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A Monte Carlo Method for Solving a Class of Integral Equations [1]

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This note describes a random walk equivalent to the Neumann series solution of an integral equation. A diffusion analogy and the problem of importance sampling are discussed briefly.

Certain types of matrices can be inverted by a Monte Carlo method that was devised by J. von Neumann and S. M. Ulam, and that appears in a paper written by G. E. Forsythe and R. A. Leibler.[2] In the following it is shown that this method, when suitably generalized, can be used to approximate the Neumann series solution of an integral equation. This procedure is then shown to be similar to those used to solve certain problems dealing with scattering of particles, which can be formulated in terms of a nonhomogeneous integral equation, and which have been described by Herman Kahn.[3]

We wish to solve the following equation for $\phi(x)$

$$\phi(x)=f(x)+\lambda\int_a^b K(x,y)\phi(y)\,dy, \tag{1}$$

where we assume, for convenience, that $K(x,y)$ is uniformly continuous and a and b are finite. A formal solution of (1), which is valid if λ is smaller in absolute value than the eigenvalue of the corresponding homogeneous equation, which is smallest in absolute value, is given by Neumann's series [4]

$$\phi(x)=f(x)+\lambda\int_a^b K(x,y)f(y)dy + \lambda^2\int_a^b K^{(2)}(x,y)f(y)\,dy+\cdots, \tag{2}$$

where

$$K^{(n)}(x,y)=\int_a^b K^{(n-1)}(x,\xi)K(\xi,y)d\xi.$$

We may write this as

$$\phi(x)=f(x)+\lambda\int_a^b L(x,y)f(y)\,dy,$$

where

$$L(x,y)=K(x,y)+\lambda K^{(2)}(x,y)+\lambda^2K^{(3)}(x,y)+\cdots.$$

We need consider hereafter only the series (2)—if we wish to obtain the resolvent kernel L, we may use the fact that L satisfies the following equation

$$L(x,y)=K(x,y)+\lambda\int_a^b K(x,\xi)L(\xi,y)\,d\xi.$$

The series (2) can be evaluated by a Monte Carlo procedure consisting of two steps: first, a random process by which a particular term of the series is selected, and second, a random process by which the multiple integral defining the term selected is approximated (see footnote 3). This, when multiplied by a suitable weighting factor, will provide an estimate of the value of $\phi(x)$ for a particular x. We notice, however, that in series (2) each term is obtained by a simple operation on the preceding one, and this allows us to construct a simple random walk for approximating (2).

This random walk is defined by a sequence of functions $P_n(x,y)$, defined for $a\leqq x\leqq b$, $a\leqq y\leqq b$, and $n=0, 1, 2, \ldots$, where $P_n(x,y) > 0$ and

$$\int_a^b P_n(x,y)\,dy<1-\delta,\quad \delta>0.$$

In terms of this sequence we also define

$$V_n(x,y)=\frac{\lambda K(x,y)}{P_n(z,y)},$$

and

$$p_n(x)=1-\int_a^b P_n(x,y)\,dy.$$

In addition, we must also require that $|\lambda|$ be smaller than the smallest eigenvalue of $K'(x,y)=|K(x,y)|$. To estimate $\phi(x)$, we start a random walk at the point x of the interval (a,b). With a probability density given by $P_0(x,x_1)$ we jump to the point x_1, or we stop the random walk, with probability $p_0(x)$. Suppose that we have made k jumps, and have reached the point x_k. Then with probability density $P_k(x_k,x_{k+1})$ we jump to the point x_{k+1}, or we stop the random walk with probability $p_k(x_k)$. If our random walk has traversed the path $\gamma: x\to x_1\to\ \ldots\ \to x_{k-1}\to x_k$, stopping at x_k, we define

$$V(\gamma/x)=V_0(x,x_1)\ldots V_{k-1}(x_{k-1},x_k)\,\frac{f(x_k)}{p_k(x)}, \tag{3}$$

and use $V(\gamma/x)$ as an estimate of $\phi(x)$. The expecta-

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[2] G. E. Forsythe and R. A. Leibler, Matrix inversion by a Monte Carlo method, MTAC **4**, No. 31, p. 127 (July 1950).

[3] Herman Kahn, RAND Corp. Report R-163, Stochastic attenuation analysis (June 14, 1949).

[4] R. Courant and D. Hilbert, Methoden der Mathematischen Physik (J. Springer, Berlin, 1924–36).

tion of $V(\gamma/x)$ is defined by

$$E(V(\gamma/x))=\int_{A_{11\gamma}} V(\gamma/x)\,dP(\gamma/x). \tag{4}$$

Since the probabilities used at each step are conditional probabilities, the probability measure defined in the space of paths with exactly k steps is given by

$$dP(\gamma/x)=P_0(x,x_1)\ldots P_{k-1}(x_{k-1},x_k)p_k(x_k)dx_1\ldots dx_k, \tag{5}$$

and thus the integral (4) can be represented by a sum of integrals, the kth of which corresponds to those γ with k steps. In this way we obtain

$$\begin{aligned}E(V(\gamma/x))&=f(x)+\lambda\int_a^b K(x,x_1)f(x_1)\,dx_1\\&\quad+\gamma^2\int_a^b\int_a^b K(x,x_1)K(x_1,x_2)f(x_2)dx_1dx_2+\ldots\\&=\phi(x),\end{aligned} \tag{6}$$

which proves that $V(\gamma/x)$ is an unbiased estimate of $\phi(x)$. Because of the condition on γ, the above integrals and series are absolutely convergent.

