An Iterative Rejection Sampling Method

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ABSTRACT: In the note we consider an iterative generalisation of the rejection sampling method. In high energy physics, this sampling is frequently used for event generation, i.e. preparation of phase space points distributed according to a matrix element squared $|M|^2$ for a scattering process. In many realistic cases $|M|^2$ is a complicated multi-dimensional function, so, the standard von Neumann procedure has quite low efficiency, even if an error reducing technique, like VEGAS, is applied. As a result of that, many of the $|M|^2$ calculations go to "waste". The considered iterative modification of the procedure can extract more "unweighted" events, i.e. distributed according to $|M|^2$. In several simple examples we show practical benefits of the technique and obtain more events than the standard von Neumann method, without any extra calculations of $|M|^2$.

KEYWORDS: Rejection sampling, Monte Carlo Simulation, Iterative algorithms .

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1. Introduction

Simulated events of particle scattering are one of the main tools both in modern theoretical research and in current experimental analyses in the high energy physics (HEP). Usually the events are prepared by means of Monte Carlo techniques. The reason for the success of the methods is very clear: current simulation problems require realistic events of the processes $2 \rightarrow N$, where N is set by the accelerator energy and is equal to several hundreds for the LHC, for instance. But even applied approximations such as partons showers and zero width decays for the final particles leave us with $N \approx 3 - 10$. This large number corresponds to a 5 - 25 dimension phase space. Owing to the large number of dimensions and complexity of the investigated functions – the matrix elements squared – we cannot rely on deterministic grid methods due to the well-known "curse of dimensionality".

The standard scheme applied is the following: at first we prepare a matrix element squared symbolically (by hand or automatically), construct an importance sampling function, again manually or automatically by applying, for example, VEGAS [1]; obtain an estimation of the total integral (the total cross section), for chosen cuts and parameters, by the classic Monte-Carlo method, find the function maximum (or an array of maxima, since stratified sampling may be worth applying), generate enough weighted events for the function, and perform the "hit-and-miss" von Neumann procedure [2]. The final step maps the weighted points, distributed according to the importance sampling function, to a subset of the sample – realistic independent unweighted events distributed according to the matrix element squared. This is the general and oversimplified scheme of functioning of almost all modern Monte-Carlo generators, see for example the review [3]. Useful information on current mathematical Monte-Carlo techniques applied in HEP can also be found in the short review by Weinzierl [4].

Although the scheme described guarantees that the unweighted events are distributed according to the function considered, the selection efficiency usually is not too high, especially if the function has lots of sharp peaks. The main reason is that importance sampling functions are simple functions and they have much smoother behaviour and describe the real function behaviour in a very crude approximation. As a result we get lots of calculated points going into the "waste bin". Since the cost calculating of the investigate function can be quite large it would be worth considering whether we can extract more information (e.g. more unweighted events) from the "waste". The most obvious way to achieve this goal is to repeat the von Neumann procedure with the rejected phase space points. It is rather clear that these points *can* be used for the task, but with worse quality. Since, at the first rejection stage, some points have been accepted and, so, removed from the sample of the weighted events, we should change the weights of all remaining points. The paper is devoted to the construction of a procedure, which gives us the possibility to use the rejected points iteratively.

In fact, the idea of using rejected points is not quite new. For example, an iterative von Neumann procedure for the extraction of random bits from an independent but biased bit array was constructed in [5]. It originates from one of von Neumann's ideas published in his famous paper [2]. In this paper we generalise another procedure set out in the paper - rejected sampling.

As we mentioned earlier the initial sample should be prepared with an importance sampling function, in order to increase selection efficiency. Since we are interested in an automated procedure, we will use the VEGAS algorithm, the de facto standard of importance sampling in HEP. It is worth noticing that VEGAS itself can be improved, as is described in Ohl's paper [6]. For some practical and historical reasons we will apply the slightly adapted VEGAS algorithm from CompHEP [7].

In Sec. 2 we give some mathematical arguments in favour of the iterative von Neumann procedure and formulate the method itself. In Sec. 3 we define a stopping rule for the method. Three model, but rather realistic, examples are considered in Sec. 4. Final remarks and conclusions are given in the section 5.

