1 Sampling Monte Carlo integrals

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1.1 Monte Carlo integrals

Let I be equal to the following 1D Monte Carlo integral:

$$I = \int\limits_{-\infty}^{\infty} f(x)g(x)\,\mathrm{d}x = \int\limits_{C} f(x)g(x)\,\mathrm{d}x \tag{1}$$

where $g(x)$ is regarded as the pay-off or the detector function of the integral. Let $g(x)$ be bounded and have compact support, limiting the integral to a finite interval: C. If $f(x)$ is non-negative, bounded and integrable on interval C, a pdf (probability density function) $\mathbb{p}(x)$ can be defined, by normalizing $f(x)$:

$$\mathbb{p}(x) = \frac{f(x)}{\int\limits_{C} f(x)\,\mathrm{d}x} \tag{2}$$

If x_i, $(x = 1, 2, ..., N)$ samples are drawn from from $\mathbb{p}(x)$ (using inverse cumulative or any other method), the estimation of the integral is the following:

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} g(x_i) \int\limits_{C} f(x)\,\mathrm{d}x = \frac{1}{N}\sum_{i=1}^{N} c_i \tag{3}$$

where c_i is the contribution of the ith particle, the obtained $\hat{I}$ is an unbiased estimation of I, i.e. $\mathbb{E}[\hat{I}] = I$.

The variance of the estimation can be estimated the following way:

$$\mathbb{D}^2[\hat{I}] = \frac{1}{N^2}\mathbb{D}^2[c_i] \approx \frac{1}{N^2}\sum_{i=1}^{N} c_i^2 - \frac{1}{N}\left(\frac{1}{N}\sum_{i=1}^{N} c_i\right)^2 \tag{4}$$

Instead of the (absolute) variance, often the relative variance: $\mathbb{r}^2[\hat{I}] = \mathbb{D}^2[\hat{I}]/\mathbb{E}^2[\hat{I}]$ is used, since it can be more informative.

1.2 Sampling exponential distribution

The cornerstone of every Monte Carlo simulation is the sampling of pdf-s, as seen in Section 1.1. One of the most commonly sampled distributions in Monte Carlo transport simulation is the exponential distribution. The reason for this is that the free path of particles between two collision sites (in homogeneous media) follows an exponential distribution, this is called the Beer-Lambert law:

$$\mathbb{p}(x) = \Sigma e^{-\Sigma x}, \quad \mathbb{P}(x) = \int_{-\infty}^{x} \mathbb{p}(x')\, \mathrm{d}x' = 1 - e^{-\Sigma x} \tag{5}$$

where Σ is the (total macroscopic) cross section of the media, $\mathbb{P}(x)$ is cdf (cumulative density function) of the distribution of the free path x. Using inverse cumulative method, equation 5 can be sampled, using a uniform (canonical) random number r, the following way:

$$x = -\frac{1}{\Sigma} \ln(1 - r) \tag{6}$$

The sampling cross section can be changed to bias the integral.

1.3 Sampling in inhomogeneous media

In inhomogeneous media the pdf and the cdf of the free path is the following:

$$\mathbb{p}(x) = \Sigma(x) e^{-\int_0^x \Sigma(x')\mathrm{d}x'}, \quad \mathbb{P}(x) = 1 - e^{-\int_0^x \Sigma(x')\mathrm{d}x'} \tag{7}$$

resulting in:

$$-\ln(1 - r) = \int_0^x \Sigma(x')\, \mathrm{d}x' \tag{8}$$

which usually can only be solved numerically, which makes the sampling difficult and inefficient.

1.4 Analog Woodcock method

Woodcock (or delta) tracking eliminates the difficulties of sampling in inhomogeneous media by introducing a majorant cross section $\Sigma_{maj} \geq \Sigma(x)$ to sample free path. The free path is sampled according to equation 6, with cross section Σ_{maj}. The sampled free path is accepted with the probability $p = \Sigma(x)/\Sigma_{maj}$, using an uniformly distributed random number, and rejected with probability $1 - p$. If a free path is rejected a virtual collision (delta scatter) happens, and the particle continues its flight without changing direction or energy to the next collision point, until a sampled free path is accepted.

The advantage of the method lies in the freedom that the flight tracking is not evaluated at every cell boundary crossing but only at the sampled collision points. On the other hand for example a small but strong absorbent with high cross section in the system results in a high majorant cross section, which makes the sampling slow and inefficient. Usually the majorant should be as low as possible, in inhomogeneous systems that means the maximum of the cross sections, in any given phase space.

