Letter to the Editor

Note on Prediction of Monte Carlo Errors

In a recent paper by Amster and Djomehri,[1] a coupled integral equation system was derived concerning the various moments of the score due to a particle starting a flight at a given phase-space point in a Monte Carlo transport calculation. In a subsequent paper, Booth and Amster[2] generalized the results of Ref. 1 to treat track-length estimators. The results of these papers are very likely among the most important recent developments in Monte Carlo theory, giving an efficient tool for variance study of Monte Carlo estimation methods.

The purpose of this Letter is to give a slightly more general formulation of equations derived in Refs. 1 and 2. Furthermore, an equation system "dual" to those given in Refs. 1 and 2 is derived. This system determines the various moments of the total score due to a particle entering a collision at a given phase-space point. Simple relations between the score moments defined in Refs. 1 and 2 and here are also established. It seems that this dual formalism is convenient in variance analysis of nonanalog games with scattering kernel biasing.

Although the results of Ref. 1 were derived for analog games, any nonanalog game being governed by positive kernels, normalized to quantities less than or equal to unity, may also be described by the resulting Eqs. (12), (13), and (14) of Ref. 1 or Eqs. (13), (14), and (15) of Ref. 2 as an analog game. The same applies to the equations derived below. In the following, the notations of Ref. 1 are used.

In Ref. 1, $p_A(\mathbf{P},s)ds$ and $p_s(\mathbf{P},s)ds$ denote the probability of a score in ds about s due to absorption and scattering at $\mathbf{P}$, respectively. In addition to these, we introduce two more probability density functions. Let $p_E(\mathbf{P},s)ds$ be the probability that the score from an endless free flight starting from $\mathbf{P}$ will be in ds about s, as also defined in Ref. 2. Furthermore, let $p_t(\mathbf{P},\mathbf{P}',s)ds$ be the probability that the score from a flight between $\mathbf{P}$ and $\mathbf{P}'$ will be in ds about s. In the generalized theory of Ref. 2, $p_s(\mathbf{P},s)$ and $p_A(\mathbf{P},s)$ are replaced by $p_s(\mathbf{P},\mathbf{P}',s)$ and $p_A(\mathbf{P},\mathbf{P}',s)$, respectively, depending on the coordinates of two successive collision points. In most practical cases, these probabilities completely describe the score distribution. However, using estimators proposed in Ref. 3 (where scattering and absorption in a given region and collisionless passage through it result in different scores), our more detailed description may be advantageous. On the other hand, this finer distinction in the score probabilities is necessary in the derivation of dual equations below.

Let $\psi(\mathbf{P},s)ds$ and $\chi(\mathbf{P},s)ds$ be the probabilities that a particle starting a flight at $\mathbf{P}$, and entering a collision at $\mathbf{P}$, respectively, will yield a total score in ds about s. Following the train of thought of Ref. 1, we obtain the equations

$$\begin{aligned}\psi(\mathbf{P},s) = {} & \left[1 - \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')\right]p_E(\mathbf{P},s) \\ & + \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')p_t(\mathbf{P},\mathbf{P}',s)*p_A(\mathbf{P}',s) \\ & \times\left[1 - \int d\mathbf{P}''E(\mathbf{P}',\mathbf{P}'')\right] \\ & + \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')\int d\mathbf{P}''E(\mathbf{P}',\mathbf{P}'') \\ & \times p_t(\mathbf{P},\mathbf{P}',s)*p_s(\mathbf{P}',s)*\psi(\mathbf{P}'',s) \end{aligned} \tag{1}$$

