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THE MONTE CARLO METHOD*

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Introduction. Briefly, the Monte Carlo method consists in formulating a game of chance or a stochastic process which produces a random variable whose expected value is the solution of a certain problem. An approximation to the expected value is then obtained by means of sampling from the resulting distribution. As in almost all numerical processes, only an approximation to the correct answer is obtained. In this case, instead of the primary source of error being due to numerical round-off, the primary source of error is due to the fact that only a finite sample can be taken. It follows, of course, that the degree of accuracy depends on the sample size.

At the end of this paper a rather extensive bibliography is given. A more complete list can be found at the end of a paper by Curtiss [1].

Two scientists from Los Alamos, Metropolis and Ulam [9], are generally credited with having given to the method the picturesque name "Monte Carlo." One of the early applications of using the sampling technique was in solving the problem of neutrons penetrating a slab. The problem, reported by Kahn [7], is essentially a problem in integral equations of the Fredholm type. Actually the knowledge of the relationship between probability problems and mathematical equations dates back to such famous mathematicians as Lagrange and Laplace. Late in the last century Lord Rayleigh proved that the solution of the "drunken walk problem" where a random path is obtained by the simple rule that every step of the inebriate is as likely a step forward as a step backward, yields an approximate solution to a parabolic type partial differential equation in one variable. In 1928, Courant, Friedrichs and Lewy [17] in their definitive article on difference equations for partial differential equations, included a treatment of the sampling technique to solve the difference equations corresponding to an elliptic differential equation.

With the advent of the high-speed computing device the picture with regard to this method of solving problems changed considerably. It suddenly became feasible to obtain large samples because of the high computing speeds available. The modern high-speed machine can generate as many as 200 random numbers from an arbitrary Gaussian distribution in one second.[1] When the method was first introduced in connection with high-

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[1] Methods by which this is done in a machine will be discussed further below.

speed computers in about 1947, statements were evoked attributing to it a panacean character. Since then a more sober outlook on the method prevails. It is generally agreed that although many questions concerning the method remain unanswered, it should be regarded as another numerical tool especially suited for certain problems.

The purpose of this article is to provide the reader with description of the many facets of the Monte Carlo Method. The subject is traversed from the most elementary to the more difficult techniques, and from the least practical (but instructive) to the most fruitful applications. One section deals with the generation of random numbers in the modern electronic computing machine. Most of the material is of an expository nature. However, the section on the solution of elliptic partial differential equations with certain boundary conditions is new. The closing section contains some general remarks on evaluating the Method.

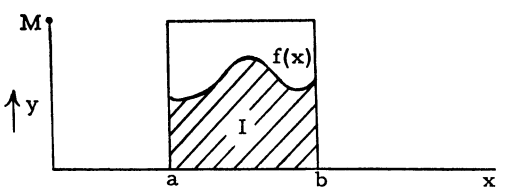
The evaluation of integrals. Consider the problem of evaluating the integral $\int f(x)dx$, where $f(x) \geqq 0$, between the limits a and b. This is equivalent to finding the area I under the curve as shown in the figure.

Consider a line $y = M$ such that $M > f(x)$ for all x in (a, b). Then, since $M(b - a)$ is the area of the rectangle, it is seen that

$$I < M(b - a) = A.$$

Consider the following game: Points (x, y) are chosen in the rectangle at random according to the rule that the choice of a point anywhere in the square is "as likely" as any other point. The number of times the point lies in the area under the curve is tallied. The ratio of the number of successes S, the points falling in I, to the total number of tries N is the random variable whose expected value is the ratio of the area under the curve (the value I) to the area A.

In actual practice the point in the rectangle can be selected by choosing from two rectangular distributions (each point equally likely) in the x and y intervals. With the value of x chosen, the quantity y is compared with $f(x)$ to determine a "success" or "failure."



According to elementary probability theory the distribution of S successes in N trials has an expected value $\bar{S} = NI/A$ and a standard deviation of

$$\sigma = \sqrt{N \frac{I}{A}\left(1 - \frac{I}{A}\right)}.$$

The standard deviation of S/N, the random variable of interest, is simply $\sigma' = \sigma/\sqrt{N}$. For large N the probable error in per cent in the ratio S/N is approximately

$$\text{Probable error in per cent} \doteq 67.45 \frac{\sigma'/\sqrt{N}}{S/N} \doteq 67.45 \sqrt{\frac{1 - I/A}{NI/A}}.$$

One sees that as N increases the probable error decreases. Also, if M is made small to increase the ratio I/A, a greater accuracy can be attained with a smaller number of tries.

