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*Design of "Random Walker" for Monte-Carlo method**

Part I (Theory)

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§1. Introduction

A model of "Random Walker", which is a sort of computor for such Monte Carlo methods as discussed in this paper, has been constructed in our institute. An outline of the mathematical principles on which it is based is given below.

Let Ω be a simply connected domain whose boundary Γ is of *arbitrary* shape. The following problems will be considered under this condition.

(I) Eigenvalue problem

$$\Delta\varphi+\lambda\varphi=0 \text{ (in } \Omega), \quad (\varphi)_\Gamma=0.$$

(II) Dirichlet problem

$$\Delta\varphi=0 \quad (\text{in } \Omega), \quad (\varphi)_\Gamma=f.$$

(III) Poisson's equation

$$\Delta\varphi=\rho \quad (\text{in } \Omega), \quad (\varphi)_\Gamma=f.$$

(IV) First-passage problems on random walk. The precise meaning of this term will be made clear later in this paper.

The computor has been designed to give the approximate characteristics to the solutions of the above problems. Of course, refinements of these results will be necessary if the exact solutions are desired.

In Part I, we will give the mathematical principles, upon which our Monte-Carlo methods are based, though the principle themselves are already known for the most part. In Part II (to be published in this journal by T. Mikami and H. Hirai) the mechanical devices required by these principles will be explained in detail. An outline of the procedure used is given below. In the 2-dimensional case, a square lattice is drawn on the surface of Braun tube. A light spot on one of the lattice points can then jump randomly to one of its four neighboring points by the instruction sent from a random number generator. A black mask, the shape of which is similar to the domain Ω is put on the surface of the tube. A light spot starting from a fixed lattice point walks randomly along the lattice lines, and after some steps appears at one of the boundary points and is thereupon detected

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by a scintilation counter. The length of path, and the number of light spots arriving at each boundary point are recorded. In the 3-dimensional case, a matrix of ferrite cores is used instead of the Braun tube. In Part III (to be published in this journal by T. Oshio) the mechanism of the random number generator will be explained. This involves a new automatic random number generator which uses the fact that the emission of gamma-rays from a Cs^{137} nucleus obeys the Poisson distribution. Here a free-running ring-gate circuit is used. Thus the order number of gate whose active period coincides with gamma-ray pulse, gives directly the random number. When higher accuracy (e.g. 10^{-20}) is necessary, appropriate pairs of random numbers thus obtained are added, and reduced by the number of the out-puts, the residue giving the required random number. Our random number generator can give 500 random numbers per second, each having the probability $1/10 \pm 10^{-20}$.

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§2. Mathematical principles.

(i) *Eigenvalue problem* (2-dimensional case). Let the ith eigenvalue and the corresponding normalized eigenfunction of the eigenvalue problem

$$\frac{1}{4}\Delta\varphi+\lambda\varphi=0 \quad (\text{in } \Omega), \qquad (1)$$
$$(\varphi)_\Gamma=0$$

be λ_i and $\varphi_i(x, y)$, respectively. Then the equation of the heat conduction

$$\frac{\partial u}{\partial t}=\frac{1}{4}\Delta u \qquad (2)$$

with the boundary condition

$$(u)_\Gamma=0 \qquad (3)$$

and the initial condition

$$u=\delta(x-x_0)\delta(y-y_0)\delta(t) \qquad (4)$$

has a solution of the form

$$u=\sum_{i=1}^{\infty} e^{-\lambda_i t}\varphi_i(x_0, y_0)\varphi_i(x, y)\,. \qquad (5)$$

Eqs (2), (3), (4), and (5) have intimate relations with probabilistic problem.

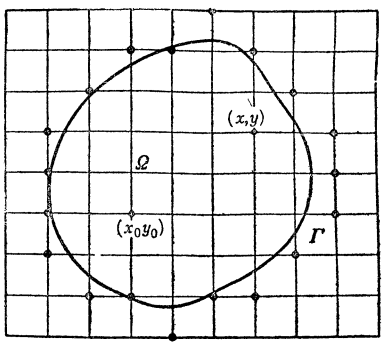

Fig. 1

In Fig. 1 we show a square containing

the domain Ω which is divided into small squares the side of which are all h in length. Γ^* is the set of lattice points which are on or nearest to the boundary Γ (the set of dots in Fig. 1). A randomly moving point (r. m. p.) starts from a fixed lattice point (x_0, y_0) in Ω and walks along the lattice lines. For simplicity, we assume that the point jumps instantaneously from one lattice point to any one of its neighboring points with equal probability ¼, and stays there for a constant time period τ. It is assumed that τ and h^2 are equal in magnitude: $\tau=h^2$. Let $P(x, y \mid n\tau)$ be the probability that a r. m. p. starting from a point (x_0, y_0) arrives at a lattice point (x, y) in Ω after n steps. Function $P(x, y \mid n\tau)$ is then one-fourth of the sum of probabilities that the r. m. p. arrives at any one of the four neighboring points after $(n-1)$ steps, i. e.,

$$P(x, y|n\tau)=\frac{1}{4}\Big[Px\{-h, y|(n-1)\tau\}+P\{x+h, y|(n-1)\tau\} +P\{x, y-h|(n-1)\tau\}+P\{x, y+h|(n-1)\tau\}\Big]. \tag{6}$$

