BIAS AND PROPAGATION OF ERRORS

Let $J(x)$ be a function and suppose we wish to compute $J(\langle f \rangle_\pi)$

TRIVIAL EXAMPLE: $J(x) = x^3$, we compute $\langle f \rangle_\pi^3$

ESTIMATOR OF $J(\langle f \rangle_\pi)$: $J(\bar{f})$

a) IS THERE A BIAS?

To answer the question we need to compute

$$\langle J(\bar{f}) \rangle_{MC} = \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} J(\bar{f}^{(i)}) \quad \text{for } N_{MC} \to \infty$$

We are not able to compute this quantity exactly in general.

For $J(x) = x^2$ we can perform the exact calculation already computed

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

$$\text{bias} = \langle f \rangle_\pi^2 - \langle \bar{f}^2 \rangle_{MC} = \frac{1}{N}\left(\langle f^2 \rangle_\pi - \langle f \rangle_\pi^2 \right)$$

The bias is of order $1/N$.

For $J(x) = x^3$ [excercise: do it!] the exact result is

$$\langle \bar{f}^3 \rangle_{MC} = \langle f \rangle_\pi^3 + \frac{3}{N}\left(\langle f^2 \rangle_\pi - \langle f \rangle_\pi^2 \right) \langle f \rangle_\pi + \frac{1}{N^2} \langle (f - \langle f \rangle_\pi)^3 \rangle_\pi$$

The bias is again of order $1/N$.

<u>Hint</u>

$$\langle \bar{f}^3 \rangle_{MC} = \frac{1}{N^3} \sum_{ijk=1}^{N} \langle f(x_i) f(x_j) f(x_k) \rangle_{MC}$$

note that there are

$N(N-1)(N-2)$ terms with $i \neq j \neq k$
$N(N-1)$ terms with $i = j \neq k$
$N(N-1)$ terms with $i = k \neq j$
$N(N-1)$ terms with $j = k \neq i$
N terms with $i = j = k$

Now the general case. In this case we assume that N is finite, but large

$$\langle J(\bar{f}) \rangle_{MC} = \langle J(\langle f \rangle_\pi + \bar{f} - \langle f \rangle_\pi) \rangle_{MC}$$

For N large, $\bar{f} - \langle f \rangle_\pi$ is small. We therefore perform a Taylor expansion

$$= J(\langle f \rangle_\pi) + J'(\langle f \rangle_\pi) \langle \bar{f} - \langle f \rangle_\pi \rangle_{MC}$$
$$+ \frac{1}{2} J''(\langle f \rangle_\pi) \langle (\bar{f} - \langle f \rangle_\pi)^2 \rangle_{MC}$$
$$+ \frac{1}{6} J'''(\langle f \rangle_\pi) \langle (\bar{f} - \langle f \rangle_\pi)^3 \rangle_{MC}$$

Now we have already computed

$$\langle \bar{f} - \langle f \rangle_\pi \rangle_{MC} = \langle \bar{f} \rangle_{MC} - \langle f \rangle_\pi = \langle f \rangle_\pi - \langle f \rangle_\pi = 0$$

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

$$\langle (\bar f - \langle f\rangle_\pi)^3\rangle_{MC} = \langle \bar f^3\rangle_{MC} - 3\langle \bar f^2\rangle_{MC}\langle f\rangle_\pi +$$
$$+3\langle \bar f\rangle_{MC}\langle f\rangle^2 - \langle f\rangle_\pi^3$$
$$= \langle f\rangle_\pi^3 + \frac{3}{N}\langle f\rangle_\pi \mathrm{Var}_\pi f + \frac{1}{N^2}\langle (f-\langle f\rangle_\pi)^3\rangle_\pi \leftarrow \langle \bar f^3\rangle_{MC}$$
$$-3\langle f\rangle_\pi\left[\langle f\rangle_\pi^2 + \frac{1}{N}\mathrm{Var}_\pi f\right] + 2\langle f\rangle_\pi^3$$
$$= \frac{1}{N^2}\langle (f-\langle f\rangle_\pi)^3\rangle_\pi$$