The above expression for the probable error in the estimate of the integral is illustrative of the errors in Monte Carlo problems. It is seen, for example, that to increase the accuracy by one additional decimal, 100 times as many samples must be taken. Third and fourth decimal accuracies in Monte Carlo processes are frequently difficult because of this relationship between accuracy and sample size.

Suppose, in the above problem that the integral

$$I_1 = \int_a^b g(x)\, dx$$

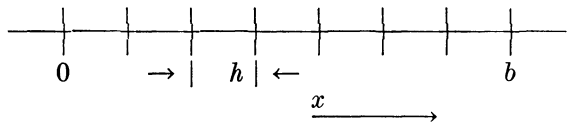
is known where $g(x)$ is an approximation to $f(x)$ and such that $f(x) < g(x)$ which makes $I_1 > I$. Then, in the above discussion, I_1 is substituted for A, and for a given number of tries, the probable error is reduced. This implies that an estimate is made of the integral and the success of the method essentially depends on the degree of approximation of I_1 to I. The formulation of the random process must be such that each point of the area represented by I_1 is "as likely" to be chosen as any other.

Another application of the sampling method lies in evaluating integrals of the Stieltjes type. If, for example, the evaluation of the integral $\int f(x)dg(x)$ is desired the procedure is entirely similar to that above except the sampling in the x coordinate is not done from a rectangular distribution but rather from a distribution which has the function $g(x)$ as a distribution function.

The method is hardly feasible for application to simple integrals of these types. However, for complicated integrals in n dimensions ($n \geqq 3$) the method becomes more attractive.

Ordinary differential equations. As another example, consider a game consisting of a series of turns played by two players G and G'. The probability that G wins a turn is p, the probability G' wins is $q = 1 - p$ and $\$h$ is at stake on each turn.

Suppose a total of $\$b$ is involved with G having $\$x$ and G' having $\$b - \$x$ initially. Graphically, a point is placed on an x-axis



and the interval $(0, b)$ is divided in equal subintervals of length h. A point starting at x moves to the right a distance h with probability p and to the left with probability $q = 1 - p$ and therefore represents the fortune of player G at any point in the game. Upon reaching b, G wins all the money and upon reaching 0, G loses all the money to G'. It can be shown [1] in a rigorous fashion that the probability $V(x)$ that G wins if he has $\$x$ at any stage of the game is the solution of the problem consisting of the difference equation

$$\frac{V(x+h) + V(x-h) - 2V(x)}{h^2} + \frac{p-q}{qh}\left[\frac{V(x+h) - V(x-h)}{h}\right] = 0$$

and the boundary conditions

$$V(0) = 0 \qquad V(b) = 1.$$

The boundary conditions correspond to the rather trivial facts that if G begins with $\$0$ he has probability 0 of winning and if he begins with $\$b$ he is certain of winning.

In showing that the probability $v(x)$ of G winning is the solution of the boundary value problem stated, the probability $V_m(x)$ of G winning in exactly m moves is expressed in terms of $V_{m-1}(x + h)$ and $V_{m-1}(x - h)$. The summation over m of both members of the resulting equation yields the expression. The procedure is universal in Monte Carlo problems of this type and is shown in detail in the proof of Theorem 1 of this paper.

If the amount of money $\$h$ involved in each move becomes smaller, and if p approaches q according to

$$p - q = h\alpha + 0(h)$$

for some α then the finite-difference problem goes formally into the problem

$$\frac{d^2u}{dX^2} + 2\alpha\frac{du}{dx} = 0$$

$$u(0) = 0, \qquad u(b) = 1.$$

Thus the game formulated gives an approximate solution to this "differential" boundary value problem if p and q are approximately equal.