Similarly we obtain for the nth moment of the $V(\gamma/x)$, (assuming the nth moment exists),

$$\left.\begin{aligned}\nu_n(x)=E(V^n(\gamma/x))&=\frac{f^n(x)}{P_0^{n-1}(x)}+\lambda\int_a^b K(x,x_1)V_0^{n-1}(x,x_1)\frac{f^n(x_1)}{P_1^{n-1}(x_1)}\,dx_1\\&\quad+\lambda^2\int_a^b K(x,x_1)K(x_1,x_2)V_0^{n-1}(x,x_1)V_0^{n-1}(x_1,x_2)\frac{f^n(x_2)}{P_2^{n-1}(x_2)}\,dx_2\,dx_1\\&\quad+\cdots.\end{aligned}\right\} \tag{7}$$

In the particular case that $P_n(x,y)$ is independent of n, that is the probabilities depend only on where we are, and not on how many steps we have taken, (7) reduces to a rather simple form. In fact, if we define $K_n(x,y)=K(x,y)V^{n-1}(x,y)$ the nth moment satisfies the following equation

$$\nu_n(x)=\frac{f^n(x)}{p^{n-1}(x)}+\lambda\int_a^b K_n(x,y)\nu_n(y)\,dy, \tag{8}$$

(assuming $|\lambda|$ is sufficiently small).

Let us now turn our attention briefly to the problem of finding a set of functions $P_n(x,y)$ such that the variance of the estimate of $\phi(x)$ will be as small as possible. We might expect that if we knew $\phi(x)$ we could find a Monte Carlo procedure that would give us the correct answer with probability 1 (see footnote 3). It is convenient to use an argument based on the two-step method mentioned earlier. In the series (2) denote the nth term by $I_n(x)$. Our Monte Carlo process gives us a set of functions $P(n,x)$ and $v(n,x)$; where $P(n,x)v(n,x)=I_n(x)$, and $P(n,x)$ is the probability of taking exactly n steps if we start at the point x. Referring to (5), we see that

$$P(n,x)=\int_a^b\cdots\int_a^b P_0(x,x_1)\cdots P_{n-1}(x_{n-1},x_n)P_n(x_n)\,dx_1\cdots dx_n.$$

We would like to choose $P(n,x)$ so that $P(n,x)=I_n(x)/\phi(x)$, as then $v(n,x)=\phi(x)$. To estimate $I_n(x)$ correctly with probability 1, we must have $K(x,y)$ and $f(x)$ non-negative, as we cannot allow negative probabilities. It may be convenient to introduce a sequence $\{U_n(x)\}$, which has a known sum $S(x)$, and estimate $\phi(x)+S(x)$ by the quantity $v^*(n,x)=v(n,x)+U_n(x)/P(n,x)$.

The above discussion is of course of little more than academic interest, but it gives an insight into the problems involved in minimizing the variance of the estimate. One thing we notice in particular is that the optimum choice of the sequence $\{P_n(x,y)\}$ will depend, in general, on the point x at which we wish to find ϕ.

As promised in the introduction, this method can be shown equivalent to Monte Carlo techniques often used to solve problems formulated in a different manner. Suppose we consider the problem, important in certain applications, of the diffusion of the neutrons through a thick slab of scattering material. Let the slab lie between the planes $x=0$ and $x=a$. Let $f(E,\theta,\phi,x)$ give the number of neutrons incident with energy E, at an angle given by θ and ϕ, which make their first collision at a distance x from the front of the slab. Let $K(E',\theta',\phi',x',E,\theta,\phi,x)$ give the probability that a neutron that makes a collision a distance x from the front of the slab, and has an initial energy E and an initial direction of travel (θ,ϕ), will proceed in the direction (θ',ϕ'), have energy E', and make its next collision at a distance x' from the front. A collision at $x>a$ corresponds to a neutron passing through the slab, and a collision at $x<0$ corresponds to a neutron reflected back, which we assume stops the process. Let $\psi(E,\theta,\phi)$ give the number of neutrons

that penetrate the slab with energy E, and have the direction of motion θ, ϕ.
Then clearly

$$\psi(E, \theta, \phi) = \int_a^\infty f(E, \theta, \phi, x)dx$$

$$+ \int_{x+a}^{x=\infty} \int_{x'=0}^{x'=a} \int_{E', \theta', \phi'} K(E, \theta, \phi, x, E', \theta', \phi', x')$$

$$\cdot f(E', \theta', \phi', x')dE'd\theta'd\phi'dx'dx \qquad (9)$$

+higher terms representing multiple collisions. This is very similar to equation (2).

The usual Monte Carlo method for evaluating (9) is to consider a randomly selected incident particle and trace its path thru the slab, using some chance device to determine the result of a collision (see footnote 3). The method we have found for evaluating series (2) corresponds to choosing a particular particle that has penetrated the slab, tracing its path backward thru the slab, and then multiplying by the density of particles that have the same entrance characteristics. Although both the position of the particle making the random walk and its final weight must be remembered from step to step, only the final weight is needed for the answer in our method, while in the other both the final position and final weight are needed, and a histogram must be plotted. Thus if an answer is desired for only a few points, our method may be simpler.

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