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Two problems of the Monte Carlo method theory

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In this paper two nonsolved problems of the Monte Carlo theory are presented. The first of them concernes the uniform boundedness of the "walk on spheres" estimates for the Helmgoltz equation. Another problem is the important example from the minimax Monte Carlo theory for evaluating of many integrals.

1. "Walk on spheres" algorithms for solving Helmholtz equation

Let us consider a three-dimensional Dirichlet problem for the Helmholtz equation

$$\Delta u + cu = 0, \quad u|_{\Gamma} = \Psi \tag{1}$$

as a main problem in a domain $D \subset X_3$ with the boundary Γ, where $c < c^*$ and $-c^*$ is the first eigenvalue of the Laplacian operator for the domain D, $r = (x, y, z) \in D$.

The conditions for the function Ψ, and Γ to be regular are assumed to be fulfilled. These conditions guarantee the existence and uniqueness of the solution of problem (1), as well as its probabilistic representation and an integral representation with making use of the Green's function for a ball (see, e.g., [1]).

Estimates to be considered below are associated with the so-called "walk on spheres" process within the domain D [2]. To describe the process, let introduce the following notation: $\overline{D}$ is a closure of domain D; $d(P)$ is a distance from the point P to the boundary Γ; Γ_ε is an ε-neighbourhood of the boundary Γ, i.e.,

$$\Gamma_\varepsilon = \{P \in \overline{D} : \ d(P) < \varepsilon\};$$

$S(P)$ is the largest sphere of those centred at the point P and entirely lying in $\overline{D}$, i.e.,

$$S(P) = \{Q \in \overline{D} : \ |Q - P| = d(P)\}.$$

In the "walk on spheres" process, every next point r_{k+1} is chosen uniformly over the surface of the sphere $S(r_k)$; the process terminates when a point finds itself inside Γ_ε.

For $c = const < c_*$, the probabilistic representation of the solution of problem (1) has the form [3]

$$E[e^{c\tau}\Psi(\xi(\tau))],$$

where $\xi(t)$ is the diffusion process originating at the point r_0 and corresponding to the Laplacian operator, τ is the instant the process leaves the domain D for the first time. Proceeding from the process being strictly Markovian, we have

$$u(r_0) = E\Big[\Psi(\xi(\tau))\prod_{i=0}^{\infty} e^{c(\tau_{i+1}-\tau_i)}\Big],$$

where τ_i is the instant the process $\xi(t)$ for the first time arrives at the surface of the i-th sphere of the corresponding "walk on the sprheres" $\{r_n\}$, $n = 0, 1, \ldots, N$, and $r_N \in \Gamma_\varepsilon$.

Let us denote by P the point of the boundary Γ closest to r_N. Using the repeated averaging procedure and the integral representation of problem (1) at the ball centre, we can easily obtain [1] that

$$u(r_0) \approx u_\varepsilon(r_0) = E\eta_\varepsilon^{(0)},$$

where

$$\eta_\varepsilon^{(0)} = \Big[\prod_{j=0}^{N-1} s(c, d_j)\Big]\Psi(P).$$

Here $d_j = d(r_j)$ and

$$s(c,d) = \begin{cases} d\sqrt{c}/\sin(d\sqrt{c}), & c \geq 0, \\ d\sqrt{c}/\mathrm{sh}(d\sqrt{c}), & c \leq 0. \end{cases}$$

If the first derivatives of the solution are bounded in $\overline{D}$, then

$$|u(r) - u_\varepsilon(r)| \leq C\varepsilon, \qquad r \in D.$$

Now let us consider the question of uniform in ε boundedness of the variance $D\eta_\varepsilon$. The variance determines the mean-square error of the resultant Monte Carlo estimate obtained by averaging the realizations of η_ε. This question will be considered here for $c > 0$, as it is quite easy to solve for $c \leq 0$ with the integral representation method [1].

In this case

$$\eta_\varepsilon \le \eta = C_2\Big[\prod_{j=0}^{\infty} s(c, d_j)\Big]$$

and $E\eta < +\infty$ for $c < c^*$ by virtue of the probabilistic representation of the solution of problem (1), by analogy with the transition from this representation to $\eta_\varepsilon^{(0)}$.

