Monte Carlo solution for the Poisson equation on the base of spherical processes with shifted centres

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Abstract. We consider a class of spherical processes rapidly converging to the boundary (so called Decentred Random Walks on Spheres or spherical processes with shifted centres) in comparison with the standard walk on spheres. The aim is to compare costs of the corresponding Monte Carlo estimates for the Poisson equation. Generally, these costs depend on the cost of simulation of one trajectory and on the variance of the estimate. It can be proved that for the Laplace equation the limit variance of the estimation doesn't depend on the kind of spherical processes. Thus we have very effective estimator based on the decentred random walk on spheres. As for the Poisson equation, it can be shown that the variance is bounded by a constant independent of the kind of spherical processes (in standard form or with shifted centres). We use simulation for a simple model example to investigate variance behavior in more details.

Keywords: Poisson equation, Laplace operator, Monte Carlo solution, spherical process, random walk on spheres, rate of convergence

1 Introduction

Consider the Poisson equation

$$\begin{cases} \Delta u = -q \\ u|_{\Gamma} = \varphi \end{cases} \tag{1}$$

in the bounded domain $G \subset \mathbb{R}^m$ with regular boundary $\Gamma = \partial G$. Let $\varphi \in \mathbf{C}(\Gamma)$ and q satisfy Hölder condition on G.

Monte Carlo scheme of $u(x) = u_{\varphi,q}(x)$ estimation is constructed on the base of a Markov chain converging to the boundary.

Thus, cost of the Monte Carlo solution includes three components:
1) rate of convergence of the Markov chain to boundary;
2) cost of one step (simulation of the Markov chain and cost of calculation of the corresponding part of the estimate)
3) variance of the estimate.

Dagstuhl Seminar Proceedings 04401
Algorithms and Complexity for Continuous Problems
http://drops.dagstuhl.de/opus/volltexte/2005/139

The most known Markov chain used for solving problems related to the Laplace operator is the spherical process, or the Random Walk on Spheres process (RWS).

We construct the Monte Carlo solution on the base of so called spherical process with shifted centres (Decentred Random Walk on Spheres, DRWS), since this process converges to boundary very fast. The aim of this paper is to describe the corresponding estimate and to investigate its cost.

2 General construction of the estimate

Let $\{w_s, \mathbf{P}_x, \theta_s, \mathcal{F}_t = \sigma(w_s, s \le t)\}$ be the Wiener family, $\tau = \inf\{t \ge 0 : w_t \in \Gamma\}$.

Consider a sequence of increasing Markov moments $\{\tau_i\}_{i=0}^{\infty}$ with respect to filtration $\mathcal{F}_t$, $\tau_0 = 0$, $\tau_i \to \tau \quad \mathbf{P}_x$-a.s. Let each point $y \in G$ be corresponded to a domain $G_y \subset G$ with regular boundary. Suppose that the Markov moment τ_1 is the exit moment: $\tau_1 = \inf\{t \ge 0 : w_t \in \partial G_{\xi_0}\}$. Put $\tau_{n+1} = \tau_1(\theta_{\tau_n}) + \tau_n$, $\xi_n = w_{\tau_n}$, $\mathcal{F}_n = \sigma(\xi_0, \dots, \xi_n)$, and

$$F(y) = \frac{1}{2}\mathbf{E}_y \int\limits_0^{\tau_1} q(w_s)ds. \tag{2}$$

Denote $\xi_\infty = \lim\limits_{n\to\infty} \xi_n = w_\tau$, $\Gamma_\varepsilon = \{y \in \overline{G} : \mathrm{dist}(y, \Gamma) < \varepsilon\}$, and $\nu_\varepsilon = \min\{n : \xi_n \in \Gamma_\varepsilon\}$. Thus, $\xi_0, \xi_1, \xi_2, \dots$ is a Markov chain embedded into the Brownian motion and ν_ε is the number of its steps before hitting the ε-boundary Γ_ε.

