In MC computation, one is often interested in computing functions of DIFFERENT mean values. To clarify the issue, we consider a simple example. We wish to estimate

$$R = \frac{\langle f \rangle_\pi}{\langle g \rangle_\pi}$$

where $f(x)$ and $g(x)$ are TWO DIFFERENT functions.

As usual, we proceed as follows.
We perform a simulation with N iterations

$$X_1 \to \dots X_i \to X_N$$ (numbers extracted with probability $\pi(x)$)

compute

$$f(X_1) \to \dots f(X_i) \dots \to f(X_N)$$
$$g(X_1) \to \dots g(X_i) \to g(X_N)$$

and

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f(X_i) \qquad \bar{g} = \frac{1}{N} \sum_{i=1}^{N} g(X_i)$$

The estimator is $R_{est} = \frac{\bar{f}}{\bar{g}}$

TWO QUESTIONS:

① BIAS ? $\quad$ $\mathrm{BIAS} = \langle R_{est} \rangle_{MC} - R$

② ERROR $\quad$ $\sigma^2 = \langle (R_{est} - \langle R_{est} \rangle_{MC})^2 \rangle_{MC}$

Computation of the bias

We compute it for large values of N

$$R_{est} = \frac{\bar{f}}{\bar{g}} = \frac{\langle f\rangle_\pi + (\bar{f} - \langle f\rangle_\pi)}{\langle g\rangle_\pi + (\bar{g} - \langle g\rangle_\pi)} = R\left(\frac{1+\Delta_f}{1+\Delta_g}\right) \qquad R = \frac{\langle f\rangle_\pi}{\langle g\rangle_\pi}$$

$$\Delta_f = \frac{\bar{f} - \langle f\rangle_\pi}{\langle f\rangle_\pi} \qquad \Delta_g = \frac{\bar{g} - \langle g\rangle_\pi}{\langle g\rangle_\pi}$$

We can assume that Δ_f, Δ_g are small.

$$R_{est} = R\,(1+\Delta_f)(1-\Delta_g+\Delta_g^2-\Delta_g^3)+\ldots =$$

$$= R\,(1+\Delta_f-\Delta_g-\Delta_f\Delta_g+\Delta_g^2+\Delta_f\Delta_g^2-\Delta_g^3+\ldots)$$

Now we know that

$$\langle \Delta_f\rangle_{MC} = \frac{1}{\langle f\rangle_\pi}\langle \bar{f} - \langle f\rangle_\pi\rangle_{MC} = 0 \qquad (\bar{f} \text{ is an unbiased estimator})$$

$$\langle \Delta_g\rangle_{MC} = \frac{1}{\langle g\rangle_\pi}\langle \bar{g} - \langle g\rangle_\pi\rangle_{MC} = 0$$

$$\langle \Delta_g^2\rangle_{MC} = \frac{1}{\langle g\rangle_\pi^2}\langle (\bar{g} - \langle g\rangle_\pi)^2\rangle_{MC} = \frac{1}{\langle g\rangle_\pi^2}\,\frac{1}{N}\,\mathrm{Var}_\pi g$$

$$\langle \Delta_g^3\rangle_{MC} = \frac{1}{\langle g\rangle_\pi^3}\langle (\bar{g} - \langle g\rangle_\pi)^3\rangle_{MC} = \frac{1}{\langle g\rangle_\pi^3}\,\frac{1}{N^2}\langle (g - \langle g\rangle_\pi)^3\rangle_\pi$$

We should now compute

$$\langle \Delta f \Delta g \rangle_{MC} = \frac{1}{\langle f\rangle_\pi \langle g\rangle_\pi} \langle (\bar f - \langle f\rangle_\pi)(\bar g - \langle g\rangle_\pi) \rangle$$

$$= \frac{1}{\langle f\rangle_\pi \langle g\rangle_\pi} \Big(\langle \bar f \bar g \rangle_{MC} - \langle f\rangle_\pi \langle \bar g\rangle_{MC} - \langle \bar f\rangle_{MC} \langle g\rangle_\pi + \langle g\rangle_\pi \langle f\rangle_\pi \Big)$$

$$= \frac{1}{\langle f\rangle_\pi \langle g\rangle_\pi} \Big(\langle \bar f \bar g \rangle_{MC} - \langle f\rangle_\pi \langle g\rangle_\pi \Big)$$

Convince yourself (the argument is the same as that given when discussing $\langle \bar f^2 \rangle_{MC}$) that

$$\langle f(x_i)\, g(x_j) \rangle_{MC} = \begin{cases} \langle fg\rangle_\pi & \text{if } i=j \\ \langle f\rangle_\pi \langle g\rangle_\pi & \text{if } i\neq j \end{cases}$$

