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QUOTA SAMPLING AND IMPORTANCE FUNCTIONS IN STOCHASTIC SOLUTION OF PARTICLE PROBLEMS

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QUOTA SAMPLING AND IMPORTANCE FUNCTIONS IN STOCHASTIC SOLUTION OF PARTICLE PROBLEMS

G. Goertzel

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A B S T R A C T

In section 1 a general stochastic particle problem is defined. Section 3 defines a quota sampling method available for simplifying the solution of such a problem. In section 4 an importance function, $Q(\alpha)$ is defined such that if it were known and could be used in the quota sampling, the solution of the stochastic problem is greatly reduced in difficulty. Thus any function $q(\alpha)$, used in quota sampling should be selected to represent $Q(\alpha)$ as closely as one's knowledge permits.

In section 5 it is shown how to set up a pair of problems, such that the solution of each is the importance function for solving the other. Thus $Q(\alpha)$ may be estimated stochastically.

QUOTA SAMPLING AND IMPORTANCE FUNCTIONS IN STOCHASTIC SOLUTION OF PARTICLE PROBLEMS

G. Goertzel June 21, 1949

NOTE: This document is intended to be a working report for the ORNL Shielding Work Session (Summer 1949) and does not have the complete set of references a final report would have. None-the-less, I feel it desirable to remark that the work herein is a logical continuation of some work of H. Kahn and T. E. Harris (various RAND Reports). Further, many of the thoughts herein arose during conferences between Mr. Kahn and me during the days June 15-17.

1. INTRODUCTION

In studying the motion of many identical particles thru a medium, one may focus one's attention on the coordinates, energy, and direction of velocity of the particle immediately before each collision. The multidimensional space thus set up (axes representing energy, velocity direction, position) is called the phase space of the particle. Points in this phase space will be indicated by α, β, γ, δ, ... and the entire space will be indicated by P.

The description of the physical processes involved is then wholly contained in the functions $P(\alpha, \beta)$ which are so defined that if a particle is at α just before its n'th collision, the probability that it will be in the small volume in phase space $d\beta$ at β just prior to its n+1'st collision is given by $P(\alpha,\beta)d\beta$. It is thus necessary that:

$$\int_P P(\alpha,\beta)d\beta \leq 1$$

where the inequality will hold if any absorption processes occur. If $P(\alpha,D)$ is the probability of absorption in a collision occuring at α, then:

$$\int_P P(\alpha,\beta)d\beta + P(\alpha,D) = 1.$$

The particle source is specified by stating the distribution in phase space of the particle just prior to its first collision, $\psi_1(\alpha)$ ($\int_P \psi_1(\alpha)\, d\alpha = 1$). Letting $\psi_n(\alpha)$ be the distribution of the particles just prior to the n'th collision, one has

$$\psi_{n+1}(\alpha) = \int \psi_n(\beta)\, P(\beta,\alpha)\, d\beta$$

whence, if the collision density is defined as

$$\psi(\alpha) = \sum_{n=1}^{\infty} \psi_n(\alpha)$$

one has

$$\psi_1(\alpha) + \sum_{n=1}^{\infty} \psi_{n+1}(\alpha) = \int_P \sum_{n=1} \psi_n(\beta)\, P(\beta,\alpha)d\beta + \psi_1(\alpha)$$

or

$$\psi(\alpha) = \int_P \psi(\beta)\, P(\beta,\alpha)\, d\beta + \psi_1(\alpha)$$

as the equation for ψ.

Now, one may pose the problem of estimating by stochastic techniques

the quantity

$$I = \int_P \psi(\alpha) \; P(\alpha,D) \quad \rho(\alpha) \, d\alpha$$

where $\psi(\alpha)\, P(\alpha,D)$ is the capture density at α and $\rho(\alpha)$ is a weight assigned to a capture at α.

In order to estimate I stochastically, one may proceed as follows for the i'th particle

(1) select α_1^i from the distribution $\psi_1(\alpha)$

$$\left[\int_P \psi_1(\alpha)\, d\alpha = 1\right]$$

(2) select α_2^i from the distribution $P(\alpha_1^i, \alpha)$, $P(\alpha_1^i, D)$

If D, cease and start again at 1) with $i+1 \rightarrow i$

If not D, to to 3).

.....

n) select α_n^i from the distribution $P(\alpha_{n-1}^i, \alpha)$, $P(\alpha_{n-1}^i, D)$

If D, cease and start again at 1) with $i+1 \rightarrow i$

If not D, go to n+1.

.....

This process is repeated for say N particles. Then, an estimate of I is given by

$$I = \frac{1}{N} \cdot \sum_{i=1}^{N} \rho(\alpha_{n_i}^i)$$

where n_i is the total number of collisions undergone by the i'th particle, so the $\alpha_{n_i}^{i}$ is the point at which the i'th particle is absorbed.

