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D.Yu.Bardin, N.D.Gagunashvili

A MONTE-CARLO METHOD FOR CALCULATING THE INTEGRAL TRANSFORMATIONS

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1. INTRODUCTION

The problem that we encounter in the experimental data analysis is the calculation of the integral transformation:

$$\phi(x') = \int_G f(x)\, p(x,x')\, dx,$$

where, e.g., $f(x)$ is a spectrum calculated within some theoretical model, which we suppose to describe the data, $f(x) \geq 0$, $p(x,x')$ is the apparatus function which defines the probability that an event with the coordinate x will be detected as an event with the coordinate x', $\int_G p(x,x')dx' = 1$, $\phi(x')$ is the distorted by a set-up model spectrum which will be compared with the measured experimental spectrum.

Usually, we are interested not in the function $\phi(x)$ but in its integrated channel content

$$I = \int_G \chi(x')\phi(x')dx' = \iint_{GG} \chi(x')f(x)p(x,x')\,dx\,dx', \qquad (1)$$

where

$$\chi(x') = \begin{cases} 1 & \text{in the subregion of } G \text{ that corresponds to the channel,} \\ 0 & \text{in other parts of the region } G. \end{cases}$$

The analytical expression for $f(x)$ is often very complicated, and the explicit expression for $p(x,x')$ is unknown completely; in these cases the Monte-Carlo method [1] is the only method for the calculation of the integral (1).

Choose the density $p(x)$ so that

$$\int_G p(x)dx = 1.$$

Define a random trajectory in the region G

$$T = (q_0 \to q_1),$$

where the point q_0 has the density $p(x)$ and the density of the point q_1 for a given q_0 is equal to $p(q_0, x)$.

Let θ denote the random variable

$$\theta = [f(q_0)/p(q_0)]\,\chi(q_1).$$

The function $w = f(q_0)/p(q_0)$ is called usually the weight.

Theorem 1.[1] The expectation value of θ equals the integral I

$$E\theta = I.$$

This theorem allows us to construct the Monte-Carlo method for estimating the integral I. So, if we play N trajectories T and for each of them calculate θ, we obtain for large enough N

$$I \approx I_N = \frac{1}{N} \sum_{i=1}^{N} \theta_i .$$

The variance of the estimation I_N is

$$DI_N = \frac{1}{N} D\theta = \frac{1}{N} [\iint_{GG} \chi(q_1) \frac{f^2(q_0)}{p(q_0)} p(q_0, q_1) dq_0 dq_1 - I^2] . \qquad (2)$$

In practice, the unbiased estimation for the variance is used

$$DI_N \approx \frac{1}{N(N-1)} \sum_{i=1}^{N} [\theta_i - I_N]^2 .$$

There are cases when the variance is large and we can reach the needed accuracy in calculating the integral I, only by increasing N. This would require a lot of the computer time, therefore one could not realize this method.

The time of generation of events by the low $p(x, x')$ (tracing) is usually much larger than the time for the generation of events by the low $p(x)$, therefore it is reasonable to trace events with the largest weight rather than all events in succession.

Let the ratio $f(x)/p(x)$ be limited by an upper bound. Than the largest weight events can be separated by the geometric method /1/.

So, let M be an arbitrary constant

$f(x)/p(x) \le M$.

Define the random variable $\theta^{(1)}$

$$\theta^{(1)} = \xi(q_0, \gamma) \chi(q_1) M,$$

where

$$\xi(q_0, \gamma) = \begin{cases} 1 \text{ for } \gamma < f(q_0)/[p(q_0)M], \\ 0 \text{ in the opposite case} \end{cases}$$

and γ is the random number. The expectation value of the random variable $\theta^{(1)}$ equals the integral I

$E\theta^{(1)} = I$.

This fact allows us to obtain the estimation for the integral

$$I \approx I_N^{(1)} = \frac{1}{N} \sum_{i=1}^{N} \theta_i^{(1)} . \qquad (3)$$

The Monte-Carlo method based on the estimation (3) may be called the method with constant weights; while the first one, the method with variable weights.

In the Monte-Carlo method with constant weights the total time for tracing decreases because of a lower number of events with nonzero weights, which only should be traced.