It can be shown that the random variable

$$\widetilde{\zeta}_\varepsilon = \sum_{n=0}^{\nu_\varepsilon - 1} F(\xi_n) + u(\xi_{\nu_\varepsilon}) \tag{3}$$

is an unbiased estimate of $u(x)$. Denote $\xi^*_{\nu_\varepsilon} \in \Gamma$ the point of boundary nearest to ξ_{ν_ε}. Then

$$\zeta_\varepsilon = \sum_{n=0}^{\nu_\varepsilon - 1} F(\xi_n) + \varphi(\xi^*_{\nu_\varepsilon}) \tag{4}$$

is a $\omega(\varepsilon)$-biased estimate of $u(x)$, where $\omega(\varepsilon)$ is a modulus of continuity of the solution $u(x)$ of the problem (1). Its variance $\mathbf{D}_x\zeta_\varepsilon$ is bounded by constant not depending on choice of the sequence of Markov moments $\{\tau_i\}_{i=0}^{\infty}$.

Moreover, for the Laplace equation with $q \equiv 0$ the asymptotic by $\varepsilon \to 0$ variance is the same for any sequence of Markov moments and equal to $\mathbf{D}_x\varphi(w_\tau) = \mathbf{D}_x\varphi(\xi_\infty)$.

3 Markov chains for estimate construction and their rates of convergence

Consider two kinds of Markov chains embedded to the Brownian motion. Since the corresponding Markov moments are moments of exits on some spheres, these processes can be called spherical processes or random walks on spheres. The question under interest is their rate of convergence to the boundary Γ.

The standard spherical process (RWS) corresponds to the case when $G_y \in G$ is the sphere with center at the point y and maximal radius.

As for the *spherical process with shifted centres* (DRWS), the center y' of the sphere G_y is $k = k(y) \geq 1$ times shifted inside away from the boundary (for the formal description see [5, 6]). Radius of the shifted sphere is equal to $k(y)d(y)$, where $d(y) = \mathrm{dist}(y, \Gamma)$. Note that the spherical process with shifted centres coincides with the standard spherical process for $k \equiv 1$.

Let's consider their rates of convergence.

Define $f(\varepsilon) = \sup\limits_{x \in G} \mathbf{E}_x \nu_\varepsilon$. Rate of convergence is determined by behaviour of $f(\varepsilon)$ in ε as $\varepsilon \to 0$.

It is well known (e.g. see [1, 2]) that for the spherical process ($k \equiv 1$) the inequality

$$f(\varepsilon) \leq C_1 |\ln \varepsilon| + C_2 \tag{5}$$

is valid for different kinds of G.

If we take a bounded shift function $k(x) \geq 1$, then the order of the upper bound is the same, but the constant before the logarithm will be asymptotically in k smaller [4].

The idea is arose to take the shift function as large as possible.

Let any point of the boundary Γ can be touched by the ball with radius $R > 0$, inside and outside. In addition, suppose that the balls touching the boundary inside lie in $\overline{G}$. We call such domains G *R-regular.*

Let us take

$$k(y) = \max(R/d(y), 1). \tag{6}$$

This shift function is infinite as $d(y) \to 0$ ($y \to \Gamma$). The corresponding spherical process is called *R-spherical with shifted centres* and reduced (near the boundary) to a random walk on shifted spheres with the same radius R. (Note that the case $R = 0$ formally corresponds to the standard spherical process (RWS).)

For such a shift function we obtain the much better rate of convergence.

Theorem 1 ([6, Th.3.1]). *The inequality*

$$f(\varepsilon) \leq C_1 \ln |\ln \varepsilon| + C_2 \tag{7}$$

holds for R-spherical family with shifted centres in R-regular domain G.

4 Variance of the estimate based on R-spherical processes

Now turn back to variance investigation. Unfortunately, $F(y)$ in (3) and (4) can not be calculated directly. Therefore, we should suggest an unbiased estimator of $F(y)$ and then to consider variance of the final realizable estimate. Let the ξ_n be a R-spherical process with the shift function (6).