Hence

$$E\eta_\varepsilon^2 \le C_2^2 E\Big[\prod_{j=0}^{\infty} s^2(c, d_j)\Big].$$

For $c > 0$ the following inequality holds [4]:

$$s^2(c/2, d) \le s(c, d)$$

with $d\sqrt{c} < \pi$. Hence the uniform in ε boundedness of the variance $D\eta_\varepsilon$ has been proved for $c < c^*/2$ at $g \equiv 0$.

On the other hand, the quantity $D\eta_\varepsilon$ should as a rule be unbounded for $c > c_0/2$, where c_0 is a solution to equation

$$s^2(c_0/2, d_{\max}) = s(c^*, d_{\max}),$$

since in this case $c_0 > c^*$, and

$$s^2(c, d) \ge s(c^*, d).$$

Moreover, here $D\eta_\varepsilon = +\infty$ for sufficiently small ε due to the above correspondence between the "walk on spheres" estimates, the diffusion-process estimates and the relation

$$c^*(D - \Gamma_\varepsilon) \to c^*(D), \quad \varepsilon \to 0.$$

Problem: *is it possible that $D\eta_\varepsilon < +\infty$ for $\varepsilon = 0$ if $c^*/2 < c < c_0/2$?*

2. Minimax estimates of the Monte Carlo method for evaluating many integrals

Monte Carlo estimates for integrals are constructed on the basis of the relations

$$I_k = \int_X f_k(x)dx = E\zeta_k, \quad \zeta_k = f_k(\xi)/p(\xi), \quad k = 1, 2, \ldots, n,$$

where $p(x)$ is the distribution density for ξ, and

$$D\zeta_k(p) = \int\limits_X \frac{f_k^2(x)dx}{p(x)} - I_k^2.$$

Let

$$F_\zeta(p) = \max_k\{D\zeta_k(p)\}.$$

We consider the following problems: find density $p = p^*(x)$ such that $\min_p F_\zeta(p) = F_\zeta(p^*)$ is attained. We formulate the known [5] relation between the minimax and the Bayes solutions in the form of the following statement.

Lemma 1. *Let $\xi_k(p)$ be random variables in a probabilistic model P of a class of admissible models, and let P_Λ be a model such that the minimum*

$$\min_P \sum_k \lambda_k D\xi_k(p) = G(\Lambda), \quad 0 \le \lambda_k < +\infty, \quad \Lambda = (\lambda_1, \dots, \lambda_n),$$

is attained, where $G(\Lambda) < \infty$ and $D\xi_k(P_\Lambda)$ is differentiable with respect to λ_i $(i, k = 1, \dots, n)$ for all Λ. Then $\min F_\xi(p)$ *is attained in P_{Λ_0}, where Λ_0 is the solution to the problem*

$$\max_\Lambda \left\{ \sum_{k=1}^n \lambda_k D\xi_k(P_\Lambda) : \ \sum_{k=1}^n \lambda_k = 1 \right\}.$$

The proof of the lemma consists in justifying the fact that the variances are equal on the support of the measure of Λ_0 and that the others do not exceed the value [6]. Then, the standard inequality [5] is applied.

Note that Lemma 1 cannot be directly derived from [5], where the set of solutions $\{P\}$ was assumed to be compact. Formally, it can be considered as a special case of the minimax theorem [5] because

$$\max_k D\xi_k = \max_\Lambda \left\{ \sum_{k=1}^n \lambda_k D\xi_k : \ \sum_k \lambda_k = 1, \ \lambda_k \ge 0 \right\}.$$

To obtain the required result, it is sufficient to invert the order of min and max. However, in the standard minimax theorem the set $\{P\}$ is also assumed to be compact; therefore, a simple proof of Lemma 1 is reasonable.

