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VARIANCE ANALYSIS OF THE MONTE CARLO PERTURBATION SOURCE METHOD IN INHOMOGENEOUS LINEAR PARTICLE TRANSPORT PROBLEMS. DERIVATION OF FORMULAE



1. Introduction

The stochastical nature of its results is known to confine the applicability of the Monte Carlo method (MC method) in solving particle transport problems. The statistical situation may become especially a precarious one if the difference of individual results is of the actual interest as it is, for example, in investigation of the dependence of a detector response on variations of a given arrangement. The applicability of the MC method is entirely called in question if the effect to be calculated goes down to the order of the statistical errors of the single results. For example, if it is yet possible to calculate with an acceptable expense the detector responses in two different states of the system with a desired accuracy of n%, then, in statistically independent calculations, already the double expense will be necessary to estimate only the sign of the difference with the same reliability if it is itself in the order of n%. On the other hand there is a potential interest to utilize the MC method in such cases,too,because often the details in geometry and in the behaviour of cross sections just must be taken into consideration to such a degree which, at least at present, is attainable without too much effort by the MC method only.

The MC method was particularly used and developed for the calculation of small effects in the field of reactor physics. But there the calculations are rendered more complicated because, in general, variations of the eigenvalue of a homogeneous transport problem are of interest. In this paper we disregard that complication and look at difference calculations for inhomogeneous problems, i.e., in particle fields with a constant outer source. However, it should be noted that the variance problems in both cases are quite similar and conclusions drawn in this paper may be immediately transferred to the reactor physical calculations.

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The main point in reducing the variances of difference estimates is the introduction of a positive correlation between the individual estimates. This is given to a high degree in the "weighting method". There, particle histories are simulated only in one state of the system, let call it the "zero" state. By an appropriate weighting according to the general biasing scheme /1-5/ these histories are simultaneously taken as randomly selected set of histories in the other state - the "one" state - of the system. This "weighting method" is applicable without approximations only then if the set of all possible particle histories in the "zero" state includes the entire set of possible histories in the "one" state. This condition considerably confines the applicability of this method. But it may be successfully utilized, for example, if the cross sections of the materials differ only slightly by small density variations in both system states. For more substantial cross section variations approximations may become necessary and it losses in effectiveness, especially, if material zones are voided. In those cases two other methods are mostly used. The practically simplest method is the "correlated sampling", where by an appropriate management of the starting random numbers the same histories are initialized in both system states. In that way all those histories which do not partake in the effect are the same in both calculations. The statistical fluctuations of the difference estimates, therefore, result only from those sets of histories which separate in both calculations in consequence of the differences in the system states, i.e., they result only from the effective histories which just cause the effect. Contrary to the "weighting method" no approximations for any cross section changes are necessary because

all effective histories are separately realized in their own system states. On the other hand, we have a loss in correlation just between the sets of effective histories. Certainly, this method could be further improved, e.g., by keeping the effective histories in the "one" state so close as possible to those of the "zero" state. However, that will be strongly confined because the joint histories are actually to realize in different system states.

Favourable possibilities to correlate the sets of effective histories seem to provide the so-called perturbation source method (PSM). Here the

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calculation of the effect is not based on two parallel, but on two sequential transport calculations each of them in one state of the system. In the first calculation the variations (perturbations⁺) of the system cause the generation of two types of source particles (perturbation particles) for the second calculation. Both types of perturbation particles then give estimates of opposite signs. The <u>common</u> generation process and the following random walk of the perturbation particles in the <u>same</u> state of the system are the features of the PSM which should give good possibilities for introducing positive correlation between the substracting estimates.

Though, all the methods are widely used in practice there is no general analysis of their efficiencies in the literature. Of course, a rigorous comparison of the methods requires the analysis as of variances as of computational expenses. This should be an attractive task for future investigations. In this paper a general variance analysis of the PSM in inhomogeneous linear particle transport problems is performed. This is done by an adequate extension of the adjoint integral formalism presented by Coveyou et al. for representing the variances of the event point estimator in analog and biased solutions of orginary particle transport problems /3/. The received results enable as the understanding of the general variance peculiarities of the PSM as to draw direct practical conclusions with respect to its improvement.

2. Uutline of the Perturbation Source Method

Let us have a time independent particle distribution which is described in the phase space by a nonnegative event density $E_0(x)$. The particle field is feeded by a given first event source $S_0(x)$ which may be assumed to be normalized

$$\int S_o(x) dx = 1. \tag{1}$$

 $E_{n}(x)$ is given as the solution of the F r e d h o l m integral equation

^{*} We emphasize that the term "perturbation" in the notation of the PSM generally is not related to an approximation in the sense of the approximative perturbation theory.

$$E_o(x) = S'_o(x) + \int K_o(x' \rightarrow x) E_o(x') dx', \qquad (2)$$

where $K_0(x \rightarrow y)$ is the nonnegative transition kernel describing the transport process of the particles in energy, flight direction and in the volume of the given system. We assume K_0 to be nonmultiplying, i.e., its normalization constant

$$G_{o}(x) \equiv \int K_{o}(x - x') dx'$$
⁽³⁾

to fulfil

$$0 \leq G_{o}(x) \leq 1.$$
 (4)