1.5 Non-analog sampling

Non-analog (not nature mimicking) sampling is an unbiased sampling technique, which allows to reduce (or increase) the variance of a Monte Carlo integral, by using alternative distributions for sampling instead of the original ones. It is also useful in case of distributions which are difficult to sample or which can only be sampled numerically.

Let $\mathbb{p}'(x)$ be the new pdf used for sampling. The x_i, $(x = 1, 2, ..., N)$ samples drawn from $\mathbb{p}'(x)$ are inserted to the new detector function: $g'(x)$, to obtain the c_i contributions to the integral:

$$c_i = g'(x_i), \quad g'(x) = g(x)\frac{f(x)}{\mathbb{p}'(x)} \tag{9}$$

By using a different notation, by introducing the particle weight w_i, the contributions become:

$$c_i = g(x_i)w(x_i) = g(x_i)w_i, \quad w(x) = \frac{f(x)}{\mathbb{p}'(x)} \tag{10}$$

thus the estimation of the integral becomes the following:

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} c_i = \frac{1}{N}\sum_{i=1}^{N} g(x_i)w_i \tag{11}$$

The variation of the estimation can be estimated the same way as in the analog case, as shown in Eq. 4.

1.6 Exponential transformation

Exponential transform (or path stretching) is a special case of non-analog sampling for sampling exponential transformation. In a homogeneous media let s be a stretching (or shrinking) factor for the cross section, thus the sampling cross section becomes: $\Sigma_{samp} = s\Sigma$. Free path can be sampled according to equation 6, using Σ_{samp}. The weight correction factor w_i in equation 10, for the sample x_i becomes the following:

$$w_i = \frac{\Sigma e^{-\Sigma x_i}}{\Sigma_{samp} e^{-\Sigma_{samp} x_i}} = \frac{1}{s} e^{-\Sigma x_i (1-s)} \tag{12}$$

INHOMOGENEOUS?

1.7 Non-analog Woodcock method

Applying the non-analog sampling to the Woodcock method results in a more general technique. In the analog Woodcock method high majorant cross section can make the sampling of the free path inefficient. Furthermore if Σ_{maj} is not a majorant cross section, the probability of accepting a collision site is greater than 1.

To solve these problems, let Σ_{samp} be and arbitrary sampling cross section, and let q be and arbitrary acceptance probability. The free path is sampled from an exponential distribution, according to equation 6, using Σ_{samp}. The sampled collision site is accepted with probability q instead of $p = \Sigma(x)/\Sigma_{samp}$, which has to be accounted for by a hit weight factor:

$$w_{(hit)} = \frac{p}{q} = \frac{1}{q}\frac{\Sigma(x)}{\Sigma_{samp}} \tag{13}$$

The sample is rejected with probability $1-q$, instead of $1-p$, thus the miss weight factor is:

$$w_{(miss)} = \frac{1-p}{1-q} = \frac{1}{1-q}\left(1 - \frac{\Sigma(x)}{\Sigma_{samp}}\right) \tag{14}$$

When the sample is rejected a virtual collision occurs and the particle continues its flight to the next sampled collision point until the sampled free path is accepted.

By using this technique and choosing proper sampling cross section the efficiency of sampling free path can be greatly increased. On the other hand using non majorant sampling cross section introduces negative weights. When $\Sigma(x) > \Sigma_{samp}$, the the miss weight factor becomes negative and changes the sign of the particle weight. It is often advised avoiding negative weights as they can increase the variance of a Monte Carlo integral.

1.8 Non-analog Woodcock Method combined with exponential transformation

Exponential transform can be applied to the Woodcock method. Let Σ_{samp} be a majorant sampling cross section in a homogeneous media, let s be a stretching factor of the sampling cross section. The samples are drawn from the pdf:

$$\mathbb{p}(x) = s\Sigma_{samp}e^{-s\Sigma_{samp}x} \tag{15}$$

Let q be the acceptance probability of a sampled collision site, instead of $p = \Sigma/\Sigma_{samp}$, thus the hit weight factor reads:

$$w_{hit} = \frac{p}{q}\frac{1}{s}e^{-\Sigma_{samp}x_i(1-s)} = \frac{\Sigma}{q\Sigma_{samp}}\frac{1}{s}e^{-\Sigma_{samp}x_i(1-s)} \tag{16}$$

The probability of rejecting the collision site is $1-q$, instead of $1-p$, thus the miss weight factor becomes:

$$w_{miss} = \frac{1-p}{1-q}\frac{1}{s}e^{-\Sigma_{samp}x_i(1-s)} = \frac{\Sigma_{samp}-\Sigma}{\Sigma_{samp}(1-q)}\frac{1}{s}e^{-\Sigma_{samp}x_i(1-s)} \tag{17}$$