Partial differential equations. Other examples of the Monte Carlo method lie in the domain of partial differential equations. Consider, for example, the Dirichlet problem of finding the numerical solution to the Laplace equation[2]

$$\nabla^2 u = 0$$

with the function values being stipulated around a boundary. The region of interest is divided into a square grid of mesh size h and it is desired to obtain the solution of the finite-difference formulas at the node points of the grid. The finite-difference formula at a node point P takes the form

$$\sum_{j=1}^{4} u(P_j) - 4u(P) = 0$$

where P_j ($j = 1, 2, 3, 4$) are the four immediate neighbors of point P. The boundary conditions can be written

$$u(R) = f(R)$$

at points R of the boundary where f is a known function.

The game to be played which produces a random function with expected value corresponding to point P which solves the boundary value problem is as follows: Random paths starting from point P and ending at the boundary are generated by the rule that upon reaching any node point the probability of proceeding to each of the four neighboring points is equally likely (i.e., each has probability $\frac{1}{4}$). The payoff upon reaching the boundary at a point R is $f(R)$, and the walk ends. The average payoff after N walks is the random variable for the point P. A proof of the validity of this procedure can be found in [17].

Curtiss [1] has published an interesting and rather complete discussion of the formulation of games for the solution of problems involving the general linear partial differential operator

$$L[u] \equiv au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y,$$

where the subscripts denote partial derivatives and the quantities a, b, c, d, and e denote constants. Also in another paper, Curtiss [23] has investigated the problem of the iteration of linear operators by the Monte Carlo method.

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[2] The operator ∇^2 is the Laplace operator. In two dimensions

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

Partial absorption boundary conditions. W. Wasow [11] has formulated and proved the validity of a random walk procedure to solve the finite-difference equations corresponding to the boundary value problem

$$\nabla^2 u(P) + g(P)u(P) = f(P)$$
$$u(R) = h(R)$$

where f and h are arbitrary functions with characteristics as described by Wasow. In this statement of the problem the differential equation holds for points P interior to a region S and the boundary condition for points (R) on the boundary B of S. It is the purpose here to extend certain of Wasow's results to boundary value problems involving the above differential equation but with the boundary condition of the form

$$n \cdot \nabla u = pu \tag{1}$$

where $n \cdot \nabla u$ is the derivative in the direction of the interior normal to the boundary and $p > 0$. The boundary condition (1) is of the type describing, for example, the transfer of heat into a constant-temperature medium.

Consider here that B is a rectangle[3] with sides parallel to the axes, and that a square lattice covers the interior. The difference equation counterpart to the boundary value problem involving condition (1) is of the form

$$\Delta u(P) + g(P)\, u(P) = f(P)$$
$$u(P_e) - u(R) = pu(R) \tag{2}$$

for points P in S, R on B, where P_e is a point interior to B and neighboring R in the direction of the normal. The symbol Δ represents the finite-difference operator

$$\Delta u = \frac{1}{h^2} \sum_{j=1}^{4} u(P_j) - 4u(P)$$

corresponding to the Laplace operator, where P_1, P_2, P_3, P_4, are the four neighboring points of P with coordinates $(x + h, y)$, $(x - h, y)$, $(x, y + h)$, and $(x, y - h)$. The quantity h is the mesh size of the square lattice.

Consider the following random walk from a point P in S: At each step the particle moves in the direction of the coordinate axes to one of its four neighboring points P_j, with the movement to each being equally likely with probability $\frac{1}{4}$. The particle has unit mass starting from point P. At

[3] The assumption of B as a rectangle is done for the sake of simplicity of exposition; it is not an essential restriction. B could be a polygon with sides parallel to the axes.

each move from a general point P', the mass is multiplied by $K(P')$ where

$$K(P') = \left[1 - \frac{h^2}{4} g(P')\right]^{-1}.$$

Upon reaching a boundary point R the probability of returning to the interior point P_e (neighboring the point R and situated in the direction of the normal) with mass unchanged is $a = 1/(1 + p)$ and the probability of being absorbed (the walk ends) is $1 - a$.

For this random walk the following theorem holds:

THEOREM 1. *The expected value $G(P, Q)$ of the mass passing through the point Q in S with walks starting from point P in S solves the problem*

$$\begin{aligned} \Delta u + g(P)u(P) &= \frac{-4}{h^2 K(P)} \delta(P, Q) \\ u(P_e) - u(R) &= pu(R) \end{aligned} \tag{3}$$

provided $G(P, Q)$ is finite. In this statement $\delta(P, Q) = 1$ if $P \equiv Q$ and $\delta(P, Q) = 0$ if $P \not\equiv Q$.