An installed detector with the response function D(x) gives the counting rate

$$A_{o} = \int \mathcal{D}(x) E_{o}(x) dx. \qquad (5)$$

The adjoint problem belonging to the particle transport problem f(2), (5)f is given by the equations

$$W_{o}(x) = D(x) + \int K_{o}(x - x') W_{o}(x') dx',$$
 (6)

$$\lambda_o = \int S_o(x) W_o(x) dx , \qquad (7)$$

where $W_{0}(x)$ is called the <u>value function</u> of the particle problem $\{(2), (5)\}/3/$. Now we change the system according to

$$K_{o}(x \rightarrow y) \implies K_{1}(x \rightarrow y)$$
 (8)

and wait for the new equilibrium event density $E_1(x)$ which is given as the solution of

$$E_{1}(x) = S_{0}(x) + \int K_{1}(x' \rightarrow x) E_{1}(x') dx'.$$
(9)

The kernel ${\rm K}_{\rm l}$ is also assumed to be nonmultiplying. The new counting rate of the detector is

$$A_{1} = \int \mathcal{D}(x) E_{x}(x) dx. \qquad (10)$$

We are interested in the Monte Carlo colculations of the effect

$$\lambda = \lambda_1 - \lambda_0 . \tag{11}$$

Performing two parallel calculations with the estimators γ ; of A_i , respectively, we have with

$$\mathcal{L} = \mathcal{L}_1 - \mathcal{L}_0 \tag{12}$$

the estimator (per particle pair) of λ . Its variance Var(2) is given by

$$Var(\gamma) = \sum_{i=0}^{4} Var(\gamma_i) - 2Cov(\gamma_0, \gamma_1), \qquad (13)$$

where the variances $\operatorname{Var}(\mathcal{J}_G)$ and the covariance $\operatorname{Cov}(\mathcal{J}_G, \mathcal{J}_I)$ are defined as usually /6/. Good estimates of λ we may expect if the variances of the estimators \mathcal{J}_i are sufficiently small and if they are positive correlated. The latter is the speciality of difference calculations.

The starting point of the PSM is now the interpretation of the effect λ as integral $\lambda = \int D(x) E(x) dx$ (14)

of the difference event density

$$E(x) = E_{1}(x) - E_{0}(x)$$
⁽¹⁵⁾

and the derivation of an equation for it. Subtracting equations (9) and (2) we get

$$E(x) = P(x) + \int K_1(x' \rightarrow x) E(x') dx'$$
 (16)

with the so-called perturbation source

$$\mathcal{P}(\mathbf{x}) = \int \left(K_1(\mathbf{x}' \rightarrow \mathbf{x}) - K_0(\mathbf{x}' \rightarrow \mathbf{x}) \right) E_0(\mathbf{x}') d\mathbf{x}'. \tag{17}$$

We point out that equation (16) may also be rewritten with K_0 instead of K_1 and defining the perturbation source with E_1 instead of E_0 . This fact is unimportant with respect to our general derivation of the variance expression for the PSM estimator in the next chapter, but it must be taken into consideration in practical applications.

Assuming that possible analytical subtractions or conversions in the difference of the kernels $\rm K_{_O}$ and $\rm K_{_1}$ have been carried out so that

$$K_{1}(x \rightarrow y) - K_{0}(x \rightarrow y) = P_{1}(x \rightarrow y) - P_{0}(x \rightarrow y)$$
⁽¹⁸⁾

with nonnegative remaining transition kernels $P_{j}(x \rightarrow y)$ we see that E(x) is also given by

$$E(x) = E_{1}(x) - E_{0}(x), \qquad (19)$$

where the $E_{\underline{i}}^{\bigstar}(x)$ are the solutions of

$$E_{i}^{*}(x) = P_{i}(x) + \int K_{1}(x \rightarrow x) E_{i}^{*}(x') dx', \quad i = 0, 1, \quad (20)$$

with the $P_i(x)$ as the constituents of the perturbation source

$$P(x) = P_1(x) - P_0(x),$$
 (21)

$$P_i(x) = \int P_i(x' - x) E_o(x') dx', \quad i = 0, 1.$$
 (22)

Therefore, λ may also be calculated as the difference

$$\lambda = \lambda_1^* - \lambda_o^* \tag{23}$$

of the counting rates

$$A_i^* = \int \mathcal{D}(x) E_i^*(x) dx$$
, $i = 0, 1.$ (24)

From equations (2) and (20) through (24) follows the general outline of the Monte Carlo procedure of the PSM(for details see chapter 3):

- Simulate the histories of <u>basic particles</u> in the "zero" state of the system according to the source and transition kernel
 - [s_,ĸ_]·
- Generate two types of new, so-called <u>perturbation particles</u> according to the definitions (22) of both perturbation source constituents during the basic histories.
- 3) Estimate λ by estimating the λ_i^* during the transport game of the perturbation particles in the "one" state of the system.