and

$$\begin{aligned}\chi(\mathbf{P},s) = {} & [1 - d\mathbf{P}'E(\mathbf{P},\mathbf{P}')]p_A(\mathbf{P},s) \\ & + \int d\mathbf{P}'E(\mathbf{P},\mathbf{P}')p_s(\mathbf{P},s)*p_E(\mathbf{P}',s) \\ & \times [1 - d\mathbf{P}''C(\mathbf{P}',\mathbf{P}'')] \\ & + \int d\mathbf{P}'E(\mathbf{P},\mathbf{P}')\int d\mathbf{P}''C(\mathbf{P}',\mathbf{P}'') \\ & \times p_s(\mathbf{P},s)*p_t(\mathbf{P}',\mathbf{P}'',s)*\chi(\mathbf{P}'',s) \quad , \end{aligned} \tag{2}$$

where

$$f(.,s)*g(.,s) = \int_{-\infty}^{\infty} ds'f(.,s')g(.,s - s') \tag{3}$$

is the convolution integral. It is heuristically obvious but it can also be derived from Eqs. (1) and (2) that the following relationship holds between the densities ψ and χ:

$$\begin{aligned}\psi(\mathbf{P},s) = {} & \left[1 - \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')\right]p_E(\mathbf{P},s) \\ & + \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')p_t(\mathbf{P},\mathbf{P}',s)*\chi(\mathbf{P}',s) \quad , \end{aligned} \tag{4}$$

while

$$\begin{aligned}\chi(\mathbf{P},s) = {} & \left[1 - \int d\mathbf{P}'E(\mathbf{P},\mathbf{P}')\right]p_A(\mathbf{P},s) \\ & + \int d\mathbf{P}'E(\mathbf{P},\mathbf{P}')p_s(\mathbf{P},s)*\psi(\mathbf{P}',s) \quad . \end{aligned} \tag{5}$$

Let $M_r(\mathbf{P})$ and $N_r(\mathbf{P})$, (r = 0, 1, . . .) be the r'th moments of the total scores corresponding to the density functions $\psi(\mathbf{P},s)$ and $\chi(\mathbf{P},s)$, respectively. Multiplying Eqs. (1) and (2) by s^r and integrating over s from $-\infty$ to $+\infty$ [with $M_0(\mathbf{P}) = N_0(\mathbf{P}) \equiv 1$] yields

$$\begin{aligned}M_r(\mathbf{P}) = {} & \left[1 - \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')\right]\int_{-\infty}^{\infty} s^r p_E(\mathbf{P},s)ds \\ & + \int d\mathbf{P}'C(\mathbf{P},\mathbf{P}')\int_{-\infty}^{\infty} s^r[p_t(\mathbf{P},\mathbf{P}',s)*p_A(\mathbf{P}',s)]ds \\ & \times\left[1 - \int d\mathbf{P}''E(\mathbf{P}',\mathbf{P}'')\right] + \sum_{n=0}^{r}\binom{r}{n}\int d\mathbf{P}'C(\mathbf{P},\mathbf{P}') \\ & \times\int_{-\infty}^{\infty} s^{r-n}[p_t(\mathbf{P},\mathbf{P}',s)*p_s(\mathbf{P}',s)]ds \\ & \times\int d\mathbf{P}''E(\mathbf{P}',\mathbf{P}'')M_n(\mathbf{P}'') \end{aligned} \tag{6}$$

[1] H. J. AMSTER and M. J. DJOMEHRI, *Nucl. Sci. Eng.*, **60**, 131 (1976).
[2] T. E. BOOTH and H. J. AMSTER, *Nucl. Sci. Eng.*, **65**, 273 (1978).
[3] E. M. GELBARD, L. A. ONDIS II, and J. SPANIER, *SIAM J. Appl. Math.*, **14**, 697 (1966).

