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Inverse Monte Carlo Analysis

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The use of the Monte Carlo method for solving inverse problems, such as those commonly encountered in radiation physics, is investigated. It is shown that a non-iterative simulation procedure employing the importance sampling concept in which samples are taken from an arbitrary probability density function (pdf) can lead to a system of equations which can be solved for a set of parameters of the true pdf. Also, under certain conditions, the uncertainty in the retrieved parameters can be estimated. Specific examples demonstrating one- and four-dimensional inversions are considered.

INTRODUCTION

Monte Carlo is a technique used widely in fields ranging from radiation transport [1–3] to business decision making [4]. In essence, it is a means of estimating expected values, and hence is a form of numerical quadrature. Although Monte Carlo can be applied to simple processes, and one-dimensional integrals, its main utility is found in simulating complex processes, and estimating multidimensional integrals. The power of the Monte Carlo technique rests in the facts that: (a) it is often more efficient than other quadrature formulas for estimating multidimensional integrals, (b) it is adaptable, in the sense that variance reduction techniques can be tailored to the specific problem, and (c) it can be applied to highly complex problems for which the definite integral formulation is not obvious and standard analytic techniques are ineffective.

Despite the wide applicability and general success of Monte Carlo in direct simulation, it has not been viewed traditionally as a good inverse technique, since an iterative simulation procedure is generally out of the question. Consider the formulation

$$r(y) = \int_{-\infty}^{\infty} z(x, y) f(x)\, dx, \tag{1}$$

in which z is a kernel, f a probability density function (pdf), and r an expectation. Monte Carlo is often used to solve the direct problem, i.e., to estimate r at discrete values of y, given z and f. However, it is not considered generally well suited to iteratively solving the inverse problem, i.e., to find f, given z and r.

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The traditional inverse approach using simulation is to search on a set of parameters, α, of the desired function, f, until some objective function, $\Omega(\alpha)$, is minimized. This requires that direct simulations for r be repeated as different values of α are searched iteratively, a procedure which can quickly become prohibitive in terms of computation effort. Here, we consider an alternative inverse Monte Carlo formulation, which requires only one direct simulation, and we demonstrate its usefulness through some simple examples. It is noted that inverse analysis is basic to many fields. Specific radiation physics applications include: remote sensing, in which unknown atmospheric or terrestrial properties (such as temperature profiles or particle size distributions) are sought; radioisotope gauging, in which material properties (such as density, thickness, or composition) may be unknown parameters; and medical radiation diagnostic testing, in which the organ burden of specific elements (such as cadmium in the kidney) is desired.

In the following section, pertinent Monte Carlo principles are reviewed and the theory of inverse Monte Carlo is presented, including a treatment of sensitivity and precision. Then, two specific simple examples are considered in order to demonstrate how particular inversions might be carried out using this procedure. Conclusions are drawn in the final section.

THEORY

Monte Carlo is a well-known technique for estimating expected values. Since an expectation can be written as a definite integral, Monte Carlo is in fact a form of numerical quadrature. It is also applied in applications where the integral formulation as an expectation is not obvious. In these cases, the Monte Carlo method can be thought of as the process of conducting a contrived mathematical experiment to estimate the expected outcome of a stochastic process by sampling from the governing probability densities, and thus as a numerical analogue to a physical experiment. As such, it is subject to the uncertainty inherent in any finite observation of a stochastic process. In principle at least, this uncertainty can be reduced to any desired degree by increasing the sample size and/or by suitably modifying the sampling process.

Preliminaries

We review a few basic concepts of Monte Carlo in order to establish the framework for what follows. Since multidimensional sampling involves successive samplings on individual variables, we limit our consideration to the case of a single random variable, x, which is governed by the pdf, $f(x)$. We also suppose z represents the outcome of a stochastic process which is a function of the random variable, x, and perhaps another independent variable, y. Then $z(x, y)$ is also a random variable, with expected value

$$\langle z(y)\rangle = \int_{-\infty}^{\infty} z(x, y) f(x)\, dx, \tag{2}$$

and variance

$$\sigma^2(z) = \int_{-\infty}^{\infty} [z(x, y) - \langle z(y)\rangle]^2 f(x)\, dx = \langle z^2(y)\rangle - \langle z(y)\rangle^2. \tag{3}$$