Denoting with $\mathbf{2}_i^{\star}$ the estimators (per basic particle) of the λ_i^{\star} the PSM estimator is given by

$$2^* = 2_1^* - 2_0^*$$
 (25)

and its variance

$$Var(q^{*}) = \sum_{i=0}^{1} Var(q^{*}_{i}) - 2Cov(q^{*}_{o}, q^{*}_{1}). \qquad (26)$$

The resulting variance Var(η^{*}) will be determined by:

the transport game of the basic particles;
 the generation procedure of the perturbation particles;

3) the transport game of the perturbation particles;

4) the estimators used for estimating the A_i^* .

What may we expect from the approach of the PSM in general? We note that the specific of the difference of two estimates is not overcome, but only transformed by the perturbation source. Obviously, we may expect a considerable improvement in the statistic of the λ -estimate, if the perturbation source becomes a nonalternate distribution. But also in the general case when the resulting perturbation source forms a difference of nonalternate distributions the PSM should be quite promising because its formulation is especially focused to the cause of the effect λ .

What in particular do our hopes found on? Let us look at the estimation of λ by performing two parallel calculations each of them in one state of the system. Positive correlation may be introduced by an appropriate management of the random numbers initializing the histories in both calculations. In that way the common part of histories in both states of the system may be kept identical and only those histories, taking part in the effect will, in general, differ after the entry in a region which was changed by the modification (8). This means that we have an undesirable loss in correlation just in the significant histories. Contrary to that the PSM seems to provide a good means to strengthen the correlation between those histories. As in the previous method one complete calculation must also be performed: the transport game of the basic particles. The generation and the transport game of

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both types of perturbation particles then correspond to that part of histories which separate in both system states and contribute to the same effect λ . The generation process of both types of perturbation particles and their following random walk in the same state of the system seem to represent favourable possibilities for introducing positive correlation between the two subtracting estimators χ_i^* and, therefore, speak in favour of this method. That they in fact take the decisive parts in the PSM we shall demonstrate in the discussion of the derived results which will be published in the next paper.

3. Variances of the Perturbation Source Method

In this chapter we derive general expressions for the variances of the PSM estimator in different versions of the method. For it we want to use the easy adjoint integral formalism of Coveyou et al./3-5/ for calculating the second moments of the estimator. Therefore, we raise some formally simplifying but generally nonrestricting suppositions.First, as estimators χ_i^* we shall use event point estimators /4/ which are based on the event chains of all perturbation particles of the type i generated during the lifetime of a basic particle. Denoting with x_1 (1=0,1,...,L) the event points of the basic particle and with x_{ni} (n=0,1,...,N) the event points of a generated "i" perturbation particle the estimators may be represented

$$\eta_{i}^{*} = \sum_{\ell=0}^{L} \sum_{n=0}^{N} w_{i}(x_{0}, x_{4}, \dots, x_{\ell}; x_{0i}, \dot{x}_{Ai}, \dots, \dot{x}_{ni}) D(x_{ni}) , \quad i = 0, 1.$$
(27)

Here is $\Psi_i(x_0, \dots, x_1; x_{1i}, \dots, x_{ni}) \ge 0$ the statistical weight of an "i" perturbation particle at its event point x_{ni} which was generated in consequence of the basic event at x_1 and after that has passed the event points x_{0i}, x_{1i} , \dots, x_{ni} . As contribution function the estimators contain the detector response D(x). Second, all the transitions in the phase space are to be considered as nonfactorized transitions, i.e., those are not devided in flights and collisions as we really do in applications /5/.

Many different simulations of a given transitional kernel $T(x \rightarrow y)$ with the normalization constant

$$t(x) = \int T(x \to x') \, dx' \tag{28}$$

may be used. In the general biasing scheme we use another nonmultiplying, but otherwise widely arbitrary kernel $\vec{1}(x \rightarrow y)$ normalized by

$$\overline{t}(x) = \int \overline{T}(x \to x') \, dx' \,. \tag{29}$$

To guarantee an unbiased simulation of $T(x \rightarrow y)$ it is necessary that $\overline{T}(x \rightarrow y) \neq 0$ for all (x,y), where $T(x \rightarrow y) \neq 0$. Then, at an event point x the biasing simulation procedure of $T(x \rightarrow y)$ is the following:

- 1) With probability $(1-\tilde{t}(x))$ there is no next event point, the history is terminated.
- 2) with probability $\overline{t}(x)$ the particle survives the event. The next event point is chosen from $\overline{T}(x - y)/\overline{t}(x)$. The statistical weight of the particle is multiplied by $T(x - y)/\overline{t}(x - y)$ after the event at x.