We now consider a square $S(x, y)$, the length of whose side is h and whose center is at the lattice point (x, y), and put

$$P(x, y|n\tau)/h^2=u(\xi, \eta|n\tau) \text{ for } (\xi,\eta)\in S(x, y).$$

Then, the function u satisfies the equation, in case of $(\xi, \eta)=(x, y)$,

$$\begin{aligned}&u(x, y|n\tau)-u(x, y|(n-1)\tau)\\&=\frac{1}{4}\{u(x+h, y|(n-1)\tau)-2u(x, y|(n-1)\tau)+u(x-h, y|(n-1)\tau)\\&\quad+u(x, y+h|(n-1)\tau)-2u(x, y|(n-1)\tau)+u(x, y-h|(n-1)\tau)\}\end{aligned}$$

Dividing the left hand side by τ and the right hand side by h^2, we get the corresponding equation when h is sufficiently small:

$$\frac{\partial u}{\partial t}=\frac{1}{4}\Delta u \tag{7}$$

where we have put $t=n\tau$.

If the r. m. p. vanishes when it arrives at the boundary Γ^*, the function P then satisfies the boundary condition $(P)_{\Gamma^*}=0$. When, however, the interval h is sufficiently small, the above condition can approxiately be written as: $(P)_\Gamma=0$. The function u now satisfies the same condition

$$(u)_\Gamma=0. \tag{8}$$

The initial condition $P=\delta_{xx_0}\delta_{yy_0}\delta(t)$ can then be replaced by

$$u=\delta(x-x_0)\delta(y-y_0)\delta(t) \tag{9}$$

Eqs. (7), (8), and (9) are to be compared with Eqs. (2), (3), and (4), respectively. The solution of (7), (8), and (9) is, therefore, given by expression (5).

The probability $P(x, y|n\tau)\equiv P(x, y|t)$ is equal to the probability that the r. m. p. enters into the small square $S(x, y)$ after time t. The probability that the r. m. p. survives during $(0, t)$ is the sum of all $P(x, y|t)$:

$$\sum_{(x,y)\in\Omega} P(x, y|t)=\int\int_{\Omega} u(x, y|t)dxdy$$
$$=\sum_{i=1}^{\infty} c_i \exp(-\lambda_i t)\varphi_i(x_0, y_0) \tag{10}$$

where

$$c_i=\int\int_{\Omega}\varphi_i(x, y)dxdy\,.$$

When N r. m. p. start at $t=0$ simultaneously from a lattice point (x_0, y_0) and N_t r. m. p. remain in Ω at t, the ratio N_t/N is, for large N, approximately equal to the probability that a r. m. p. remains in Ω at t. N_t/N is then nearly equal to the series given by (10):

$$\frac{N_t}{N}=\sum_{i=1}^{\infty} c_i \mathrm{ext}(-\lambda_i t)\varphi_i(x_0, y_0). \tag{11}$$

Let N r. m. p. start at $t=0$ from each lattice point in Ω simultaneously, then we have

$$q(t)=\frac{1}{N}\int\int_{\Omega} N_t dxdy=\sum_{i=1}^{\infty} c_i^2 \exp(-\lambda_i t) \tag{12}$$

Practically N r. m. p. start from each (x_0, y_0) successivly, and the number of steps of each r. m. p. is counted.

Both the curves of N_t/N and $q(t)$ vs. t are the superpositions of exponential curves of the form $e^{-\lambda i t}$. The resolution of curve $q(t)$ gives the eigenvalues $\lambda_i (i=1, 2, 3, \cdots)$. Using these eigenvalues, the values of the eigenfunctions $c_i\varphi_i(x, y)$ at the starting point (x_0, y_0) are obtained from expression (11).

Resolution of curves. The points N_t/N plotted for each value of $t=n\tau$, will be on the smooth curve (11) when t is not large, but, for large values of t it scatters from the curve (see Fig. 2). This is due to the smallness of the sample N_t for large

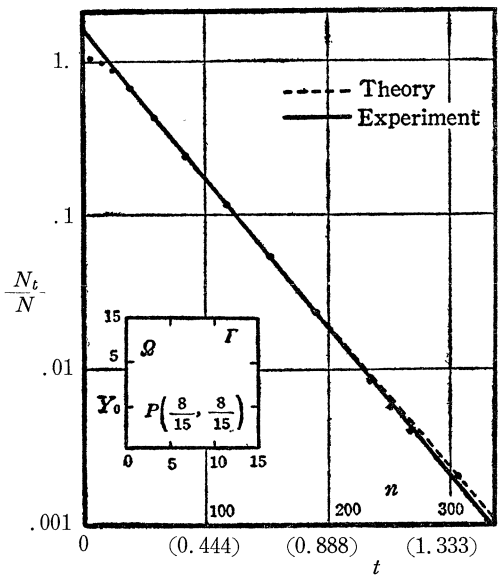

Fig. 2

value of t. The values of $q(t)$ will behave in a like manner. The number N must therefore be sufficiently large. The following theorems will be useful for the resolution of our curves.