2. Iterative von Neumann procedure

We start from the standard "hit-and-miss" von Neumann procedure applied to a nonnegative function $f(\bar{x})$, where $\bar{x} = \{x_1, ..., x_d\}$ is a point in the *d*-dimension phase space. For simplicity we limit ourselves to a bounded domain \mathcal{D} in the phase space. At first, we prepare a sample of N phase space points $\{\bar{x}_i\}_N$, i = 0, ..., N-1 in \mathcal{D} , distributed according to an importance sampling distribution $g(\bar{x})$, where $g(\bar{x})$ is a positive function normalised with the condition $\int_{\mathcal{D}} g(\bar{x}) d\bar{x} = 1$. So, the corresponding weight ω_i of each point is equal to $f(\bar{x}_i)/g(\bar{x}_i)$. Having the weights we can estimate the total integral

$$I_{tot} = \int_{\mathcal{D}} f(\bar{x}) d\bar{x} \approx \langle f \rangle_{\bar{1}} = \langle f/g \rangle_{\bar{g}} = \frac{1}{N} \sum_{i=0}^{N-1} \omega_i,$$

where we denote an estimation of the integral with a sample of uniformly distributed points $\langle \cdot \rangle_{\bar{1}}$. We can also obtain an estimation of the accuracy given by $\sigma^2 = \langle \omega^2 \rangle_{\bar{g}} - \langle \omega \rangle_{\bar{g}}^2$ – the standard deviation. The next step is to pick out a subset of the point distributed according to $f(\bar{x})$ from $\{\bar{x}_i\}_N$. Let us formulate the standard rejection sampling procedure¹:

- Generate a random number $0<\xi<1$
- Compare $W_i = \omega_i / \omega_0$, if $W_i > \xi$ accept the point to the final sample.
- Repeat the procedure for all points in the sample.

It is obvious that the final sample of accepted points is distributed according to $f(\bar{x})$. But we also obtain the second sample of the *rejected* points. Usually the sample is much larger than the sample of accepted points. So, the main question of this note is whether we can extract something useful from analyzing the rejected points. Our answer is affirmative. Namely, we will construct a procedure, which "returns" the rejected point sample to (almost) the initial position before the von Neumann procedure was applied. Thus, we will build an iterative Monte-Carlo rejection sampling.

The possibility of the procedure is based on two observations. First, we can apply the "hit-and-miss" algorithm for points distributed according to any importance sampling function. The only conditions we require is our ability to calculate the function at each point in the initial sample and the positivity of the function, since $g(\bar{x}_i)$ goes to denominator. Certainly, the acceptance efficiency will be strongly dependent on the chosen function. The second observation (or, strictly speaking, a limitation) is the relevance of the maximum value of $f(\bar{x})$ at \bar{x}_0 . If we take ω_0 for the "hit-and-miss" procedure the point will be accepted by construction, since the acceptance probability of the point is equal to 1.0. So, the rejected points will describe the region near \bar{x}_0 worse then any other region, and further samples constructed at the next rejection steps will become worse and worse. Thus, we must formulate a simple criterion which ensures a sufficiently reasonable description of the region around the "maximum" in the new accepted sample and stops iteration if the description becomes "too poor" (see more details of the criterion in the next section). Therefore, our goal is twofold. First, we must construct a distribution function for the rejected points (we make it in this section). After that, we have to see whether the rejected points are still able to describe $f(\bar{x})$ without serious drawbacks, especially in the region around f_{max} .

The first problem can be solved by considering the densities of points in three samples: a) the initial one, b) the sample of accepted points after the "hit-and-miss" procedure, and c) the sample of rejected points. The densities are equal to

$$\rho_{ini}(\bar{x}) = N \cdot g(\bar{x}) \equiv N \cdot g_0(\bar{x}),$$
$$\rho_{acc}(\bar{x}) = \alpha \cdot N_{acc} \cdot f(\bar{x}),$$
$$\rho_{rej}(\bar{x}) = N_{rej} \cdot g_1(\bar{x}),$$

¹We will assume the point \bar{x}_0 has the maximum weight $\omega_0 = f(\bar{x}_0)/g(\bar{x}_0)$ in the sample.