With respect to the transport games especially two simulations are of interest. Those are the <u>analoy</u> and the <u>EV-biasing</u> simulations. Both are included in the more general survival-biasing, where

$$\overline{T}(x \rightarrow y) = \overline{E}(x) * T(x \rightarrow y)/t(x)$$
⁽³⁰⁾

is used with $\overline{t}(x)$ as arbitrary survival probability. The special choices $\overline{t}(x) \equiv t(x)$ and $\overline{t}(x) \cong 1$ give the analog and the EV-biasing simulations, respectively. Therefore, we shall derive all the formulas for the whole class of survival-biasing games and only in the discussion extract the special cases. In the EV-biasing transport game a history must be suitably terminated, e.g.,by a Russian Roulette procedure after the statistical weight was fallen down under a given minimum amount /4/. Contrary to the transport games the generation process according to the transition kernels $P_i(x \rightarrow y)$ will be dealt with in the general biasing technique.

A FORTRAN-like outline of the PSM procedure as it will be considered in this paper is set forth in Fig.1 through Fig.5. Fig.3 through Fig.5 show different generation procedures at an event point x of a basic particle having

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(START)
$$\eta^* = \eta^*_1 = \eta^*_0$$

Choose x from $S_0(x)$.
w=1
(1) Generation procedure at x.
Transport game of all the generated perturbation
particles including the summations of the η^*_1 .
With probability $(1 - \overline{\mathcal{G}}_0(x))$, go to (2).
w=w * $\mathcal{G}_0(x)/\overline{\mathcal{G}}_0(x)$
Choose y from $K_0(x \rightarrow y)/\mathcal{G}_0(x)$.
x=y
Go to (1)
(2) $\eta^* = \eta^*_1 - \eta^*_0$

Fig. 1. The PSM procedure

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First event points x_i and starting weights w_i (i=0,1)

are given from the generation procedure at x.

(START) i=0

(1) If w_i=0, go to (3).

(2) \eta_i^* = \eta_i^* + w_i * D(x_i)

With probability (1 - \overline{\mathfrak{S}}_1(x_i)), go to (3).

w_i = w_i * \overline{\mathfrak{S}}_1(x_i) / \overline{\mathfrak{S}}_1(x_i)

Choose y_i from K_i(x_i - y_i) / \overline{\mathfrak{S}}_1(x_i).

x_i = y_i

Go to (2).

(3) If i=1, STOP.

i=i+1

Go to (1)
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Fig. 2. The perturbation transport game including the event point estimation.

(START) i=0 (1) $w_i = 0$ With probability $(1 - \overline{p}_i(x))$, go to (2). Choose x_i from $\overline{p}_i(x \rightarrow x_i)$. $w_i = w \neq P_i (x \rightarrow x_i) / (\overline{p}_i(x) \neq \overline{p}_i(x \rightarrow x_i))$ (2) If i=1, STOP. i=i+1Go to (1).

Fig. 3. Generation procedure (A)

(START) $\psi_0 = \psi_1 = 0$ With probability (1- $\overline{p}(x)$), STOP. i = 0 (1) Choose x_i from $\overline{p}_i(x \rightarrow x_i)$. $\psi_i = \psi + P_i(x \rightarrow x_i)/(\overline{p}(x) + \overline{p}_i(x \rightarrow x_i))$ If i=1, STOP. i=i+1 Go to (1).

Fig. 4. Generation procedure (B)

(START)
$$\Psi_0 = \Psi_1 = 0$$

With probability $(1 - \overline{p}(x))$, STOP.
Choose x_1 from $\overline{p}(x \rightarrow x_1)$.
 $\Psi_1 = \Psi \neq (P_1(x \rightarrow x_1) - P_0(x \rightarrow x_1))/(\overline{p}(x) + \overline{p}(x \rightarrow x_1))$

Fig. 5. Generation procedure (C)

the weight w. They will be explained in more detail in the further derivation. It is of importance to point out that we explicitly consider only statistically independent transport games of the perturbation particles. The possibilities of correlated games should be investigated for the future. Their doubtless usefulness, however, becomes evident in our results.

Let us start with the analysis of the event point estimation carried out during a survival-biasing transport game in the "one" state of the system. For that we define $\overline{\boldsymbol{\zeta}}(x)$ to be a random variable whose value is the

total contribution to the estimate, present and future, made by a particle of unit weight experiencing an event in dx near $\times /3/$. At such an event point we have the following balance:

Balance (I)

Event and probability Value of $\overline{\xi}_{1}(x)$ 1) With probability (1- $\overline{\sigma}_{1}(x)$) the history is terminated. D(x) 2) With probability $\overline{\sigma}_{1}(x) * K_{1}(x \rightarrow \gamma) dy / \tilde{\sigma}_{1}(x)$

the particle survives and has the next event in dy near y.

 $D(x) + \overline{S}_{4}(y) * \overline{S}_{4}(x) / \overline{S}_{4}(x)$

From this balance we find for the expected value $M[\bar{S}_{i}(x)]$ the equation

$$\mathcal{M}\left[\overline{S}_{1}(x)\right] = \mathcal{D}(x) + \int \mathcal{K}_{1}(x \rightarrow x') \mathcal{M}\left[\overline{S}_{1}(x)\right] dx'. \quad (31)$$

This function

$$W_{1}(\mathbf{x}) \equiv \mathcal{M}\left[\bar{\mathcal{F}}_{1}(\mathbf{x})\right] \tag{32}$$

is the <u>value function</u> of a particle transport problem in a system K_{1} with a detector U(x) = /3, 4/.