The basis for direct Monte Carlo follows from the Strong Law of Large Numbers [1, 5, 6], which states that the quantity

$$\hat{z}(y) = \frac{1}{N} \sum_{i=1}^{N} z_i(y), \tag{4}$$

where $z_i(y) = z(\xi_i, y)$ and ξ_i is a random sample from $f(x)$, is an unbiased estimator for $\langle z(y)\rangle$. The quantity $\hat{z}$ is a Monte Carlo estimate of $\langle z\rangle$, and has the form of a numerical quadrature in which the ξ are nodes and the weights are of equal value, $1/N$.

Because most simulation processes are inefficient, techniques have been devised [7, 8] for reducing the number of trials required to obtain a result with a given variance. For our purposes, it is sufficient to consider only one such technique, importance sampling, which provides a means for altering the sampling process by allowing the nodes to be chosen from an arbitrary pdf. In direct Monte Carlo, importance sampling is a technique to reduce the variance by using a knowledge of the physical processes involved or some other a priori information to choose the ξ_i from a pdf which will favor histories that lead to successes. Consider the pdf, $f^*(x)$, and the function

$$z^*(x, y) = z(x, y)\, W(x), \tag{5}$$

where

$$W(x) = f(x)/f^*(x). \tag{6}$$

It is easily shown that the expected value of z^* with respect to f^* is the same as the expected value of z with respect to f, although the variances may be different. Thus, we can estimate $\langle z(y)\rangle$ by using Monte Carlo to estimate $\langle z^*(y)\rangle$. This leads to a quadrature having the more standard form

$$\langle z(y)\rangle = \int_{-\infty}^{\infty} z(x, y) f(x)\, dx \cong \hat{z^*}(y) = \frac{1}{N} \sum_{i=1}^{N} z(\xi_i, y)\, W_i, \tag{7}$$

in which the nodes are obtained by sampling from f^* and the weights are given by

$$W_i = f(\xi_i)/f^*(\xi_i).$$

This is the standard importance sampling process. Sampling from f^* introduces a bias which is accounted for by the weight factor, $W = f/f^*$, so that the estimate z^* is also an unbiased estimator for $\langle z\rangle$.

Inverse Monte Carlo

Now, we consider the use of importance sampling in inverse analysis. A general inverse problem can be expressed in the form of a Fredholm Equation of the First Kind, i.e.,

$$r(y) = \int_{-\infty}^{\infty} z(x, y) f(x)\, dx, \tag{8}$$

in which the function f is unknown and r can be measured at n discrete values of y, yielding the vector $\mathbf{r}$. The objective is to find $m \leqslant n$ parameters of f by inversion. These parameters, $\boldsymbol{\alpha}$, may be disjoint in x such that

$$\begin{aligned} f(x) &= \alpha_i, x \in (x_i, x_{i+1}), \qquad i = 1, 2, \ldots, m, \\ &= 0, \qquad\qquad\qquad\quad \text{otherwise}, \end{aligned} \tag{9}$$

where

$$x_1 \leqslant x_2 \leqslant \cdots \leqslant x_{m+1}, \tag{10}$$

or overlapping in x such that

$$f(x) = f(\boldsymbol{\alpha}, x), \tag{11}$$

where $\boldsymbol{\alpha}$ is a column vector of m global parameters in some assumed functional form for f. If a suitable quadrature can be applied, the problem is effectively transformed to a system of n equations in m unknowns, the specific form of which will depend on the kernel, z, and on the quadrature scheme. The traditional simulation approach is to choose an intial estimate for $\boldsymbol{\alpha}$, use a simulation model to construct estimates, $\hat{\mathbf{r}}$, of $\mathbf{r}$ by sampling from the assumed f, and iterate in order to find the $\boldsymbol{\alpha}$ which best matches $\hat{\mathbf{r}}$ to $\mathbf{r}$ in some sense. This is obviously costly since multiple simulations are required.