and

$$N_r(\boldsymbol{P}) = \left[1 - \int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}')\right]\int_{-\infty}^{\infty} s^r p_A(\boldsymbol{P},s)ds + \int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}')\int_{-\infty}^{\infty} s^r[p_s(\boldsymbol{P},s)*p_E(\boldsymbol{P}',s)]\,ds \times\left[1 - \int d\boldsymbol{P}''C(\boldsymbol{P}',\boldsymbol{P}'')\right] + \sum_{n=0}^{r}\binom{r}{n}\int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}') \times\int d\boldsymbol{P}''C(\boldsymbol{P}',\boldsymbol{P}'')\int_{-\infty}^{\infty} s^{r-n}[p_s(\boldsymbol{P},s)*p_t(\boldsymbol{P}',\boldsymbol{P}'',s)] \times ds N_n(\boldsymbol{P}'') \quad . \tag{7}$$

In derivation of Eqs. (6) and (7), we have made use of the identity

$$\int_{-\infty}^{\infty} s^r[f(.,s)*g(.,s)]ds = \sum_{n=0}^{r}\binom{r}{n}\left[\int_{-\infty}^{\infty} s^{r-n}f(.,s)ds\right] \times\left[\int_{-\infty}^{\infty} s^n g(.,s)ds\right] \quad .$$

It can be seen from Eq. (6) that the scattering and absorption score densities of Ref. 2 are related to our densities according to the relations

$$p_s(\boldsymbol{P},\boldsymbol{P}',s) = p_t(\boldsymbol{P},\boldsymbol{P}',s)*p_s(\boldsymbol{P}',s)$$

and

$$p_A(\boldsymbol{P},\boldsymbol{P}',s) = p_t(\boldsymbol{P},\boldsymbol{P}',s)*p_A(\boldsymbol{P}',s) \quad .$$

According to Eqs. (4) and (5), the moments M_r and N_r are related as

$$M_r(\boldsymbol{P}) = \left[1 - \int d\boldsymbol{P}'C(\boldsymbol{P},\boldsymbol{P}')\right]\int_{-\infty}^{\infty} s^r p_E(\boldsymbol{P},s)ds + \sum_{n=0}^{r}\binom{r}{n}\int d\boldsymbol{P}'C(\boldsymbol{P},\boldsymbol{P}') \times\int_{-\infty}^{\infty} s^{r-n}p_t(\boldsymbol{P},\boldsymbol{P}',s)ds N_n(\boldsymbol{P}') \quad , \tag{8}$$

while

$$N_r(\boldsymbol{P}) = \left[1 - \int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}')\right]\int_{-\infty}^{\infty} s^r p_A(\boldsymbol{P},s)ds + \sum_{n=0}^{r}\binom{r}{n}\int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}') \times\int_{-\infty}^{\infty} s^{r-n}p_s(\boldsymbol{P},s)ds M_n(\boldsymbol{P}') \quad . \tag{9}$$

In the case when the scores are deterministic, i.e., if

$$p_k(\boldsymbol{P},s) = \delta[s - f_k(\boldsymbol{P})] \quad , \quad (k = E,A,s) \quad ,$$
$$p_t(\boldsymbol{P},\boldsymbol{P}',s) = \delta[s - f_t(\boldsymbol{P},\boldsymbol{P}')] \quad ,$$

then Eqs. (8) and (9) become

$$M_r(\boldsymbol{P}) = \left[1 - \int d\boldsymbol{P}'C(\boldsymbol{P},\boldsymbol{P}')\right]f_E^r(\boldsymbol{P}) + \int d\boldsymbol{P}'C(\boldsymbol{P},\boldsymbol{P}') \times[f_t(\boldsymbol{P},\boldsymbol{P}') + f_A(\boldsymbol{P}')]^r\left[1 - \int d\boldsymbol{P}''E(\boldsymbol{P}',\boldsymbol{P}'')\right] + \sum_{n=0}^{r}\binom{r}{n}\int d\boldsymbol{P}'C(\boldsymbol{P},\boldsymbol{P}')\,[f_t(\boldsymbol{P},\boldsymbol{P}') + f_s(\boldsymbol{P}')]^{r-n} \times\int d\boldsymbol{P}''E(\boldsymbol{P}',\boldsymbol{P}'')M_n(\boldsymbol{P}'') \tag{10}$$