where we assume the importance sampling functions are normalised to 1.0 and α is responsible for normalisation of $f(\bar{x})$: $\alpha = 1/\int f(\bar{x})d\bar{x} \approx 1/I_{tot}$. N_{acc} and N_{rej} are the numbers of accepted and rejected points correspondingly and $N = N_{acc} + N_{rej}$. Our first problem is to find the function $g_1(\bar{x})$. Since the samples of accepted and rejected points are obtained from the initial sample we can make use of the following key equation:

$$\rho_{ini}(\bar{x}) = \rho_{acc}(\bar{x}) + \rho_{rej}(\bar{x}) \tag{2.1}$$

Substituting our expressions for the densities we obtain

$$g_1(\bar{x}_i) = (N - \alpha \cdot N_{acc} \cdot \omega_i)g_0(\bar{x}_i)/N_{rej},$$

where ω_i is the initial weight of the i-th point (for the importance sampling function $g_0(\bar{x}) \equiv g(\bar{x})$). Since the proper weights of the rejected points distributed according to $g_1(\bar{x})$ are $f(\bar{x}_i)/g_1(\bar{x}_i)$ we can obtain the final formula for the weight of the point \bar{x}_i (if it has been rejected):

$$\omega_i' = \frac{(1-\epsilon) \cdot \omega_i}{1-\epsilon \cdot \omega_i/I_{tot}},\tag{2.2}$$

where ω_i is the point weight *before* rejection sampling, ω'_i is its weight according to the distribution $g_1(\bar{x})$, and ϵ is the acceptance efficiency for the sample.

The first consequence of the formula is that we do not need to calculate the new importance sampling function $g_1(\bar{x})$ for the next iteration at all. The new weights of the rejected points are calculated from the old ones by means of a very simple function $f(z) = A \cdot z/(1 - B \cdot z)$. Thus, we come back to the first step and can repeat the von Neumann rejection procedure based on the new weights. Obviously, the second iteration will bring less points since larger weights became larger and vice versa.

Accordingly the iterative Monte-Carlo "hit-and-miss" procedure has a very simple formulation:

- 1. Prepare a sample of points $\{\bar{x}_i\}_N$ with weights $\omega_i = f(\bar{x}_i)/g(\bar{x}_i)$ and estimate I_{tot}
- 2. Perform the von Neumann procedure for the sample.
- 3. Re-calculate the weights of the rejected points according the formula (2.2) and find the point with the maximum weight. It will be the next \bar{x}_0 .
- 4. Check whether the sample satisfy a stopping condition. If not, repeat the iterations starting from point 2.

It is interesting to mention that the transformation (2.2) is stable during iterations. If we perform m iterations and accept $N_{acc}^{(1)}, ..., N_{acc}^{(m)}$ points in the iterations, then we obtain

$$\omega_i^{(n)} = \frac{(1 - \epsilon^{(n)}) \cdot \omega_i}{1 - \epsilon^{(n)} \cdot \omega_i / I_{tot}},$$

where $\epsilon^{(n)} = \sum_{i=1}^{m} \epsilon^{(i)} \sum_{i=1}^{m} N_{acc}^{(i)}/N.$

Let's estimate the a priori number of events, which would be accepted at the $(n+1)^{\text{th}}$ iteration, if we know the information from the previous stage. In order to accept a point, we compare its weight with a uniformly distributed number ξ . So, we can say that ω_i/ω_0 is the probability of the point to be accepted. Since the transformation (2.2) does not change the maximum point, we can write down

$$N_{acc}^{(n+1)} = N_{rej}^{(n)} \frac{I_{tot}}{\omega_{0,rej}^{(n),'}} = I_{tot} \left(\frac{N_{tot}^{(n)}}{\omega_{0,rej}^{(n)}} - N_{acc}^{(n)} \right) = N_{tot}^{(n)} (1/\omega_{0,rej}^{(n)} - 1/\omega_{0,tot}^{(n)}),$$

where $N_{tot}^{(n)}$, $N_{acc}^{(n)}$, and $N_{rej}^{(n)}$ are the numbers of points in the sample before nth iteration, and the numbers of accepted and rejected points at the iteration. $\omega_{0,tot}^{(n)}$, $\omega_{0,rej}^{(n)}$ and $\omega_{0,rej}^{(n),'}$ are the maximum weight in the whole sample before the nth iteration, the maximum weight of rejected points only and the point weight calculated according to (2.2). In the formula we use an approximate equality for the a priori and a posteriori acceptance efficiency at the nth iteration: $\epsilon_{est} = I_{tot}/\omega_0 \approx \epsilon_{real} = N_{acc}/N$.