We now present an alternative approach which involves simulating the process only once using an assumed from, f^*, for f in the importance sampling manner. This requires the weighting of each history by the ratio f/f^*, which is a function of $\boldsymbol{\alpha}$, leading to a quadrature approximation of the form

$$\mathbf{r} \cong \hat{\mathbf{r}} = \frac{1}{N} \sum_{i=1}^{N} \frac{\mathbf{z}(\xi_i) f(\boldsymbol{\alpha}, \xi_i)}{f^*(\xi_i)}, \tag{12}$$

in which all quantities are known except the $\boldsymbol{\alpha}$. If f is linear in the $\boldsymbol{\alpha}$, this has the matrix form

$$\mathbf{r} = \mathbf{A}\boldsymbol{\alpha}, \tag{13}$$

and a straightforward matrix inversion is possible. If f is nonlinear in the $\boldsymbol{\alpha}$, a nonlinear inversion is necessary. Hence, the importance sampling concept of direct

Monte Carlo can be used to derive a system of equations in a single-step procedure which in principle can be solved, at least numerically, for the parameters, $\boldsymbol{\alpha}$, of the unknown function f. Of course, the domain of f^* must include that of the actual pdf in the sense that f^* is nonzero where zf is nonzero, so that all regions of x which contribute to the expectation are sampled.

This is a single-step procedure in the sense that it is non-iterative. However, since there are n different elements of the vector $\mathbf{r}$, it may be necessary to perform separate simulations to construct estimates of different members, depending on the specific experiment. If a given simulation history can lead to any one of the n outcomes, then all elements of $\mathbf{r}$ can be simulated in one ensemble of histories by proper scoring; however, if, for instance, different initial conditions are required for different elements of $\mathbf{r}$, then separate simulations may be required. In either situation, the proposed inverse formulation is non-iterative.

The advantages of this formulation are similar to those of direct Monte Carlo. They include: (a) the need to perform the direct simulation only once; (b) the ability to choose the importance function, f^*, to suit the problem; (c) the fact that the simulation does not require the explicit Fredholm Equation formulation as long as the physics of the problem are known; and (d) the ability to handle complex kernels, which may pose significant difficulties for analytic approaches.

Not only can we generate a system of equations for $\boldsymbol{\alpha}$, by Monte Carlo, but we can often estimate the uncertainty in their solution. Recall that in direct Monte Carlo the variance of the mean, commonly denoted σ^2/N, can be estimated by the quantity

$$\frac{s^2}{N} = \frac{1}{N(N-1)} \sum_{i=1}^{N} (r_i - \hat{r})^2 = \frac{1}{N-1} (\bar{r^2} - \hat{r}^2), \tag{14}$$

where $\hat{r}$ is the Monte Carlo estimate of the mean and r_i is the score of the ith history. Thus, we can construct a measure of the uncertainty in the estimate $\hat{\mathbf{r}}$, namely,

$$\sigma(\hat{r}_i) = \left[\frac{s^2}{N}\right]^{1/2} \cong \frac{\sigma}{\sqrt{N}}, \qquad i = 1, 2, \ldots, n. \tag{15}$$

If the r_i are measurements, they will also be subject to uncertainty, which we denote by the standard deviations $\sigma(r_i)$. Hence, the comparison of r_i with $\hat{r}_i$, given in Eq. (12), will be subject to a combined standard deviation given by

$$\sigma_i = [\sigma^2(\hat{r}_i) + \sigma^2(r_i)]^{1/2}. \tag{16}$$

Assuming the r_i are independent, this uncertainty is propagated through Eq. (12) to give an uncertainty in the calculated α_j which can be estimated by the standard formula, given by Jaffey [9],

$$\sigma(\alpha_j) = \left[\sum_{i=1}^{n} \left(\frac{\partial \alpha_j}{\partial r_i}\right)^2 \sigma_i^2\right]^{1/2}, \qquad j = 1, 2, \ldots, m. \tag{17}$$

We note that $\partial\alpha_j/\partial r_i$ is to be evaluated at r_i, and is merely an estimate of the sensitivity of the solution for α_j to variations in the response about the point r_i. However, it may often be simpler to evaluate $\partial r_i/\partial\alpha_j$ than $\partial\alpha_j/\partial r_i$, expecially if Eq. (12) is not linear in the $\boldsymbol{\alpha}$. In these cases, $\sigma(\alpha_j)$ can be estimated by replacing the $\partial\alpha_j/\partial r_i$ in Eq. (17) with $(\partial r_i/\partial\alpha_j)^{-1}$, which can be obtained, at least numerically, from the system to be inverted, i.e., from Eq. (12).