Proof: Let $L_{m,r}(P, Q)$ be a particular path from P to Q which consists of m steps interior to B and r returns from the boundary. Let $M_{m,r}(P, Q)$ be the mass upon arrival at Q for this path. The probability of movement along such a path is $4^{-m}a^r$. The expected mass upon arrival at Q with paths consisting of m steps and r returns is

$$g_{m,r}(P, Q) = \frac{a^r}{4^m} \sum_{[L_{m,r}(P,Q)]} M_{m,r}(P, Q) \tag{4}$$

the summation being over all such paths.

According to the rules of the walk

$$M_{m,r}(P, Q) = K(P) M_{m-1,r}(P_j, Q)$$

where P_j is a neighboring point of P and where the path for $M_{m-1,r}(P_j, Q)$ is contained in the one for $M_{m,r}(P, Q)$. By (4) and since there are four neighbors P_j

$$\begin{aligned} g_{m,r}(P, Q) &= \frac{K(P)a^r}{4^m} \sum_{j=1}^{4} \sum_{[L_{m-1,r}(P,Q)]} M_{m-1,r}(P_j, Q) \\ &= \frac{K(P)}{4} \sum_{j=1}^{4} g_{m-1,r}(P_j, Q). \end{aligned} \tag{5}$$

From the rules of the walk $g_{00}(P, Q) = \delta(P, Q)$ and, since P is not on the boundary B, $g_{0r}(P, Q) = 0$ for all r. Since

$$G(P, Q) = \lim_{m,r\to\infty} \sum_{i,j=0}^{m,r} g_{ij}(P, Q)$$

from (5) it is seen that

$$G(P, Q) - \delta(P, Q) = \frac{K(P)}{4} \sum_{j=1}^{4} G(P_j, Q)$$

or $G(P, Q)$ satisfies the difference equation in (3).

Next it is seen that

$$g_{m,r-1}(P_e, Q) = \frac{a^{r-1}}{4^m} \sum_{[L_{m,r-1}(P_e,Q)]} M_{m,r-1}(P_e, Q)$$

$$= \frac{a^{r-1}}{4^m} \sum_{[L_{m,r}(R,Q)]} M_{m,r}(R, Q).$$

The latter equality holds because a path which has one more return from the boundary than the path starting at P_e must necessarily have started from the boundary point R and must result in the same mass at the point Q. Therefore

$$g_{mr}(R, Q) = a g_{m,r-1}(P_e, Q)$$

and, since $g_{mo}(R, Q) = 0$ for all m, taking the limiting sum of both members produces

$$G(R, Q) = aG(P_e, Q).$$

That is, $G(R, Q)$ satisfies the boundary condition in (3), and the proof of the theorem is completed.

Except for the factor $-\frac{1}{4}h^2K(P)$ the function $G(P, Q)$ is the Green's function of the problem (2). Thus the solution of (2) can be written

$$u(P) = \frac{-h^2}{4} \sum_{Q \in B} G(P, Q)K(Q) f(Q).$$

Therefore, the following random walk procedure produces a random variable whose expected value solves (2): At each point Q in the walk from P as described above, the amount of mass is multiplied by $K(Q)f(Q)$ and the products added until absorption takes place on the boundary. The random variable for N walks starting at P is the cumulative sum multipled by $-h^2/4N$.

The proof of the following establishes the validity of the random walk procedure for the problem (2):

THEOREM 2. *If $g(P) < 0$ for all P in S the expected value $G(P, Q)$ represented by the sum*

$$G(P, Q) = \lim_{m,r \to \infty} \sum_{i,i}^{m,r} g_{ij}(P, Q) \tag{6}$$

exists.

