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Short note

Monte Carlo efficiency improvement by multiple sampling of conditioned integration variables

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ABSTRACT

We present a technique that permits to increase the efficiency of multidimensional Monte Carlo algorithms when the sampling of the first, unconditioned random variable consumes much more computational time than the sampling of the remaining, conditioned random variables while its variability contributes only little to the total variance. This is in particular relevant for transport problems in complex and randomly distributed geometries. The proposed technique is based on an new Monte Carlo estimator in which the conditioned random variables are sampled more often than the unconditioned one. A significant contribution of the present Short Note is an automatic procedure for calculating the optimal number of samples of the conditioned random variable per sample of the unconditioned one. The technique is illustrated by a current research example where it permits to increase the efficiency by a factor 100.

1. Introduction

Monte Carlo integration is used in many research fields (*e.g.* radiation transport physics, quantum mechanics, financial computing [1,2]) to evaluate multidimensional integrals that can be written as the expectation $\mathcal{A}$ of a random variable W:

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$$\mathcal{A} = E[W] = \int_{\mathcal{D}_X} dx\, p_X(x) \int_{\mathcal{D}_Y(x)} dy\, p_Y(y;x)\, \hat{w}(x,y) \tag{1}$$

where X and Y are (vector) random variables (defined by their domains $\mathcal{D}_X$ and $\mathcal{D}_Y(x)$ as well as their associated probability densities p_X and $p_Y(y;x)$), and W is the random variable defined by the function $\hat{w}$ that to X and Y associates $W = \hat{w}(X,Y)$. Monte Carlo integration permits to evaluate an unbiased estimator of $\mathcal{A}$ by sampling n independent and identically distributed (IID) random variables X_i and Y_i (where all the X_i are IID as X, and all the $Y_i(x)$ are IID as $Y(x)$). The plain Monte Carlo estimator A_n is defined by

$$\mathcal{A} = E[A_n] \text{ with } A_n = \frac{1}{n}\sum_{i=1}^{n} \hat{w}(X_i, Y_i). \tag{2}$$

The practical use of Monte Carlo integration is sometimes limited by the prohibitive computational cost required to obtain an estimate with the required precision (the standard deviation σ_{A_n} of the Monte Carlo estimate being inverse proportional to $\sqrt{n}$). This has motivated research to increase the efficiency, which is a quality measure for a Monte Carlo estimator taking into account both its precision and its computational cost [3]:

$$\epsilon_{A_n} = \frac{1}{\sigma^2_{A_n} C_{A_n}} \tag{3}$$

where $\sigma^2_{A_n}$ is the variance of A_n, and C_{A_n} the computational cost required to calculate A_n. Depending on the specific problem, several variance reduction techniques might permit to increase the efficiency (*e.g.*, importance sampling, stratified sampling, control variates and antithetic sampling [2]). The present Short Note presents a technique that increases the Monte Carlo efficiency for problems where the sampling of the unconditioned random variable X is computationally expensive (compared to the sampling of the conditioned random variable Y) whereas the variability of X contributes only little to the variance of W (compared to the variability of Y). This will be quantified in Sec. 2. Such a situation is encountered, *e.g.*, in transport problems in complex geometries where the geometry is statistically distributed (see Sec. 3 for a practical example). The principle is to consider a new Monte Carlo estimator in which Y is sampled more often than X. To our knowledge, despite the simplicity of this technique, it has never been explicitly reported in the Monte Carlo literature. Its formal investigation in the present Short Note permits us in particular to provide an easy-to-implement procedure to automatically compute the optimal number of samples of Y per sample of X (at the end of Sec. 2).

2. Efficiency-optimized Monte Carlo algorithm

We propose to use the new estimator A_{n,n_Y} of $\mathcal{A}$ defined by

$$\mathcal{A} = E[A_{n,n_Y}] \text{ with } A_{n,n_Y} = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{n_Y}\sum_{j=1}^{n_Y} \hat{w}(X_i, Y_{ij}). \tag{4}$$

where all the $Y_{ij}(x)$ are IID as $Y_i(x)$. A_{n,n_Y} is indeed an estimator of $\mathcal{A}$ since $E[\hat{w}(X_i,Y_{ij})] = E[\hat{w}(X_i,Y_i)]$ for all j. Note that the plain Monte Carlo estimator A_n corresponds to $n_Y = 1$ in Eq. (4). The Monte Carlo algorithm corresponding to Eq. (4) is:

1. repeat n times (for i from 1 to n):
   (a) realize a sample x_i of X_i;
   (b) repeat n_Y times (for j from 1 to n_Y):
      i. realize a sample y_{ij} of Y_{ij};
      ii. calculate $\hat{w}_{ij} = \hat{w}(x_i, y_{ij})$;
   (c) calculate the Monte Carlo weight $\hat{f}_i = \frac{1}{n_Y}\sum_{j=1}^{n_Y} \hat{w}_{ij}$;
2. calculate the Monte Carlo estimate $a_{n,n_Y} = \frac{1}{n}\sum_{i=1}^{n} \hat{f}_i$ and the standard error $\sigma_{A_{n,n_Y}} = \frac{1}{\sqrt{n-1}}\sqrt{\frac{1}{n}\sum_{i=1}^{n}\hat{f}_i^2 - \left(\frac{1}{n}\sum_{i=1}^{n}\hat{f}_i\right)^2}$.

Let us now determine the efficiency increase permitted by this technique. Therefore we first have to express the contributions of X and Y to the total variance $\sigma^2_{A_{n,n_Y}}$ and the total computational cost $C_{A_{n,n_Y}}$ of the proposed Monte Carlo estimator A_{n,n_Y}. Denoting $\sigma^2_X = Var_X[E_Y[W|X]]$ the explained variance (which is the contribution of X) and $\tilde{\sigma}^2_Y = E_X[Var_Y[W|X]]$ the unexplained variance (which is the contribution of Y) of the random variable W, and then applying successively the law of total variance and the Lindeberg–Levy central limit theorem, leads to

$$\sigma^2_{A_{n,n_Y}} = \frac{1}{n}\left(\sigma^2_X + \frac{1}{n_Y}\tilde{\sigma}^2_Y\right). \tag{5}$$