3. The stopping rule for iterations

The procedure constructed in the previous section lacks only one element – a reasonable stopping rule. In order to find the condition let us look at the formula (2.2) in more detail. It fails to produce sensible weights if the function $f(\omega) = 1 - \epsilon \cdot \omega / I_{tot}$ is less than or equal to zero. It is clear that the worst case happens if we substitute the maximum weight ω_0 . Let us show that $1 - \epsilon \cdot \omega_0 / I_{tot} = 0$ "on the average". As we pointed out above, the probability of a point to be accepted is equal $W_i = \omega_i / \omega_0$. Since any accepted point increases the accepted point sample, the average number of accepted point is $N_{acc} = \sum_{i=0}^{N} W_i = N \cdot I_{tot}/\omega_0$ or $1 - \epsilon \cdot \omega_0 / I_{tot} = 0$. So, it looks as the standard von Neumann procedure picks out all possible points and already the first re-weighting brings us to an inapplicable state of the iterative method. But, the solution of the drawback happens automatically, merely due to the definition of the von Neumann procedure. By construction, \bar{x}_0 always falls within the accepted point sample, and for almost all rejected points the formula (2.2) gives a finite answer. It also makes clear the source of the extra events. We effectively lower the normalised factor $\omega_0 \to \omega_{0,rej} < \omega_0$, so there is a room for more accepted events. But the reduction is rather smart and does not spoil the statistical sense of accepted events. Certainly the rejected events give a cruder estimation of the function and in realistic cases there exists a neighbourhood of \bar{x}_0 where we do not have any rejected points at all. So, we lose some part of the total integral. As we see in the next section the total integral in iteration tends to decrease and, thus, further iterations give an underestimated simulation of our function $f(\bar{x})$.

Not we can formulate a natural criterion of the stopping condition for the iterative procedure. At the beginning we have a sample which gives us an estimation of the total integral with some error. It is estimated from the standard deviation calculated using the sample. We can continue the iterations as long as the integral estimations at the first and *m*-th steps $I_{tot}^{(0)}$ and $I_{tot}^{(m)}$ satisfy the following inequality

$$|I_{tot}^{(0)} - I_{tot}^{(m)}| \le \sigma_0 + \sigma_m, \tag{3.1}$$

where $\sigma_{0,m}$ are the standard deviations at the first and *m*-th steps. In this case, we still properly estimate the function $f(\bar{x})$ at the *m*-th step, in general, and can extract points distributed according to the function. Now we are able to formulate the algorithm completely:

- 1. Prepare a sample of points $\{\bar{x}_i\}_N$ with calculated weights $\omega_i = f(\bar{x}_i)/g(\bar{x}_i)$ and estimate I_{tot}
- 2. Perform the von Neumann procedure for the sample
- 3. Re-calculate weights of the rejected points according the formula (2.2) and find the point with the maximum weight. It will be the next \bar{x}_0
- 4. Check whether all the calculated weights are positive. If not, stop iteration
- 5. Estimate the total integral value and check whether the inequality (3.1) holds true. If yes, repeat the iteration starting from point 2, otherwise stop.

The final problem we come across is the question whether we can mix accepted events obtained in the all iterations. In fact, it is easy to prove that the accepted events have equal weights $I_{tot} = \langle f \rangle_{\bar{1}} = \langle \omega \rangle_{\bar{g}(x)}$. The points are distributed according to $g(\bar{x}) = f(\bar{x})/\langle f \rangle$, if we substitute the expression to the weight formula $\omega_i = f(\bar{x}_i)/g(\bar{x}_i) = \langle f \rangle$. In each step in the algorithm we obtained events with different weights, but they are distributed within the sample statistical error and can be considered as statistically the same.