Proof: Since $g(P) < 0$ for all P in S, there exists a number M such that

$$\max_{P \in S} [K(P)] = M < 1.$$

Also,

$$M_{m,r}(P, Q) \leqq M^m.$$

If $N_m(P, Q)$ is the number of distinct paths from P to Q with exactly m interior moves then

$$g_{m,r}(P, Q) = \frac{a^r}{4^m} \sum_{[L_{m,r}(P,Q)]} M_{m,r}(P, Q)$$

$$\leqq \frac{a^r}{4^m} N_m(P, Q) M^m < a^r M^m.$$

The last inequality holds because $N_m(P, Q) < 4^m$ since the total number of distinct paths consisting of m interior moves to *any* point in S is 4^m. The existence of $G(P, Q)$ follows readily under the realization that the double sequence of partial sums involved in the sum (6) is monotone nondecreasing in m and r and the sum is termwise less than the double sum with terms of the form $a^r M^m$ which certainly coverges since $0 < a < 1$ and $0 < M < 1$.

Random number generation. Since all Monte Carlo techniques require a random number source, the subject of generating the random numbers is most important. Perhaps the first extensive project in the generation of random sequences of numbers was that undertaken by the RAND Corporation in 1947 and reported by G. W. Brown [20]. The technique used consisted of generating random digits by counting electronically pulses from a random frequency pulse source and periodically punching digits on IBM cards. Some one million random digits were obtained and tabulated by this "electronic roulette wheel."

With the advent of the stored program computer, however, and its awkwardness in storing and handling extensive tables of numbers compared to its arithmetic speed, a method of generating random numbers as needed was seen as necessary. With the technique generally in use a sequence of "random" numbers is generated by the arithmetic process of performing successive multiplications and discarding many of the digits, usually the high or the high and low order digits. A scheme[4] in extensive use can be described by the formula

$$y_i = 5^{2q+1} y_{i-1} (\text{mod } 2^s)$$
$$y_0 = 1 \tag{7}$$

[4] Another technique, based on Fibonacci sequences, is described by Taussky and Todd [26].

where q is a nonnegative integer, and s is the number of binary digits useful or desirable in the number produced. This method produces positive odd integers s binary digits in length in the range $2^s > y \geqq 0$. Sequences of such numbers are pseudo-random with uniform distribution in the range if s is large.

As reported in a paper by Moshman [24], by classical number theory one may deduee that the period for the sequence of numbers thus produced is 2^{s-2}. In most cases s is on the order of 40, making possible large sets of pseudo-random numbers. Calling the least significant digit $n = 1$, the nth digit has a period 2^{n-2}; the more significant digits are more nearly random.

The method of producing sequences of numbers which correspond to normal or Gaussian distributions consists in averaging subsequences of the numbers y_i obtained from (7). In so doing a standard theorem on the distribution of means is involved: If y has a distribution of mean m and standard deviation σ for which the moment generating function exists then the random variable y formed by taking the average value $\bar{y}$ of n samples of y according to

$$x = (\bar{y} - m)\frac{\sqrt{n}}{\sigma} \tag{8}$$

approaches a standard distribution as n is large. Fortunately n need not be large to satisfy most requirements. Kendall and Babington-Smith [19] have treated many of these questions with considerable thoroughness.

In practice with large scale binary computing machines like the IBM 704 or the Remington-Rand 1103A, s is taken to be as large as possible, namely 35, so that maximum periodicity is obtained. In most cases q is chosen so that 5^{2q+1} is as large as possible while still less than 2^s. It is convenient, though not necessary, to take y_0 equal to 5^{2q+1} itself. For obtaining deviates from the normal distribution according to (8), n is usually taken to be about 10 but it can be chosen smaller. Very often a subroutine for the computer is prepared which, when used, produces a number from a distribution corresponding to the standard distribution (zero mean and unit standard deviation). Multiplying the numbers thus obtained by an arbitrary σ produces deviates from the normal distribution of standard deviation σ. All writers on the subject conclude that the numbers obtained from this technique satisfactorily pass all tests of randomness. Moshman [24] reports on extensive tests performed on a slight variation of the method of (7) suitable for a decimal computer where the numbers were chosen modulo 10^s and 7^{4q+1} was used instead of 5^{2q+1}.

It is sometimes convenient to choose the parameter q in (7) so that 5^{2q+1} is considerably less than 2^s. F. Meek [21] reports on a subroutine for producing normally distributed deviates prepared for the 1103 computer

with $q = 2$ and $n = 6$. In this case 5^5 was desirable since that number in binary form contains few binary ones and the multiplication is consequently faster on the 1103. The chi-squared test for these numbers x_i, showed them to conform satisfactorily to a Gaussian distribution. The numbers x_i can be chosen at the rate of 217 per second.

