AN EXPLICIT FORMULATION OF THE GENERALIZED ANTITHETIC TRANSFORMATION FOR MONTE CARLO INTEGRATION

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ABSTRACT

The method of "antithetic variates" for Monte Carlo sampling was invented by Hammersley and Morton, and has been generalized by Halton and Handscomb, and by Laurent, who described the most economical general transformations without giving their explicit forms (except for a few of the simplest cases). The present paper gives a derivation of the full explicit forms of the Laurent transforms of any order.

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We consider the evaluation of an integral of the form

$$\theta = \int_0^1 f(x)\, dx \qquad (1)$$

by Monte Carlo sampling[3]. If ξ denotes a *canonical random variable* (that is, a random variable distributed with uniform probability density in the unit interval $U = [0, 1)$), then *crude Monte Carlo* consists in sampling the (*primary*) estimator $f(\xi)$, which, by repeated independent trials, yields the (*secondary*) estimate

$$\psi_k(\xi_1, \xi_2, \ldots, \xi_k) = \frac{1}{k} \sum_{i=1}^{k} f(\xi_i); \qquad (2)$$

and, since the expectations are

$$E[\psi_k] = E[f] = \theta, \qquad (3)$$

Kolmogorov's form of the Strong Law of Large Numbers[2] shows that

$$\psi_k \to \theta \text{ (almost surely) as } k \to \infty. \qquad (4)$$

If we further suppose that the integral

$$\int_0^1 f(x)^2\, dx = \theta^2 + \mathrm{var}[f] \qquad (5)$$

exists, then the variance

$$\mathrm{var}[\psi_k] = \mathrm{var}[f]/k \to 0 \text{ as } k \to \infty. \qquad (6)$$

Results such as Chebyshev's inequality and the Central Limit Theorem indicate a probable rate of convergence of ψ_k of the order of the standard deviation, $\surd(\mathrm{var}[f]/k)$, and the slow decrease of this quantity with k has spurred much effort to reduce the basic variance factor $\mathrm{var}[f]$, arising from the observation that the answer θ may be obtained equally well by replacing the function f by any other function g, so long as

$$\int_0^1 g(x)\ dx = \int_0^1 f(x)\ dx = \theta. \tag{7}$$

Much ingenuity has been devoted to devising techniques for transforming functions f into functions g so as to reduce the variance factor var$[g]$ appreciably while preserving the integral θ. One such technique is that of *antithetic variates*, devised by Hammersley and Morton[5] and developed and generalized by Halton and Handscomb[4] and by Laurent[7]. Basically, this involves the construction of relatively simple transformations of the form (linear in f)

$$\underline{\underline{A}}f(x) = \sum_{m=0}^{n-1} \kappa_m f(\lambda_m + \mu_m x), \tag{8}$$

and sampling the primary estimator $\underline{\underline{A}}f(\xi)$ in repeated trials to yield the secondary estimate

$$\underline{\underline{A}}^k\psi_k(\xi_1, \xi_2, \ldots, \xi_k) = \frac{1}{k}\sum_{i=1}^{k} \underline{\underline{A}}f(\xi_i). \tag{9}$$

In order that

$$\underline{\underline{A}}^k\psi_k \to \theta \text{ (a. s.) as } k \to \infty. \tag{10}$$

it is necessary and sufficient that

$$\mathrm{E}[\underline{\underline{A}}^k\psi_k] = \mathrm{E}[\underline{\underline{A}}f] = \theta; \tag{11}$$

and this is achieved when

$$\sum_{m=0}^{n-1} \kappa_m \int_0^1 f(\lambda_m + \mu_m x)\ dx = \sum_{m=0}^{n-1} \frac{\kappa_m}{\lambda_m} \int_{\lambda_m}^{\lambda_m+\mu_m} f(y)\ dy = \theta. \tag{12}$$

In particular, all these authors consider the transformations (which satisfy (8) and (12))

$$\underline{\underline{D}}f(x) = \frac{1}{2}[f(x) + f(1 - x)] \tag{13}$$

and

$$\underline{\underline{U}}_n f(x) = \frac{1}{n}\sum_{m=0}^{n-1} f\left(\frac{x + m}{n}\right); \tag{14}$$

and they prove that

$$\mathrm{var}[\underline{\underline{U}}_n f] = \sum_{r,s\geq 0} \frac{(-1)^r \Delta_r \Delta_s B_{r+s+2}}{(r+s+2)!\ n^{r+s+2}} = \frac{\Delta_0^2}{12n^2} + \frac{\Delta_1^2 - 2\Delta_0\Delta_2}{720\ n^4} + \frac{\Delta_2^2 - 2\Delta_1\Delta_3 + 2\Delta_0\Delta_4}{30240\ n^6} + \ldots, \tag{15}$$

where the B_m are the Bernoulli numbers[1] and

$$\Delta_j = \Delta_j f = f^{(j)}(1) - f^{(j)}(0), \quad f^{(j)}(x) = \frac{d^j f}{dx^j}. \tag{16}$$