4. Numerical examples

In order to check the practicality of the method we consider three different numerical examples of application of the method to complicated multidimensional functions.

The first example is a sum of two Gaussians

$$f_1(\bar{x}) = A_{norm} \cdot \left[\exp\left(-\frac{(\bar{x} - \bar{a}_1)^2}{2 \cdot \sigma_1^2}\right) + \xi_6 \cdot \exp\left(-\frac{(\bar{x} - \bar{a}_2)^2}{2 \cdot \sigma_2^2}\right) \right]$$
(4.1)

in a 6-dimensional unit hypercube. For calculations we chose the following values of the parameters: $A_{norm} = 1.0, \xi_6 = 729.0, \sigma_1 = 0.06, \sigma_2 = 0.02, \bar{a}_1 = (0.2, 0.2, 0.2, 0.2, 0.2, 0.2),$ and $\bar{a}_2 = (0.7, 0.7, 0.7, 0.7, 0.7, 0.7)$. We chose $A_2 = 729.0$ in order to compensate for the difference in the Gaussian widths.

At first, we prepared the VEGAS grid (10 iterations of the grid customization were done) for the function and generated the initial sample of points; it contained approximately $4.5 \cdot 10^6$ points. After that, the iterative von Neumann procedure was carried out with the sample. By definition, the first iteration corresponds to the standard von Neumann selection. On the whole we made 25 iterations. No zero or negative weights were calculated in the iterations. Fig 1 displays the total integrals and cumulative numbers of points selected at each iteration. As we see our stopping rule 3.1 is satisfied at the 15th iteration. Fig. 2 illustrates the quality of fitting of the two obtained samples. We fit the histogram dN_{point}/dx_0 with the original function (certainly, in 1 dimension). The upper plot corresponds to the first iteration sample only (the standard procedure), and the distribution for the sample of points combined for fifteen iterations is depicted in the lower plot. The latter sample is 6.5 times bigger then the former sample. Although the quality of fit for the iterative sample is slightly lower, all parameters of the original function are reconstructed better than for the standard sample. So, we can conclude the built iterative method works properly in this particular example.



Figure 1: Values of the total integral and the cumulative number of selected events at iterations of the iterative von Neumann procedure for the function (4.1).

The second example is a combination of two Breit-Wigner peaks in the 8-dimensional unit hypercube. The exact formula is the following:

$$f_2(\bar{x}) = A_{norm} \cdot \left[\frac{1}{(a_1 - Y)^2 + \Gamma_1^2} + \frac{\xi}{(a_2 - Y)^2 + \Gamma_2^2} \right], \tag{4.2}$$

where we introduce the resonance variable $Y = \sum_{i=0}^{3} x_i$. Again, we prepared a sample of points in the phase space. The sample size was $2.8 \cdot 10^6$ points for the function with

parameters $A_{norm} = 60.0$, $\xi = 0.167$, $\Gamma_1 = 0.01$, and $\Gamma_2 = 0.02$. The two peaks are located at the points $a_1 = 0.2$ and $a_2 = 0.75$. The resonances are taken for the sum of four variables $Y = \sum_{i=0}^{3} x_i$ in order to make the function less sensitive for the VEGAS customization. By definition, the first iteration of the iterative von Neumann procedure gave the standard selection with the a posteriori efficiency $\epsilon_{eff} = 2.57\%$. After that we repeated the procedure 16 times for the re-calculated weights (at each step). The total integral values and numbers of selected points are reported in Fig. 3. Owing to the stopping rule (3.1) we should combine samples of the first 6 iterations only. This results in the total cumulative efficiency $\epsilon_{eff} = 4.41\%$. Again, we fit the histogram dN_{point}/dY with the original formula². We see the iterative sample results in a better fit, i.e a smaller χ^2 and more precise values of the function parameters.