Once one has noted the simple process of generating numbers from a uniform distribution according to (7), many other schemes are possible. Von Neumann [25] suggested a method for generating numbers satisfying a nonuniform, arbitrary probability distribution $f(x)dx$ on (0, 1). In this method one normalizes $f(x)$ by choosing an a such that $\max_{x\in(0,1)}[af(x)] = 1$. Numbers x_i and y_i are generated from a uniform distribution on (0, 1) and x_i is accepted or rejected as a deviate depending on whether $y_i \leqq af(x_i)$ or $y_i > af(x_i)$. The accepted x_i's have the required distribution. Other tricks are, of course, possible.

Linear systems and matrix inversion. Elliptic partial differential equations, when solved numerically, are, of course, nothing more than a specialized system of linear algebraic equations. For this reason the discussions lead directly to the solution of linear systems by Monte Carlo techniques. Forsythe and Leibler [18] have reported on a method by Von Neumann and Ulam for solving linear systems and inverting matrices. Included in this paper is an expression for the variance of the random variable, the expected value of which is the solution. Wasow [22] has carried this a step further and has shown that the problem can be formulated in terms of a "mass" of the moving point as was done in the section on random walk boundary conditions.

An interesting question concerns the relationship between the proof of the preceding section and the proof of Forsythe and Leibler [18] of the general formulation. In discussing this, consider B the matrix whose inverse is desired and let $A = I - B$ where I is the unit matrix. The condition advanced by Forsythe and Leibler for the validity (convergence) of the procedure is that

$$\max_r \mid \lambda_r(\bar{A}) \mid < 1$$

where $\bar{A}_{ij} = \mid A_{ji} \mid$ and $\lambda_r(A)$ denotes the rth eigenvalue of A. In the above section the off-diagonal elements of A are $[4 - g(p)]^{-1}$ and there are four such elements in each row. Thus by Gerschgorin's theorem[5] the eigen-

[5] Gerschgorin's theorem states that, for a matrix of order n with elements A_{ij}, the eigenvalues lie in the union of the n circles of radius

$$r = \sum_{j=1}^{n} \mid A_{ij} \mid - \mid A_{ii} \mid$$

and with centers at A_{ii}.

values of A are certainly less than one in magnitude as long as $g(p) < 0$, the condition advanced for the validity of the procedure.

It is clear that the condition of Forsythe and Leibler concerning the size of the eigenvalues is less stringent that the condition of the preceding section, that $g(p) < 0$. However, since Gerschgorin's theorem is usually, in practice, applied in these matters, the conditions are practically equivalent.

Remarks. Probably the most fruitful application of the method has not been mentioned above, however. In the above discussions the emphasis was placed on the solution of a categorical mathematical problem, already formulated. Very frequently one formulates the Monte Carlo process from the physical process without first translating the process into a type of mathematical expression. The difference in approach is not trivial, however, since it happens frequently that the mathematical formulation of the complete problem is not feasible, or if the formulation is feasible, the solution by standard techniques is not possible because of problem nonlinearities.

As a case in point, consider the problem of a guided missile trajectory or, more specifically, the impact point of the missile. The impact point is a random variable because of random variables in the guidance primarily due to radar propagation anomalies but also due to electrical circuit "noise." In this case sampling is done directly; simulation of the trajectory is performed on the basis of the character of the distribution of the random variables.

There are, however, advantages in using the Monte Carlo scheme for certain standard mathematical problems. For example, in the solution of elliptic partial differential equations "local solutions" or solutions at a given point are possible. This makes possible the solution in certain restricted areas, or at certain points, without the necessity of solving the equations for all unknowns simultaneously as with the usual classical methods of solving linear equations. Therefore, computer storage requirements are considerably lightened and computer time may be saved.

Certain advancements in the techniques and theory of the method are called for. In particular, analytical work is necessary to obtain estimates of the accuracies obtained for a sample of a given size, and thereby obtain estimates for the time required for computation. Certain techniques such as "importance sampling," that technique by which sampling is carried out to a greater extent in "areas" which affect the answer the most, need to be exploited further. Finally, experimental evidence in the form of machine-solved problems is needed to give weight to the feasibility of the method in certain cases.

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