Next, quite similarly we prepare the statistical analysis of the basic game in the system state K_0 including a generation process of perturbation particles whose histories then contribute to the estimate. Let us define $\overline{\zeta}_0(x)$ to be a random variable whose value is, for each possible basic particle of unit weight experiencing an event in dx near x, the total contribution to the estimate, present and future, resulting from the particle during its further random walk in the system K_0 by generating perturbation particles which then directly contribute to the estimate. Furthermore, let $\overline{\mathcal{J}}(x)$ be a random variable whose value is the contribution to the estimate, made by a perturbation particle which is possibly generated in consequence of an event of a basic particle with unit weight in dx near x. Hence, for an event point of a basic particle with unit weight in dx near x we may set up the following balance for $\overline{\zeta}_n(x)$: Balance (II)

 $\overline{\mathcal{F}}(x) + \overline{\mathcal{F}}(y) * \overline{\mathcal{G}}(x) / \overline{\mathcal{G}}(x)$

S(r)

- 1) With probability (1- $\overline{\mathfrak{S}}_{0}(x)$) the history is termintated.
- 2) With probability $\overline{G}_{o}(\mathbf{x}) \star K_{o}(\mathbf{x} \rightarrow \mathbf{y}) d\mathbf{y} / G_{o}(\mathbf{x})$ the basic particle survives and has the next event in dy near y,

The next relation we have to find is that between $\hat{J}(x)$ and $\hat{f}_1(x)$. It is determined by the simulation procedure of the generation process. Only for a little while, we digress now from the original PSM and assume, for convenience, instead of equation (21) a single nonnegative generation process, i.e.,

$$P(\mathbf{x}) = \int P(\mathbf{x}' \rightarrow \mathbf{x}) E_o(\mathbf{x}') d\mathbf{x}'. \tag{33}$$

Here $P(x \rightarrow y)$ is to be a nonnegative transition kernel describing the generation of perturbation particles caused by an event of a basic particle at x and the transition to its first event point y. $P(x \rightarrow y)$ is simulated according to the general biasing technique where we explicitly write the biasing kernel $\overline{P}(x \rightarrow y)$ as the product of a generation probability $\overline{p}(x)$ and a normalized probability density function $\overline{p}(x \rightarrow y)$

$$\overline{P}(x \rightarrow y) = \overline{p}(x) * \overline{p}(x \rightarrow y). \tag{34}$$

Then we find:

Balance (III) Event and probability 1) With probability (1-p(x)) no perturbation

particle is generated.

2) With probability $\overline{p}(x) + \overline{p}(x \rightarrow y) dy$

a perturbation particle is generated and experiences its first event in dy near y.

 $\overline{\tilde{S}}_{1}(y) * \frac{P(x \to y)}{\overline{p}(x) * \overline{p}(x \to y)}$

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Value of $\overline{\mathcal{F}}(x)$

Hence, for the expected value $W(x) = M[\overline{s}(x)]$ (35)

we get the equation

$$W(\mathbf{x}) = M[\overline{\mathcal{F}}(\mathbf{x})] + \int K_o(\mathbf{x} - \mathbf{x}') W(\mathbf{x}') d\mathbf{x}' \qquad (36)$$

and, furthermore, with definition (32)

$$M[\overline{\mathcal{S}}(x)] = \int P(x \to x') W_1(x') dx' . \tag{37}$$

The expected value of the event point estimator χ^{\star} is given by

$$\mathcal{M}[p^*] = \int \mathcal{S}'_o(x) \mathcal{M}[\overline{\mathcal{S}}_o(x)] dx. \tag{38}$$

It is not hard to see that

$$M[p^*] = \int M[\overline{\mathcal{J}}(x)]E_o(x) dx$$

= $\int P(x) W_1(x) dx$ (39)
= $(D(x) E(x) dx - 1)$

 $= \int \mathcal{Q}(x) E(x) \, \partial(x) = \lambda \quad ,$ i.e., that χ^* is an unbiased estimator of λ . Now we direct our attention to the variance

$$Var(p^*) \equiv M[p^{*^2}] - \lambda^2 , \qquad (40)$$

where $M[2^{*2}]$ is the second moment and is given by

$$\mathcal{M}[\eta^{*2}] = \int \mathcal{S}_{0}(x) \mathcal{M}[\overline{\mathcal{S}}(x)] dx \qquad (41)$$