It follows

$$\langle \bar f \bar g \rangle_{MC} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle f(x_i)\, g(x_j) \rangle_{MC} \qquad \left(\begin{array}{c}\text{we use}\\ \text{the definition}\\ \text{of } \bar f, \bar g\end{array}\right)$$

$$= \frac{1}{N^2} \sum_{i=1}^{N} \langle f(x_i) g(x_i) \rangle_{MC} + \frac{1}{N^2} \sum_{i\neq j} \langle f(x_i) g(x_j) \rangle_{MC}$$

$$= \frac{1}{N^2} N \langle fg\rangle_\pi + \frac{1}{N^2} N(N-1) \langle f\rangle_\pi \langle g\rangle_\pi$$

$$= \langle f\rangle_\pi \langle g\rangle_\pi + \frac{1}{N} \Big(\langle fg\rangle_\pi - \langle f\rangle_\pi \langle g\rangle_\pi \Big)$$

We thus get

$$\langle \Delta f \Delta g \rangle = \frac{1}{\langle f \rangle_\pi \langle g \rangle_\pi} \frac{1}{N} \left(\langle fg \rangle_\pi - \langle f \rangle_\pi \langle g \rangle_\pi \right)$$

We define the <u>covariance</u> of f and g with respect to π

$$\begin{aligned} \mathrm{Cov}_\pi(f,g) &= \int dx\, \pi(x) \left(f(x) g(x) - \langle f \rangle_\pi \langle g \rangle_\pi \right) \\ &= \langle fg \rangle_\pi - \langle f \rangle_\pi \langle g \rangle_\pi \end{aligned}$$

$$\langle \Delta f \Delta g \rangle = \frac{1}{\langle f \rangle_\pi \langle g \rangle_\pi} \frac{1}{N} \mathrm{Cov}_\pi(f,g)$$

We do not go into the details but one can prove that

$$\langle \Delta f \Delta g^2 \rangle \sim \frac{1}{N^2}$$

Thus

$$\begin{aligned} \langle R_{est} \rangle_{MC} = R + \frac{R}{N} \Big(&- \frac{1}{\langle f \rangle_\pi \langle g \rangle_\pi} \mathrm{Cov}_\pi(f,g) + \\ &+ \frac{1}{\langle g \rangle_\pi^2} \mathrm{Var}_\pi\, g \Big) + O(N^{-2}) \end{aligned}$$

R_{est} is a BIASED estimator of R

$$\text{BIAS} \sim \frac{1}{N} \qquad \text{(as usual)}$$

ERROR ON THE RATIO

$$\sigma^2 = \langle (R_{est} - \langle R_{est} \rangle_{MC})^2 \rangle_{MC}$$
$$= \langle R_{est}^2 \rangle_{MC} - \langle R_{est} \rangle_{MC}^2$$

To compute $\langle R_{est}^2 \rangle_{MC}$

$$R_{est}^2 = R^2 (1 + \Delta_f)^2 (1 - \Delta_g + \Delta_g^2)^2$$
$$= R^2 (1 + 2\Delta_f + \Delta_f^2)(1 - 2\Delta_g + 3\Delta_g^2)$$
$$= R^2 (1 + 2\Delta_f - 2\Delta_g + \Delta_f^2 - 4\Delta_f \Delta_g + 3\Delta_g^2)$$

we only keep terms up to power 2 [R_{est}^2 up to $O(N^{-1})$]

$$\langle R_{est}^2 \rangle_{MC} = R^2 (1 + \langle \Delta_f^2 \rangle_{MC} - 4 \langle \Delta_f \Delta_g \rangle_{MC} + 3 \langle \Delta_g^2 \rangle_{MC})$$

The previous calculations give

$$\langle R_{est} \rangle_{MC} = R (1 - \langle \Delta_f \Delta_g \rangle_{MC} + \langle \Delta_g^2 \rangle_{MC})$$

It follows

$$\sigma^2 = R^2 (1 + \langle \Delta_f^2 \rangle_{MC} - 4 \langle \Delta_f \Delta_g \rangle_{MC} + 3 \langle \Delta_g^2 \rangle_{MC}) \leftarrow \langle R_{est}^2 \rangle_{MC}$$
$$- R^2 (1 - 2 \langle \Delta_f \Delta_g \rangle_{MC} + 2 \langle \Delta_g^2 \rangle_{MC}) \leftarrow \langle R_{est} \rangle_{MC}^2$$
$$= R^2 (\langle \Delta_f^2 \rangle_{MC} - 2 \langle \Delta_f \Delta_g \rangle_{MC} + \langle \Delta_g^2 \rangle_{MC})$$
$$\downarrow$$
$$\sigma^2 = \frac{1}{N} R^2 \left(\frac{Var_\pi f}{\langle f \rangle_\pi^2} - 2 \frac{Cov_\pi (f, g)}{\langle f \rangle_\pi \langle g \rangle_\pi} + \frac{Var_\pi g}{\langle g \rangle_\pi^2} \right)$$

Comments

a) $\sigma \sim \frac{1}{\sqrt{N}}$ as obvious

b) It depends on the variance of f an g (that as on the errors on $\bar{f}, \bar{g}$) but also on the COVARIANCE of f and g

AN APPROXIMATE FORMULA :

THE INDEPENDENT ERROR FORMULA

We simply neglect the covariance and write

$$\sigma^2_{ind} = \frac{1}{N} R^2 \left(\frac{Var_\pi f}{\langle f \rangle_\pi^2} + \frac{Var_\pi g}{\langle g_\pi \rangle^2} \right)$$

$$= R^2 \left(\frac{\sigma_f^2}{\langle f \rangle_\pi^2} + \frac{\sigma_g^2}{\langle g \rangle_\pi^2} \right)$$

σ_f error on $\bar{f}$

σ_g error on $\bar{g}$

This formula follows from a general ERROR PROPAGATION FORMULA.