Unfortunately, the calculation of the $\sigma(\hat{r}_i)$ and $\partial r_i/\partial\alpha_j$ requires that the value of $\boldsymbol{\alpha}$ be known. This situation can be handled in any of several ways, e.g.: (a) complete a preliminary inverse Monte Carlo calculation for $\boldsymbol{\alpha}$, then use this value to estimate the $\sigma(\hat{r}_i)$ (if necessary, in a subsequent inverse Monte Carlo calculation); (b) assume a value for $\boldsymbol{\alpha}$, for the purpose of estimating $\sigma(\hat{r}_i)$, from the interval over which the solution is expected; or (c) assume $\sigma(\hat{r}_i) \cong \sigma(r_i)$, so that $\sigma_i^2 = 2\sigma^2(r_i)$. Option (a) can be employed in the following manner. Identify the desired sample size, N. Run a simulation using $N/2$ histories and calculate $\boldsymbol{\alpha}_1$. Run a second simulation of $N/2$ histories to compute $\boldsymbol{\alpha}_2$ and, using $\boldsymbol{\alpha}_1$, the $\sigma(\alpha_j)$. Finally, average the results of the two simulations to obtain an $\boldsymbol{\alpha}$ based on the desired sample of N histories.

If desired, a composite standard deviation can be formed from

$$\sigma(\boldsymbol{\alpha}) = \left[\sum_{j=1}^{m} w_j \sigma^2(\alpha_j)\right]^{1/2}, \tag{18}$$

where w_j is a weight factor associated with the solution for α_j and provides a measure of the relative importance of the solution for the jth parameter. Then clearly the quantity $\sigma(\boldsymbol{\alpha})$ provides a measure of the quality of a particular inverse formulation. The specific choice of the importance function, f^*, affects both the sensitivities and the standard deviations in the estimates, $\sigma(\hat{r}_i)$, and hence provides a means for constructing an optimal system of equations for inversion.

Application

In order to demonstrate the application of inverse Monte Carlo analysis, we first consider a simple example in radiative transfer. Let a semi-infinite, homogeneous, isotropic, plane-parallel gray atmosphere of unit optical thickness be subject to a steady, uniform, isotropic incident radiation field on the left face. Let A and B be the albedo and transmission, respectively, and $\bar{A}$ and $\bar{B}$ be measurements of these quantities, i.e.,

$$\bar{A} \cong A = \frac{\int_0^{-1} \Psi(0, \mu, \omega)\mu \, d\mu}{\int_0^1 \Psi(0, \mu)\mu \, d\mu} = 2\int_0^1 \Psi(0, -\mu; \omega)\mu \, d\mu \tag{19}$$

and

$$\bar{B} \cong B = 2\int_0^1 \Psi(1, \mu; \omega)\mu \, d\mu, \tag{20}$$

where Ψ is radiation intensity, x is the optical variable, μ is the direction cosine of the propogating radiation with respect to the positive x-direction, ω is the single scatter albedo, and

$$\Psi(0, \mu) = 1, \qquad \mu > 0, \tag{21}$$

$$\Psi(1, \mu) = 0, \qquad \mu < 0. \tag{22}$$

We wish to find the scattering probability, ω, from either of the measurements $\bar{A}$ or $\bar{B}$. We note that Eqs. (19) and (20) are not directly in the form of Eq. (8), although the problem could be so posed; here we simulate the physics of the problem.