It is known that F can be expressed through integral of a Green function g for the corresponding domain:

$$F(y) = \int\limits_{G_y} g(y, z)q(z)dz,$$

where G_y is the $k(y)$-shifted ball with centre y'. If $d(y) < R$, then radius of the ball G_y is equal to R and

$$g(y, z) = \frac{1}{\sigma_m} \left(\frac{1}{|y - z|^{m-2}} - \left(\frac{R}{|y - y'|} \frac{1}{|y^* - z|} \right)^{m-2} \right),$$

where

$$y^* = y' + \frac{R}{|y - y'|^2}(y - y')$$

and σ_m is the area of a sphere with unit radius in $\mathbb{R}^m$. If $d(y) \geq R$, then

$$g(y, z) = \frac{1}{\sigma_m} \left(\frac{1}{|y - z|^{m-2}} - \frac{1}{d^{m-2}(y)} \right).$$

Let us take an unbiased estimate of $F(y)$ instead of its exact value. Define $a(y) = (R^2 - |y - y'|^2)/2m$ for $d(y) < R$ and $a(y) = d^2(y)/2m$ for $d(y) \geq R$. Let the random variable λ_n has the distribution density $\pi(y, z) = g(y, z)/a(y)$ under the condition $\xi_n = y$. It can be shown that

$$\zeta^\varepsilon = \sum_{n=0}^{\nu_\varepsilon - 1} a(\xi_n)q(\lambda_n) + \varphi(\xi^*_{\nu_\varepsilon}), \tag{8}$$

is a realizable $\omega(\varepsilon)$-biased estimate of $u(x)$.

Denote

$$\zeta^\infty = \sum_{n=0}^{\infty} a(\xi_n)q(\lambda_n) + \varphi(\xi_\infty). \tag{9}$$

The following proposition can be proved analogously to [3, Th. 2.5.1].

Proposition 1. *Under the conditions of Theorem 1 variance of the estimate* ζ^ε *is bounded by a constant not depending on choice of admissible* R *in (6):*

$$\mathbf{D}_x\zeta^\varepsilon \leq \mathbf{D}_x\zeta^\infty + O(\omega(\varepsilon)),$$

where

$$\mathbf{D}_x\zeta^\infty \leq u_{\varphi^2,0}(x) + ||a||\, u_{0,q^2}(x) + 2||u_{\varphi,q}||\, u_{0,q}(x) - u^2_{\varphi,q}.$$

Let's decompose the estimates (8) and (9): $\zeta^\varepsilon = \zeta_1^\varepsilon + \zeta_2^\varepsilon$ and correspondingly $\zeta^\infty = \zeta_1^\infty + \zeta_2^\infty$. Here ζ_1^ε (and ζ_1^∞) is an estimate of the solution of (1) with $\varphi \equiv 0$ and ζ_2^ε (and ζ_2^∞) is an estimate of the solution of (1) with $q \equiv 0$. Denote $\mathbf{D}\zeta_1^\infty = \mathrm{VAR_q}(R)$, $\mathbf{D}\zeta_2^\infty = \mathrm{VAR}_\varphi(R)$ and the resultant variance $\mathbf{D}\zeta^\infty = \mathrm{VAR}(R)$.

Evidently, for the Laplace equation with $q \equiv 0$ the asymptotic by $\varepsilon \to 0$ variance $\mathrm{VAR}_\varphi(R)$ is the same for any admissible value of R and equal to $\mathbf{D}_x \varphi(\xi_\infty) = u_{\varphi^2,0} - u_{\varphi,0}^2$.

For the case $q \neq 0$ the situation is not so evident. Numerical experiments show that variance for some $R > 0$ can be either smaller or bigger than one for RWS (i.e. $R = 0$). Moreover, $\mathrm{VAR_q}(R)$ can be bigger and the resultant variance $\mathrm{VAR}(R)$ can be smaller because of different correlations between ζ_1^ε and ζ_2^ε (ζ_1^∞ and ζ_2^∞) for different values of R.

