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Exact Monte Carlo Solution of Elliptic Partial Differential Equations *

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A continuous random walk procedure is developed for solving some elliptic partial differential equations with constant coefficients. The Monte Carlo method described here is exact (except possibly at the boundary) in the sense that the only error involved is the inherent statistical sampling error, that tends to zero as the sample size increases.

INTRODUCTION

Elliptic partial differential equations are commonly solved by making a finite-difference approximation for the derivatives, resulting in a system of linear equations to solve. It is well known [1, p. 483; 2] that these finite-difference equations can be solved by Monte Carlo techniques. However, there are two errors introduced in solving elliptic partial differential equations in this manner. First, there is the statistical sampling error inherent in any Monte Carlo calculation and second, there is the error introduced by the finite-difference approximation. Haji-Sheikh [3] showed that Laplace's equation could be solved directly by Monte Carlo, without first introducing a finite-difference approximation; that is, the solves the *differential* equation rather than the finite-difference equations. The only error made in the interior is the inherent statistical sampling error, that tends to zero as the sample size increases.

Following Haji-Sheikh, I show how to solve some partial differential equations of the form:

$$u_{xx} + u_{yy} - \lambda u = 0, \qquad \lambda \text{ constant.} \tag{1}$$

This is an important class of partial differential equations because *any* elliptic partial differential equation with constant coefficients can be reduced, by suitable transformations [1, p. 75], to the canonical form of Eq. (1).

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DIRICHLET PROBLEM

We shall consider solving Eq. (1), with u specified on the boundary, by Monte Carlo. Equation (1) can be rewritten in polar coordinates as [4]

$$u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} - \lambda u = 0. \tag{2}$$

Separating variables,

$$u(r, \theta) = R(r)\, \Theta(\theta), \tag{3}$$

results in two ordinary differential equations (separation constant β^2),

$$r^2 \frac{R''(r)}{R(r)} + \frac{rR'(r)}{R(r)} - \lambda r^2 = \beta^2, \tag{4}$$

$$\Theta''(\theta) + \beta^2 \Theta(\theta) = 0. \tag{5}$$

The angular equation has solutions

$$\Theta(\theta) = a_\beta \cos \beta\theta + b_\beta \sin \beta\theta, \tag{6}$$

where a_β and b_β are independent of θ. Requiring $\Theta(\theta)$ to be periodic in 2π, so that $u(r, \theta)$ be single valued, results in

$$\beta = n = \text{integer}. \tag{7}$$

Thus the radial equation becomes

$$R''(r) + \frac{1}{r} R'(r) + \left(-\lambda - \frac{n^2}{r^2}\right) R(r) = 0. \tag{8}$$

This is Bessel's equation with solutions $I_n(\lambda^{1/2}r)$ and $K_n(\lambda^{1/2}r)$. We require $u(r, \theta)$ to be finite when r is zero, so we must throw out the K_n solution because of a singularity at zero. Thus the solution to Eq. (2) is

$$u(r, \theta) = a_0 I_0(\alpha r) + \sum_{n=1}^{\infty} I_n(\alpha r)(a_n \cos n\theta + b_n \sin n\theta). \tag{9}$$

where

$$\alpha = \lambda^{1/2}. \tag{10}$$

Integrating Eq. (9) over θ results in

$$\int_0^{2\pi} u(r, \theta)\, d\theta = 2\pi a_0 I_0(\alpha r). \tag{11}$$

Note that $u(0, \theta) = u(0)$ is independent of θ if u is to be single valued at r equal to zero. Setting r to zero in Eq. (11) and noting $I_0(0) = 1$ results in

$$a_0 = u(0). \tag{12}$$

Substituting Eq. (12) into Eq. (11) yields

$$u(0) = \frac{1}{I_0(\alpha r)} \frac{1}{2\pi} \int_0^{2\pi} u(r, \theta)\, d\theta, \tag{13}$$

or, changing variables to $\gamma = i\alpha$ (for $\lambda < 0$)

$$u(0) = \frac{1}{J_0(\gamma r)} \frac{1}{2\pi} \int_0^{2\pi} u(r, \theta)\, d\theta. \tag{14}$$

Inspecting Eq. (13) we see that u at the center of a circle of radius r is the average value of u on the circle multiplied by a factor $1/I_0(\alpha r)$, depending only on the radius of the circle. Thus u at the center of a circle can be computed by randomly sampling $u/I_0(\alpha r)$ on the circle. In Monte Carlo parlance, we let a particle take a random jump to any point $P(\theta)$ on the circle, multiply the particle's statistical weight by $w = 1/I_0(\alpha r)$, and $wu(P(\theta))$ becomes one particle's estimate of $u(0)$. Averaging over a large number of one-particle estimates will give an accurate value for $u(0)$.