Therefore

$$\langle J(\bar f)\rangle_{MC} = J(\langle f\rangle_\pi) + \frac{1}{2N} J''(\langle f\rangle_\pi)\,\mathrm{Var}_\pi f + O(N^{-2})$$

The bias is always of order $1/N$.

b) Computation of the error

$$\sigma^2 = \left\langle \left(J(\bar f) - \langle J(\bar f)\rangle_{MC}\right)^2 \right\rangle_{MC}$$

Again we assume N finite but large

$$J(\bar f) - \langle J(\bar f)\rangle_{MC} =$$
$$\cancel{J(\langle f\rangle_\pi)} + J'(\langle f\rangle_\pi)(\bar f - \langle f\rangle_\pi) + \frac{1}{2}J''(\langle f\rangle_\pi)(\bar f - \langle f\rangle_\pi)^2 + \dots$$
$$-\left[\cancel{J(\langle f\rangle_\pi)} + \frac{1}{2N}J''(\langle f\rangle_\pi)\,\mathrm{Var}_\pi f + O(N^{-2})\right]$$

[first line = expansion of $J(\bar f)$]

Now we square the prevrous expression
[we set $J_1 = J'(\langle f\rangle_\pi)$, $J_2 = J''(\langle f\rangle_\pi)$]
and take the average

$$\sigma^2 = J_1^2 \langle (\bar{f} - \langle f\rangle_\pi)^2\rangle_{MC} \longrightarrow \text{order } \frac{1}{N}$$

$$+ \frac{1}{4} J_2^2 \langle (\bar{f} - \langle f\rangle_\pi)^4\rangle_{MC} \longrightarrow \text{order } \frac{1}{N^2} \left(\begin{array}{l}\text{it can be} \\ \text{proved} \\ \text{computing } \langle \bar{f}^4\rangle\end{array}\right)$$

$$+ \frac{1}{4N^2} J_2^2 (\mathrm{Var}_\pi f)^2 \longrightarrow \text{order } \frac{1}{N^2}$$

$$+ J_1 J_2 \langle (\bar{f} - \langle f\rangle_\pi)^3\rangle_{MC} \longrightarrow \text{order } \frac{1}{N^2}$$

$$+ \frac{1}{N} J_1 J_2 \mathrm{Var}_\pi f \, \langle \bar{f} - \langle f\rangle_\pi \rangle_{MC} \longrightarrow \left(\text{order } \frac{1}{N}\right) \cdot 0 = 0$$

$$+ \frac{1}{2N} J_2^2 \mathrm{Var}_\pi f \, \langle (f - \langle f\rangle_\pi)^2\rangle_{MC} \longrightarrow \text{order } \frac{1}{N}\cdot\frac{1}{N} = \frac{1}{N^2}$$

$$= J_1^2 \langle (\bar{f} - \langle f\rangle_\pi)^2\rangle_{MC} + O(N^{-2})$$

$$= J_1^2 \frac{1}{N} \mathrm{Var}_\pi f$$

$$\text{error su } J(\bar{f}) = \underbrace{\left| \left(\frac{\partial J(x)}{\partial x}\right)\Big|_{x=\bar{f}} \right|} \times (\text{error on } \bar{f})$$

NOTE : i) absolute value

ii) we replace $J'(\langle f\rangle_\pi)$ with $J'(\bar{f})$; the difference between the two terms is of order $1/N$

ERROR PROPAGATION FORMULA

Meaning of bias

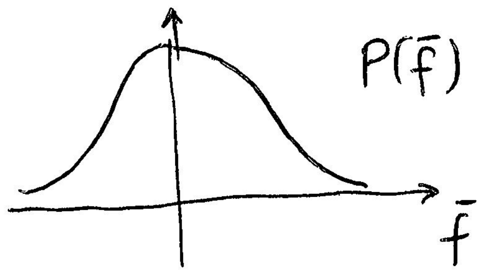
Roughly speaking (confusing mean with median) the presence of a bias means that it is more probable to obtain a result larger than the mean value than smaller or vice versa.