We construct a simple algorithm to estimate A and B by direct Monte Carlo. The incident distribution is equivalent to a surface source of strength

$$Q_S = \mu I(0, \mu) = \mu, \qquad \mu > 0. \tag{23}$$

Thus, the incident direction cosine, μ_0, of a source particle is sampled from the pdf

$$f(\mu_0) = 2\mu_0, \qquad \mu_0 \in [0, 1). \tag{24}$$

The distance to the first interaction point is determined in the usual manner, and the particle is forced to scatter at the interaction point. This is the importance sampling step which allows the inverse calculation for ω, and corresponds to sampling from the assumed pdf,

$$\begin{aligned} f^* &= 1, \qquad \text{scatter}, \\ &= 0, \qquad \text{absorption}, \end{aligned} \tag{25}$$

instead of the true pdf,

$$\begin{aligned} f &= \omega, \qquad \text{scatter}, \\ &= 1 - \omega, \qquad \text{absorption}. \end{aligned} \tag{26}$$

This requires weighting at each interaction point by the factor $W = \omega$. A new direction, assuming isotropic scattering, is then chosen and the particle followed to its next interaction point or to escape. In order to improve the efficiency of the calculation, last-flight estimation [3] is applied. This consists in extending each flight path to force escape, and adjusting by the weight factor

$$\begin{aligned} W &= e^{x/\mu}, \qquad \mu < 0, \\ &= e^{-(1-x)/\mu}, \qquad \mu < 0. \end{aligned} \tag{27}$$

At each interaction point, a scatter is forced, a new direction is chosen and last-flight estimation is employed. Thus, we obtain estimates for A of the form

$$\hat{A} = \frac{1}{N} \sum_{i=1}^{N} W_i, \tag{28}$$

where the history weight is the product of weights at each interaction point, i.e.,

$$W_i = \prod_{j=1}^{J_i} \omega \exp(x_j/\mu_j)_i, \tag{29}$$

x_j is the optical depth at which the jth scatter occurs, μ_j is the direction cosine after the jth scatter and J_i is the number of interactions during history i before escape from the slab. After N histories have been simulated, this leads to a polynomial equation of the form

$$\hat{A} = a_1\omega + a_2\omega^2 + \cdots + a_v\omega^v, \tag{30}$$

where

$$v = \max(J_i), \qquad i = 1, 2, \ldots, N. \tag{31}$$

The quantity $a_j\omega^j$ represents the contribution to the total albedo from particles which undergo j scatters before escape through the left face. Similarly, for the transmission, we obtain an equation of the form

$$\hat{B} = b_0 + b_1\omega + b_2\omega^2 + \cdots + b_v\omega^v. \tag{32}$$

It is then necessary only to find the zeros of a polynomial of degree v in order solve the inverse problem.

The results of a series of inverse Monte Carlo runs for the case $\omega = 0.8$ are given in Table I. For these runs, the values $\bar{A} = 0.2802$ and $\bar{B} = 0.4162$, obtained by the F_N method [10], were input and the simulations were terminated after a specified number of scatters, v. The uncertainties in the $\bar{A}$ and $\bar{B}$ were assumed negligible and the true value, $\omega = 0.8$, was used in the calculation of $\sigma(\omega)$. The results demonstrate that the single scatter albedo can be estimated fairly accurately in a reasonable number of histories. Also, the results do not appear to be very sensitive to the value of v used, above about $v = 8$, indicating that the contributions to the albedo and transmission quickly decrease with increasing number of scatters.

TABLE I

The Inverse Solution for the Single Scatter Albedo, $\omega = 0.8$

Number of histories, N	Number of scatters allowed, v	Eq.	ω	$\sigma(\omega)$
10,000	6	(30)	0.8004	0.0051
20,000	8	(30)	0.8022	0.0035
40,000	10	(30)	0.8012	0.0025
10,000	6	(32)	0.8090	0.0060
20,000	8	(32)	0.8004	0.0040
40,000	10	(32)	0.8003	0.0029

We note that all but one of the calculated values of ω are within the indicated standard deviations of the true value, $\omega = 0.8$. Further, it is apparent that the calculated standard deviations, $\sigma(\omega)$, vary approximately as $1/\sqrt{N}$, as expected. Interestingly, although the direct simulations for the transmission are more precise than those for the albedo, the inverse calculations for ω using the albedo are more precise than those using the transmission. This occurs because the sensitivity of Eq. (30), $dA/d\omega$, is sufficiently greater than that of Eq. (32), $dB/d\omega$, for the case considered. It is also noted that although this was a rather simple example, extensions to more complicated geometries or to nonuniform boundary conditions, which may pose significant problems for traditional inverse approaches, present only technical difficulties for the Monte Carlo method.