From balance (II) we find the equation for $M(\overline{s}(x))$

$$\mathsf{M}[\overline{\mathfrak{F}}_{\mathfrak{s}}^{2}(\mathfrak{k})] = \mathsf{M}[\overline{\mathfrak{F}}(\mathfrak{k})](\mathcal{H}(\mathfrak{k}) - \mathsf{M}[\overline{\mathfrak{F}}(\mathfrak{k})]) + \mathsf{Var}(\overline{\mathfrak{F}}(\mathfrak{k})) + \frac{\mathsf{G}_{\mathfrak{s}}(\mathfrak{k})}{\mathsf{G}_{\mathfrak{s}}(\mathfrak{k})} \int \mathsf{K}_{\mathfrak{s}}(\mathfrak{k} - \mathfrak{k}) \mathsf{M}[\overline{\mathfrak{F}}_{\mathfrak{s}}^{2}(\mathfrak{k})] d\mathfrak{k}_{\mathfrak{s}}^{\prime}(\mathfrak{k}_{2})$$

where we have defined a nonnegative variance function of $\overline{\mathcal{J}}(\kappa)$

$$\operatorname{Var}(\overline{\mathcal{F}}(x)) = M[\overline{\mathcal{F}}(x)] - M^{2}[\overline{\mathcal{F}}(x)] . \tag{43}$$

With the help of a new distribution function $\overline{F}_{\mathcal{S}}(\mathbf{x}) \geq \mathbf{0}$ as solution of

$$\overline{F}_{o}(x) = S_{o}(x) + \int \frac{G_{o}(x')}{\overline{G}_{o}(x')} K_{o}(x' - x) \overline{F}_{o}(x') dx' \qquad (44)$$

$$M[2^{*2}] = \int M[\overline{J}(x)] (x) W(x) - M[\overline{J}(x)]) \widetilde{F}(x) dx' + \int Var(\overline{J}(x)) \widetilde{F}_{0}(x) dx'.$$
(45)

Note that for the analog basic game $\vec{F}_0(x) = E_0(x)$.

The second moment $M[\mathcal{F}(x)]$ is easily calculated from balance (III)

$$M[\overline{\mathcal{F}}_{(x)}^{2}] = \frac{1}{\overline{p}(x)} \int \frac{p(x \to x')}{\overline{p}(x \to x')} M[\overline{\mathcal{F}}_{1}(x)] dx' \qquad (46)$$

and from balance (I) we find the equation for $M(S_1(\alpha))$

$$M[\overline{\mathfrak{F}}_{4}^{2}(\mathfrak{x})] = \mathcal{D}(\mathfrak{x})(\mathcal{Z}W(\mathfrak{x}) - \mathcal{D}(\mathfrak{x})) + \frac{G_{4}(\mathfrak{x})}{G_{4}(\mathfrak{x})}\int K_{4}(\mathfrak{x} - \mathfrak{x}')M[\overline{\mathfrak{F}}_{4}^{2}(\mathfrak{x}')]d\mathfrak{x}'. \quad (47)$$

Now we return to the actual PSM with the double generation process. For its variance analysis let us define $\overline{S}_{0}(x)$ ($\overline{S}_{1}(x)$) to be a random variable whose value is the contribution to the estimate, made by a "zero" ("one") particle w hich is possibly generated in consequence, of an event of a basic particle with unit weight in dx near x. The relation of both variables to $\overline{S}_{1}(x)$ from the basic game is also given by balance (II) but with the redefinition

$$\overline{\mathcal{F}}(\mathbf{x}) = \overline{\mathcal{F}}_{\mathbf{x}}(\mathbf{x}) - \overline{\mathcal{F}}_{\mathbf{x}}(\mathbf{x}) . \tag{48}$$

As before we have

$$M[\eta^*] = \int S_0(x) W(x) dx \tag{49}$$

but now W(x) is the solution of equation (36) with the source term

$$M[\overline{f}(k)] = M[\overline{f}_{k}(k)] - M[\overline{f}_{k}(k)] . \qquad (50)$$

Likewise equation (37), the double generation procedure must guarantee that

$$M[\overline{J}_{i}(x)] = \int P_{i}(x - x') W_{1}(x') dx', \quad i = 0, 1.$$
 (51)

Taking into account the redefinition (48) resulting in the modification (50) with equations (51) the second moment of the PSM estimator (25) is also given by equations (41), (42) or (45). The quantity, which yet has to be newly calculated is the variance function $Var(\mathbf{J}(x))$. Now we shall do this for the double generation procedures shown in Fig.3 through Fig.5.