Note that the solution to the problem of optimization of estimates for integrals according to the criterion based on the weighted sum of variance is well-known and is given by the relations

$$\min_p \sum_{k=1}^n \lambda_k D\xi_k(p) = \sum_{k=1}^n \lambda_k D\xi_k(P_\Lambda) = G_n(\Lambda),$$

where

$$P_\Lambda(x) = c\left[\sum_{k=1}^{n} \lambda_k f_k^2(x)\right]^{1/2}, \qquad c^{-1} = \int \left[\sum_{k=1}^{n} \lambda_k f_k^2(x)\right]^{1/2} dx,$$

$$G_n(\Lambda) = \left\{ \int \left[\sum_{k=1}^{n} \lambda_k f_k^2(x)\right]^{1/2} dx \right\}^2 - \sum_{k=1}^{n} \lambda_k I_k^2.$$

Here the nature of the space X and of the integration measure is not important. However, we assume for simplicity that X is a finite-dimensional Euclidean space, and the integrals are taken with respect to the Lebesgue measure in X. Below, we consider the statements concerning the minimax of the variances of estimates of n integrals (see [6]).

Lemma 2. *Let*

$$P_0 = \int \sup_k |f_k(x)| dx < +\infty.$$

Then the optimal density is given by

$$p^*(x) = p_{\Lambda^*}(x),$$

where Λ^* is a maximum point for $G_n(\Lambda)$.

Consider also the case, where $f_\sigma = f(x,\sigma)$ depends continuously on σ, $\sigma \in [\sigma^{(1)}, \sigma^{(2)}]$. Introduce the following notation: Λ is a probabilistic measure on $[\sigma^{(1)}, \sigma^{(2)}]$, $\zeta_\sigma(p) = \zeta(p,\sigma)$

$$P_0 = \int \left[\sup_\sigma |f(x,\sigma)|\right] dx, \quad \varphi^2(x) = \inf_k \int f^2(x,\sigma)\Lambda_k^*(d\sigma),$$

where $\Lambda_k^* = (\lambda_1^*, \dots, \lambda_{k+1}^*)$ is the optimal (in the sense of Lemma 2) discrete measure for the set of values of σ coinciding with the $k+1$ nodes of the uniform network of $[\sigma^{(1)}, \sigma^{(2)}]$.

Lemma 3. *Let $P_0 < +\infty$, $|f(x,\sigma) f'_\sigma(x,\sigma)| \leq h(x)$,*

$$\int \frac{f^2(x,\sigma)}{\varphi(x)} dx < c_1 < +\infty, \quad \int \frac{h(x)}{\varphi(x)} dx < c_2 < +\infty.$$

Then,

$$p^*(x) = p(x,\Lambda^*) = c\left[\int f^2(x,\sigma)\Lambda^*(d\sigma)\right]^{1/2},$$

where Λ^* is a maximum point for

$$G(\Lambda) = \left\{ \int \left[\int f^2(x,\sigma)\Lambda(d\sigma) \right]^{1/2} dx \right\}^2 - \int I^2(\sigma)\Lambda(d\sigma).$$

Proof see in [6].

Consider a case [6] important for the minimax theory of the weight Monte Carlo algorithms

$$f(x,\sigma) = \sigma \exp(-\sigma x), \quad X = [0,+\infty), \quad 0 < \sigma_1 < \sigma_2 < \infty.$$

Calculations carried out for a large set of values of σ_1 and σ_2 show that the optimal density p^* coincides in this case with the density p_{12}^* obtained by changing the segment $[\sigma_1, \sigma_2]$ with the two-element set $\{\sigma_1, \sigma_2\}$, and has the form

$$p_{12}^*(x) = c\big[\lambda\sigma_1^2 \exp(-2\sigma_1 x) + (1-\lambda)\sigma_2^2 \exp(-2\sigma_2 x)\big]^{1/2},$$

where λ is determined from the condition

$$D\zeta(p_{12}^*, \sigma_1) = D\zeta(p_{12}^*, \sigma_2) = D_{12}^*(\sigma_1, \sigma_2), \quad 0 \le \lambda \le 1.$$

Calculations were used to verify the inequality

$$D\zeta(p_{12}^*, \sigma) \le D_{12}^*(\sigma_1, \sigma_2), \quad \sigma_1 \le \sigma \le \sigma_2.$$

According to the reamak to Lemma 1 this Lemma makes it possible for p_{12}^* to solve the minimax problem on the segment $[\sigma_1, \sigma_2]$. However, *we have no strict proof of the sought inequality.*

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