and

$$N_r(\boldsymbol{P}) = \left[1 - \int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}')\right]f_A^r(\boldsymbol{P}) + \int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}') \times[f_s(\boldsymbol{P}) + f_E(\boldsymbol{P}')]^r\left[1 - \int d\boldsymbol{P}''C(\boldsymbol{P}',\boldsymbol{P}'')\right] \times\sum_{n=0}^{r}\binom{r}{n}\int d\boldsymbol{P}'E(\boldsymbol{P},\boldsymbol{P}')\int d\boldsymbol{P}''C(\boldsymbol{P}',\boldsymbol{P}'') \times[f_s(\boldsymbol{P}) + f_t(\boldsymbol{P}',\boldsymbol{P}'')]^{r-n}N_n(\boldsymbol{P}'') \quad . \tag{11}$$

Equations (6) and (10) are slightly generalized forms of Eqs. (13) and (55) of Ref. 1 and Eqs. (13), (14), and (15) of Ref. 2. Equations (7) and (11) together with relation (8) may be advantageous in the efficiency study of nonanalog games with scattering kernel biasing. For example, in the MELP method,[4] the score densities are

$$p_s(\boldsymbol{P},s) = p_A(\boldsymbol{P},s) = \delta(s)$$

and

$$p_t(\boldsymbol{P},\boldsymbol{P}',s) = p_E(\boldsymbol{P},s) = \delta[s + f(\boldsymbol{P}) + f(\overline{\boldsymbol{P}}) - 1] \quad , \tag{12}$$

with

$$\overline{\boldsymbol{P}} = T(\boldsymbol{P}) \quad , \quad 0 \le f(\boldsymbol{P}) \le \frac{1}{2} \quad ,$$

where T is a transformation of the phase space. (In Ref. 4, T is the inversion of the particle's direction.) Denoting the unbiased and biased scattering kernels by $E(\boldsymbol{P},\boldsymbol{P}')$ and $\hat{E}(\boldsymbol{P},\boldsymbol{P}')$, respectively, the following relation holds[4]:

$$\hat{E}(\boldsymbol{P},\boldsymbol{P}') = 2E(\boldsymbol{P},\boldsymbol{P}')f(\boldsymbol{P}')/[f(\boldsymbol{P}') + f(\overline{\boldsymbol{P}}')] \quad , \tag{13}$$

provided that transformation T in Eq. (12) is such that

$$E(\boldsymbol{P},\boldsymbol{P}') = E(\boldsymbol{P},\boldsymbol{P}') \quad .$$

If $C(\boldsymbol{P}',\boldsymbol{P}'')$ is the unbiased transport kernel, the biased kernel has the form[4]

$$\hat{C}(\boldsymbol{P}',\boldsymbol{P}'') = C(\boldsymbol{P}',\boldsymbol{P}'')/2f(\boldsymbol{P}') \quad . \tag{14}$$

The weight of a particle at $\boldsymbol{P}''$ scattering at $\boldsymbol{P}$ with a weight of unity will be[4]

$$w(\boldsymbol{P}'') = f(\boldsymbol{P}') + f(\overline{\boldsymbol{P}}') \quad . \tag{15}$$

Expressions (13), (14), and (15) can easily be introduced into an equation of the form of Eq. (11) concerning the biased game[5] to compare the score moments with those of the corresponding unbiased game, whereas a similar insertion into Eq. (10) leads to an equation containing the values of $f(\boldsymbol{P})$ at different arguments.

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[4] H. BORGWALDT, "Comparison of Three Methods to Control the Leakage of Particles in a Monte Carlo Game," *Proc. Conf. Developments in Reactor Mathematics and Applications*, CONF-710302, Vol. I, p. 857, U.S. Atomic Energy Commission (1971).

[5] I. LUX, "Systematic Study of Some Standard Variance Reduction Techniques," to be published in *Nucl. Sci. Eng.*