It is clear from (15) that $\text{var}[\underline{\underline{U}}_n f] = \underline{O}(n^{-2M})$ if we can arrange that

$$\Delta_j = 0 \text{ for } j = 0, 1, 2, \ldots, M - 1. \tag{17}$$

Halton and Handscomb[4] observed that, since

$$\Delta_j \underline{\underline{D}} f = \frac{1}{2}[1 - (-1)^j]\Delta_j f \quad [=0 \text{ if } j \text{ is even}] \tag{18}$$

and
$$\Delta_j \underline{\underline{U}}_n f = n^{-j-1}\, \Delta_j f, \tag{19}$$

the condition (17) can be achieved by a preliminary transformation of f consisting of the successive application of linear combinations of the $\underline{\underline{U}}_n$ and of $\underline{\underline{D}}$. Laurent[7] [who gives (18) with an incorrect coefficient; but this is unimportant] saw that much simpler transformations than those of Halton and Handscomb would suffice; namely,

$$\underline{\underline{H}}_M f = \sum_{m=1}^{M+1} \alpha_m \underline{\underline{U}}_m f \quad \text{and} \quad \underline{\underline{K}}_{2N+1} f = \sum_{n=1}^{N+1} \beta_n \underline{\underline{U}}_n \underline{\underline{D}} f. \tag{20}$$

However, he does not explicitly obtain the coefficients α_m and β_n, except in a few of the simplest cases. The purpose of this note is to supply the full solution. It then becomes possible to compute $g(\xi) = \underline{\underline{U}}_n \underline{\underline{H}}_M f(\xi)$ or $g'(\xi) = \underline{\underline{U}}_n \underline{\underline{K}}_M f(\xi)$, so that $\text{var}[g]$ or $\text{var}[g']$ is $\underline{O}(n^{-2M})$ yielding accurate secondary estimates with very few repeated trials.

Since $\underline{\underline{D}}$ and $\underline{\underline{U}}_n$ satisfy (11), (18), and (19), we see from (20) that (11) and (17) will apply to $\underline{\underline{H}}_M$ and $\underline{\underline{K}}_{2N+1}$ if the coefficients α_m and β_n satisfy the equations

$$\sum_{m=1}^{M+1} m^{-i}\alpha_m = \delta_{i0} \quad \text{and} \quad \sum_{n=1}^{N+1} n^{-2j}\beta_n = \delta_{j0}; \tag{21}$$

with $i = 0, 1, 2, \ldots, M$; $j = 0, 1, 2, \ldots, N$; and $\delta_{k0} = 1$ if $k = 0$ and $= 0$ otherwise. Let us define the Vandermonde determinant[6]

$$\phi_{rst}(x) = \begin{vmatrix} 1 & 1 & \dots & 1 & 1 & 1 & \dots & 1 \\ 1 & 2^{-t} & \dots & (r-1)^{-t} & x & (r+1)^{-t} & \dots & (s+1)^{-t} \\ 1 & 2^{-2t} & \dots & (r-1)^{-2t} & x^2 & (r+1)^{-2t} & \dots & (s+1)^{-2t} \\ & & \dots & & \dots & & \dots & \\ 1 & 2^{-st} & \dots & (r-1)^{-st} & x^s & (r+1)^{-st} & \dots & (s+1)^{-st} \end{vmatrix}$$

Then it is clear that, by Cramer's rule, the solutions of the equations (21) are, respectively,

$$\alpha_m = \phi_{mM1}(0)/\phi_{mM1}(m^{-1}) \quad \text{and} \quad \beta_n = \phi_{nN2}(0)/\phi_{nN2}(n^{-2}). \qquad (23)$$

But we note that $\phi_{rst}(x)$ is a polynomial in x of degree s, which vanishes when $x = 1, 2^{-t}, \dots, (r-1)^{-t}, (r+1)^{-t}, \dots, (s+1)^{-t}$; whence, for some C_{rst} independent of x,

$$\phi_{rst}(x) = C_{rst}(x-1)(x-2^{-t})\dots[x-(r-1)^{-t}][x-(r+1)^{-t}] \dots[x-(s+1)^{-t}]; \qquad (24)$$

and therefore, by (23), we get, after a little simplification, that

$$\alpha_m = (-1)^{M-m+1}\, m^M \,/\, (m-1)!\,(M-m+1)! \qquad (25)$$

$$\beta_n = 2\,(-1)^{N-n+1}\, n^{2N+2} \,/\, (N-n+1)!\,(N+n+1)! \qquad (26)$$

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