A second example, similar to one posed by Chahine [11], is considered in order to demonstrate a multivariable inversion. Here, the problem is posed and solved in a strictly mathematical sense, without considering a specific physical process. We assume f satisfies

$$I(v) = \int_0^1 H(x - v) f(x)\, dx, \qquad v \in [0, 1), \tag{33}$$

where $H(x - v)$ is the unit step function,

$$\begin{aligned} H(x - v) &= 0, \qquad x < v, \\ &= 1, \qquad x \geqslant v. \end{aligned} \tag{34}$$

We further assume f has the step-wise form

$$\begin{aligned} f(x) = \alpha_1, &\qquad x \in \Delta_1 = [0, 0.2), \\ \alpha_2, &\qquad x \in \Delta_2 = [0.2, 0.4), \\ \alpha_3, &\qquad x \in \Delta_3 = [0.4, 0.8), \\ \alpha_4, &\qquad x \in \Delta_4 = [0.8, 1), \\ 0, &\qquad \text{otherwise.} \end{aligned} \tag{35}$$

Then, given "measurements"

$$\begin{aligned} \bar{I}(0) &= 1, \\ \bar{I}(0.2) &= 0.92, \\ \bar{I}(0.4) &= 0.76, \end{aligned}$$

and

$$\bar{I}(0.8) = 0.08, \tag{36}$$

we seek to obtain the α_i. The solution is easily obtained by standard techniques and is seen to be

$$\begin{aligned} \alpha_1 &= 0.4, \\ \alpha_2 &= 0.8, \\ \alpha_3 &= 1.7, \\ \alpha_4 &= 0.4. \end{aligned} \tag{37}$$

We wish to demonstrate the inverse Monte Carlo principle for a four-dimensional inversion by attempting to retrieve these parameters. We begin by sampling from the unit rectangular pdf

$$\begin{aligned} f^*(x) &= 1, \qquad x \in [0, 1), \\ &= 0, \qquad \text{otherwise}, \end{aligned} \tag{38}$$

which is defined over the appropriate interval, [0, 1). Then, we construct Monte Carlo estimates, $\hat{I}$, of $\bar{I}$ each of the form

$$\hat{I}_j = \frac{1}{N} \sum_{i=1}^{N} H(\xi_i - v_j) f(\xi_i), \qquad j = 1, 2, 3, 4, \tag{39}$$

where the ξ_i are sampled from f^* and the v_j assume the values

$$\begin{aligned} v_1 &= 0, \\ v_2 &= 0.2, \\ v_3 &= 0.4, \\ v_4 &= 0.8. \end{aligned} \tag{40}$$

Substituting $\bar{I}$ for $\hat{I}$, we obtain

$$\bar{I} = \mathbf{A}\boldsymbol{\alpha}, \tag{41}$$

where

$$\mathbf{A} = (a_{ji})_{4 \times 4}, \tag{42}$$

$$a_{ji} = \frac{1}{N} \sum_{k=1}^{N_i} H(\xi_k - v_j), \tag{43}$$

and N_i is the number of sampled values, ξ_i, within Δ_i, where the Δ_i are defined in Eq. (35).

The solution of Eq. (41) is easily obtained by matrix inversion. The results of a sequence of simulations employing increasing sample populations, N, are given in Table II and show clearly the convergence toward the true pdf. For the calculation of