5 Cost of simulation for *R*-spherical processes

Consider the three-dimensional case ($m = 3$).

We should compare costs of simulation of random variables entering to the estimation formula (8), i.e., distributions on the (de)centred sphere ($\xi_{n+1} \sim p(y,z)$) and in the (de)centred ball ($\lambda_n \sim \pi(y,z)$) under the condition $\xi_n = y$. Certainly, these costs depend on the way of simulation. Therefore, we consider only one of possible variants.

For the Random Walk on Spheres process ($R = 0$), the exit point of the Wiener process has uniform distribution on the centred sphere, i.e., $p(y,z) = 1$ in respect to the uniform distribution on the sphere. Therefore, we can simulate the uniform distribution on a diameter of the sphere and then the uniform distribution on the corresponding circle. To obtain realization of λ_n in the centred ball, we can simulate radius value with density $6\sigma(d(y) - \sigma)/d^3(y)$ and then the uniform distribution on the sphere with the obtained radius.

For Decentred Random Walk on Spheres process ($R > 0$), the exit point of the Wiener process from the decentred sphere has density

$$p(y,z) = \frac{k(y)(2k(y)-1)d^3(y)}{|z-y|^3} \tag{10}$$

with respect to the uniform distribution on the sphere with $k(y)$-shifted centre y', where $k(y)$ is the shift coefficient, $d(y) = \mathrm{dist}(y, \Gamma)$. Therefore, we can simulate the distribution with density

$$\frac{1}{2d(y)} \frac{2k(y)-1}{(1 + 2(k(y)-1)v/d(y))^{3/2}}$$

on the diameter that contains y and then simulate the uniform distribution on the corresponding circle.

Simulation of the distribution with density π in the decentred ball of radius R is more complicated. Let $d(y) < R$ (otherwise the ball is centred and this case is described above).

Let us introduce new coordinates for z: $\omega = |y - z|$, $\sigma = |y' - z|$, θ denotes the angle between some fixed plane containing the axe (y, y') and the plane containing points y, y', z ($g(y, z)$ doesn't depend on θ). In new coordinates (θ, σ, ω), $\sigma \in [0, R]$, $\omega \in [|r - \sigma|, r + \sigma]$, $\theta \in [0, 2\pi)$, where $r = ||y - y'||$, we have

$$\pi(y, (\theta, \sigma, \omega)) = \left(\frac{1}{2\pi}\right) \times \left(\frac{6\sigma}{r(R^2 - r^2)} \left(\min(r, \sigma) - \sigma r/R\right)\right) \times$$

$$\times \left(\left(2(\min(r, \sigma) - \sigma r/R)\right)^{-1} \left(1 - \left(1 + \frac{R^2 - r^2}{\omega^2}\left(1 - \frac{\sigma^2}{R^2}\right)\right)^{-\frac{1}{2}}\right)\right) =$$

$$= \pi_1(\theta) \times \pi_2(\sigma) \times \pi_3(\omega|\sigma).$$

The distribution with density $\pi_1(\theta)$ is uniform on $[0, 2\pi)$. Two other density can be simulated by the rejection method with appropriate constants, for example.

Thus, simulation of the corresponding random variables for DRWS has more cost in comparison with RWS. However, the difference isn't too big.

6 Numerical results

6.1 Comparison by convergence rate

Consider the Poisson equation (1), where $G \in \mathbb{R}^3$ is the sphere with centre at $(0, 0.2, 0)$ and unit radius, $q(y) = 20||y||^2$, $\varphi(y) = (1 - ||y||^4) \mid_\Gamma$. Then the solution is $u(x) = 1 - ||x||^4$.