The variance of the estimation $I_N^{(1)}$ is the following

$$DI_N^{(1)} = \frac{1}{N} D\theta^{(1)} = \frac{1}{N} [M \iint_{GG} \chi(q_1) f(q_0) p(q_0, q_1) dq_0 dq_1 - I^2] = \frac{1}{N} [MI - I^2];$$

it is larger than the variance of the estimation I_N in the variable-weight method

$DI_N^{(1)} \ge DI_N$.

In many cases the first method is nonrealizable and the second one gives the unsufficient accuracy for the same values of N.

Below we propose a generalization of the constant weight method that allows us to achieve a reasonable compromise, to calculate the integral with the acceptable accuracy, having a rather small number of events with nonzero weights.

2. METHOD WITH FRACTIONAL WEIGHTS

For every $k = 1, 2, \ldots$ introduce the random variable

$$\theta^{(k)} = \frac{1}{k} \sum_{\ell=1}^{k} \xi(q_0, \gamma_\ell) \chi(q_1) M,$$

with $\gamma_1, \ldots, \gamma_k$ random numbers. The expectation value of the random variable $\theta^{(k)}$ is equal to the integral I

$E\theta^{(k)} = I$

which allows us to obtain the estimation of the integral

$$I \approx I_N^{(k)} = \frac{1}{N} \sum_{i=1}^{N} \theta_i^{(k)} .$$

The variance of the estimation $I_N^{(k)}$ in the fractional-weight method is

$$DI_N^{(k)} = \frac{1}{N} D\theta^{(k)} = \frac{1}{N} (D\theta + \frac{D\theta^{(1)} - D\theta}{k}). \qquad (4)$$

We see that as $k \to \infty$ the accuracy of the fractional-weight method tends to the accuracy of the method with variable weights, and for $k=1$ this method coincides with the constant - weight method.

The efficiency of a Monte-Carlo method can be characterized by the labour content quantity T /1/

$T = tD\eta$,

where $D\eta$ is the variance of the random variable η for which we calculate the expectation value, and t is the time for calculating of one value of η.

The calculation time needed for reaching a given accuracy is proportional to the labour content [1].

It is natural in the fractional weight method to use such k that the labour content T(k) be minimum.

3. OPTIMIZATION OF THE LABOUR CONTENT

Let t_0 is the time for calculating q_0 and $f(q_0)/p(q_0)$, t_1 is the time for calculating q_1 and $\chi(q_1)$ and t_2 is the time for calculating $\xi(q_0,\gamma)$.

Then the calculation time of $\theta^{(k)}$ on the average is equal to

$$t^{(k)} = t_0 + [1-(1-g)^k]\, t_1 + k\, t_2 ,$$

where

$$g = E\{f(q_0)/[p(q_0)M]\} = \frac{1}{M}\int_G f(x)\,dx$$

is the average probability of the event $[\xi(q_0,\gamma)=1]$. Thus, the labour content of the fractional weight method is the following:

$$T(k) = \{t_0+[1-(1-g)^k]\,t_1 + k\,t_2\}\{D\theta + \frac{D\theta^{(1)}-D\theta}{k}\}.$$

The value of k corresponding to the minimum of the labour content can be found from the equation:

$$\frac{dT(k)}{dk} = 0. \qquad (5)$$

In practice, $t_2 \ll t_0, t_1$ and $g \ll 1$; in that case the solution of eq. (5) reads

$$k = \left(\frac{1}{g}\cdot\frac{D\theta^{(1)}-D\theta}{D\theta}\cdot\frac{t_0}{t_1}\right)^{1/2}. \qquad (6)$$

An example of the calculation of an optimum k for a concrete problem will be presented at the end of this paper.

