During the random walk on spheres and balls simulation, when the path falls into  $\Gamma_{\varepsilon}$  at a step with a random number N, the chain terminates and the estimator for  $U(\mathbf{w}_N)$  multiplied by the weight  $Q^N$  is added to the counter. As a result, the following estimator for  $U(\mathbf{w}_0)$  is obtained:

$$\zeta(\mathbf{w}_0) = \sum_{n=0}^{N-1} Q^n G(\mathbf{w}_n) + Q^N U(\mathbf{w}_N), \ Q^{n+1} = Q^n \cdot Q_{j_n j_{n+1}}^{(c)}, \ Q^0 = 1.$$

**Theorem 1.** If  $-c^*$  is the first eigenvalue of the Laplace operator in  $\Omega$  and for any  $r \in \Omega$  the following assumptions hold:  $|\kappa^2 - c(r)| + 3|v(r)|/R(r) \leq 2c_0/3$ ,  $c_0 < 6c^*/\pi^2 \simeq 0.6079c^*$ , then there exists a unique bounded solution to the equation (3) that admits a representation by a Neumann series and equals the solution to the BVP (1)-(2): U(r,0) = u(r),  $U(r,1) = R(r)u'_v(r)/3$ .

**Boundary condition.** Since the values of  $U(\mathbf{w})$  in  $\Gamma_{\varepsilon}$  are indeterminate, the corresponding estimators are obtained as follows. For  $j_N = 0$  and  $r \in \Gamma_{1\varepsilon}$  one can set  $U(r, 0) = \psi_1(r^*)$ , where  $r^* \in \Gamma_1$ ,  $|r - r^*| = R(r)$ . For  $r \in \Gamma_{2\varepsilon}$  the following representation holds:

$$U(r,0) = \frac{1 + \alpha \cdot d_{\gamma}(r)}{1 + \alpha \cdot (d_{\gamma}(r) + \varepsilon)} U(r - \varepsilon\gamma, 0) + \frac{\varepsilon}{1 + \alpha \cdot (d_{\gamma}(r) + \varepsilon)} \psi(\pi(r)) + \mathcal{O}(\varepsilon^2),$$

here  $d_{\gamma}(r)$  is the distance between r and  $\Gamma_2$  along the vector field  $\gamma$ , and  $\pi(r)$  is the projection of the point  $r \in \Gamma_{2\varepsilon}$  onto  $\Gamma_2$  along the vector field  $\gamma$ . According to the latter representation the algorithm with reflection should be applied. Assuming that the first derivatives of the solution are bounded in  $\Omega$ , and therefore  $R(r)u'_v(r) = \mathcal{O}(\varepsilon)$  for  $r \in \Gamma_{\varepsilon}$ , one can approximately set U(r, 1) = 0for  $j_N = 1$ . As a result, the realizable but biased estimator  $\zeta_{\varepsilon}(\mathbf{w}_0)$  is obtained for  $U(\mathbf{w}_0)$ .

**Theorem 2.** If the first derivatives of u(r) are bounded in  $\Omega$ , then there exists  $\mathbf{E}\zeta_{\varepsilon}(r,0) = u_{\varepsilon}(r)$  and  $|u(r) - u_{\varepsilon}(r)| = \mathcal{O}(\varepsilon), \ \varepsilon > 0, \ r \in \Omega$ . Moreover, there exists  $\mathbf{E}\zeta_{\varepsilon}(r,1) = f_{\varepsilon}(r)$  and  $|R(r)u'_{v}(r)/3 - f_{\varepsilon}(r)| = \mathcal{O}(\varepsilon), \ \varepsilon > 0, \ r \in \Omega$ .

Simulation of the probability densities in (3). The function  $F_S$  is the probability density of uniform distribution on the sphere:  $F_S(\varphi, \theta) dS = d\varphi \sin(\theta) d\theta/4\pi$ , here  $\theta \in (0, \pi)$ ,  $\varphi \in (0, 2\pi)$ ,  $\rho = |r' - r| \in (0, R)$  are coordinates of the local (with the origin at the point r) spherical coordinate system. The probability densities  $F_0$  and  $F_1$  are factorable in this coordinate system:  $F_j(r, r')dr' = F_S(\varphi, \theta) d\varphi d\theta \cdot F_j^{\rho}(\rho) d\rho$ , j = 0, 1; and the factors  $F_j^{\rho}(\rho)$  have the following form:

$$F_0^{\rho}(\rho) = \frac{6C_{01}^{-1}(\kappa R)}{R^2 \sinh{\{\kappa R\}}} \rho \sinh{\{\rho_{\kappa}\}}, \quad F_1^{\rho}(\rho) = \frac{4C_{11}^{-1}(\kappa R)}{R^2 \sinh{\{\kappa R\}}} \left[\kappa \rho \cosh{\{\rho_{\kappa}\}} + \sinh{\{\rho_{\kappa}\}} - \frac{\kappa \rho^3}{R^2}\right],$$

here  $\rho_{\kappa} \equiv \kappa(R - \rho)$ . We can use the von Neumann rejection method for sampling the probability density  $F_0^{\rho}(\rho)$ . A majorant function can be chosen in two ways:

$$g_0(\rho) \equiv \rho \sinh \{\rho_\kappa\} / \sinh \{\kappa R\} \leqslant \rho \exp(-\kappa \rho) \equiv g_1(\rho) \leqslant R \exp(-\kappa \rho) \equiv g_2(\rho).$$

If the function  $g_1$ , which is proportional to the gamma distribution with parameters  $(2, \kappa)$ , is also sampled by the rejection method (i. e. rejecting the values of  $\rho$  which is greater than R), then the ratio of the corresponding computational costs is the following:  $S_2/S_1 = \kappa R(1 - e^{-\kappa R})$ . Therefore, if  $S_2 < S_1$  (it holds when  $\kappa R < 1.35$ ) then we use the majorant function  $g_2$  or else we use  $g_1$ .

if  $S_2 < S_1$  (it holds when  $\kappa R < 1.35$ ) then we use the majorant function  $g_2$  or else we use  $g_1$ . For the probability density  $F_1^{\rho}(\rho)$  we have  $\kappa \rho \cosh\{\rho_{\kappa}\} + \sinh\{\rho_{\kappa}\} - \kappa \rho^3/R^2 \leq (\kappa R+1) \cosh\{\rho_{\kappa}\}$ . If  $\alpha$  is a uniform random variable on (0, 1) and variable  $\eta$  is the solution to the equation  $\sinh\{\kappa(R-\eta)\} = \alpha \sinh\{\kappa R\}$  then  $\eta$  has the probability density  $A_{\kappa,R} \cosh\{\rho_{\kappa}\}$  on (0, R).

The similar technique with Green's function for Laplace operator  $\Delta$  is described in [1].

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