If, however, $\rho(\alpha)$ is of appreciable magnitude only for such α that are large space distances from the points where $\psi_1(\alpha)$ is appreciable, a very small proportion of the points $\alpha_{n_i}^{i}$ will contribute to the estimation of I and the process is extremely inefficient.

To overcome this difficulty a method of quota sampling is introduced, based on an estimation of the Green's function. This is treated below, following a brief Green's function discussion.

2. THE GREEN'S FUNCTION AND ITS ADJOINT

If the particle source $\psi_1(\alpha)$ in the equation

$$\psi(\alpha) = \int_P \psi(\beta)\, P(\beta,\alpha)\, d\beta + \psi_1(\alpha)$$

is taken to be a particle which is born at σ (i.e. which is at σ just before the 1'st collision), one may write for the Green's function of the present problem

$$g(\sigma,\alpha) = \int_P g(\sigma,\beta)\, P(\beta,\alpha)\, d\beta + \delta(\sigma-\alpha);$$

calling $g(\sigma,\alpha)$ a Green's function is justified by the result

$$\psi(\alpha) = \int_P \psi_1(\sigma)\, g(\sigma,\alpha)\, d\sigma.$$

Since $P(\beta,\alpha) \neq P(\alpha,\beta)$ in general,

$$g(\sigma,\alpha) \neq g(\alpha,\sigma).$$

However if an adjoint function is defined

$$g^+(\sigma,\alpha) = \int_P P(\alpha,\beta)\, g^+(\sigma,\beta)\, d\beta + \delta(\alpha-\sigma)$$

one immediately sees, by evaluating $\int g(T,\alpha)\, g^+(\sigma,\alpha)\, d\alpha$ from the defining equation for g and also from that for g^+

$$\int \delta(\alpha-\sigma)\, g(T,\alpha)\, d\alpha = \int \delta(\alpha-T)\, g^+(\sigma,\alpha)\, d\alpha$$

or

$$g(T,\sigma) = g^+(\sigma,T).$$

Clearly the equation for g^+ differs from that for g in that

$$P(\alpha,\beta) \neq P(\beta,\alpha).$$

3. QUOTA SAMPLING

The stochastic procedure of the end of section 1 may be modified as follows. An arbitrary function $q(\alpha)$ is introduced. In the work below it is given physical meaning, but for the present q is of purely formal significance. The weight $W(\alpha,\beta)$ is defined as

$$W_o(\alpha) = \int \frac{\psi_1(\gamma)\, q(\gamma)\, d\gamma}{q(\alpha)}$$

$$W(\alpha,\beta) = \int \frac{P(\alpha,\gamma)\, q(\gamma)\, d\gamma + P(\alpha,D)\, \rho(\alpha)}{q(\beta)}$$

$$W(\alpha,D) = \int \frac{P(\alpha,\gamma)\, q(\gamma)\, d\gamma + P(\alpha,D)\, \rho(\alpha)}{\rho(\alpha)}$$

If then

$$\tilde{\psi}_1(\alpha) = \frac{\psi_1(\alpha)}{W_o(\alpha)}$$

$$\tilde{P}(\alpha,\beta) = \frac{P(\alpha,\beta)}{W(\alpha,\beta)}$$

$$\tilde{P}(\alpha,D) = \frac{P(\alpha,D)}{W(\alpha,D)}$$

and one carries out the procedure at the end of section 1 using $\tilde{\psi}_1$, $\tilde{P}$ instead of ψ_1, P, the corresponding estimate for I becomes

$$I = \frac{1}{N} \sum_{i=1}^{N} \rho(\alpha_{n_i}^{i})\; W_o(\alpha_1^i)\; W(\alpha_1^i, \alpha_2^i) \ldots W(\alpha_{n_{i-1}}, \alpha_{n_i}^i)\; W(\alpha_{n_i}^i, D)$$

where n_i again is the total number of collisions undergone by the i'th particle.

This transformation has not changed the expected value of I.

4. IMPORTANCE FUNCTION

It will now be shown that by a proper choice of $q(\alpha)$, which special choice we will write $Q(\alpha)$, the estimated value of I is always the same and therefore the exact value (since the expectation value is the exact value).

It follows from this, that if $q(\alpha)$ is taken as close as possible to $Q(\alpha)$, one may expect to obtain an estimate of I with little work.