TABLE II

Retrieval of Step-wise PDF Parameters

Parameter	Number of histories, N			Actual values
	2500	10,000	40,000	
α_1	0.408	0.392	0.418	0.4
$\sigma(\alpha_1)$	0.088	0.046	0.023	—
α_2	0.666	0.803	0.765	0.8
$\sigma(\alpha_2)$	0.101	0.054	0.026	—
α_3	1.74	1.70	1.70	1.7
$\sigma(\alpha_3)$	0.041	0.020	0.010	—
α_4	0.414	0.389	0.405	0.4
$\sigma(\alpha_4)$	0.016	0.008	0.004	—
$\sigma(\boldsymbol{\alpha})$	0.141	0.074	0.036	—

the $\sigma(\alpha_i)$, the true values of α_i were used, since they were known, and the $\sigma[\bar{I}(v_i)]$ were taken to be zero. We note that 8 of the 12 retrieved values (or 67%) were within the indicated standard deviations of the true values, and that the standard deviations vary approximately as $1/\sqrt{N}$, as expected. The $\sigma(\boldsymbol{\alpha})$ were calculated from Eq. (18) with the $w_j = 1$. We also note that since $H(x)$, $H(x-0.2)$, $H(x-0.4)$, and $H(x-0.8)$ form a basis for f, we are able in principle to retrieve f completely, in the limit as $N \to \infty$.

Because the α_i in Table II are only estimates, their substitution into Eq. (35) will not give a properly normalized pdf. The results of applying two normalization schemes to the values obtained in the 40,000-history simulation of Table II are shown in Table III. In the first scheme (S1), the values were simply scaled by the normalization factor 1.0024. In the second scheme (S2), the parameter with the largest standard deviation, α_2, was recalculated by subsituting the retrieved values for the other three parameters into the normalization condition. Regardless of which procedure is preferred, it is clear that the inverse Monte Carlo technique can be applied to the multidimensional retrieval of a pdf.

TABLE III

Normalization of Retrieved Parameters

Parameter	Retrieved values ($N = 40{,}000$)	S1 values	S2 values	True values
α_1	0.418	0.419	0.418	0.400
α_2	0.765	0.767	0.777	0.800
α_3	1.70	1.70	1.70	1.70
α_4	0.405	0.406	0.405	0.400

CONCLUSIONS

Inversion by Monte Carlo need not involve iterative forward solutions of the direct problem as parameters are varied through some search procedure. Instead, a system of equations can be developed in terms of the desired parameters using only one direct simulation in which an arbitrary pdf is sampled in place of the unknown one. Thus, there are an infinite number of inverse formulations possible, as determined by the specific pdf employed in the importance sampling scheme. Undoubtedly, certain choices will lead to more well-behaved systems than others, for a given number of histories in the forward simulation.

In radiation applications, for example, it is usually possible to write the appropriate radiative transfer or radiation transport equations and boundary or initial conditions, although it is often difficult to solve them analytically. Monte Carlo simulation provides a way to construct "solutions" to either the direct or inverse problem. Given the phase function (the pdf describing the radiation scattering) one can simulate to obtain estimates of the radiation flux or intensity; alternatively, given measurements of the intensity or related quantities one can sample from an arbitrary phase function to construct a system of equations which can be solved to obtain estimates of parameters of the true phase function.

This inverse Monte Carlo technique is general, in that it can be applied to any problem which can be adequately posed and for which the physical data are available. In this sense, it allows the simulation of experiments which might be expensive, time-consuming, or too idealized to run in the laboratory or in the field. Hence, the inverse Monte Carlo approach can be used to lead the experimenter toward optimal experiment design. Another aspect of its generality is the fact that, in principle at least, it can be applied where the physical experiment is constrained to conditions for which an analytic inverse model is difficult to develop. Thus, it can be matched to the physical situation. The inverse Monte Carlo method is also selective, since it can be used to study particular aspects of a problem, the effects of which might not be easily isolated experimentally. Thus, for instance, the portion of a response coming from a particular region of parameter space can be identified by suitable scoring of a simulation, even if separation of the response into components might be difficult experimentally.

The simple examples considered demonstrate the principle for single-dimensional and multidimensional retrievals. Clearly, extension to higher dimensionality is straightforward, though perhaps cumbersome in some cases. It is realized that inverse Monte Carlo will not be the universally preferred technique and that other inverse formulations will prove preferable in certain circumstances. However, this technique does provide a means of generating an invertible system of equations in a single-step direct simulation, and does provide an approach which may prove useful when other formulations fail, are suspect, or are difficult to apply.

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