We shall now see how a more general boundary value problem can be solved with Monte Carlo, first intuitively and then more formally. Consider the closed and connected region D shown in Fig. 1 (u—specified on boundary ∂D, $u_{xx} + u_{yy} - \lambda u = 0$ in D). Suppose that we wish the solution of Eq. (1) at a point P_0 and suppose that u is specified on the boundary ∂D. To estimate $u(P_0)$, a point P_1 is sampled uniformly on the largest circle C_0 (centered on P_0, radius r_0) lying entirely within D, $u(P_1)/I_0(\alpha r_0)$ is then one particle's estimate of $u(P_0)$. If P_1 lies "on" (within some small ε of) ∂D, then $u(P_1)$ is known and $u(P_1)/I_0(\alpha r_0)$ is taken as one particle's estimate of $u(P_0)$. However, in general P_1 will not lie on ∂D, so that $u(P_1)$ is not known; in this case, $u(P_1)$ is estimated in the same fashion as $u(P_0)$. That is, a point P_2 is sampled uniformly on the largest circle C_1 (centered on P_1, radius r_1) lying within D; $u(P_2)/I_0(\alpha r_1)$ is then an estimate of $u(P_1)$ and hence, $u(P_2)/(I_0(\alpha r_0)\, I_0(\alpha r_1))$ is an estimate of $u(P_0)$. If P_2 lies "on" ∂D, then $u(P_2)$ is known and $u(P_2)/(I_0(\alpha r_0) I_0(\alpha r_1))$ is one particle's estimate of $u(P_0)$. If P_2 does not lie "on" ∂D,

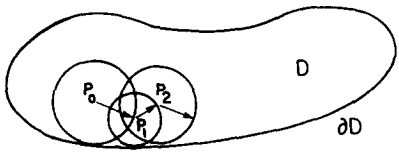


FIGURE 1

this procedure is repeated until the walk terminates "on" the boundary at the nth step, whereupon

$$u(P_n)/(I_0(ar_0)\cdots I_0(ar_n)) \tag{15}$$

is taken as one particle's estimate of $u(P_0)$.

Now let us consider this boundary value problem in a more formal manner. We define a small parameter $\varepsilon > 0$ such that if P is a point within ε of the closest boundary point P^*, then we take $u(P) = u(P^*)$.[1] Thus using Eq. (13) yields

$$u(P_n) = H(\varepsilon - r_n)u(P_n^*) + \frac{\bar{H}(r_n - \varepsilon)}{I_0(ar_n)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_n u(P_{n+1}), \tag{16}$$

where

$$\begin{aligned} H(x) &= 0, \quad \text{if} \quad x < 0, \\ &= 1, \quad \text{if} \quad x \geqslant 0, \\ \bar{H}(x) &= 0, \quad \text{if} \quad x \leqslant 0, \\ &= 1, \quad \text{if} \quad x > 0, \\ P_n &= (x_n, y_n), \\ P_{n+1} &= (x_n + r_n\cos\theta_n, y_n + r_n\sin\theta_n), \\ &= r_n(x_n, y_n) = \text{distance to closest boundary point.} \end{aligned}$$

Writing Eq. (16) for point P_0 yields

$$u(P_0) = H(\varepsilon - r_0)u(P_0^*) + \frac{\bar{H}(r_0 - \varepsilon)}{I_0(ar_0)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_0 u(P_1), \tag{17}$$

and substituting Eq. (16) for $u(P_1)$ into Eq. (17) yields

$$\begin{aligned} u(P_0) = H(\varepsilon - r_0)u(P_0^*) &+ \frac{\bar{H}(r_0 - \varepsilon)}{I_0(ar_0)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_0 \\ &\times \left[H(\varepsilon - r_1)u(P_1^*) + \frac{\bar{H}(r_1 - \varepsilon)}{I_0(ar_1)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_1 u(P_2)\right], \end{aligned} \tag{18}$$

and substituting Eq. (16) for $u(P_2)$ into Eq. (18) yields

$$\begin{aligned} u(P_0) = H(\varepsilon - r_0)u(P_0^*) &+ \frac{\bar{H}(r_0 - \varepsilon)}{I_0(ar_0)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_0 \\ &\times \left[H(\varepsilon - r_1)u(P_1^*) + \frac{\bar{H}(r_1 - \varepsilon)}{I_0(ar_1)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_1 \right. \\ &\times \left.\left\{H(\varepsilon - r_2)u(P_2^*) + \frac{\bar{H}(r_2 - \varepsilon)}{I_0(ar_2)}\frac{1}{2\pi}\int_0^{2\pi} d\theta_2 u(P_3)\right\}\right]. \end{aligned} \tag{19}$$

[1] This means that this method is not exact at the boundary, but only in the interior.