Suppose that there are two quantities that take value A and B, respectively, with error σ_A, σ_B. The C is a function F(A,B)

What is the error on C

$$\sigma_c^2 = \left(\frac{\partial F}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial F}{\partial B}\right)^2 \sigma_B^2$$

· This formula assumes the absence of correlations between A, B

Let us apply this equation to our case

$$C = \frac{A}{B}$$

$$\sigma_C^2 = \frac{1}{B^2}\sigma_A^2 + \frac{A^2}{B^4}\sigma_B^2 = \left(\frac{A}{B}\right)^2\left(\frac{\sigma_A^2}{A^2} + \frac{\sigma_B^2}{B^2}\right)$$

Same expression $\begin{pmatrix} A = \langle f \rangle_\pi \\ B = \langle g \rangle_\pi \end{pmatrix}$

The error σ_{ind} may be larger or smaller than the correct error (the covariance may be positive or negative)

AN UPPER BOUND : THE WORST-ERROR FORMULA

It is easy to prove that

$$|\mathrm{Cov}_\pi(f,g)| \le [\mathrm{Var}_\pi f \cdot \mathrm{Var}_\pi g]^{1/2}$$

so that

$$-\frac{\mathrm{Cov}_\pi(f,g)}{\langle f \rangle_\pi \langle g \rangle_\pi} \le \frac{[\mathrm{Var}_\pi f \cdot \mathrm{Var}_\pi g]^{1/2}}{|\langle f \rangle_\pi|\,|\langle g \rangle_\pi|}$$

Thus

$$\sigma^2 \le \frac{R^2}{N}\left(\frac{\mathrm{Var}_\pi f}{\langle f \rangle_\pi^2} + \frac{2[\mathrm{Var}_\pi f \cdot \mathrm{Var}_\pi g]^{1/2}}{|\langle f \rangle_\pi|\,|\langle g \rangle_\pi|} + \frac{\mathrm{Var}_\pi g}{\langle g \rangle_\pi^2}\right)$$

$$= \frac{R^2}{N}\left(\frac{\sqrt{\mathrm{Var}_\pi f}}{|\langle f \rangle_\pi|} + \frac{\sqrt{\mathrm{Var}_\pi g}}{|\langle g \rangle_\pi|}\right)^2 = R^2\left(\frac{\sigma_f}{|\langle f \rangle_\pi|} + \frac{\sigma_g}{|\langle g \rangle_\pi|}\right)^2$$

WORST-ERROR FORMULA

$$\sigma \leq \sigma_{WE} = |R| \left(\frac{\sigma_f}{|\langle f \rangle_\pi|} + \frac{\sigma_g}{|\langle g \rangle_\pi|} \right)$$

For the general case

$$\sigma_{WE,C} = \left| \frac{\partial F}{\partial A} \right| \sigma_A + \left| \frac{\partial F}{\partial B} \right| \sigma_B$$

It is usually a poor approximation : it significantly overestimates the error

$$\sigma^2 = \frac{1}{N} R^2 \left(\frac{\langle f^2\rangle_\pi - \langle f\rangle_\pi^2}{\langle f\rangle_\pi^2} - \frac{2\langle fg\rangle_\pi - 2\langle f\rangle_\pi \langle g\rangle_\pi}{\langle f\rangle_\pi \langle g\rangle_\pi} + \frac{\langle g^2\rangle_\pi - \langle g\rangle_\pi^2}{\langle g\rangle_\pi^2} \right)$$

cancel

$$= \frac{1}{N} R^2 \left(\frac{\langle f^2\rangle_\pi}{\langle f\rangle_\pi^2} - 1 - \frac{2\langle fg\rangle_\pi}{\langle f\rangle_\pi \langle g\rangle_\pi} + 2 + \frac{\langle g^2\rangle_\pi}{\langle g\rangle_\pi^2} - 1 \right)$$

$$= \frac{1}{N} R^2 \underbrace{\left\langle \left(\frac{f}{\langle f\rangle_\pi} - \frac{g}{\langle g\rangle_\pi} \right)^2 \right\rangle_\pi}_{O}$$

Estimator of O

$$O = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{f_i}{\bar{f}} - \frac{g_i}{\bar{g}} \right)^2$$

This is a <u>BIASED</u>, <u>CORRECT</u> estimator of O.