Generation procedure (A)

The "i" particles are statistically independent generated using the generation probabilities $\overline{p}_i(x)$ and transfer functions $\overline{p}_i(x - y)$. We find the following balance:

Balance (IV)

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Event and probability	$\overline{\mathcal{S}}(x)$ Value of $\overline{\mathcal{S}}_1(x)$
l) With probability $(1-\overline{p}_1(x))$ no "one"	
particle is generated.	0
1.1) With probability $(i-\overline{p_0}(x))$ no	
"zero" particle is generated.	0
l.2) With probability p _o (x)∉p _o (x→y)dy _o	
a "zero" particle is generated	
and has its first event in dy, $\overline{\mathbf{y}}$	(y) + <u>P(x - y)</u>
near y _o .	(a) + p(a + y_a)
2) With probability $\vec{p}_1(x) \cdot \vec{p}_1(x - y_1) a y_1$	
the "one" particle is generated and	
experiences its first event in dy $_{ m l}$	E(4)* Pa(x+y1)
near y _l .	54 4 Fq(x) + Fq(x-ya)
2.1) With probability $(1-\overline{p}_{0}(x))$	•
no "zero" particle is gene-	
rated.	0
2.2) With probability $\overline{p}_{0}(x) * \overline{p}_{0}(x - y_{0}) dy_{0}$	
the "zero" particle is generated	
and has its first event in dy _o	$\overline{\overline{S}}_{n}(y_{0})^{*} \frac{P_{0}(x^{*} + y_{0})}{\overline{\sigma}(x)^{*}} \overline{\overline{\sigma}(x)^{*}} \overline{\overline{\sigma}(x)^{*}}$
near y _o .	20 Per 20
$M[\overline{\mathcal{F}}_{(x)}^{2}] = \sum_{i=0}^{4} \frac{1}{\overline{p}_{i}(x)} \int \frac{P_{i}^{2}(x-x')}{\overline{p}_{i}(x-x')} M[\overline{\mathcal{F}}_{2}^{2}(x')]a$	4.
$-2 \int \mathcal{P}_{0}(x \to x') \mathcal{P}_{1}(x \to x'') \mathcal{M}[\overline{S}_{1}(x \to x'')] \mathcal{M}[\overline{S}_{1$	(') <u>\$</u> (x")]dx'dx".

With that the variance function (43) may be written

$$\operatorname{Var}(\overline{\mathcal{J}}(\mathbf{x})) = \operatorname{Var}(\overline{\mathcal{J}}(\mathbf{x})) + \operatorname{Var}(\overline{\mathcal{J}}_{4}(\mathbf{x})) - 2\operatorname{Cov}(\overline{\mathcal{J}}(\mathbf{x}), \overline{\mathcal{J}}_{4}(\mathbf{x})) , \quad (53)$$

where

$$V_{ar}(\overline{J}_{i}(t)) = M[\overline{J}_{i}(t)] - M[\overline{J}_{i}(t)], \quad i = 0, 1, \quad (54)$$

$$Cov(\overline{\mathcal{F}}(k),\overline{\mathcal{F}}_{1}(k)) = M[\overline{\mathcal{F}}(k)\overline{\mathcal{F}}_{1}(k)] - M[\overline{\mathcal{F}}(k)]M[\overline{\mathcal{F}}_{1}(k)]$$
⁽⁵⁵⁾

with

$$M[\vec{J}_{i}(\vec{x})] = \frac{1}{\vec{p}_{i}(x)} \int \frac{P_{i}(x \to x')}{\vec{p}_{i}(x \to x')} M[\vec{s}_{i}(x')] dx', \quad i = 0, 1, (56)$$

and
$$M[\overline{f}_{a}(x)] = \iint P_{a}(x \to x') P_{a}(x \to x'') M[\overline{f}_{a}(x')] \overline{f}_{a}(x'')] dx' dx''. \tag{57}$$
Generation procedure (B)

The perturbation particles are generated in pairs using a pair generation probability $\vec{p}(x)$ but after that they will be transferred to their first event points by statistically independent selecting from the distribution functions $\vec{p}_i(x \rightarrow y)$. For this procedure we find the balance:

Balance(V)

Event and probability
$$\overline{\mathbf{X}}(\mathbf{x})$$
Value of $\overline{\mathbf{X}}(\mathbf{x})$ 1) With probability (1- $\overline{p}(\mathbf{x})$) no pair of
perturbation particles is generated.002) With probability $\overline{p}(\mathbf{x}) = \overline{p}_0(\mathbf{x} - \mathbf{y}) = \overline{p}_1(\mathbf{x} - \mathbf{y}_1) d\mathbf{y}_0 d\mathbf{y}_1$
a pair of perturbation particles is
generated and they experience their
first events in $d\mathbf{y}_0$ and $d\mathbf{y}_1$ near \mathbf{y}_0
and \mathbf{y}_1 , respectively. $\overline{\mathbf{X}}(\mathbf{x}) = \frac{\overline{p}_0(\mathbf{x} - \mathbf{y}_0)}{\overline{\mathbf{X}}(\mathbf{x}) = \overline{p}_0(\mathbf{x} - \mathbf{y}_0)}$

Then we get

 $M[\overline{J}_{i}(x)] = \frac{1}{\overline{p}(x)} \left(\frac{P_{i}^{2}(x - x')}{\overline{p}(x - x')} M[\overline{J}_{i}(x)]dx', \quad i = 0, 1, (58) \right)$

and

 $M[\overline{\mathcal{F}}_{0}(x),\overline{\mathcal{F}}_{n}(x)] = \frac{1}{\overline{\rho}(x)} \left(\left(\mathcal{P}_{0}(x \rightarrow x') \mathcal{P}_{n}(x \rightarrow x'') \mathcal{M}[\overline{\mathcal{F}}_{n}(x'),\overline{\mathcal{F}}_{n}(x'')] dx' dx'' \right) \right)$ (59)