Repetitively substituting yields

$$u(P_0) = H(\varepsilon - r_0)u(P_0^*) + \sum_{n=1}^{\infty} \frac{\bar{H}(r_0-\varepsilon)}{I_0(\alpha r_0)} \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 \frac{\bar{H}(r_1-\varepsilon)}{I_0(\alpha r_1)} \frac{1}{2\pi}\int_0^{2\pi} d\theta_1 \frac{\bar{H}(r_2-\varepsilon)}{I_0(\alpha r_2)} \cdots \frac{1}{2\pi}\int_0^{2\pi} d\theta_{n-2} \frac{\bar{H}(r_{n-1}-\varepsilon)}{I_0(\alpha r_{n-1})} \frac{1}{2\pi}\int_0^{2\pi} d\theta_{n-1} H(\varepsilon - r_n)u(P_n^*), \quad (20)$$

provided the sum converges, a question treated later.

Now let us investigate the random walk procedure described earlier. The probability, $p(P_n \to P_{n+1})dP_{n+1}$ of going from P_n to dP_{n+1} about P_{n+1} (see Fig. 2) is

$$p(P_n \to P_{n+1})dP_{n+1} = \bar{H}(r_n - \varepsilon)\frac{d\theta_n}{2\pi}; \quad (21)$$

and the probability of terminating at the nth step is $H(\varepsilon - r_n)$. Thus the probability of the walk P_0, P_1, in dP_1, P_2 in dP_2,..., P_n in dP_n, p_n^* in dP_n^* is

$$\bar{H}(r_0-\varepsilon)\frac{d\theta_0}{2\pi}\bar{H}(r_1-\varepsilon)\frac{d\theta_1}{2\pi}\cdots\bar{H}(r_{n-1}-\varepsilon)\frac{d\theta_{n-1}}{2\pi}H(\varepsilon - r_n). \quad (22)$$

The weight multiplier at the nth step is $1/I_0(\alpha r_n)$ if the particle does not hit the boundary, and one if the particle hits the boundary. Thus the particle's score upon hitting the boundary, for the given walk, is

$$[I_0(\alpha r_0)I_0(\alpha r_1)\cdots I_0(\alpha r_{n-1})]^{-1}u(P_n^*). \quad (23)$$

The mth moment of the score, S_m, generated by a particle at P_0 is the integral, over all possible random walks, of the walk's probability multiplied by the mth power of the walk's score. Thus

$$S_m = H(\varepsilon - r_0)[u(P_0^*)]^m + \sum_{n=1}^{\infty}\int_0^{2\pi} d\theta_0\int_0^{2\pi} d\theta_1\cdots\int_0^{2\pi} d\theta_{n-1} \times\left[\frac{\bar{H}(r_0-\varepsilon)}{2\pi}\frac{\bar{H}(r_1-\varepsilon)}{2\pi}\cdots\frac{\bar{H}(r_{n-1}-\varepsilon)}{2\mu}H(\varepsilon - r_n)\right] \times[\{I_0(\alpha r_0)I_0(\alpha r_1)\cdots I_0(\alpha r_{n-1})\}^{-1}u(P_n^*)]^m, \quad (24)$$

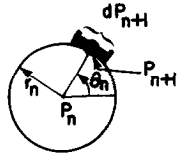


FIGURE 2

where the first term is all random walks of zero steps and the rest of the terms are random walks of n steps. Comparing Eq. (24) with Eq. (20) yields (for $m = 1$)

$$\text{Mean Score} = u(P_0). \tag{25}$$

It is sufficient, though not necessary, that $\lambda \geqslant 0$ (α real) for the sum in Eq. (24) to converge. To see this note that $r_k > \varepsilon$ for all $k < n$, thus $0 < I_0^{-1}(\alpha r_k) < I_0^{-1}(\alpha\varepsilon) \equiv \eta < 1$ because $I_0(x)$ is a positive increasing function of $|x|$ with a minimum value of 1. If $|u(P_n^*)| < M$ for all P_n^* on ∂D then the sum converges absolutely because it is bounded by

$$M^m \sum_{n=1}^{\infty} (\eta^m)^n$$

which converges because $\eta < 1$. For $\lambda < 0$, α is imaginary and the I_0 function becomes J_0. The convergence conditions for $\lambda < 0$ have not been determined; there are cases where the sum converges and where it does not. The case for λ complex has not been studied.

