Uncertainty estimation

Premise in Monte Carlo simulations:

Large enough MC simulations should converge to the "real value" . Khintchine's theorem:

$$\mu = \int_{x_0}^{x_{\max}} \mathrm{d}x \; T(x) = \int_{x_0}^{x_{\max}} \mathrm{d}x \; x p(x)$$

$$P\left\{ \left| \frac{T^1 + T^2 + \cdots + T^{N_\mathrm{h}}}{N_\mathrm{h}} \right| - \mu > \epsilon \right\} \longrightarrow 0$$

Uncertainty estimation

How fast MC simulations converge?

Central Limit Theorem. In the limit of large N_h:

$$P\left(\frac{\tilde{T}-\mu}{\sigma/\sqrt{N_\mathrm{h}}} < \beta\right) \longrightarrow \Re(\beta)$$

$$N_\mathrm{h} \gg \sigma^6/\langle x^3\rangle^2$$

Uncertainty estimation

Direct uncertainty estimation.

N-history run to determine the expected value of X

$$\overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$s_x^2 = \frac{1}{N-1}\sum_{i=1}^{n}(x_i - \overline{x})^2 = \frac{1}{N-1}\sum_{i=1}^{n}(x_i^2 - \overline{x}^2)$$

$$s_{\overline{x}}^2 = \frac{s_x^2}{N} \qquad\qquad x = \overline{x} \pm s_{\overline{x}}.$$

$$s_x^2 = \frac{1}{n-1}\sum_{j=1}^{n}(x_j - \overline{x})^2 = \frac{1}{n-1}\sum_{j=1}^{n}(x_j^2 - \overline{x}^2)$$

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Uncertainty estimation by batches.

A run with N histories is divided into n batches. Then, the expected value of X can be found as follows:

$$x_j = \sum_{i=1}^{N/n} x_i \qquad \overline{x} = \frac{1}{N}\sum_{j=1}^{n} x_j$$

$$s_x^2 = \frac{1}{n-1}\sum_{j=1}^{n}(\overline{x}_j - \overline{x})^2 \approx \frac{1}{n-1}\sum_{j=1}^{n}(\overline{x}_j^2 - \overline{x}^2)$$

$$s_{\overline{x}}^2 = \frac{s_x^2}{n} \qquad x = \overline{x} \pm s_{\overline{x}}$$

Uncertainty estimation

Combination of independent calculation uncertainties

N_k is the total number of histories of the k run.

$$\overline{x} = \sum_{k=1}^{m} \left(\frac{N_k}{N}\right) \overline{x}_k$$

m is the number of runs.

$\overline{x}_k$ s the expected value of the x run.

N is the total number of histories.

$$N = \sum_{k=1}^{m} N_k$$

Uncertainty estimation

Combination of independent calculation uncertainties (cont.)

Combined variance obtained by uncertainty propagation

$$s_{\overline{x}}^2 = \sum_{k=1}^{m} \left(\frac{N_k}{N}\right)^2 s_{\overline{x}_k}^2$$

Example for m=2

$$\overline{x} = \left(\frac{N_1}{N}\right)\overline{x}_1 + \left(\frac{N_2}{N}\right)\overline{x}_2$$

$$N = N_1 + N_2$$

$$s_{\overline{x}} = \sqrt{\left(\frac{N_1}{N}\right)^2 s_{\overline{x}_1}^2 + \left(\frac{N_2}{N}\right)^2 s_{\overline{x}_2}^2}$$

Uncertainty estimation

Relation between the sample variance and the variance of the mean

μ is the population mean

$$: \overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \approx \mu$$

If x_i are independent variables

$$s_{\overline{x}}^2 = \sum_{i=1}^{N}\left(\frac{\partial \overline{x}}{\partial x_i}\right)^2 \sigma^2 \approx \sum_{i=1}^{N}\left(\frac{\partial \overline{x}}{\partial x_i}\right)^2 s_x^2$$

$$\frac{\partial \overline{x}}{\partial x_j} = \frac{1}{N}\sum_{i=1}^{N}\frac{\partial x_i}{\partial x_j} = \frac{1}{N}\sum_{i=1}^{N}\delta_{ij} = \frac{1}{N}$$

$$s_{\overline{x}}^2 = \frac{1}{N^2}\sum_{i=1}^{N}\sigma^2 = \frac{1}{N}\sigma^2 \approx \frac{1}{N}s_x^2$$