Generation procedure (C)

We may extend the pair generation procedure (B) by using the same distribution $\overline{p}(x \rightarrow y)$ for selecting the first event points of both perturbation particles. In that way we arrive at a single generation procedure where the one generated perturbation particle now directly represents the difference of both perturbation source terms. With regard to a comparison with the foregoing two-particle generations it is useful to deal with this single generation procedure formally in the same framework, i.e., so as would we have two perturbation particles with different starting weights, but with identical histories. Thus we may set up the following balance. Balance (VI)

Event and probability

- 1) With probability $(1-\overline{p}(x))$ no pertur-
- bation is generated.
- With probability p(x)xp(x→y)dy the perturbation particle is generated and experiences its first event in dy near y.

0

In Value of Jack)

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 $\overline{\xi}_{1}(y) = \frac{\overline{P_{0}}(x \rightarrow y)}{\pi(x) + \pi(x \rightarrow y)} \qquad \overline{\xi}_{1}(y) = \frac{\overline{P_{0}}(x \rightarrow y)}{\overline{F(x)} + \overline{F(x \rightarrow y)}}$

From that we get

$$\mathcal{M}\left[\overline{\mathcal{J}}_{i}^{2}(x)\right] = \frac{1}{\overline{p}(x)} \int \frac{\mathcal{P}_{i}^{2}(x \to x')}{\overline{p}(x \to x')} \mathcal{M}\left[\overline{\mathcal{J}}_{i}^{2}(x')\right] dx', \quad i = 0, 1 \quad (60)$$

and

$$\mathbf{M}[\overline{\mathbf{J}}(\mathbf{x})\overline{\mathbf{J}}_{\mathbf{x}}(\mathbf{x})] = \frac{1}{\overline{p}(\mathbf{x})} \int \frac{B(\mathbf{x} + \mathbf{x}') B_{\mathbf{x}}(\mathbf{x} + \mathbf{x}')}{\overline{p}(\mathbf{x} + \mathbf{x}')} M[\overline{\mathbf{J}}_{\mathbf{x}}(\mathbf{x}')] d\mathbf{x}'. \tag{61}$$

We point out yet the special case where $W_1(x)$ is known. Then the PSM procedure may be terminated at the first events of the perturbation particles.

This is easily to realize with the help of equations (20) through (24) and (31), (32) arriving at

$$\lambda = \int W_{1}(x) \left[\int E_{0}(x') (P_{1}(x'+x)) - P_{0}(x'-x)) dx' \right] dx' \qquad (62)$$

The representation of λ by equation (62) makes clear its interpretation as an ordinary functional of the total first event density of perturbation particles. Simulating the latter the event point estimators Z_{i}^{*} must be used with $W_{1}(x)$ as the contribution function. The variance analysis of that case is easily accomplished. For this end, in the balances of the generation procedures considered above instead of the random variable $\overline{\xi}(g)$ we have to use its mean value $W_{1}(y)$. We find:

- for the generation procedure (A)

$$\mathcal{M}[\overline{f_i(k)}] = \frac{1}{\overline{p_i}(k)} \int \frac{\mathcal{P}_i^2(k - x')}{\overline{p_i}(k - x')} W_1^2(k') dx', \qquad i = 0, 1, (63)$$

$$Cov(\overline{f_o(k)}, \overline{f_a(k)}) = 0.$$
(64)

- for the generation procedure (B)

$$M[\overline{J}_{i}^{2}(x)] = \frac{1}{\overline{p}(x)} \int \frac{P_{i}^{2}(x \to x')}{\overline{P_{i}}(x \to x')} W_{1}^{2}(x')dx', \qquad i = \partial_{i} 1, \quad (65)$$

$$C_{OV}(\overline{J}_{0}(x), \overline{J}_{1}(x)) = \left(\frac{1}{\overline{p}(x)} - 1\right) M[\overline{J}_{0}(x)] M[\overline{J}_{1}(x)]. \quad (66)$$

- for the generation procedure (C)

$$\mathcal{N}\left[\overline{\mathcal{J}}_{i}^{2}(\mathbf{x})\right] = \frac{1}{\overline{p}(\mathbf{x})} \int \frac{\overline{P}_{i}^{2}(\mathbf{x} \rightarrow \mathbf{x}')}{\overline{p}(\mathbf{x} \rightarrow \mathbf{x}')} W_{1}^{2}(\mathbf{x}')d\mathbf{x}', \qquad i = 0, 1, \quad (67)$$

$$M[\overline{f}_{6}(x)\overline{f}_{4}(x)] = \frac{1}{\overline{p}(x)} \int \frac{\underline{R}(x-x')P_{4}(x-x')}{\overline{p}(x-x')} W_{4}^{2}(x')dx'.$$
(68)

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