1. *Rayleigh's theorem*[1]. The lowest eigenvalue λ_1 of (1) is not smaller than that of the circle whose area is equal to that of the domain Ω, i.e.

$$\lambda_1 \geqq \frac{1}{4}(\pi/A)j^2, \tag{13}$$

where A is the area of Ω, and $j=2.4048$ is the first zero point of the Bessel function $J_0(x)$. The equality holds valid only for the circle. For the second eigenvalue λ_2, we have the inequality

$$\lambda_2 \geqq \frac{1}{4}(2\pi/A)j^2. \tag{14}$$

2. Let Ω' be an arbitrary domain containing Ω, and μ_n be the nth eigenvalue of the problem

$$\frac{1}{4}\Delta\varphi+\lambda\varphi=0 \quad (\text{in } \Omega')$$

$$\frac{\partial\varphi}{\partial n}=0 \quad \text{on the boundary of } \Omega',$$

then we have the inequality

$$\mu_n \leqq \lambda_n . \tag{15}$$

3. For arbitrary natural number n, the inequality

$$\lambda_{n+1} \leqq 3\lambda_n \tag{16}$$

holds valid.

The resolution of curves N_t/N and $q(t)$ may be executed statistically, developing the idea used in the so-called Prony's interpolation.

Our model of computor uses the random numbers punched on a tape, and also a mechanical counter. For this reason, the speed of the random walk cannot be made greater than 4 steps per second. As an experimental example of our method for the eigenvalue problem, we have chosen a square for Ω. Dividing the side

Table 1.

Boundary	Division number of one side or radius	Starting point (x_0, y_0)	Number of random paths	λ_1		$c_1\varphi_1(x_0, y_0)$	
				Theor. value	Exp. value	Theor. value	Exp. value
Square	15	(8.8)	1,000	4.93	5.01	1.64	1.59
〃	15	(6.6)	100	4.93	—	1.46	1.30
〃	15	(4.4)	100	4.93	—	0.89	0.98
circle	7	Center	500	1.44	1.41	1.09	1.14

into 15 equal parts, 1000 r.m.p.'s have been started from a lattice point $\left(\frac{8}{15}, \frac{8}{15}\right)$. It took about an hour for the whole random walks. A similar experiment was carried for a circle. The results are tabulated in Table 1.

(ii) *Dirichlet problem.* Let the equation be

$$\Delta\varphi=0 \quad (\text{in } \Omega)$$

and the boundary condition be $\varphi=f(Q)$, $(Q\in\Gamma)$.

$\omega(Q, P)$ is the probability that a r.m.p. starting from a lattice point P in the domain Ω dies out at a point Q of Γ^*. We can then write approximately[2]

$$\varphi(P)\cong\sum f(Q)\omega(Q, P), \quad (Q\in\Gamma^*) \tag{17}$$

$\omega(Q, P)$ is estimated from N_t/N, where N is the number of r.m.p. starting from P, and N_t is the number of r.m.p. terminating at Q. Here, N is assumed to be sufficiently large.

As an example of the application of this method, it is possible to find a practical method of maping a simply connected closed domain conformally onto a unit circle.

(iii) *Poisson's equation.* The formula used in this case is[2]

$$\varphi(P)\cong\sum_{Q\in\Gamma^*} f(Q)\omega(Q, P)+h^2\sum_{Q\in\Omega}\rho(Q)G(Q, P), \tag{18}$$

where

$$G(Q,P)=\sum_{n=0}^{\infty}\frac{\alpha_n(Q, P)}{4^{n+1}} \tag{19}$$

and $\alpha_n(Q, P)$ is the probability that a r.m.p. starting from P arrives at Q after n steps. $\alpha_n(Q, P)$ and $G(Q, P)$ are symmetric with respect to Q and P, i.e.

$$\alpha_n(P, Q)=\alpha_n(Q, P), \quad G(P, Q)=G(Q, P).$$

By using a sufficiently large number of r.m.p., we can estimate the values of $G(Q, P)$ for arbitrary pairs of Q and P in Ω. Poisson's equation can then be solved by using formula (18).

(iv) *Problem of first passage.* The probability that a r.m.p. starting from a lattice point P in Ω comes to a lattice point Q in Ω or Γ^* after n steps without crossing the boundary of Ω, and the probability that a r.m.p. starting from P comes to Q *for the first time*, after n steps, can be obtained by using a sufficiently large number of r.m.p.

From the mathematical point of view, the above mentioned problems may easily be extended to the 3-dimensional case. The problem of constructing such a computor along this extension may not necessarily be easy. However, a number of the difficulties in the construction may be resolved by the use of a matrix of ferrite cores. Such a development is now being carried on and it is anticipated thatthe pro-

blems discussed in this paper will be solved practically in the 2-and 3-dimensional spaces.

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