

Q1: What is the principle of the correlated sampling method?

Ans:

Correlated sampling can be used when one must calculate the difference between two very similar models  $g_1$  and  $g_2$ ,

$$Y_1 = g_1(X), Y_2 = g_2(X)$$

Commonly,  $g_2$  is a slightly modified model  $g_1$ . Since the difference

$$E[Y_1] - E[Y_2]$$

maybe exceedingly small, the simple sampling would need to calculate  $E[Y_1]$  and  $E[Y_2]$  to a particularly good accuracy, which would require a large computational time.

The method can efficiently resolve this problem by studying the random variable.

$$Z = Y_1 - Y_2 = (g_1 - g_2)(X)$$

The variance of  $Z$  is

$$Var[Z] = Var[Y_1] + Var[Y_2] - 2COV[Y_1, Y_2]$$

Thus, if  $Y_1$  and  $Y_2$  are strongly positively correlated to each other, which is likely when  $g_1$  and  $g_2$  are very similar, then simple sampling of  $Z$  is more efficient than sampling  $Y_1$  and  $Y_2$  separately using independent input random variables  $X_1$  and  $X_2$ .

Q2: What is the principle of stratified sampling?

Ans:

$X$  is divided into  $L$  strata (value groups,  $X_i, i = 1, \dots, L$ ), and  $Y$  is sampled within these groups (which also divides  $Y$  into strata).

Strata may be designed so that the variance of  $Y_i$  within the strata is slight (some knowledge is needed here).

Dividing  $X$  into strata  $X_i$  causes  $Y$  be also divided into corresponding strata  $Y_i$ , i.e., samples  $x$  from  $X_i$  will generate samples  $y = g(x)$  from  $Y_i$ .

Since we know exactly the probability that a random number  $X$  falls into some group  $X_i$  we also know that with the same probability  $\omega_i$  samples of  $Y$  fall into  $Y_i$ .

It can be shown that

$$E[Y] = \sum_{i=1}^L \omega_i E[Y_i]$$

And

$$Var[m_Y] = \sum_{i=1}^L \omega_i^2 \frac{Var[Y_i]}{n_i}$$

Where  $n_i$  is the total number of samples  $x$  in  $X_i$ .

Since  $E[Y_i]$  is not known for any  $i$ , the expectation value must be estimated by

$$m_Y = \sum_{i=1}^L \omega_i m_{Y_i}$$

If strata are designed well then it is likely that  $Var[m_Y]$  get smaller compared to the value obtained from simple sampling. On the other hand, a poor stratification will result in an increased variance.

\*\*\*The variance obtained by stratified sampling is minimised when the samples are distributed in strata according to the *Neyman allocation*

$$n_i = n \frac{\omega_i \sigma_{Y_i}}{\sum_{j=1}^L \omega_j \sigma_{Y_j}} \text{ where } \sigma_{Y_i} \text{ is the standard deviation of } Y_i.$$

These deviations  $\sigma_{Y_i}$  are not known at the beginning of the calculation, therefore, the simulation is commonly divided into batches; the strata in the first batch may contain equal number of samples. In the following batches,  $\sigma_{Y_i}$  can be estimated for all  $i$ , and samples can be distributed more efficiently.

Nevertheless, there is a risk of estimating  $\sigma_{Y_i}$  incorrectly in the first batch, which could result in a wrong distribution of the following batches!

Q3: What is the principle of the importance sampling?

Ans:

The method samples  $X$  from a new pdf  $f_Z$ , which is corrected by multiplying the sampled values of  $Y$  by a correction factor

$$\frac{f_X(x)}{f_Z(x)}.$$

The computed random variable  $Z$

$$Z = g(x) \frac{f_X(x)}{f_Z(x)}$$

has the expectation value  $E[Z]$  equal to  $E[Y]$ :

$$E[Z] = \int_x g(x) \frac{f_X(x)}{f_Z(x)} f_Z(x) dx = \int_x g(x) f_X(x) dx = E[Y]$$

**\*\*Ideal pdf  $f_Z$**

The variance of  $Z$  is

$$Var[Z] = E[Z^2] - (E[Z])^2 = \int_x g^2(x) \frac{f_X^2(x)}{f_Z(x)} dx - (E[Y])^2$$

Thus, if the importance function is chosen such that

$$f_Z(x) = \frac{g(x)f_X(x)}{E[Y]}$$

then  $Var[Z] = 0!$

In this ideal case, only one sample would be sufficient to obtain the precise value of  $E[Y]$  (with a zero variance). Therefore, this method is sometimes called the *zero-variance scheme*.

**\*\*We can't know the ideal pdf  $f_Z$ .**

- Computing the precise importance function  $f_Z(x)$  is computationally equivalent to computing the value of  $E[Y]$ . Therefore, in practice, the importance function must be derived using numerical models much simpler than  $g(x)$ , so the zero variance is never obtained (although the variance can be sufficiently reduced).
- The correction factors must be computed for each sample, which may be computationally expensive, and it may negatively reflect into FOM.
- There is a risk that this technique will increase the variance if the importance function is wrong!