The proposed $Q(\alpha)$ is given by

$$Q(\alpha) = \int_P g(\alpha, \beta)\, P(\beta, D)\, \rho(\beta)\, d\beta$$

whence

$$Q(\beta)\, W(\alpha,\beta) = \int_P\int_P P(\alpha,\gamma)\, g(\gamma,\beta)\, P(\beta,D)\, \rho(\beta)\, d\gamma\, d\beta + P(\alpha, D)\, \rho(\alpha)$$

$$= \int_P\int_P P(\alpha,\gamma)\, g^{+}(\beta,\gamma)\, P(\beta, D)\, \rho(\beta)\, d\gamma\, d\beta + P(\alpha,D)\, \rho(\alpha)$$

But $\int_P P(\alpha,\gamma)\, g^{+}(\beta, \gamma)\, d\gamma = g^{+}(\beta, \alpha) - \delta(\beta - \alpha)$

whence

$$Q(\beta)\, W(\alpha, \beta) = \int_P \left[g(\alpha,\gamma) - \delta(\alpha - \gamma)\right] P(\gamma,D)\, \rho(\gamma)\, d\gamma + P(\alpha, D)\, \rho(\alpha)$$

$$= Q(\alpha)$$

or $$W(\alpha,\beta) = \frac{Q(\alpha)}{Q(\beta)}\ ;\ W(\alpha,D) = \frac{Q(\alpha)}{\rho(\alpha)}\ ;\ W_0(\alpha) = \int_P \psi_1(\alpha)\, Q(\alpha)\, d\alpha.$$

Thus for this choice of q,

$$I = \frac{1}{N} \sum_{i=1}^{N} \int_P \psi_1 (\alpha)\, Q(\alpha)\, d\alpha = \int_P \psi_1 (\alpha)\, Q(\alpha)\, d\alpha$$

as was to be shown. Further, this agrees with the previous definition of I, since

$$\int_P \psi_1 (\alpha)\, Q(\alpha)\, d\alpha$$

$$= \iint \psi_1 (\alpha)\; g(\alpha, \beta)\; P(\beta, D)\; \rho(\beta)\; d\alpha\, d\beta$$

$$= \int \psi(\beta)\; P(\beta, D)\; \rho(\beta)\, d\beta \equiv I$$

where use was made of the result

$$\psi(\alpha) = \int \psi_1 (\beta)\, g(\beta, \alpha)\, d\beta.$$

The $Q(\alpha)$ used above is clearly a measure of the importance (to I) of a neutron at α. This follows from the definition of $Q(\alpha)$ directly or from the result

$$I = \int_P \psi_1 (\alpha)\; Q(\alpha)\, d\alpha.$$

We may thus use the term importance function (coined by Harry Soodak in a similar situation) to describe $Q(\alpha)$ and its guessed at approximation $q(\alpha)$.

5. THE ADJOINT SITUATION

Clearly, if one computes I as above, in general he can obtain at the same time an estimate of $\psi(\alpha)$. However $\psi(\alpha)$ is not readily related to $Q(\alpha)$, so that it is difficult to use the information on $\psi(\alpha)$ to improve $q(\alpha)$. On the other hand, if a pair of problems is set up as below, one may circumvent the above difficulty and calculate $\psi(\alpha)$ and $Q(\alpha)$ side by side.

$$g(\alpha, \beta) = \int_P g(\alpha, \gamma) \; P(\gamma, \beta)\, d\gamma + \delta(\alpha - \beta)$$

$$g^+(\alpha, \beta) = \int_P g^+(\alpha, \gamma) \; P(\beta, \gamma)\, d\gamma + \delta(\alpha - \beta)$$

where, as shown before

$$g^+(\alpha, \beta) = g(\beta, \alpha)$$

$$Q(\alpha) = \int_P g(\alpha, \beta) \; P(\beta, D) \; \rho(\beta) \; d\beta$$

$$= \int_P P(\beta, D) \; \rho(\beta) \; g^+(\beta, \alpha)\, d\beta.$$

From which

$$\int P(\alpha,\gamma) \; Q(\gamma)\, d\gamma + P(\alpha, D)\, \rho(\alpha) = Q(\alpha).$$

This is a stochastic problem equivalent to the one for $\psi(\alpha)$,

$$\int \psi(\gamma) \; P(\gamma, \alpha)\, d\gamma + \psi_1(\alpha) = \psi(\alpha),$$

and may be solved by similar processes using as importance function $q^+(\alpha)$ given by

$$q^+(\alpha) = \int_P g^+(\alpha, \beta)\, \psi_1(\beta)\, d\beta$$

$$= \int_P g(\beta, \alpha)\, \psi_1(\beta)\, d\beta = \psi(\alpha)$$

as is suggested by the results found above:

$$I = \int_P \psi_1(\alpha)\, Q(\alpha)\, d\alpha = \int_P P(\alpha, D)\, \rho(\alpha)\, \psi(\alpha)\, d\alpha.$$

Thus, the problem of determining I may be solved by solving in parallel the stochastic problems for $\psi(\alpha)$ and $Q(\alpha)$ and using them to estimate $q(\alpha)$ and $q^+(\alpha)$ as one proceeds, thus improving the computation of $\psi(\alpha)$ using the result of the computation of $Q(\alpha)$ and vice-versa.

6. CONCLUSIONS

The general considerations above give a procedure for quota sampling which consists of estimating $q(\alpha)$ to match the definition of $Q(\alpha)$ in section 4, using one's best judgment, and then carrying out the stochastic process as specified in section 3. The procedure of section 5 should be further investigated to determine in what problems it is useful.