4. THE FRACTIONAL-WEIGHT METHOD WITH THE SELECTION BY THE SAMPLING MAXIMUM

In those cases when the upper bound for the weight $f(x)/p(x)$ is unknown, we can calculate the integral I by the fractional - weight method using the sampling maximum of the weights. Let $q_{01},\dots,q_{0N}$ be the points independently distributed with density $p(x)$. Let us find the maximum value of the weight reached on this set of points

$$\tilde M(q_{01},\dots,q_{0N}) = \max_{1\le i\le N}\left[\frac{f(q_{0i})}{p(q_{0i})}\right].$$

Let $\tilde\theta_i^{(k)}$ denote the random variable

$$\tilde\theta_i^{(k)} = \frac{1}{k}\sum_{\ell=1}^{k} \xi(q_{0i},\gamma_{\ell i})\,\chi(q_{1i})\,\tilde M,$$

where

$$\xi(q_{0i},\gamma_{\ell i}) = \begin{cases} 1 \text{ for } \gamma < f(q_{0i})/[p(q_{0i})\tilde M], \\ 0 \text{ in the opposite case.}\end{cases}$$

Let $\tilde I_N^{(k)}$ denote the estimation of the integral

$$\tilde I_N^{(k)} = \frac{1}{N}\sum_{i=1}^{N}\tilde\theta_i^{(k)}.$$

Theorem 2. The expectation value of the estimation $\tilde I_N^{(k)}$ is equal to the integral

$$E\tilde I_N^{(k)} = I.$$

Proof. For proving let us calculate this expectation value

$$E\tilde I_N^{(k)} = \frac{1}{Nk}\sum_{i=1}^{N}\sum_{\ell=1}^{k} E[\xi(q_{0i},\gamma_{\ell i})\,\chi(q_{1i})\tilde M] =$$

$$= \frac{1}{Nk}\sum_{i=1}^{N}\sum_{\ell=1}^{k}\underbrace{\int_G\int_G\cdots\int_G\int_G}_{N}\int_0^1 \xi(q_{0i},\gamma_{\ell i})\,\chi(q_{1i})\,\tilde M(q_{01},\dots,q_{0N})\times$$

$$\times\, p(q_{01})\dots p(q_{0N})\,p(q_{0i},q_{1i})\,dq_{01}\dots dq_{0N}\,dq_{1i}\,d\gamma_{\ell i} = I.$$

Thus, theorem 2 grounds the Monte-Carlo method with fractional weights, where the upper bound M is changed by the sampling maximum of the weights.

Theorem 3. The random variables $\tilde\theta_i^{(1)}$ and $\tilde\theta_j^{(1)}, i\neq j$ do not correlate.

Proof. For proving we calculate the expectation value for the product of these random variables

$$E\tilde\theta_i^{(1)}\tilde\theta_j^{(1)} = \underbrace{\int_G\int_G\cdots\int_G\int_G\int_G}_{N}\int_0^1\int_0^1 \xi(q_{0i},\gamma_i)\,\xi(q_{0j},\gamma_j)\,\chi(q_{1i})\times$$

$$\times\,\chi(q_{1j})\,\tilde M(q_{01},\dots,q_{0N})\,p(q_{01})\dots p(q_{0N})\,p(q_{0i},q_{1i})\,p(q_{0j},q_{1j})\times$$

$$\times\, dq_{01}\dots dq_{0N}\,dq_{1i}\,dq_{1j}\,d\gamma_i\,d\gamma_j =$$

$$= \underbrace{\int_G\int_G\cdots\int_G\int_G\int_G}_{N}\frac{f(q_{0i})f(q_{0j})}{p(q_{0i})p(q_{0j})}\,\chi(q_{1i})\,\chi(q_{1j})\times$$

$$\times\, p(q_{01})\dots p(q_{0N})\,p(q_{0i},q_{1i})\,p(q_{0j},q_{1j})\,dq_{01}\dots dq_{0N}\,dq_{1i}\,dq_{1j} = I^2.$$

From the absence of correlation of $\tilde{\theta}_i^{(1)}$ and $\tilde{\theta}_j^{(1)}$ it follows that the variance of the estimation $\tilde{I}_N^{(1)}$ is

$$D\tilde{I}_N^{(1)}=\frac{1}{N}D\tilde{\theta}_1^{(1)}=\frac{1}{N}[\underbrace{\iint\ldots\iint}_{\substack{GG\quad GG\\ N}}\chi(q_{11})f(q_{01})\tilde{M}(q_{01},\ldots,q_{0N})\times$$

$$\times\, p(q_{02})\ldots p(q_{0N})p(q_{01},q_{11})\,dq_{01}\ldots dq_{0N}\,dq_{11}-I^2]$$

and the variance of the estimation $\tilde{I}$

$$D\tilde{I}_N^{(k)}=\frac{1}{N}D\tilde{\theta}_1^{(k)}=\frac{1}{N}(D\theta+\frac{D\tilde{\theta}_1^{(1)}-D\theta}{k}). \qquad (7)$$