For later zero variance optimisation scheme, a different notation can be used. Let o be the oversampling factor of the majorant cross section Σ_{maj}, such that: $\Sigma_{samp} = o\Sigma_{maj}$. Also Σ/Σ_{samp} is always a factor of the weight hit factor, which introduces weight fluctuations the inhomogeneous case, thus the acceptance probability q can be redefined the following way:

$$q = Q\frac{\Sigma}{\Sigma_{samp}} = Q\frac{\Sigma}{o\Sigma_{maj}} \tag{18}$$

With these redefined quantities, the effective sampling cross section in equation 6. becomes: $Qs\Sigma$. The redefined weight factors are:

$$w_{hit} = \frac{p}{q}\frac{1}{s}e^{-o\Sigma_{maj}x_i(1-s)} = \frac{1}{Qs}e^{-o\Sigma_{maj}x_i(1-s)} \tag{19}$$

for a hit, and

$$w_{miss} = \frac{1-p}{1-q}\frac{1}{s}e^{-o\Sigma_{maj}x_i(1-s)} = \frac{o\Sigma_{maj}-\Sigma}{o\Sigma_{maj}-Q\Sigma}\frac{1}{s}e^{-o\Sigma_{maj}x_i(1-s)} \tag{20}$$

for a miss. In case of both notations after a collision site is rejected a virtual scatter occurs and the particle continues its flight until a sampled collision site is accepted.

1.9 Zero variance solution

According to the non-analog sampling theory described in section 1.5. the analytic form of the variance of the contributions to the integral is:

$$\mathbb{D}^2[c_i] = \mathbb{D}^2[c] = \int \left(g(x)\frac{f(x)}{\mathbb{p}'(x)}\right)^2 \mathbb{p}'(x)\,\mathrm{d}x - \left(\int f(x)g(x)\,\mathrm{d}x\right)^2 \tag{21}$$

If this variance is set equal to 0, the equation can be solved for $\mathbb{p}'(x)$, yielding:

$$\mathbb{p}'(x) = \frac{f(x)g(x)}{\int f(x)g(x)\,\mathrm{d}x} = \frac{f(x)g(x)}{I} \tag{22}$$

By sampling $\mathbb{p}'(x)$ a zero variance sampling can be achieved, which means that one single sample is enough to calculate the integral. The calculation still requires sampling the distribution, but the outcome will not be stochastic in nature. The c_i contribution of the sample x_i, sampled from $\mathbb{p}'(x)$ is the following:

$$c_i = g(x)\frac{f(x_i)}{\frac{f(x_i)g(x_i)}{\int f(x)g(x)\,\mathrm{d}x}} = \int f(x)g(x)\,\mathrm{d}x = I \tag{23}$$

It can be seen that every contribution equals the exact value of the integral, but to achieve this the integral has to appear in $\mathbb{p}'(x)$, as a normalizing factor, as seen in equation 22. But apart from the most simple cases the ideal $\mathbb{p}'(x)$ can only be sampled numerically, which already ruins the zero variance sampling.

For these reasons this zero variance sampling method has only a theoretical significance. In reality zero variance is rarely achievable, only in special cases set up for demonstrating this phenomena.

2 Zero variance transport Monte Carlo

The optimally biased Monte Carlo transport kernel (ref) is the following:

$$T'(r' \to r, E, \underline{\Omega}) = T(r' \to r, E, \underline{\Omega})\frac{\psi^*(r, E, \underline{\Omega})}{\chi^*(r', E, \underline{\Omega})} \tag{24}$$

where T is the unbiased free flight transport kernel, ψ^* is the adjoint collision density of particles entering a reaction, χ^* is the adjoint collision density of particles leaving the collision, r' is the starting spacial position of the particle, r is the endpoint of the free flight. $\chi^*(r', E, \underline{\Omega})$ is the expected total contribution of a particle starting a free flight at r', $\psi^*(r, E, \underline{\Omega})$ is the expected total contribution of a particle entering a collision at r. Given the link between ψ^* and χ^*:

$$\chi^*(r', E, \underline{\Omega}) = \int T(r' \to r, E, \underline{\Omega})\psi^*(r, E, \underline{\Omega})\,\mathrm{d}r \tag{25}$$

T' is normalized, and is the pdf of r

2.1 qZ

2.2 qZ=Qs decomposition

2.3 id Q

$$\frac{1}{s}\frac{o\Sigma_{maj}-\Sigma}{o\Sigma_{maj}-Q\Sigma}=1 \tag{26}$$

and

$$q_Z = Qs \tag{27}$$

solve for Q:

$$Q_{id} = q_Z\frac{o\Sigma_{maj}}{o\Sigma_{maj}+(q_Z-1)\Sigma} \tag{28}$$