Inhomogeneous Dirichlet Problem

Consider Eq. (2) with a constant source term q, that is,

$$u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta} - \lambda u = q. \tag{26}$$

An obvious particular solution to Eq. (26), for $\lambda \neq 0$ is

$$u_p = -q/\lambda \tag{27}$$

so that the general solution of Eq. (26) is, taking the homogeneous solution from Eq. (9), (recall $\alpha = \lambda^{1/2}$)

$$u(r, \theta) = a_0 I_0(\alpha r) + \sum_{n=1}^{\infty} I_n(\alpha r)(a_n \cos n\theta + b_n \sin n\theta) - q/\lambda. \tag{28}$$

Integrating Eq. (28) over θ results in

$$\int_0^{2\pi} u(r, \theta)\, d\theta = 2\pi a_0 I_0(\alpha r) - 2\pi q/\lambda. \tag{29}$$

Note that $u(0, \theta) = u(0)$ is independent of θ if u is to be single valued when r is zero. Setting r to zero in Eq. (29), and noting $I_0(0) = 1$ results in

$$a_0 = u(0) + q/\lambda. \tag{30}$$

Substituting Eq. (30) into Eq. (29) yields (for $\lambda \neq 0$)

$$u(0) = \frac{1}{I_0(\alpha r)} \frac{1}{2\pi} \int_0^{2\pi} u(r, \theta)\, d\theta + Q(r), \tag{31}$$

where

$$Q(r) = -(1 - 1/I_0(\alpha r))q/\lambda. \tag{32}$$

Thus u, at the center of a circle of radius r, is equal to $Q(r)$, plus the average of $u(r, \theta)/I_0(\alpha r)$ on the circle. The only modification to the previous random walk procedure is that the particle now scores its weight times $Q(r)$ at each step, in addition to scoring when the particle reaches the boundary. In other words, the integral of Eq. (31) is estimated by random sampling, as before, and an additional term, $Q(r)$, is added.

We now discuss the case when $\lambda = 0$ in Eq. (26), that is, Poisson's equation. For this case a particular solution of Eq. (26) is

$$u_p = +qr^2/4, \tag{33}$$

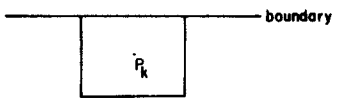
and following the procedure in the preceding paragraph we obtain, for $\lambda = 0$ (note that Eq. (34) is the limit as $\lambda \to 0$ of Eq. (31))

$$u(0) = \frac{1}{2\pi} \int_0^{2\pi} u(r, \theta)\, d\theta - qr^2/4. \tag{34}$$

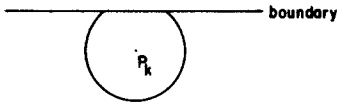
Haji-Sheikh also treats this case.

Comments on Boundary Treatment

As noted earlier, the method is exact in the interior but approximate at the boundary because random walking on circles only allows the particle to get arbitrarily close to the boundary, instead of actually landing on the boundary. A circle was chosen only because the Green's function for the boundary is quite simple, namely $(2\pi I_0(\alpha r))^{-1}$ (see Eq. (13)) for every point on the circle. There is no fundamental reason why other shapes cannot be used; as long as the Green's function for the shape is known, points can be selected at random on the shape. Thus for sampling near straight boundaries one could sample from a rectangle,



or perhaps a "chopped circle"



Sampling from the Green's function for either of these shapes produces a nonzero probability of landing on the boundary. Thus in principle it is possible to have an exact treatment where the particles actually terminate on, not just near, the boundary. This obviates approximating $u(P_n)$ by $u(P_n^*)$. I have not investigated alternate shapes but Troubetzkoy *et al.* [6] have used rectangles for solving the heat equation.

Application to Higher Dimensions

Although this paper has only treated two-dimensional domains there appears[2] to be no reason the method should not be applicable, with suitable restrictions, to n-dimensional domains (Haji-Sheikh [3] solves Laplace's equation in three dimensions). Courant and Hilbert [5] state that every solution of

$$u_{x_1x_1} + \cdots + u_{x_nx_n} + \lambda u = 0$$

that is regular in the domain satisfies the mean value relation

$$u(0) = \frac{1}{p(r)} \frac{1}{A} \iint_A u \, dA,$$

where r is the radius of the n-dimensional sphere, A is the surface area of the n-dimensional sphere, and

$$p(r) = \frac{\Gamma(n/2) J_{(n-2)/2}(\lambda^{1/2} r)}{(r\lambda^{1/2}/2)^{(n-2)/2}},$$

so that a point is sampled uniformly on a $(n-1)$-dimensional sphere of area A (radius r) and multiplied by the leading weight factor.

Conclusions

This paper provides an alternative Monte Carlo method for the solution of some elliptic partial differential equations. For the class of problems [2] where Monte Carlo solution is preferred over direct solution of the finite-difference equations, the method described here offers two advantages. First, there is no error introduced by a

[2] I have not investigated this in depth.

finite-difference approximation and second, the boundary is usually reached with short random walks because the step size is always adjusted to be as large as possible. While only Dirichlet boundary conditions have been discussed here, Haji-Sheikh [3] discusses derivative boundary conditions as well.

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