We take 1000000 realizations, $x = (0, 0.8, 0)$. Then consider the standard spherical process (RWS) and R-spherical processes with $R = 0.5$ and $R = 1$. Evidently, the case $R = 1$ corresponds to just one step before hitting the boundary of the chosen G due to its spherical shape.

To illustrate the advantage of R-spherical process with shifted centres from the viewpoint of convergence rate, Fig. 1 is represented. The figure shows that the RWS process needs to do approximately 60 steps before hitting 10^{-9}-boundary whereas the R-spherical process with $R = 0.5$ needs just 6 steps.

6.2 Comparison by simulation cost

It follows from Sect. 5 that simulation of one step of the R-spherical process is generally more complex in comparison with RWS; this difference is constant and doesn't depend on ε. Fast convergence of the R-spherical process to the boundary overcomes this shortcoming as $\varepsilon \to 0$. For the given realization (not optimal) of the simulation procedure the time for simulation of one trajectory of R-spherical process with $R = 0.5$ becomes smaller for $\varepsilon \leq 10^{-3}$.

It should be mentioned that additional difficulties can be caused by the form of the domain G, since we need to know value of R such that G is R-regular. As for the example under consideration this problem is trivial.

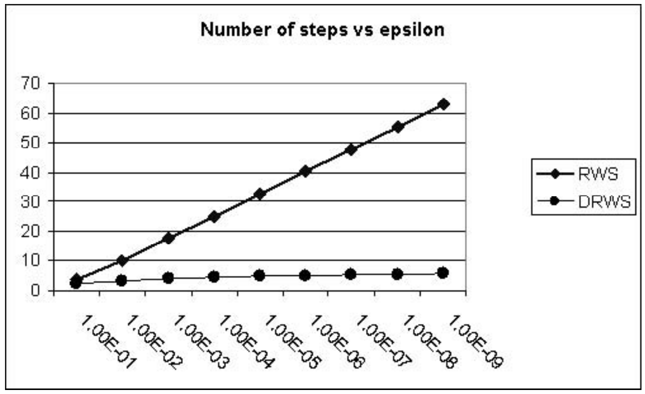

Fig. 1. Rates of convergence for RWS and DRWS

6.3 Comparison by variance

Unfortunately, there are no theoretical results for dependence on R of variances of estimates based on R-spherical processes except the facts formulated in Sect. 4.

Numerical results for the considered example are represented in Table 1. Indeed, the estimate of VAR_φ doesn't depend on kind of the process and equal to 3.8. For this example, the bigger R is the smaller $\mathrm{VAR}_q(R)$ (for several other examples with positive functions q the dependence $\mathrm{VAR}_q(R)$ of R is the same; however, for q changing its sign on G this dependence isn't confirmed).

Table 1. Estimates of variance

	$R = 0$ (RWS)	$R = 0.5$	$R = 1$
VAR_q	2.6	2.1	1.1
VAR_φ	3.8	3.8	3.8
VAR	2.3	2.0	4.9

The smallest value of $\mathrm{VAR}_q(R)$ is reached at $R = 1$. Recall that for the considered example the case $R = 1$ corresponds to just one step of the Markov chain before hitting the boundary; therefore ζ_1^ε and ζ_2^ε are uncorrelated and the resultant variance VAR of ζ^ε is equal to sum of VAR_q and VAR_φ. On the other side, for $R < 1$ the random variables ζ_1^ε and ζ_2^ε (ζ_1^∞ and ζ_2^∞) have positive correlation and the resultant variance VAR(1) is biggest.

7 Conclusions

Thus, theoretical results confirm that for small ε the estimate of the solution of the Poisson equation (1) based on the R-spherical process with shifted centres is better in comparison with the conventional Monte Carlo estimate.

Smallness of the threshold depends on efficiency of simulation procedures and also on functions q and φ. Numerical experiments show that there are no clear results related to dependence on R of the variance of the estimate based on the R-spherical process with shifted centres. Still there is a chance to obtain the result under some limitations on q and φ.

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