- An extreme case

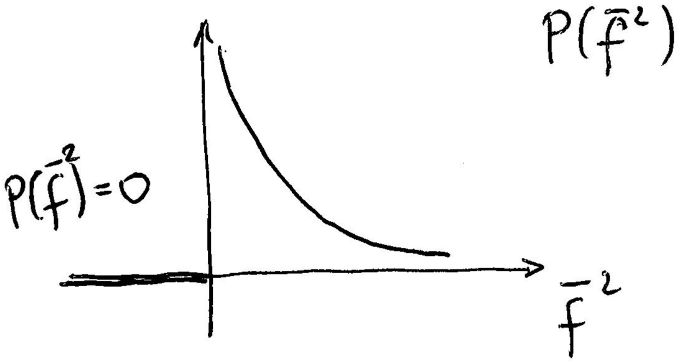
Suppose $\langle f \rangle_\pi = 0$ so that $\langle f \rangle_\pi^2 = 0$

Suppose you do not know the result and use our numerical method to estimate $\langle f \rangle_\pi$

$\bar{f}$ will have a distribution centered in 0



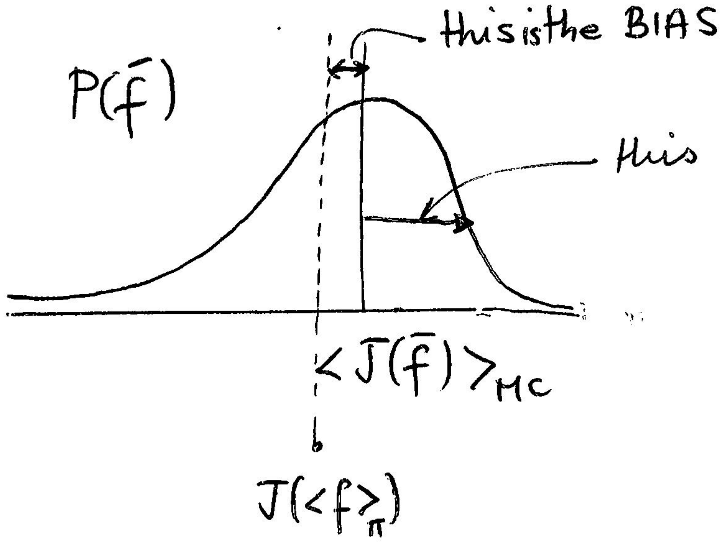
We get positive and negative values for $\bar{f}$ with equal probability ($\bar{f}$ is UNBIASED)



Of course $P(\bar{f}^2)=0$ for $\bar{f}^2<0$

All estimates are larger (they are positive) than the correct value.

Why the bias is irrelevant for large values of N?

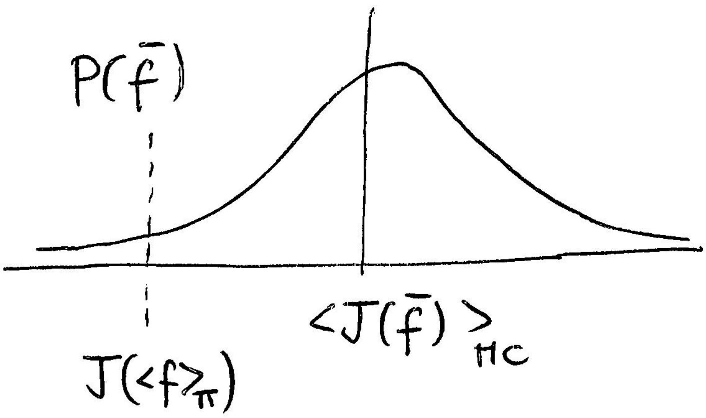


In this situation (bias $\ll$ error) the bias is negligible. This situation always occur for N large since

$$\text{error} \sim \frac{1}{\sqrt{N}} \qquad \text{bias} \sim \frac{1}{N}$$

(the bias decreases more rapidly than the error)

The bias is relevant if



This may occur when N is small