Q4: What procedures are involved in the simulation of a single neutron history?

Ans:

Simulation of a single neutron history (assuming we know its initial position, direction, and energy):

- i. Sample the distance to next collision.
- ii. If the neutron moves outside the system (with black BC) then end this history.
- iii. Select the nuclide for the collision.
- iv. Select the reaction type.
- v. If the selected reaction is:
  - capture then end this neutron history.
  - fission then end this neutron history and simulate the histories of the new fission neutrons (stable solution is obtained only for sub-critical systems).
  - scattering then transform the neutron direction and energy and go to step i.

Q5: What is the transition kernel?

Ans:

The transition kernel  $T$  is the pdf of the distance  $s$  to next collision

$$T = \Sigma_t(\vec{r}, E)e^{-\Sigma_t s}$$

Q6: How can we sample the distance to the next collision in a homogeneous system?

Ans:

Sampling the distance  $s$  to the next collision by the inverse method for homogeneous material:

The cdf function,  $F_s = \int_0^s \Sigma_t(\vec{r}, E)e^{-\Sigma_t s'} ds' = 1 - e^{-\Sigma_t s}$

Generate random number  $u$  from (0,1)

Solve  $u = 1 - e^{-\Sigma_t s}$  for  $s$ :

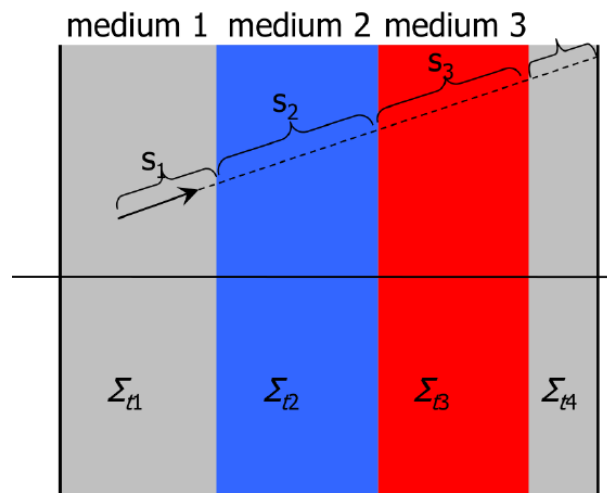
$$s = -\frac{1}{\Sigma_t} \ln(1 - u)$$

Since  $1 - u$  is also a random number from (0,1)

$$\Rightarrow s = -\frac{1}{\Sigma_t} \ln(u)$$

Q7: How can we sample the distance to next collision in inhomogeneous media?

Ans:



Q8: How can we select the nuclide on which the neutron collides?

Ans:

A collision occurs in a material. Hence, we assume we have a list of nuclides with their respective nuclide concentrations (and macroscopic cross section).

- We can assign a neutron collision probability to each nuclide  $i$  as

$$p(i) = \frac{\Sigma_{t,i}(\vec{r}, E)}{\Sigma_t(\vec{r}, E)}$$

- Knowing the collision probabilities on various nuclides, we can sample the nuclide type by the inverse transform method.

Q9: How can we select the type of the collision reaction?

Ans:

- For the selected nuclide type  $i$ , we can assign probabilities to various neutron interactions  $j$  as

$$p(j|i) = \frac{\Sigma_{j,i}(\vec{r}, E)}{\Sigma_{t,i}(\vec{r}, E)}$$

- Knowing the probabilities for various neutron interactions, we can again sample the interaction type by the inverse transform method.

Q10: What are the principal problems in criticality simulations?

Ans:

- In criticality simulations the fission source is not known. The fission source is given by the steady-state neutron flux itself (which is the solution of the problem).
- Moreover, the steady-state solution in fissile systems without an external source of neutrons is possible only in exactly critical systems.

Q11: How are criticality problems simulated by Monte Carlo?

Ans:

- We can divide neutron histories into generations (called cycles in Monte Carlo terminology).
- We guess the distribution of the source in the first cycle.
- During each cycle, we collect the new fission neutrons, and we use them as the source for the next cycle.
- The source will converge over the cycles to the steady-state distribution.
- Once the source is converged, we can start to collect unbiased results.
- Cycles are therefore divided into “inactive” cycles (having only the function of converging the source) and “active” cycles (that are used for computing the result)



Q12: How is the multiplication factor calculated in criticality calculations?

Ans:

- The multiplication factor represents the average number of fission neutrons produced during a single neutron history.
- We can estimate the multiplication factor at each cycle based on the neutron histories simulated at the actual cycle. However, we have artificially changed the fission cross sections, so we need to correct the multiplication factor being computed (by multiplying it with the multiplication factor used for changing the fission cross sections).
- The fission cross sections in the very first cycle need to be divided by a multiplication factor set by the user in the input file.