The third example represents a non-symmetric function in a 20-dimensional hypercube:

$$f_2(\bar{x}) = \frac{A_{norm}}{(a_1 + x_0)^{20}}.$$
(4.3)

Since $x_0 \geq 0$ in the hypercube and the function approaches infinity at $x_0 = -a_1$, we simulate the right-hand slope of the function, if $a_1 > 0$. We chose the following values of the function parameters: $A_{norm} = 10^{-55}$ and $a = 10^{-3}$. The initial sample had $2.23 \cdot 10^6$ points. The first (standard) iteration gave the a posteriori efficiency $\epsilon_{eff} = 3.29\%$. We repeated the selection ten times and combined selected points in the final samples for the five iterations, according to our sopping rule. The final efficiency is equal to 7.28\%. The total integral values and numbers of selected points are reported in Fig. 5. Since we cannot improve the accuracy of A_{norm} by our method, we are interested in the quality of the reconstruction of a only. We fit the histogram dN_{point}/dx_0 with the original formula. Again, we see that the iterative sample results in smaller χ^2 and more precise value of a(see Fig. 6).

5. Discussion and Conclusions

A simple generalisation of the standard von Neumann procedure has been constructed. The method is based on the observation that in realistic Monte-Carlo calculations we always have an uncertainty in the estimation of the total integral. This means we can repeat the standard von Neumann rejection sampling several times until we are within limits of the uncertainty. As soon as we exceed the limit the final sample will start to give worse results. Since we exclude some points in the rejection sampling we must rearrange weights of points in the rejected sample. We found that the transformation is universal (it does not depend on the function considered) and extremely simple – the key formula (2.2). The second obstacle which can prevent iteration is negative weights of some points. This can

²Strictly speaking, for the fitting procedure we must multiply the expression (4.2) by Y^3 since we prepared the sample parametrised with $\{x_0, ..., x_7\}$, but the resonance variable is the combination $Y = \sum_{i=0}^{3} x_i$. If we transform the initial parametrisation into the most natural one, which contains Y, integration over the other re-defined variables gives us an extra factor Y^{N-1} in the numerator. In our case, N is equal to 4.

happen especially in the case of very low selection efficiency. So, we formulated a stopping rule for the iterative procedure, which permits one to stay within a well-defined statistical interpretation of selected points and to combine all samples obtained in the iterations into one.

It is worth stressing that, by definition of our method, we cannot improve the accuracy of the total integral or, in other words, the quality of the reconstruction of the total normalization constant of a function under consideration. Moreover, since we select points with larger weights, the rejected point sample gives a biased estimation of the total integral. Of course we can prevent bad behaviour of the iteration process by application of the stopping rule (3.1).

Three numerical examples show the procedure can really bring practical benefits in calculations. Owing to the simplicity of the procedure it can have a very broad area of application. In fact, almost every sampler, satisfying the condition that we should be able to prepare a set of independently generated points with weights, can be supplemented with a code producing more points iteratively. The method can be easily generalised to stratified sampling, since it can be applied independently in each stratum.

As the first realistic application we are going to implement the method in the Monte-Carlo generators CompHEP [8] and Herwig++ [9]. Certainly, the method can be adopted by other popular codes (e.g. PYTHIA, MadGraph, Alpgen, Sherpa) [10].

6. Acknowledgements

I would like to thank Bryan Webber and Deirdre Black for useful discussions and remarks. I would like to acknowledge the British STFC for the award of a Responsive Research Associate position, RFBR (the RFBR grant 07-07-00365-a), and European Union Marie Curie Research Training Network MCnet (contract MRTN-CT-2006-035606) for partial support of the project.

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Figure 2: The dN_{point}/dx_0 distribution for the example (4.1) for two approaches, the standard von Neumann procedure (upper plot) and the iterative von Neumann procedure (lower plot). Both curves are fitted with the original function (for 1 dimension). It is worth noticing that $\xi = \sqrt[6]{\xi_6}$, since this is an one-dimensional histogram. -11 –



Figure 3: Values of the total integral and the cumulative number of selected events at iterations of the iterative von Neumann procedure for the function (4.2).



Figure 4: The dN_{point}/dY distribution for the example (4.2) fitted for two approaches, the standard von Neumann procedure (upper plot) and the iterative von Neumann procedure (lower plot).



Figure 5: Values of the total integral and the cumulative number of selected events at iterations of the iterative von Neumann procedure for the function (4.3).



Figure 6: The dN_{point}/dx_0 distribution for the example (4.3) fitted for two approaches, the standard von Neumann procedure (upper plot) and the iterative von Neumann procedure (lower plot).