From the absence of correlation it follows also that the sampling variance is the unbiased estimation of the variance

$$DI_N^{(k)}\approx\frac{1}{N(N-1)}\sum_{i=1}^{N}[\tilde{\theta}_i^{(k)}-\tilde{I}_N^{(k)}]^2.$$

Comparing the expression for the variance in the simple method of fractional weight (4) with those in its latter modification (7) we see that for the same N and k

$$D\tilde{I}_N^{(k)}\le DI_N^{(k)},$$

because always

$$\tilde{M}(q_{01},\ldots,q_{0N})\le M.$$

Thus, this method provides a better accuracy than the simple fractional weight method. The shortcoming of the latter is that it is necessary to storage all points $q_{01},\ldots,q_{0N}$ with their weights during the calculations.

5. A PRACTICAL EXAMPLE OF THE APPLICATION OF THE FRACTIONAL WEIGHT METHOD

This work was initiated by the necessity to calculate the background from electromagnetic three-muon events (tridents) in analysing multimuon spectra measured in an experiment on deep inelastic muon-nucleon scattering /2/. For calculations of the background we generated 468 312 events with their weights using the program TRIDENT /3/. The accuracy in the definition of the total cross section of the trident production is equal to 1.3%. It is impossible to process 468 312 events through programs of tracing /4-6/ because for tracing of one event one needs, on the average, 2.5 s at CDC-6500. At k = 1 the number of events with the nonzero weight is equal to 520 which gives 4.8% accuracy of the total cross section. The calculation of the optimum k was done by the approximate formula (6).

In our case

$$\frac{D\theta^{(1)}-D\theta}{D\theta}\approx 13,\quad g=\frac{520}{468312}\approx 1.1\cdot 10^{-3},\quad \frac{t_0}{t_1}\approx 0.009$$

so that $k\approx 10$.

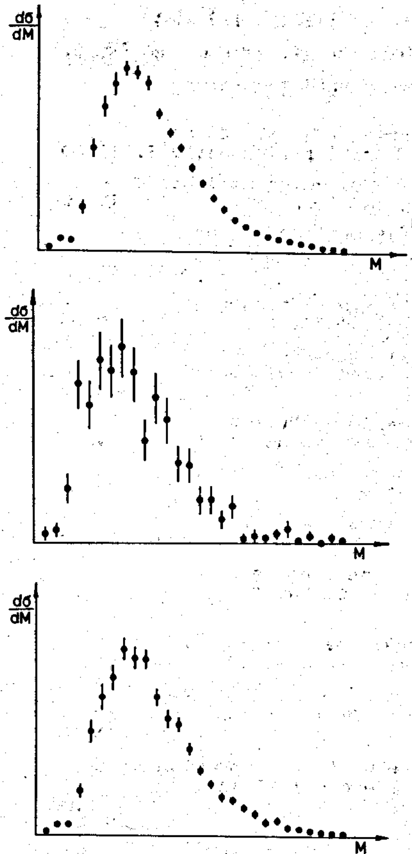

Fig. The spectra of effective dimuon masses calculated a) in the variable-weight method, b) in the constant-weight method, c) in the fractional-weight method.

If we take the labour content of the variable weight method equal to 1: $T(\infty)=1$ then $T(1)=0.14$ and $T(10)=0.05$, and the ratio $T(\infty)/T(10)\approx 20$. The number of events with nonzero weights is not yet very large and is equal to 4113 what provides the accuracy 2%.

In the figure we presented the spectra of effective dimuon masses from electromagnetic tridents calculated in the variable weight method (a), in the constant-weight method (b), and in the fractional-weight method, k = 10 (c). Some geometrical cuts simulating the set-up were applied, the dimuon mass was calculated using the 4-momentum of μ^- and μ^+ with the lowest momentum.

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